



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 12:38 AM UTC

PDB ID : 1IDN / pdb_00001idn
Title : MAC-1 I DOMAIN METAL FREE
Authors : Baldwin, E.T.
Deposited on : 1998-06-10
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

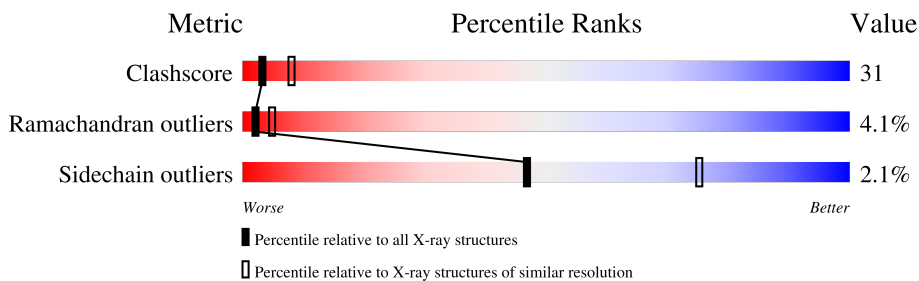
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	1	190	35% 47% 15% .
1	2	190	31% 46% 21% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3238 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 CD11B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	190	Total	C	N	O	S	0	0	0
			1530	975	271	281	3			
1	2	190	Total	C	N	O	S	0	0	0
			1530	975	271	281	3			

- Molecule 2 is water.

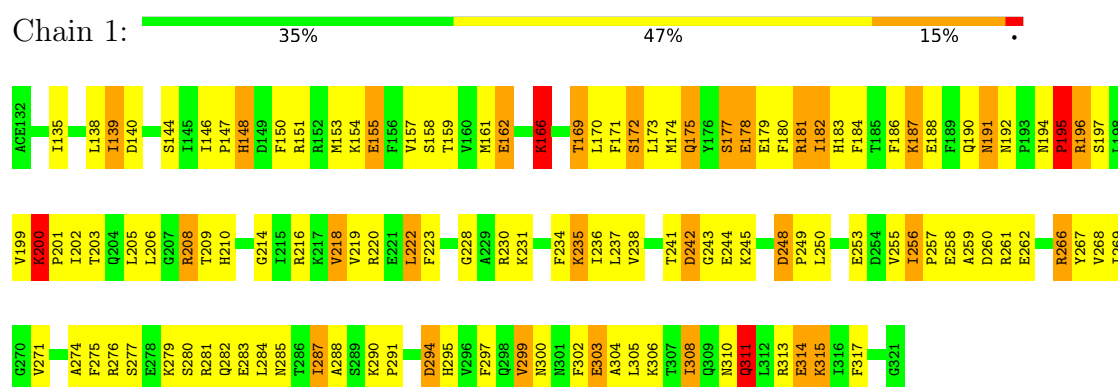
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	129	Total	O	0	0
			129	129		
2	2	49	Total	O	0	0
			49	49		

3 Residue-property plots

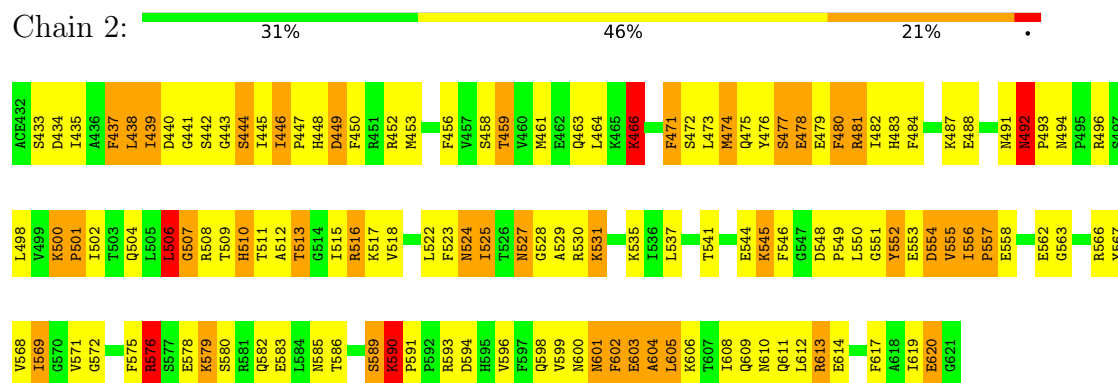
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CD11B



• Molecule 1: CD11B



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	49.32Å 124.05Å 76.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	68.0 (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ, XTALVIEW	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3238	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: ACE

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	1	1.36	4/1557 (0.3%)	2.50	100/2095 (4.8%)
1	2	1.32	4/1557 (0.3%)	2.49	110/2095 (5.3%)
All	All	1.34	8/3114 (0.3%)	2.50	210/4190 (5.0%)

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	2	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	593	ARG	CD-NE	-6.95	1.36	1.46
1	1	266	ARG	CA-CB	5.96	1.61	1.53
1	2	509	THR	CA-CB	5.84	1.61	1.53
1	2	524	ASN	N-CA	5.74	1.52	1.45
1	1	288	ALA	CA-CB	5.63	1.62	1.53
1	2	502	ILE	CA-CB	5.33	1.59	1.54
1	1	209	THR	CA-CB	5.24	1.60	1.52
1	1	166	LYS	N-CA	5.02	1.52	1.46

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	613	ARG	CD-NE-CZ	18.01	149.61	124.40
1	1	216	ARG	CD-NE-CZ	17.30	148.62	124.40
1	2	593	ARG	CD-NE-CZ	16.66	147.72	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	151	ARG	CD-NE-CZ	14.77	145.08	124.40
1	2	594	ASP	CA-CB-CG	13.46	126.06	112.60
1	1	148	HIS	CA-CB-CG	13.08	126.88	113.80
1	1	216	ARG	NE-CZ-NH2	11.91	129.92	119.20
1	2	491	ASN	CA-CB-CG	11.88	124.47	112.60
1	1	200	LYS	CB-CG-CD	11.69	138.18	111.30
1	1	315	LYS	CA-CB-CG	11.62	137.34	114.10
1	1	200	LYS	CG-CD-CE	11.53	137.81	111.30
1	1	195	PRO	CA-C-N	11.19	135.72	120.38
1	1	195	PRO	C-N-CA	11.19	135.72	120.38
1	1	300	ASN	CA-CB-CG	11.13	123.73	112.60
1	2	449	ASP	CA-CB-CG	10.48	123.08	112.60
1	1	200	LYS	CA-CB-CG	9.96	134.02	114.10
1	2	566	ARG	CD-NE-CZ	9.89	138.25	124.40
1	1	181	ARG	CA-CB-CG	9.80	133.71	114.10
1	1	184	PHE	CA-CB-CG	9.78	123.58	113.80
1	2	617	PHE	CA-CB-CG	9.36	123.16	113.80
1	2	590	LYS	CA-CB-CG	9.34	132.78	114.10
1	2	585	ASN	CA-CB-CG	9.31	121.91	112.60
1	2	500	LYS	CA-CB-CG	9.28	132.65	114.10
1	1	256	ILE	O-C-N	9.21	126.31	120.42
1	2	546	PHE	CA-CB-CG	9.01	122.81	113.80
1	2	548	ASP	CA-CB-CG	8.99	121.59	112.60
1	2	478	GLU	N-CA-C	-8.92	102.17	113.23
1	1	261	ARG	N-CA-CB	8.87	123.16	110.12
1	2	593	ARG	CG-CD-NE	8.86	131.49	112.00
1	2	562	GLU	CA-CB-CG	8.80	131.71	114.10
1	1	242	ASP	CA-CB-CG	8.78	121.38	112.60
1	1	288	ALA	N-CA-C	8.71	123.37	110.48
1	2	434	ASP	CB-CA-C	8.54	125.94	111.68
1	1	177	SER	CA-CB-OG	8.50	128.10	111.10
1	1	317	PHE	CA-CB-CG	8.46	122.26	113.80
1	2	555	VAL	N-CA-C	8.33	121.69	113.53
1	1	310	ASN	N-CA-C	8.32	120.35	111.28
1	2	602	PHE	CA-CB-CG	-8.29	105.51	113.80
1	2	494	ASN	CA-CB-CG	8.20	120.80	112.60
1	1	299	VAL	CA-C-N	7.83	131.82	120.38
1	1	299	VAL	C-N-CA	7.83	131.82	120.38
1	2	479	GLU	CB-CG-CD	7.81	125.87	112.60
1	2	571	VAL	N-CA-C	7.77	119.05	108.17
1	1	206	LEU	N-CA-C	7.70	121.98	112.58
1	2	553	GLU	CA-CB-CG	7.69	129.48	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	481	ARG	N-CA-C	7.67	120.90	108.41
1	2	613	ARG	NE-CZ-NH2	7.63	126.07	119.20
1	2	444	SER	CA-C-O	7.46	126.96	118.97
1	1	243	GLY	CA-C-O	7.45	128.96	121.29
1	1	162	GLU	CB-CG-CD	7.43	125.24	112.60
1	2	471	PHE	CA-CB-CG	7.41	121.21	113.80
1	1	314	GLU	CB-CG-CD	7.32	125.04	112.60
1	1	175	GLN	N-CA-CB	7.31	122.54	110.85
1	2	572	GLY	CA-C-N	7.20	135.28	121.54
1	2	572	GLY	C-N-CA	7.20	135.28	121.54
1	1	219	VAL	N-CA-C	7.19	117.96	110.62
1	2	444	SER	CA-C-N	7.19	132.34	122.93
1	2	444	SER	C-N-CA	7.19	132.34	122.93
1	2	553	GLU	CB-CG-CD	7.14	124.74	112.60
1	1	178	GLU	N-CA-C	-7.09	104.27	114.12
1	1	139	ILE	N-CA-C	7.04	118.43	108.36
1	2	446	ILE	CB-CA-C	7.00	118.73	110.68
1	2	474	MET	N-CA-CB	6.96	124.48	111.53
1	1	258	GLU	N-CA-CB	6.96	120.46	110.16
1	2	576	ARG	CG-CD-NE	6.92	127.22	112.00
1	1	172	SER	CA-C-O	-6.86	113.31	120.99
1	1	179	GLU	CA-C-O	-6.80	113.08	121.78
1	1	177	SER	N-CA-CB	6.77	121.94	110.49
1	1	303	GLU	CA-CB-CG	6.71	127.53	114.10
1	1	235	LYS	CA-CB-CG	6.70	127.49	114.10
1	2	446	ILE	CA-C-N	6.68	128.19	119.84
1	2	446	ILE	C-N-CA	6.68	128.19	119.84
1	1	216	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	1	175	GLN	CA-CB-CG	6.68	127.46	114.10
1	2	513	THR	N-CA-CB	6.67	120.07	110.06
1	1	255	VAL	N-CA-C	6.63	117.27	111.90
1	2	492	ASN	CA-CB-CG	6.62	119.22	112.60
1	2	506	LEU	CA-CB-CG	6.59	139.36	116.30
1	2	506	LEU	CA-C-O	-6.54	111.16	120.51
1	1	182	ILE	N-CA-CB	6.54	119.44	111.60
1	1	175	GLN	CA-C-O	-6.51	113.80	121.16
1	1	260	ASP	CA-CB-CG	6.49	119.08	112.60
1	2	553	GLU	CB-CA-C	-6.47	100.05	110.79
1	1	256	ILE	N-CA-CB	6.47	114.85	110.52
1	1	287	ILE	CA-C-N	6.46	132.11	121.39
1	1	287	ILE	C-N-CA	6.46	132.11	121.39
1	2	482	ILE	N-CA-CB	6.45	118.31	112.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	294	ASP	CA-CB-CG	-6.43	106.17	112.60
1	1	191	ASN	CA-CB-CG	6.41	119.01	112.60
1	1	186	PHE	O-C-N	6.40	129.71	122.22
1	2	589	SER	CA-C-O	-6.40	113.56	121.88
1	2	481	ARG	CA-CB-CG	6.36	126.81	114.10
1	1	186	PHE	CA-CB-CG	6.35	120.15	113.80
1	2	524	ASN	CA-CB-CG	6.35	118.95	112.60
1	1	285	ASN	CA-CB-CG	-6.33	106.27	112.60
1	2	569	ILE	CA-C-O	-6.31	113.82	120.57
1	2	601	ASN	CA-CB-CG	6.31	118.91	112.60
1	1	315	LYS	CB-CG-CD	6.30	125.79	111.30
1	1	295	HIS	CA-CB-CG	-6.29	107.51	113.80
1	2	569	ILE	CB-CG1-CD1	6.27	126.97	113.80
1	2	586	THR	N-CA-C	6.25	119.37	111.69
1	2	598	GLN	CA-CB-CG	6.24	126.58	114.10
1	2	439	ILE	CA-C-N	6.24	131.28	121.99
1	2	439	ILE	C-N-CA	6.24	131.28	121.99
1	1	253	GLU	CA-CB-CG	6.21	126.51	114.10
1	1	311	GLN	CA-CB-CG	6.18	126.47	114.10
1	2	605	LEU	N-CA-C	-6.18	105.90	113.50
1	2	516	ARG	CD-NE-CZ	6.17	133.04	124.40
1	2	567	TYR	CA-CB-CG	6.17	125.00	113.90
1	2	554	ASP	CA-CB-CG	6.16	118.76	112.60
1	2	437	PHE	CA-CB-CG	6.14	119.94	113.80
1	2	510	HIS	CA-CB-CG	6.12	119.92	113.80
1	2	556	ILE	CA-C-O	6.10	122.78	118.69
1	1	166	LYS	CB-CA-C	6.09	121.95	110.62
1	2	504	GLN	CB-CG-CD	6.08	122.93	112.60
1	1	192	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	1	203	THR	CA-C-N	6.04	129.28	120.71
1	1	203	THR	C-N-CA	6.04	129.28	120.71
1	2	590	LYS	CB-CG-CD	6.03	125.17	111.30
1	2	563	GLY	CA-C-N	6.01	130.51	122.93
1	2	563	GLY	C-N-CA	6.01	130.51	122.93
1	2	524	ASN	CB-CA-C	5.97	119.66	109.80
1	2	482	ILE	O-C-N	5.96	128.98	122.36
1	1	155	GLU	CG-CD-OE1	5.92	132.01	118.40
1	1	155	GLU	CB-CG-CD	5.89	122.61	112.60
1	1	218	VAL	N-CA-C	-5.88	104.18	110.36
1	2	531	LYS	N-CA-C	5.85	117.65	111.28
1	2	501	PRO	N-CA-C	5.84	121.52	113.98
1	1	242	ASP	N-CA-CB	5.84	119.40	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	181	ARG	N-CA-C	5.83	118.23	108.73
1	1	208	ARG	CD-NE-CZ	-5.83	116.24	124.40
1	1	148	HIS	N-CA-CB	5.82	118.87	110.20
1	2	439	ILE	N-CA-C	5.79	116.92	108.53
1	2	558	GLU	O-C-N	5.78	130.87	122.43
1	1	206	LEU	CA-C-O	-5.77	113.64	120.57
1	2	596	VAL	N-CA-C	5.77	116.90	108.53
1	1	238	VAL	CA-C-O	-5.75	114.38	120.53
1	2	608	ILE	N-CA-C	5.72	118.39	112.90
1	1	243	GLY	N-CA-C	5.71	119.41	110.91
1	2	508	ARG	CD-NE-CZ	5.71	132.39	124.40
1	1	191	ASN	N-CA-CB	5.69	118.47	110.90
1	1	317	PHE	N-CA-CB	5.68	118.85	110.33
1	1	248	ASP	O-C-N	5.64	127.62	121.36
1	2	562	GLU	CB-CG-CD	5.63	122.17	112.60
1	1	196	ARG	N-CA-C	5.61	118.12	111.33
1	1	208	ARG	CB-CG-CD	5.54	124.05	111.30
1	2	576	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	2	548	ASP	CB-CA-C	5.51	116.86	109.42
1	2	478	GLU	CA-CB-CG	5.50	125.10	114.10
1	1	157	VAL	CA-C-O	-5.49	115.71	121.41
1	1	196	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	1	222	LEU	N-CA-C	5.45	117.22	111.28
1	2	545	LYS	N-CA-CB	-5.44	101.30	110.49
1	2	619	ILE	CB-CA-C	5.44	120.21	111.29
1	2	459	THR	CA-C-O	-5.43	115.12	120.82
1	2	438	LEU	CA-C-N	-5.42	116.10	123.10
1	2	438	LEU	C-N-CA	-5.42	116.10	123.10
1	1	235	LYS	CB-CG-CD	5.42	123.76	111.30
1	1	315	LYS	N-CA-CB	5.42	119.64	110.49
1	2	509	THR	N-CA-C	5.41	117.57	107.99
1	2	525	ILE	CB-CG1-CD1	5.41	125.16	113.80
1	2	572	GLY	N-CA-C	5.40	123.79	112.45
1	2	568	VAL	CA-CB-CG1	5.38	119.55	110.40
1	1	216	ARG	CB-CA-C	-5.35	102.48	110.88
1	1	230	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	1	181	ARG	CB-CG-CD	5.32	123.53	111.30
1	2	444	SER	N-CA-C	-5.29	107.19	113.97
1	2	578	GLU	CB-CA-C	5.29	118.86	109.65
1	1	169	THR	CA-CB-OG1	-5.29	101.66	109.60
1	2	552	TYR	CA-C-N	5.29	127.37	120.28
1	2	552	TYR	C-N-CA	5.29	127.37	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	603	GLU	CA-CB-CG	5.28	124.66	114.10
1	2	591	PRO	CA-C-N	5.28	124.79	119.19
1	2	591	PRO	C-N-CA	5.28	124.79	119.19
1	2	579	LYS	N-CA-CB	5.28	118.17	110.47
1	1	258	GLU	O-C-N	5.26	128.15	122.15
1	1	158	SER	N-CA-CB	5.23	117.73	109.94
1	2	474	MET	O-C-N	5.23	129.34	123.27
1	1	294	ASP	CA-C-O	-5.23	112.95	119.38
1	2	466	LYS	CA-CB-CG	5.23	124.56	114.10
1	2	481	ARG	CB-CA-C	-5.22	101.49	110.16
1	2	527	ASN	CA-CB-CG	-5.22	107.38	112.60
1	1	267	TYR	O-C-N	5.21	130.01	123.23
1	2	458	SER	N-CA-CB	5.21	117.56	110.01
1	1	299	VAL	CB-CA-C	5.20	119.71	110.71
1	2	610	ASN	CB-CA-C	5.20	119.19	110.92
1	2	480	PHE	CA-C-N	5.18	130.30	123.00
1	2	480	PHE	C-N-CA	5.18	130.30	123.00
1	1	150	PHE	N-CA-CB	5.17	118.18	110.22
1	1	260	ASP	CA-C-O	-5.16	115.38	120.70
1	2	478	GLU	CB-CA-C	5.16	120.02	109.55
1	1	236	ILE	CA-C-O	-5.15	114.65	120.67
1	2	598	GLN	CB-CG-CD	5.15	121.35	112.60
1	1	190	GLN	CA-C-N	5.14	130.30	122.24
1	1	190	GLN	C-N-CA	5.14	130.30	122.24
1	2	459	THR	N-CA-CB	5.12	117.43	110.01
1	1	159	THR	N-CA-C	5.09	116.83	111.28
1	1	231	LYS	N-CA-C	5.09	117.23	111.02
1	1	178	GLU	O-C-N	5.08	128.16	122.27
1	1	196	ARG	CB-CG-CD	5.07	122.96	111.30
1	1	255	VAL	CA-C-O	-5.06	115.54	120.30
1	2	512	ALA	CA-C-O	-5.06	115.50	121.07
1	1	276	ARG	CB-CA-C	-5.03	100.56	110.11
1	1	202	ILE	N-CA-C	5.02	115.71	108.93
1	2	567	TYR	CA-C-O	-5.02	114.92	120.24
1	1	234	PHE	N-CA-CB	5.02	117.25	110.38
1	2	605	LEU	O-C-N	5.01	129.21	122.49
1	2	474	MET	CA-CB-CG	5.01	124.11	114.10
1	2	479	GLU	CG-CD-OE1	5.00	129.91	118.40
1	2	602	PHE	CA-C-O	-5.00	115.55	120.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	576	ARG	Sidechain

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	1	1530	0	1550	95	0
1	2	1530	0	1550	97	1
2	1	129	0	0	13	0
2	2	49	0	0	6	1
All	All	3238	0	3100	189	1

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 31.

All (189) 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)
1:1:181:ARG:HG2	1:1:205:LEU:HD11	1.29	1.11
1:2:439:ILE:HD11	1:2:473:LEU:HD21	1.29	1.10
1:2:518:VAL:HG13	1:2:522:LEU:HD12	1.45	0.98
1:1:183:HIS:HB3	2:1:824:HOH:O	1.62	0.98
1:2:609:GLN:HB2	2:2:42:HOH:O	1.68	0.93
1:1:311:GLN:HE21	1:1:311:GLN:H	1.11	0.91
1:1:294:ASP:O	1:1:315:LYS:NZ	2.06	0.88
1:1:218:VAL:HG11	1:1:237:LEU:HD13	1.56	0.86
1:1:277:SER:C	1:1:279:LYS:H	1.85	0.81
1:2:472:SER:OG	1:2:522:LEU:HD22	1.80	0.80
1:1:311:GLN:H	1:1:311:GLN:NE2	1.79	0.80
1:1:242:ASP:OD1	2:1:61:HOH:O	1.98	0.79
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.63	0.79
1:1:194:ASN:HD22	1:1:197:SER:H	1.33	0.75
1:1:306:LYS:HD2	1:1:306:LYS:H	1.52	0.74
1:2:599:VAL:HG11	1:2:605:LEU:HD23	1.71	0.73
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.25	0.72
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.71	0.71
1:1:306:LYS:H	1:1:306:LYS:CD	2.03	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:466:LYS:HE3	1:2:620:GLU:HG2	1.72	0.71
1:1:306:LYS:HD2	1:1:306:LYS:N	2.05	0.71
1:2:518:VAL:HG11	1:2:537:LEU:HD13	1.72	0.71
1:2:513:THR:OG1	1:2:550:LEU:HD13	1.91	0.70
1:1:162:GLU:HA	2:1:53:HOH:O	1.90	0.70
1:2:609:GLN:CG	2:2:42:HOH:O	2.39	0.69
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.75	0.68
1:1:155:GLU:OE2	2:1:915:HOH:O	2.11	0.68
1:2:609:GLN:CB	2:2:42:HOH:O	2.36	0.68
1:1:195:PRO:O	1:1:199:VAL:HG23	1.95	0.67
1:1:178:GLU:HG3	1:1:208:ARG:H	1.59	0.67
1:2:545:LYS:NZ	1:2:551:GLY:HA2	2.10	0.67
1:2:442:SER:C	1:2:444:SER:H	2.03	0.66
1:1:166:LYS:NZ	1:1:166:LYS:HB2	2.12	0.65
1:1:178:GLU:OE2	1:1:208:ARG:HG3	1.96	0.65
1:1:144:SER:O	2:1:810:HOH:O	2.15	0.65
1:1:277:SER:O	1:1:281:ARG:HG2	1.97	0.64
1:1:155:GLU:OE1	1:1:196:ARG:NH1	2.31	0.64
1:2:466:LYS:HE3	1:2:620:GLU:CG	2.28	0.63
1:2:449:ASP:OD2	1:2:602:PHE:HD2	1.82	0.63
1:1:244:GLU:OE2	1:1:280:SER:HB3	1.98	0.63
1:1:194:ASN:HD22	1:1:197:SER:N	1.98	0.62
1:1:181:ARG:HG2	1:1:205:LEU:CD1	2.20	0.62
1:1:162:GLU:CA	2:1:53:HOH:O	2.47	0.61
1:1:173:LEU:HD23	1:1:174:MET:N	2.15	0.61
1:2:609:GLN:CD	2:2:42:HOH:O	2.43	0.61
1:2:603:GLU:O	1:2:606:LYS:HG2	2.01	0.61
1:1:269:ILE:HA	1:1:297:PHE:O	2.00	0.61
1:1:308:ILE:HA	1:1:311:GLN:NE2	2.14	0.61
1:1:166:LYS:HB2	1:1:166:LYS:HZ2	1.66	0.60
1:2:437:PHE:HB2	1:2:473:LEU:HD12	1.83	0.60
1:2:545:LYS:HZ1	1:2:551:GLY:HA2	1.68	0.59
1:1:220:ARG:NH1	2:1:59:HOH:O	2.35	0.58
1:2:440:ASP:C	1:2:440:ASP:OD1	2.47	0.58
1:2:439:ILE:HD11	1:2:473:LEU:CD2	2.18	0.58
1:2:477:SER:OG	1:2:478:GLU:N	2.36	0.57
1:2:444:SER:HA	2:2:36:HOH:O	2.04	0.57
1:2:459:THR:HG22	1:2:463:GLN:HE21	1.70	0.57
1:1:181:ARG:NE	1:1:205:LEU:HD21	2.21	0.56
1:1:266:ARG:NH2	2:1:858:HOH:O	2.38	0.56
1:2:513:THR:O	1:2:517:LYS:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:178:GLU:CD	1:1:208:ARG:HG3	2.31	0.55
1:2:443:GLY:N	1:2:506:LEU:HA	2.21	0.55
1:2:473:LEU:HG	1:2:474:MET:N	2.20	0.55
1:1:148:HIS:HB2	2:1:816:HOH:O	2.06	0.55
1:1:187:LYS:HB3	1:1:228:GLY:HA3	1.88	0.55
1:1:138:LEU:HA	1:1:174:MET:O	2.07	0.55
1:1:180:PHE:N	2:1:837:HOH:O	2.32	0.55
1:2:531:LYS:HA	2:2:47:HOH:O	2.06	0.55
1:2:511:THR:O	1:2:515:ILE:HG13	2.07	0.55
1:2:448:HIS:HD2	1:2:452:ARG:CZ	2.20	0.54
1:1:274:ALA:O	1:1:280:SER:OG	2.19	0.54
1:2:445:ILE:CG2	1:2:450:PHE:HB2	2.33	0.53
1:1:194:ASN:O	1:1:195:PRO:C	2.52	0.52
1:2:459:THR:HG22	1:2:463:GLN:HG3	1.92	0.52
1:2:556:ILE:HB	1:2:557:PRO:HD3	1.90	0.52
1:1:172:SER:OG	1:1:222:LEU:HD22	2.10	0.52
1:2:524:ASN:O	1:2:529:ALA:HB3	2.10	0.52
1:2:544:GLU:HA	1:2:583:GLU:OE1	2.09	0.52
1:1:279:LYS:O	1:1:282:GLN:HB3	2.10	0.51
1:2:550:LEU:HA	1:2:554:ASP:OD2	2.10	0.51
1:1:290:LYS:HA	1:1:291:PRO:C	2.36	0.51
1:1:177:SER:O	1:1:210:HIS:HB2	2.11	0.51
1:2:443:GLY:HA2	1:2:506:LEU:CD2	2.41	0.51
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.41	0.51
1:1:169:THR:HG22	1:1:170:LEU:N	2.26	0.50
1:1:299:VAL:CG2	1:1:304:ALA:HB3	2.42	0.50
1:2:456:PHE:HE2	1:2:605:LEU:O	1.94	0.50
1:1:135:ILE:O	1:1:171:PHE:HA	2.11	0.50
1:1:294:ASP:HB3	2:1:15:HOH:O	2.12	0.50
1:1:277:SER:O	1:1:279:LYS:N	2.44	0.50
1:1:308:ILE:HD12	1:1:308:ILE:C	2.37	0.49
1:1:256:ILE:O	1:1:259:ALA:HB3	2.12	0.49
1:2:506:LEU:O	1:2:507:GLY:O	2.30	0.49
1:2:552:TYR:O	1:2:556:ILE:HG12	2.12	0.49
1:1:244:GLU:HA	1:1:283:GLU:OE1	2.12	0.49
1:1:313:ARG:NE	1:1:314:GLU:OE2	2.46	0.49
1:1:166:LYS:NZ	1:1:166:LYS:CB	2.75	0.49
1:1:146:ILE:HB	1:1:147:PRO:HD2	1.94	0.49
1:2:556:ILE:N	1:2:557:PRO:CD	2.76	0.49
1:1:153:MET:CE	1:1:302:PHE:HE2	2.26	0.49
1:1:256:ILE:HB	1:1:257:PRO:HD3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:443:GLY:HA2	1:2:506:LEU:HD23	1.94	0.48
1:2:498:LEU:O	1:2:501:PRO:HD2	2.14	0.48
1:2:516:ARG:NH1	1:2:550:LEU:HD21	2.28	0.48
1:1:275:PHE:HA	1:1:280:SER:OG	2.14	0.48
1:2:496:ARG:O	1:2:500:LYS:HG2	2.14	0.48
1:2:511:THR:HG22	1:2:515:ILE:HD11	1.96	0.47
1:2:456:PHE:CE2	1:2:605:LEU:O	2.68	0.47
1:1:214:GLY:O	1:1:218:VAL:HG23	2.13	0.47
1:1:144:SER:HB2	2:1:810:HOH:O	2.15	0.47
1:2:611:GLN:OE1	1:2:611:GLN:N	2.44	0.47
1:2:530:ARG:O	1:2:535:LYS:NZ	2.42	0.47
1:2:599:VAL:HG13	1:2:604:ALA:O	2.14	0.47
1:1:281:ARG:C	1:1:283:GLU:N	2.73	0.46
1:1:303:GLU:O	1:1:306:LYS:HD3	2.15	0.46
1:2:516:ARG:HB2	1:2:555:VAL:HG11	1.97	0.46
1:2:477:SER:O	1:2:510:HIS:HB2	2.15	0.46
1:2:453:MET:HE3	1:2:602:PHE:CE1	2.51	0.46
1:1:245:LYS:HD2	1:1:248:ASP:HB3	1.98	0.46
1:1:299:VAL:HG11	1:1:305:LEU:HD23	1.96	0.46
1:1:223:PHE:CD1	1:1:235:LYS:HD2	2.51	0.45
1:1:302:PHE:HE1	2:1:808:HOH:O	1.99	0.45
1:1:194:ASN:ND2	1:1:197:SER:H	2.09	0.45
1:2:464:LEU:HD21	1:2:613:ARG:HA	1.97	0.45
1:2:552:TYR:OH	1:2:583:GLU:OE2	2.29	0.45
1:2:480:PHE:CZ	1:2:513:THR:HG22	2.51	0.45
1:1:268:VAL:HG12	1:1:284:LEU:HD22	1.99	0.45
1:2:439:ILE:HG12	1:2:473:LEU:HD11	1.98	0.45
1:1:139:ILE:HG13	1:1:175:GLN:CB	2.46	0.45
1:2:611:GLN:HA	1:2:614:GLU:HG2	1.98	0.45
1:1:249:PRO:HB2	1:2:550:LEU:HD11	1.98	0.45
1:2:459:THR:CG2	1:2:463:GLN:HE21	2.28	0.45
1:2:600:ASN:O	1:2:601:ASN:HB3	2.17	0.44
1:1:169:THR:O	1:1:170:LEU:HD23	2.17	0.44
1:2:464:LEU:HD23	1:2:613:ARG:HG3	2.00	0.44
1:2:589:SER:C	1:2:590:LYS:HE3	2.42	0.44
1:2:446:ILE:HD11	1:2:449:ASP:OD1	2.18	0.44
1:1:161:MET:HE3	1:1:171:PHE:CB	2.48	0.44
1:1:161:MET:HE3	1:1:171:PHE:HB3	1.99	0.44
1:1:311:GLN:HE21	1:1:311:GLN:N	1.95	0.44
1:2:576:ARG:O	1:2:576:ARG:HG2	2.18	0.44
1:1:138:LEU:HD22	1:1:218:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:575:PHE:HA	1:2:580:SER:OG	2.18	0.44
1:2:439:ILE:CD1	1:2:473:LEU:HD11	2.47	0.44
1:2:439:ILE:CD1	1:2:473:LEU:HD21	2.21	0.44
1:2:579:LYS:O	1:2:582:GLN:HB3	2.18	0.43
1:2:484:PHE:HA	1:2:488:GLU:OE2	2.18	0.43
1:1:256:ILE:N	1:1:257:PRO:CD	2.81	0.43
1:2:443:GLY:CA	1:2:506:LEU:HD22	2.48	0.43
1:1:155:GLU:CD	1:1:196:ARG:HH12	2.26	0.43
1:1:299:VAL:CG1	1:1:305:LEU:HD23	2.48	0.43
1:2:541:THR:HG23	1:2:575:PHE:CZ	2.54	0.43
1:1:250:LEU:CD1	1:2:549:PRO:HB2	2.48	0.43
1:1:262:GLU:OE1	1:1:262:GLU:HA	2.19	0.43
1:2:461:MET:HE3	1:2:471:PHE:CB	2.49	0.43
1:2:487:LYS:HB2	1:2:528:GLY:N	2.33	0.43
1:1:249:PRO:CB	1:2:550:LEU:HD11	2.49	0.42
1:2:483:HIS:O	1:2:484:PHE:HB3	2.19	0.42
1:2:550:LEU:H	1:2:550:LEU:HD12	1.84	0.42
1:1:287:ILE:HD13	1:1:287:ILE:HG21	1.85	0.42
1:1:139:ILE:HG13	1:1:175:GLN:HB3	2.01	0.42
1:1:281:ARG:C	1:1:283:GLU:H	2.28	0.42
1:2:492:ASN:H	1:2:493:PRO:HD3	1.84	0.42
1:1:153:MET:HE3	1:1:302:PHE:CE2	2.55	0.42
1:1:188:GLU:HA	1:1:191:ASN:HD22	1.83	0.42
1:2:435:ILE:O	1:2:471:PHE:HA	2.19	0.42
1:2:545:LYS:HZ2	1:2:551:GLY:HA2	1.82	0.42
1:2:438:LEU:HD12	1:2:474:MET:HG3	2.02	0.42
1:1:139:ILE:O	1:1:175:GLN:HB2	2.20	0.41
1:1:140:ASP:CB	1:1:241:THR:HA	2.50	0.41
1:1:174:MET:HE2	1:1:182:ILE:HG12	2.01	0.41
1:1:271:VAL:CG2	1:1:305:LEU:HD21	2.50	0.41
1:2:441:GLY:HA3	1:2:475:GLN:OE1	2.21	0.41
1:2:449:ASP:OD2	1:2:602:PHE:CD2	2.68	0.41
1:2:476:TYR:CD1	1:2:476:TYR:C	2.99	0.41
1:1:248:ASP:OD1	1:1:249:PRO:HD2	2.20	0.41
1:1:154:LYS:HE3	1:1:199:VAL:O	2.21	0.41
1:1:169:THR:CG2	1:1:170:LEU:N	2.84	0.41
1:1:218:VAL:CG1	1:1:237:LEU:HD13	2.40	0.41
1:2:474:MET:HB2	1:2:481:ARG:O	2.21	0.41
1:2:476:TYR:HB2	1:2:480:PHE:CD1	2.56	0.41
1:2:433:SER:HB3	1:2:435:ILE:HG13	2.03	0.40
1:2:492:ASN:ND2	1:2:498:LEU:HD21	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:525:ILE:C	1:2:527:ASN:H	2.29	0.40
1:1:200:LYS:HB3	1:1:201:PRO:HD3	2.03	0.40
1:1:314:GLU:O	1:1:315:LYS:C	2.64	0.40
1:2:437:PHE:HB2	1:2:473:LEU:CD1	2.48	0.40
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.62	0.40
1:2:569:ILE:HD11	1:2:612:LEU:HD22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:590:LYS:O	2:2:34:HOH:O[2_555]	2.13	0.07

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	1	49/190 (26%)	40 (82%)	8 (16%)	1 (2%)	6	16
1	2	172/190 (90%)	142 (83%)	22 (13%)	8 (5%)	2	3
All	All	221/380 (58%)	182 (82%)	30 (14%)	9 (4%)	2	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	492	ASN
1	2	506	LEU
1	2	507	GLY
1	2	466	LYS
1	2	604	ALA
1	2	620	GLU
1	2	477	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	523	PHE
1	1	195	PRO

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	1	168/168 (100%)	163 (97%)	5 (3%)	36	66
1	2	168/168 (100%)	166 (99%)	2 (1%)	63	84
All	All	336/336 (100%)	329 (98%)	7 (2%)	47	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	166	LYS
1	1	187	LYS
1	1	200	LYS
1	1	308	ILE
1	1	311	GLN
1	2	557	PRO
1	2	590	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	191	ASN
1	1	194	ASN
1	1	285	ASN
1	1	298	GLN
1	1	309	GLN
1	1	311	GLN
1	2	448	HIS
1	2	463	GLN
1	2	491	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	492	ASN
1	2	510	HIS
1	2	585	ASN
1	2	601	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](#)

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

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.