



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:07 PM UTC

PDB ID : 1CID / pdb_00001cid
Title : CRYSTAL STRUCTURE OF DOMAINS 3 & 4 OF RAT CD4 AND THEIR
RELATIONSHIP TO THE NH2-TERMINAL DOMAINS
Authors : Brady, R.L.; Dodson, E.J.; Lange, G.
Deposited on : 1993-01-28
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

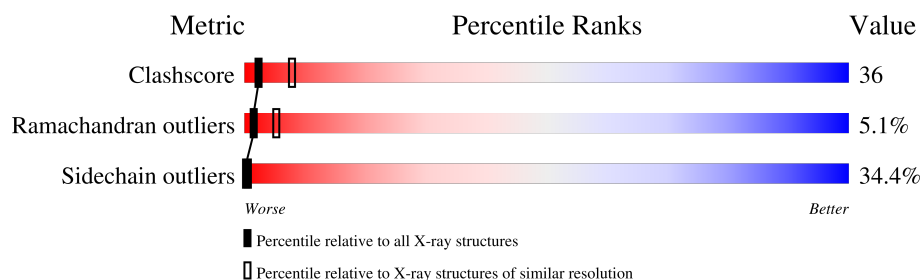
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	177	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1396 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 T CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	9	0	0
			1381	867	232	276	6			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	S	0	0
			1	1		

- Molecule 3 is water.

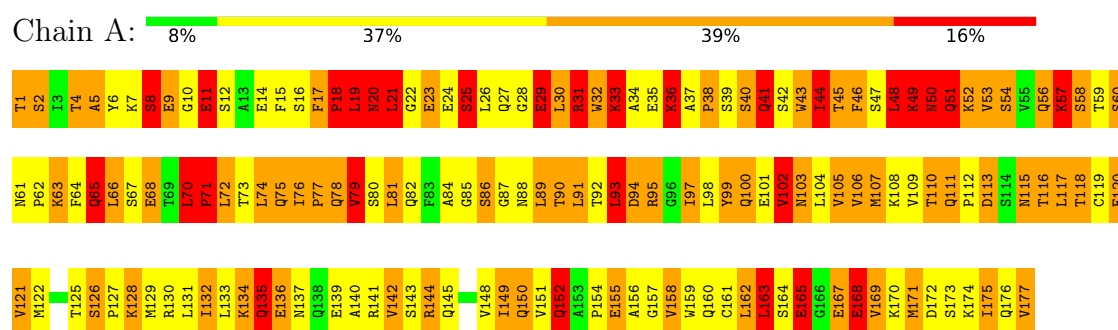
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: T CELL SURFACE GLYCOPROTEIN CD4



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.80Å 77.80Å 82.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1396	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.61	6/1402 (0.4%)	3.95	333/1895 (17.6%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	SER	CA-CB	-7.08	1.43	1.52
1	A	17	PHE	CA-CB	-6.95	1.44	1.53
1	A	37	ALA	N-CA	6.16	1.52	1.46
1	A	70	LEU	N-CA	5.62	1.54	1.46
1	A	157	GLY	N-CA	5.22	1.51	1.44
1	A	94	ASP	CA-C	5.13	1.59	1.52

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	61	ASN	O-C-N	24.91	136.22	121.27
1	A	94	ASP	N-CA-C	-21.39	88.18	111.07
1	A	93	LEU	CA-C-O	18.26	146.62	120.51
1	A	24	GLU	CA-C-N	15.77	144.76	123.00
1	A	24	GLU	C-N-CA	15.77	144.76	123.00
1	A	113	ASP	CA-C-O	-14.71	109.60	120.19
1	A	70	LEU	O-C-N	14.65	138.17	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASN	CA-C-O	-14.26	105.65	120.63
1	A	75	GLN	CA-C-O	-13.66	105.76	120.24
1	A	168	GLU	CA-C-O	13.20	134.48	120.36
1	A	78	GLN	CB-CG-CD	12.97	134.66	112.60
1	A	24	GLU	CA-C-O	12.85	135.28	121.15
1	A	88	ASN	CA-CB-CG	12.60	125.20	112.60
1	A	5	ALA	O-C-N	12.59	138.04	123.31
1	A	78	GLN	CA-CB-CG	12.41	138.93	114.10
1	A	115	ASN	N-CA-C	-12.08	99.02	113.88
1	A	104	LEU	O-C-N	11.79	138.37	123.28
1	A	75	GLN	N-CA-CB	-11.78	92.27	110.77
1	A	79	VAL	CA-CB-CG2	-11.45	90.93	110.40
1	A	70	LEU	CA-C-O	-11.41	104.53	120.16
1	A	103	ASN	O-C-N	11.38	136.94	123.17
1	A	130	ARG	NE-CZ-NH2	11.16	129.24	119.20
1	A	143	SER	CA-CB-OG	11.04	133.17	111.10
1	A	169	VAL	O-C-N	11.03	137.53	122.97
1	A	92	THR	CA-C-N	10.99	142.53	121.54
1	A	92	THR	C-N-CA	10.99	142.53	121.54
1	A	171	MET	O-C-N	10.94	134.23	123.29
1	A	92	THR	CA-C-O	10.89	133.85	121.11
1	A	71	PRO	N-CA-C	10.77	140.10	112.10
1	A	79	VAL	CA-CB-CG1	10.69	128.57	110.40
1	A	77	PRO	N-CA-C	10.54	132.66	114.75
1	A	24	GLU	N-CA-C	10.39	124.88	110.24
1	A	40	SER	N-CA-CB	10.30	125.57	109.71
1	A	27	GLN	N-CA-C	-10.27	92.66	109.40
1	A	75	GLN	CA-CB-CG	10.13	134.35	114.10
1	A	35	GLU	CB-CG-CD	10.04	129.67	112.60
1	A	40	SER	CA-C-O	10.03	132.21	120.58
1	A	75	GLN	CB-CA-C	9.78	125.79	110.14
1	A	57	LYS	CA-C-O	9.70	134.38	120.51
1	A	11	GLU	O-C-N	-9.61	110.32	122.43
1	A	111	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	A	158	VAL	CA-C-O	-9.47	110.27	120.59
1	A	145	GLN	N-CA-CB	-9.38	99.56	110.35
1	A	105	VAL	CA-C-N	9.35	134.78	123.19
1	A	105	VAL	C-N-CA	9.35	134.78	123.19
1	A	101	GLU	N-CA-CB	9.35	125.86	110.63
1	A	59	THR	N-CA-CB	9.22	124.89	111.05
1	A	117	LEU	CA-C-O	-9.15	109.04	120.20
1	A	167	GLU	CA-CB-CG	9.11	132.31	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	VAL	CA-C-O	-9.09	93.73	121.00
1	A	11	GLU	CA-C-N	9.07	134.98	122.19
1	A	11	GLU	C-N-CA	9.07	134.98	122.19
1	A	133	LEU	CA-C-N	9.05	136.80	122.59
1	A	133	LEU	C-N-CA	9.05	136.80	122.59
1	A	65	GLN	CA-C-O	-9.04	110.28	120.32
1	A	117	LEU	N-CA-CB	9.03	125.49	110.77
1	A	144	ARG	CD-NE-CZ	8.99	136.99	124.40
1	A	93	LEU	CA-C-N	8.98	132.11	120.44
1	A	93	LEU	C-N-CA	8.98	132.11	120.44
1	A	103	ASN	CA-CB-CG	8.97	121.57	112.60
1	A	105	VAL	N-CA-CB	8.93	123.39	111.25
1	A	134	LYS	CB-CG-CD	-8.87	90.90	111.30
1	A	78	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	A	148	VAL	CB-CA-C	8.68	120.31	110.41
1	A	60	SER	CA-CB-OG	8.67	128.44	111.10
1	A	111	GLN	CG-CD-OE1	8.66	138.13	120.80
1	A	119	CYS	CA-C-O	-8.62	109.67	120.28
1	A	64	PHE	CA-CB-CG	8.52	122.31	113.80
1	A	42	SER	CA-C-O	-8.47	110.92	120.32
1	A	70	LEU	CB-CA-C	8.45	126.83	110.17
1	A	17	PHE	CA-CB-CG	8.44	122.24	113.80
1	A	67	SER	CA-C-O	-8.43	110.80	120.58
1	A	46	PHE	O-C-N	8.42	132.78	123.10
1	A	26	LEU	CA-C-N	8.38	135.51	122.94
1	A	26	LEU	C-N-CA	8.38	135.51	122.94
1	A	85	GLY	CA-C-O	-8.33	115.16	120.91
1	A	141	ARG	CA-C-N	8.33	133.84	123.10
1	A	141	ARG	C-N-CA	8.33	133.84	123.10
1	A	19	LEU	CA-C-N	8.32	137.42	121.54
1	A	19	LEU	C-N-CA	8.32	137.42	121.54
1	A	56	GLN	N-CA-C	-8.29	95.72	109.07
1	A	59	THR	O-C-N	8.29	134.79	122.94
1	A	11	GLU	N-CA-CB	-8.28	97.18	110.51
1	A	8	SER	N-CA-CB	8.17	123.95	110.63
1	A	25	SER	CA-C-O	8.17	129.28	120.38
1	A	109	VAL	O-C-N	8.12	132.04	123.03
1	A	130	ARG	CD-NE-CZ	8.11	135.75	124.40
1	A	173	SER	N-CA-CB	-8.11	96.64	110.99
1	A	105	VAL	CA-C-O	-8.08	111.92	120.48
1	A	43	TRP	CB-CG-CD1	8.07	139.01	126.90
1	A	36	LYS	CA-C-O	-8.01	110.23	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLN	CB-CA-C	7.95	123.47	109.72
1	A	65	GLN	O-C-N	7.94	132.60	123.31
1	A	115	ASN	CA-C-N	-7.89	111.48	122.93
1	A	115	ASN	C-N-CA	-7.89	111.48	122.93
1	A	18	PRO	N-CA-CB	-7.88	94.98	103.25
1	A	78	GLN	N-CA-C	-7.83	94.11	110.80
1	A	155	GLU	CG-CD-OE1	-7.83	100.39	118.40
1	A	65	GLN	CB-CA-C	-7.83	95.53	109.70
1	A	135	GLN	CA-C-O	-7.82	111.98	121.36
1	A	120	GLU	N-CA-CB	7.73	125.90	111.53
1	A	115	ASN	O-C-N	7.72	132.70	122.36
1	A	78	GLN	CB-CA-C	7.71	125.75	110.42
1	A	110	THR	CA-C-N	7.70	134.39	123.30
1	A	110	THR	C-N-CA	7.70	134.39	123.30
1	A	29	GLU	N-CA-CB	-7.68	97.22	111.13
1	A	169	VAL	CA-C-O	-7.67	112.23	120.59
1	A	168	GLU	CA-C-N	-7.66	113.10	122.90
1	A	168	GLU	C-N-CA	-7.66	113.10	122.90
1	A	109	VAL	CA-C-O	-7.65	112.39	120.57
1	A	87	GLY	CA-C-O	-7.61	112.78	121.68
1	A	46	PHE	CA-C-O	-7.59	113.33	121.45
1	A	52	LYS	N-CA-CB	7.52	122.38	110.65
1	A	174	LYS	CB-CA-C	-7.51	95.62	109.37
1	A	126	SER	CA-CB-OG	7.48	126.06	111.10
1	A	109	VAL	N-CA-CB	7.43	119.91	110.99
1	A	86	SER	CA-CB-OG	-7.43	96.24	111.10
1	A	137	ASN	CA-CB-CG	7.41	120.01	112.60
1	A	169	VAL	CB-CA-C	7.39	121.11	110.98
1	A	29	GLU	CB-CG-CD	-7.39	100.04	112.60
1	A	136	GLU	CA-C-O	-7.39	109.94	120.51
1	A	35	GLU	CA-C-N	-7.39	107.93	121.52
1	A	35	GLU	C-N-CA	-7.39	107.93	121.52
1	A	11	GLU	CG-CD-OE2	7.38	135.38	118.40
1	A	14	GLU	N-CA-CB	7.38	122.36	110.77
1	A	19	LEU	N-CA-C	7.34	120.98	109.96
1	A	104	LEU	CA-C-N	-7.34	114.08	123.19
1	A	104	LEU	C-N-CA	-7.34	114.08	123.19
1	A	20	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	84	ALA	CA-C-O	-7.27	112.76	121.05
1	A	10	GLY	N-CA-C	-7.23	105.34	115.32
1	A	4	THR	O-C-N	7.23	132.63	123.23
1	A	52	LYS	CB-CG-CD	7.22	127.91	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	CA-CB-CG	7.21	128.52	114.10
1	A	160	GLN	CB-CA-C	7.21	123.53	109.33
1	A	156	ALA	CA-C-O	-7.20	113.92	121.55
1	A	8	SER	N-CA-C	-7.19	98.60	110.17
1	A	82	GLN	CA-C-O	-7.17	110.57	119.38
1	A	65	GLN	CB-CG-CD	-7.16	100.44	112.60
1	A	44	ILE	CA-C-O	-7.14	113.00	120.64
1	A	149	ILE	O-C-N	7.13	130.17	122.76
1	A	113	ASP	N-CA-C	-7.07	100.36	108.49
1	A	165	GLU	CB-CG-CD	-7.07	100.58	112.60
1	A	68	GLU	CA-CB-CG	7.07	128.24	114.10
1	A	36	LYS	CA-C-N	-7.04	110.97	123.08
1	A	36	LYS	C-N-CA	-7.04	110.97	123.08
1	A	155	GLU	CA-CB-CG	-7.03	100.04	114.10
1	A	76	ILE	CB-CA-C	7.03	124.14	111.36
1	A	35	GLU	CA-C-O	-7.01	110.48	120.51
1	A	45	THR	CA-C-O	-7.01	113.28	120.71
1	A	159	TRP	CA-C-N	-6.99	111.83	122.81
1	A	159	TRP	C-N-CA	-6.99	111.83	122.81
1	A	137	ASN	CA-C-N	6.99	134.89	121.54
1	A	137	ASN	C-N-CA	6.99	134.89	121.54
1	A	176	GLN	CB-CG-CD	6.96	124.44	112.60
1	A	130	ARG	CA-C-O	-6.84	113.43	121.44
1	A	120	GLU	O-C-N	6.84	131.20	123.27
1	A	106	VAL	N-CA-C	6.83	117.74	108.17
1	A	103	ASN	CB-CG-ND2	-6.80	106.19	116.40
1	A	134	LYS	CB-CA-C	-6.80	95.84	109.79
1	A	95	ARG	CD-NE-CZ	6.75	133.86	124.40
1	A	163	LEU	CA-CB-CG	6.75	139.94	116.30
1	A	152	GLN	CA-C-O	6.73	128.36	120.69
1	A	95	ARG	CA-CB-CG	6.71	127.53	114.10
1	A	149	ILE	CA-C-O	-6.70	114.08	121.92
1	A	84	ALA	O-C-N	6.70	130.91	123.01
1	A	14	GLU	CB-CA-C	-6.69	99.43	110.14
1	A	57	LYS	CA-C-N	6.69	132.89	121.86
1	A	57	LYS	C-N-CA	6.69	132.89	121.86
1	A	149	ILE	CA-CB-CG2	-6.68	99.14	110.50
1	A	51	GLN	CA-C-N	-6.64	113.63	123.00
1	A	51	GLN	C-N-CA	-6.64	113.63	123.00
1	A	9	GLU	N-CA-CB	-6.63	99.15	109.69
1	A	142	VAL	CA-C-O	-6.62	113.17	120.72
1	A	36	LYS	O-C-N	6.62	131.76	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	LEU	O-C-N	6.56	129.68	122.20
1	A	4	THR	N-CA-CB	6.56	122.24	110.83
1	A	57	LYS	N-CA-C	6.54	124.73	110.80
1	A	8	SER	CA-C-N	-6.53	111.70	120.90
1	A	8	SER	C-N-CA	-6.53	111.70	120.90
1	A	165	GLU	N-CA-CB	6.50	120.97	110.77
1	A	105	VAL	O-C-N	6.49	129.99	123.18
1	A	130	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	A	120	GLU	OE1-CD-OE2	6.48	138.46	122.90
1	A	50	ASN	O-C-N	-6.48	114.52	122.55
1	A	59	THR	N-CA-C	-6.47	99.90	109.81
1	A	141	ARG	CD-NE-CZ	-6.46	115.35	124.40
1	A	41	GLN	CB-CG-CD	6.45	123.57	112.60
1	A	150	GLN	CA-C-O	-6.45	113.56	121.11
1	A	151	VAL	N-CA-CB	6.45	122.02	111.58
1	A	32	TRP	N-CA-C	6.44	119.90	109.40
1	A	43	TRP	CB-CG-CD2	-6.43	117.80	126.80
1	A	156	ALA	O-C-N	6.41	130.69	122.81
1	A	175	ILE	CA-C-O	6.40	127.80	120.76
1	A	130	ARG	O-C-N	6.37	131.43	123.15
1	A	15	PHE	CA-C-O	-6.37	113.72	121.36
1	A	22	GLY	CA-C-N	-6.36	111.63	122.56
1	A	22	GLY	C-N-CA	-6.36	111.63	122.56
1	A	116	THR	CA-C-N	6.36	131.80	122.39
1	A	116	THR	C-N-CA	6.36	131.80	122.39
1	A	46	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	42	SER	N-CA-CB	6.35	121.78	110.80
1	A	104	LEU	CA-C-O	-6.34	112.46	120.20
1	A	78	GLN	O-C-N	6.33	131.00	122.59
1	A	117	LEU	O-C-N	6.28	131.32	123.28
1	A	53	VAL	N-CA-C	-6.27	103.21	110.05
1	A	18	PRO	N-CA-C	6.27	125.39	112.47
1	A	5	ALA	N-CA-CB	6.22	121.55	110.80
1	A	12	SER	CA-C-O	-6.16	113.58	120.54
1	A	74	LEU	CB-CA-C	6.15	120.45	109.38
1	A	65	GLN	N-CA-CB	6.14	121.42	110.80
1	A	73	THR	N-CA-C	-6.14	98.99	109.24
1	A	1	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	162	LEU	CA-CB-CG	6.11	137.70	116.30
1	A	159	TRP	CA-C-O	-6.06	114.27	121.66
1	A	102	VAL	O-C-N	6.06	129.61	123.07
1	A	85	GLY	N-CA-C	-6.05	102.41	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	GLU	CA-C-N	6.04	129.41	120.90
1	A	23	GLU	C-N-CA	6.04	129.41	120.90
1	A	23	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	73	THR	CB-CA-C	6.02	121.28	109.35
1	A	125	THR	CA-C-O	-5.98	114.37	120.71
1	A	145	GLN	CA-C-N	5.97	133.64	123.01
1	A	145	GLN	C-N-CA	5.97	133.64	123.01
1	A	160	GLN	CA-C-O	-5.97	114.36	121.11
1	A	162	LEU	O-C-N	5.96	130.58	123.24
1	A	11	GLU	CA-CB-CG	5.96	126.02	114.10
1	A	100	GLN	CA-C-O	-5.96	113.45	120.60
1	A	20	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	119	CYS	O-C-N	5.90	130.56	123.36
1	A	32	TRP	CA-C-N	-5.90	114.46	123.07
1	A	32	TRP	C-N-CA	-5.90	114.46	123.07
1	A	163	LEU	O-C-N	5.89	130.10	123.27
1	A	163	LEU	N-CA-CB	5.88	119.83	110.65
1	A	8	SER	CA-C-O	5.85	128.19	121.28
1	A	28	GLY	N-CA-C	-5.85	100.08	111.03
1	A	152	GLN	CB-CG-CD	5.85	122.54	112.60
1	A	92	THR	N-CA-C	5.81	118.67	109.50
1	A	158	VAL	O-C-N	5.78	130.60	122.97
1	A	48	LEU	O-C-N	5.78	130.07	123.31
1	A	37	ALA	CB-CA-C	5.77	116.65	110.65
1	A	132	ILE	N-CA-CB	-5.76	102.25	111.58
1	A	74	LEU	N-CA-C	-5.76	100.32	109.59
1	A	97	ILE	CA-C-N	5.74	129.63	121.42
1	A	97	ILE	C-N-CA	5.74	129.63	121.42
1	A	144	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	A	167	GLU	N-CA-CB	5.72	118.91	110.56
1	A	155	GLU	CB-CG-CD	-5.71	102.89	112.60
1	A	9	GLU	CA-CB-CG	-5.70	102.69	114.10
1	A	100	GLN	CA-C-N	-5.70	112.94	122.64
1	A	100	GLN	C-N-CA	-5.70	112.94	122.64
1	A	151	VAL	CA-C-O	5.67	126.60	120.43
1	A	143	SER	N-CA-C	-5.66	97.97	107.32
1	A	72	LEU	N-CA-CB	5.65	120.04	110.49
1	A	160	GLN	N-CA-CB	-5.65	101.42	111.08
1	A	76	ILE	CA-CB-CG2	5.63	120.07	110.50
1	A	50	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	107	MET	O-C-N	5.60	130.32	123.21
1	A	4	THR	CA-C-O	-5.56	114.69	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASN	N-CA-CB	-5.56	101.95	110.85
1	A	137	ASN	CA-C-O	5.56	125.74	119.18
1	A	72	LEU	CA-C-N	-5.55	113.73	122.73
1	A	72	LEU	C-N-CA	-5.55	113.73	122.73
1	A	118	THR	CA-C-N	-5.54	113.02	122.33
1	A	118	THR	C-N-CA	-5.54	113.02	122.33
1	A	16	SER	CB-CA-C	5.53	119.72	109.70
1	A	151	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	91	LEU	CA-CB-CG	5.51	135.60	116.30
1	A	14	GLU	OE1-CD-OE2	5.50	136.11	122.90
1	A	116	THR	N-CA-CB	-5.50	101.84	110.69
1	A	109	VAL	CB-CA-C	-5.49	103.38	110.84
1	A	128	LYS	CA-C-O	5.46	128.32	120.51
1	A	18	PRO	CA-C-N	5.45	128.59	120.95
1	A	18	PRO	C-N-CA	5.45	128.59	120.95
1	A	66	LEU	CA-CB-CG	5.45	135.38	116.30
1	A	98	LEU	O-C-N	-5.45	116.58	123.01
1	A	4	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	88	ASN	O-C-N	-5.44	116.31	123.16
1	A	17	PHE	O-C-N	5.43	128.35	121.12
1	A	171	MET	CA-C-O	-5.43	115.47	121.28
1	A	34	ALA	CB-CA-C	5.41	119.17	110.29
1	A	136	GLU	N-CA-CB	5.41	119.63	110.49
1	A	68	GLU	O-C-N	-5.40	115.41	122.59
1	A	12	SER	CA-CB-OG	-5.40	100.31	111.10
1	A	113	ASP	CA-CB-CG	5.38	117.97	112.60
1	A	78	GLN	CG-CD-OE1	5.37	131.54	120.80
1	A	24	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	64	PHE	N-CA-C	-5.36	103.06	110.35
1	A	32	TRP	CD2-CE3-CZ3	5.35	125.56	118.60
1	A	33	LYS	N-CA-CB	5.35	119.11	110.65
1	A	29	GLU	CG-CD-OE2	5.34	130.68	118.40
1	A	66	LEU	CA-C-N	5.34	128.93	121.24
1	A	66	LEU	C-N-CA	5.34	128.93	121.24
1	A	73	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	58	SER	O-C-N	5.33	128.72	121.74
1	A	52	LYS	N-CA-C	-5.31	99.75	108.41
1	A	48	LEU	N-CA-CB	-5.30	101.62	110.80
1	A	97	ILE	N-CA-CB	5.29	118.02	111.41
1	A	62	PRO	CA-N-CD	-5.29	104.10	111.50
1	A	115	ASN	N-CA-CB	5.27	117.60	110.59
1	A	5	ALA	N-CA-C	-5.26	99.87	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CA-CB-CG	5.25	124.60	114.10
1	A	103	ASN	CA-C-N	-5.25	114.62	122.39
1	A	103	ASN	C-N-CA	-5.25	114.62	122.39
1	A	154	PRO	N-CD-CG	-5.25	95.33	103.20
1	A	135	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	A	115	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	135	GLN	N-CA-C	-5.24	101.99	110.32
1	A	139	GLU	N-CA-C	5.23	118.20	110.46
1	A	140	ALA	N-CA-CB	-5.23	101.69	109.69
1	A	116	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	72	LEU	CD1-CG-CD2	-5.20	99.36	110.80
1	A	122	MET	CB-CG-SD	-5.18	97.15	112.70
1	A	80	SER	CB-CA-C	5.17	119.63	110.16
1	A	103	ASN	CA-C-O	-5.16	115.57	121.40
1	A	38	PRO	CB-CA-C	5.12	120.01	111.56
1	A	174	LYS	CA-C-N	5.11	130.07	122.71
1	A	174	LYS	C-N-CA	5.11	130.07	122.71
1	A	36	LYS	N-CA-CB	5.11	117.99	110.33
1	A	40	SER	CA-C-N	5.10	131.28	121.54
1	A	40	SER	C-N-CA	5.10	131.28	121.54
1	A	80	SER	CA-C-N	5.08	127.80	120.38
1	A	80	SER	C-N-CA	5.08	127.80	120.38
1	A	33	LYS	CG-CD-CE	5.08	122.98	111.30
1	A	49	LYS	CB-CG-CD	5.06	122.93	111.30
1	A	100	GLN	O-C-N	5.05	129.44	123.33
1	A	168	GLU	OE1-CD-OE2	5.05	135.02	122.90
1	A	33	LYS	CB-CG-CD	5.04	122.90	111.30
1	A	31	ARG	CB-CG-CD	5.04	122.90	111.30
1	A	111	GLN	CG-CD-NE2	-5.03	108.85	116.40
1	A	107	MET	CG-SD-CE	5.02	111.94	100.90
1	A	37	ALA	O-C-N	5.02	126.15	120.68
1	A	176	GLN	CA-C-O	5.00	125.71	120.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	LEU	Peptide,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	1381	0	1402	99	0
2	A	1	0	0	0	0
3	A	14	0	0	2	0
All	All	1396	0	1402	99	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 36.

All (99) 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:57:LYS:O	3:A:222:HOH:O	1.61	1.14
1:A:32:TRP:HZ3	1:A:102:VAL:HG12	1.28	0.97
1:A:25:SER:HA	1:A:48:LEU:O	1.71	0.89
1:A:49:LYS:O	1:A:50:ASN:ND2	2.05	0.88
1:A:41:GLN:HG3	1:A:43:TRP:CH2	2.09	0.88
1:A:1:THR:O	1:A:100:GLN:OE1	1.93	0.86
1:A:32:TRP:CZ3	1:A:102:VAL:HG12	2.13	0.84
1:A:112:PRO:HG2	1:A:116:THR:CG2	2.13	0.78
1:A:129:MET:HG3	1:A:165:GLU:HB2	1.65	0.77
1:A:36:LYS:O	1:A:38:PRO:HD3	1.83	0.77
1:A:19:LEU:O	1:A:21:LEU:HD23	1.85	0.76
1:A:32:TRP:HZ3	1:A:102:VAL:CG1	1.99	0.72
1:A:33:LYS:HE2	1:A:40:SER:HB2	1.72	0.71
1:A:8:SER:O	1:A:11:GLU:HB2	1.91	0.70
1:A:111:GLN:CD	1:A:177:VAL:HG13	2.17	0.70
1:A:6:TYR:C	1:A:7:LYS:HG2	2.16	0.69
1:A:30:LEU:O	1:A:43:TRP:HA	1.95	0.66
1:A:57:LYS:NZ	1:A:58:SER:O	2.27	0.66
1:A:41:GLN:HG3	1:A:43:TRP:CZ3	2.31	0.66
1:A:131:LEU:HB3	1:A:149:ILE:HD13	1.79	0.65
1:A:115:ASN:HB3	1:A:152:GLN:HE22	1.61	0.65
1:A:21:LEU:HD13	1:A:70:LEU:HD13	1.81	0.62
1:A:99:TYR:HD1	1:A:100:GLN:N	1.97	0.62
1:A:112:PRO:HG2	1:A:116:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:NZ	1:A:40:SER:OG	2.18	0.61
1:A:108:LYS:HE3	1:A:110:THR:HG21	1.83	0.60
1:A:1:THR:C	1:A:100:GLN:OE1	2.44	0.60
1:A:46:PHE:HB2	1:A:54:SER:O	2.03	0.59
1:A:142:VAL:HG13	1:A:144:ARG:HD3	1.85	0.59
1:A:47:SER:HB3	1:A:56:GLN:OE1	2.04	0.58
1:A:120:GLU:HG2	3:A:226:HOH:O	2.04	0.58
1:A:50:ASN:C	1:A:51:GLN:HG2	2.28	0.58
1:A:29:GLU:CD	1:A:31:ARG:HE	2.12	0.58
1:A:111:GLN:NE2	1:A:177:VAL:HG13	2.19	0.58
1:A:99:TYR:CD1	1:A:100:GLN:N	2.73	0.57
1:A:136:GLU:HB2	1:A:158:VAL:HB	1.88	0.56
1:A:44:ILE:HD12	1:A:58:SER:HB3	1.88	0.54
1:A:112:PRO:HG2	1:A:116:THR:HG22	1.90	0.54
1:A:50:ASN:O	1:A:51:GLN:HG2	2.08	0.53
1:A:33:LYS:HZ1	1:A:40:SER:CB	2.19	0.53
1:A:44:ILE:HA	1:A:58:SER:HA	1.90	0.53
1:A:126:SER:O	1:A:129:MET:HB2	2.09	0.52
1:A:108:LYS:HE3	1:A:110:THR:CG2	2.40	0.52
1:A:112:PRO:HD2	1:A:116:THR:HB	1.90	0.52
1:A:46:PHE:HA	1:A:54:SER:O	2.10	0.52
1:A:46:PHE:CA	1:A:54:SER:O	2.58	0.51
1:A:135:GLN:O	1:A:136:GLU:C	2.53	0.51
1:A:106:VAL:O	1:A:121:VAL:HA	2.11	0.50
1:A:81:LEU:HD23	1:A:106:VAL:HG12	1.93	0.50
1:A:46:PHE:CB	1:A:54:SER:O	2.59	0.49
1:A:90:THR:HG22	1:A:97:ILE:CG2	2.41	0.49
1:A:4:THR:HG22	1:A:5:ALA:N	2.28	0.49
1:A:111:GLN:OE1	1:A:177:VAL:HG13	2.12	0.49
1:A:1:THR:O	1:A:100:GLN:CD	2.55	0.48
1:A:86:SER:HB2	1:A:102:VAL:O	2.13	0.48
1:A:164:SER:HB3	1:A:169:VAL:HG22	1.94	0.48
1:A:112:PRO:HD2	1:A:116:THR:C	2.38	0.48
1:A:47:SER:CB	1:A:56:GLN:OE1	2.62	0.47
1:A:112:PRO:HD2	1:A:116:THR:O	2.14	0.47
1:A:46:PHE:HZ	1:A:89:LEU:HD11	1.79	0.47
1:A:81:LEU:HD23	1:A:106:VAL:CG1	2.44	0.47
1:A:165:GLU:HB3	1:A:170:LYS:HE2	1.96	0.47
1:A:164:SER:HA	1:A:168:GLU:O	2.16	0.46
1:A:32:TRP:CZ3	1:A:102:VAL:CG1	2.86	0.46
1:A:136:GLU:CD	1:A:158:VAL:HG11	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:CB	1:A:102:VAL:O	2.65	0.45
1:A:19:LEU:C	1:A:21:LEU:HD23	2.42	0.45
1:A:45:THR:O	1:A:56:GLN:O	2.34	0.45
1:A:8:SER:O	1:A:9:GLU:C	2.60	0.45
1:A:53:VAL:HG12	1:A:54:SER:N	2.30	0.45
1:A:1:THR:O	1:A:100:GLN:NE2	2.50	0.45
1:A:65:GLN:HE22	1:A:77:PRO:HG3	1.82	0.45
1:A:107:MET:HE3	1:A:171:MET:HE3	1.98	0.44
1:A:117:LEU:HD11	1:A:175:ILE:HG21	1.99	0.44
1:A:163:LEU:HD12	1:A:170:LYS:HB2	1.99	0.44
1:A:52:LYS:HE2	1:A:68:GLU:HB3	2.00	0.44
1:A:47:SER:N	1:A:54:SER:O	2.46	0.44
1:A:144:ARG:HB2	1:A:149:ILE:HG21	2.00	0.44
1:A:41:GLN:HG3	1:A:43:TRP:HH2	1.76	0.43
1:A:31:ARG:NH1	1:A:31:ARG:HB3	2.33	0.43
1:A:17:PHE:HA	1:A:18:PRO:HD3	1.56	0.43
1:A:52:LYS:NZ	1:A:68:GLU:HB3	2.34	0.43
1:A:11:GLU:O	1:A:79:VAL:HB	2.19	0.43
1:A:41:GLN:CG	1:A:43:TRP:CZ3	3.02	0.42
1:A:63:LYS:O	1:A:77:PRO:HD3	2.20	0.42
1:A:90:THR:HG22	1:A:97:ILE:HG21	2.00	0.42
1:A:131:LEU:C	1:A:132:ILE:HG13	2.43	0.42
1:A:161:CYS:O	1:A:172:ASP:HA	2.19	0.42
1:A:113:ASP:OD1	1:A:116:THR:N	2.52	0.42
1:A:168:GLU:CD	1:A:170:LYS:HZ2	2.28	0.42
1:A:70:LEU:HA	1:A:71:PRO:HA	1.26	0.42
1:A:128:LYS:O	1:A:165:GLU:HA	2.20	0.41
1:A:19:LEU:H	1:A:19:LEU:HG	1.47	0.41
1:A:48:LEU:HD11	1:A:70:LEU:HD21	2.02	0.41
1:A:71:PRO:O	1:A:72:LEU:HB3	2.21	0.41
1:A:33:LYS:HE2	1:A:40:SER:CB	2.45	0.40
1:A:144:ARG:HB2	1:A:149:ILE:CG2	2.51	0.40
1:A:163:LEU:CD1	1:A:170:LYS:HB2	2.52	0.40
1:A:41:GLN:HA	1:A:43:TRP:CZ3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	175/177 (99%)	150 (86%)	16 (9%)	9 (5%)	1 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	20	ASN
1	A	21	LEU
1	A	41	GLN
1	A	39	SER
1	A	93	LEU
1	A	57	LYS
1	A	18	PRO
1	A	71	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/160 (100%)	105 (66%)	55 (34%)	0 0

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	8	SER

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Mol	Chain	Res	Type
1	A	11	GLU
1	A	19	LEU
1	A	20	ASN
1	A	21	LEU
1	A	23	GLU
1	A	25	SER
1	A	29	GLU
1	A	30	LEU
1	A	31	ARG
1	A	33	LYS
1	A	36	LYS
1	A	41	GLN
1	A	44	ILE
1	A	48	LEU
1	A	49	LYS
1	A	50	ASN
1	A	51	GLN
1	A	54	SER
1	A	57	LYS
1	A	60	SER
1	A	63	LYS
1	A	65	GLN
1	A	66	LEU
1	A	70	LEU
1	A	71	PRO
1	A	74	LEU
1	A	75	GLN
1	A	76	ILE
1	A	78	GLN
1	A	79	VAL
1	A	89	LEU
1	A	90	THR
1	A	91	LEU
1	A	93	LEU
1	A	94	ASP
1	A	95	ARG
1	A	99	TYR
1	A	102	VAL
1	A	103	ASN
1	A	105	VAL
1	A	118	THR
1	A	121	VAL

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Mol	Chain	Res	Type
1	A	127	PRO
1	A	134	LYS
1	A	135	GLN
1	A	150	GLN
1	A	152	GLN
1	A	155	GLU
1	A	162	LEU
1	A	163	LEU
1	A	165	GLU
1	A	167	GLU
1	A	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	88	ASN
1	A	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is modelled with single atom - 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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.