



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 1BHO / pdb_00001bho
Title : MAC-1 I DOMAIN MAGNESIUM COMPLEX
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

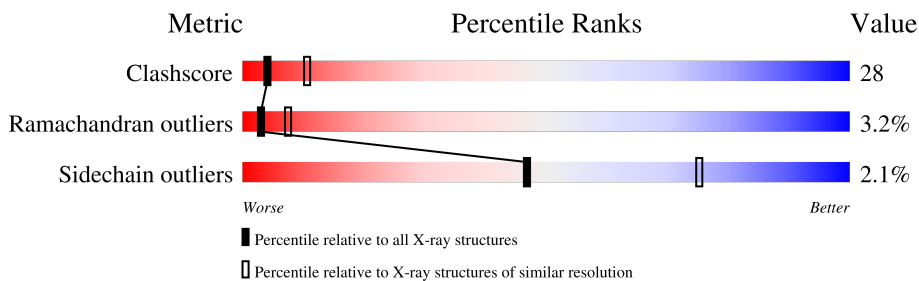
1 Overall quality at a glance

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	36% 41% 21% .
1	2	190	39% 44% 17% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3187 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	Mg	0	0
			1	1		
2	2	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

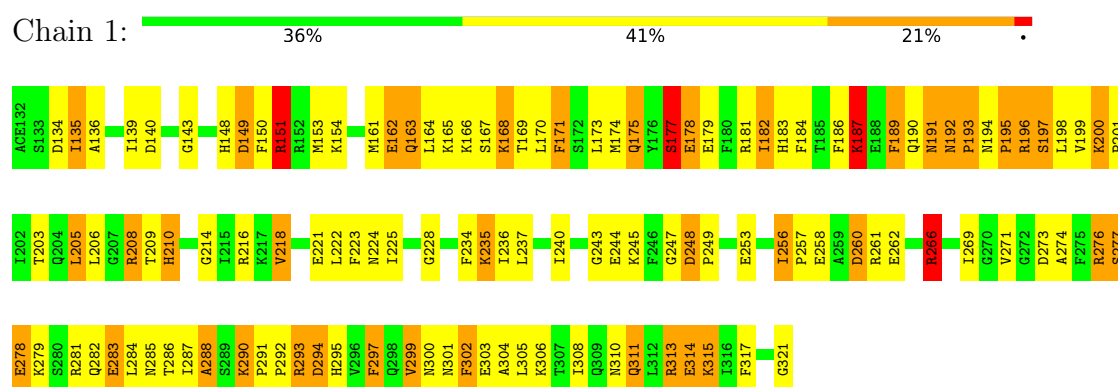
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	90	Total	O	0	0
			90	90		
3	2	35	Total	O	0	0
			35	35		

3 Residue-property plots

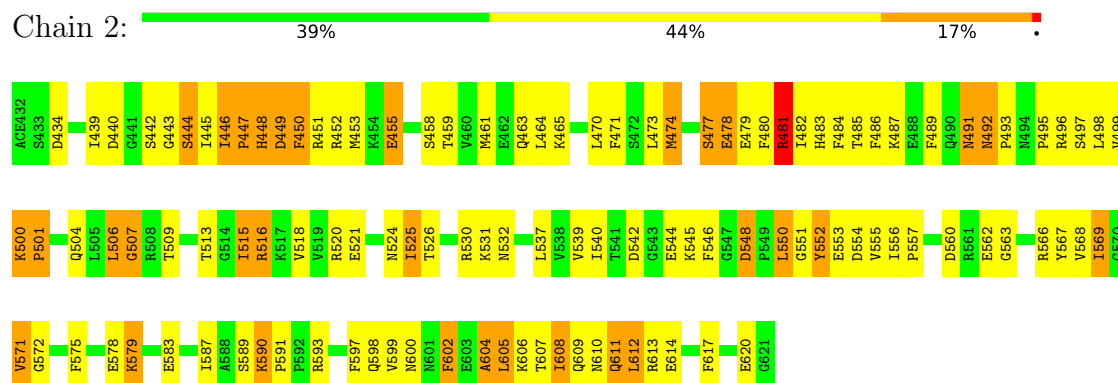
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	48.59Å 123.27Å 75.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	60.4 (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3187	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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, MG

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	1.32	3/1557 (0.2%)	2.42	109/2095 (5.2%)
1	2	1.32	2/1557 (0.1%)	2.42	88/2095 (4.2%)
All	All	1.32	5/3114 (0.2%)	2.42	197/4190 (4.7%)

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	1	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	209	THR	CA-CB	6.88	1.61	1.52
1	2	478	GLU	CA-CB	-6.40	1.45	1.54
1	1	208	ARG	CA-CB	-6.11	1.45	1.53
1	1	266	ARG	CA-CB	5.63	1.62	1.53
1	2	509	THR	CA-CB	5.17	1.60	1.53

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	491	ASN	CA-CB-CG	15.88	128.48	112.60
1	2	593	ARG	CD-NE-CZ	15.47	146.06	124.40
1	2	521	GLU	CA-CB-CG	14.52	143.14	114.10
1	2	546	PHE	CA-CB-CG	12.32	126.12	113.80
1	1	317	PHE	CA-CB-CG	11.27	125.07	113.80
1	2	449	ASP	CA-CB-CG	11.11	123.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	293	ARG	CD-NE-CZ	11.04	139.86	124.40
1	1	148	HIS	CA-CB-CG	10.58	124.38	113.80
1	1	315	LYS	CB-CG-CD	10.39	135.19	111.30
1	1	216	ARG	CD-NE-CZ	10.16	138.62	124.40
1	2	590	LYS	CB-CG-CD	9.98	134.25	111.30
1	1	317	PHE	N-CA-CB	9.72	123.51	110.59
1	2	571	VAL	N-CA-C	9.24	121.24	107.75
1	2	590	LYS	CA-CB-CG	9.20	132.50	114.10
1	1	184	PHE	CA-CB-CG	9.13	122.93	113.80
1	1	299	VAL	CB-CA-C	9.02	126.31	110.71
1	1	195	PRO	CA-C-N	9.01	134.34	120.82
1	1	195	PRO	C-N-CA	9.01	134.34	120.82
1	2	444	SER	CA-C-N	8.95	134.04	122.95
1	2	444	SER	C-N-CA	8.95	134.04	122.95
1	1	175	GLN	N-CA-CB	8.93	125.07	110.69
1	1	243	GLY	N-CA-C	8.86	125.27	110.56
1	2	471	PHE	CA-CB-CG	8.84	122.64	113.80
1	1	260	ASP	CA-CB-CG	8.49	121.09	112.60
1	2	478	GLU	CA-CB-CG	8.49	131.08	114.10
1	2	602	PHE	CA-CB-CG	-8.46	105.34	113.80
1	1	206	LEU	N-CA-C	8.42	123.13	112.86
1	2	478	GLU	N-CA-C	-8.40	103.47	114.31
1	2	500	LYS	CA-CB-CG	8.40	130.90	114.10
1	2	474	MET	N-CA-CB	8.35	127.06	111.53
1	2	566	ARG	CD-NE-CZ	8.32	136.05	124.40
1	1	256	ILE	O-C-N	8.29	125.72	120.42
1	2	554	ASP	CA-CB-CG	8.24	120.84	112.60
1	2	597	PHE	CA-CB-CG	8.18	121.97	113.80
1	1	277	SER	N-CA-C	8.17	122.19	109.52
1	2	560	ASP	CA-CB-CG	8.10	120.70	112.60
1	1	140	ASP	CA-CB-CG	8.06	120.66	112.60
1	2	515	ILE	N-CA-CB	8.05	119.08	110.62
1	1	209	THR	N-CA-C	7.94	122.90	107.98
1	2	544	GLU	CB-CG-CD	7.92	126.06	112.60
1	1	165	LYS	CA-C-N	7.81	135.26	121.75
1	1	165	LYS	C-N-CA	7.81	135.26	121.75
1	2	562	GLU	CA-CB-CG	7.75	129.59	114.10
1	2	548	ASP	CB-CA-C	7.46	118.27	109.47
1	1	294	ASP	N-CA-C	7.44	120.27	111.71
1	1	178	GLU	N-CA-C	-7.39	104.51	113.97
1	1	315	LYS	CA-CB-CG	7.38	128.85	114.10
1	1	236	ILE	CA-C-O	-7.35	112.07	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	208	ARG	CA-CB-CG	7.30	128.70	114.10
1	1	253	GLU	CA-CB-CG	7.24	128.57	114.10
1	1	175	GLN	CA-C-O	-7.16	113.12	120.71
1	1	261	ARG	N-CA-CB	7.10	122.48	110.49
1	2	602	PHE	CB-CA-C	7.08	122.59	110.84
1	1	256	ILE	N-CA-CB	7.06	115.25	110.52
1	2	572	GLY	CA-C-N	7.06	130.05	120.38
1	2	572	GLY	C-N-CA	7.06	130.05	120.38
1	2	521	GLU	N-CA-CB	7.04	122.59	110.34
1	1	175	GLN	O-C-N	7.00	132.10	123.21
1	2	509	THR	N-CA-C	6.96	120.31	107.99
1	2	491	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	1	299	VAL	CA-C-N	6.93	129.45	120.44
1	1	299	VAL	C-N-CA	6.93	129.45	120.44
1	1	182	ILE	N-CA-CB	6.89	120.03	111.41
1	1	149	ASP	CA-CB-CG	6.89	119.49	112.60
1	1	295	HIS	CA-CB-CG	-6.79	107.01	113.80
1	1	216	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	1	243	GLY	CA-C-O	6.75	128.78	121.56
1	2	477	SER	N-CA-CB	6.74	121.89	110.49
1	1	177	SER	N-CA-CB	6.74	121.88	110.49
1	2	531	LYS	N-CA-C	6.73	118.70	111.36
1	2	598	GLN	CB-CG-CD	6.72	124.03	112.60
1	2	602	PHE	CA-C-O	-6.72	113.16	121.02
1	2	448	HIS	CA-CB-CG	-6.70	107.10	113.80
1	1	208	ARG	CD-NE-CZ	-6.64	115.10	124.40
1	2	516	ARG	CD-NE-CZ	6.59	133.63	124.40
1	1	258	GLU	N-CA-CB	6.59	119.81	110.12
1	1	234	PHE	N-CA-CB	6.56	120.42	110.45
1	1	189	PHE	N-CA-C	-6.54	104.08	111.07
1	1	192	ASN	CA-CB-CG	6.51	119.11	112.60
1	1	200	LYS	CA-CB-CG	6.46	127.03	114.10
1	2	600	ASN	N-CA-C	6.44	120.35	112.23
1	2	566	ARG	NE-CZ-NH2	6.44	124.99	119.20
1	2	449	ASP	N-CA-C	-6.43	104.32	111.71
1	2	589	SER	N-CA-C	-6.41	101.29	110.59
1	1	177	SER	CA-CB-OG	6.40	123.89	111.10
1	2	593	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	1	210	HIS	CA-C-N	6.28	129.21	120.29
1	1	210	HIS	C-N-CA	6.28	129.21	120.29
1	2	481	ARG	N-CA-C	6.20	118.97	107.99
1	1	266	ARG	N-CA-C	6.20	119.04	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	290	LYS	CB-CG-CD	6.19	125.53	111.30
1	2	478	GLU	CB-CA-C	6.18	119.40	109.02
1	2	608	ILE	N-CA-C	6.17	118.82	112.90
1	1	224	ASN	CA-CB-CG	6.10	118.70	112.60
1	2	552	TYR	CA-C-N	6.07	129.54	120.31
1	2	552	TYR	C-N-CA	6.07	129.54	120.31
1	1	135	ILE	N-CA-C	6.04	116.56	107.80
1	2	524	ASN	CB-CA-C	6.02	120.54	109.71
1	1	189	PHE	O-C-N	6.02	128.27	122.07
1	1	203	THR	CA-C-N	6.01	129.37	120.95
1	1	203	THR	C-N-CA	6.01	129.37	120.95
1	2	539	VAL	CA-C-O	-6.01	113.84	121.48
1	2	491	ASN	CB-CA-C	6.01	121.74	111.46
1	1	191	ASN	CA-CB-CG	5.99	118.58	112.60
1	2	520	ARG	CA-C-O	-5.97	114.56	120.82
1	2	506	LEU	CA-C-O	-5.94	112.02	120.51
1	2	571	VAL	N-CA-CB	-5.93	103.93	111.64
1	2	579	LYS	CB-CG-CD	5.89	124.85	111.30
1	2	479	GLU	N-CA-C	-5.86	101.05	110.14
1	2	590	LYS	CG-CD-CE	5.83	124.71	111.30
1	1	134	ASP	CA-CB-CG	5.82	118.42	112.60
1	1	253	GLU	CB-CG-CD	5.80	122.45	112.60
1	2	471	PHE	CA-C-N	5.78	132.38	121.69
1	2	471	PHE	C-N-CA	5.78	132.38	121.69
1	1	293	ARG	CG-CD-NE	5.77	124.70	112.00
1	2	568	VAL	N-CA-C	5.77	116.17	107.75
1	1	235	LYS	CB-CG-CD	5.76	124.54	111.30
1	2	455	GLU	CB-CG-CD	5.72	122.33	112.60
1	1	136	ALA	CA-C-N	5.71	131.21	122.93
1	1	136	ALA	C-N-CA	5.71	131.21	122.93
1	2	444	SER	N-CA-C	-5.70	106.19	114.12
1	2	575	PHE	N-CA-C	5.66	119.27	112.93
1	1	297	PHE	N-CA-CB	5.61	120.02	110.71
1	2	550	LEU	N-CA-CB	5.59	118.10	110.38
1	2	497	SER	CA-C-N	5.58	130.12	120.58
1	2	497	SER	C-N-CA	5.58	130.12	120.58
1	1	222	LEU	N-CA-C	5.58	117.44	111.36
1	2	477	SER	O-C-N	5.58	130.00	122.59
1	2	553	GLU	CB-CG-CD	5.58	122.08	112.60
1	1	297	PHE	CA-CB-CG	5.57	119.37	113.80
1	2	444	SER	CA-C-O	5.52	124.98	118.90
1	1	193	PRO	CA-C-N	-5.51	115.43	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	193	PRO	C-N-CA	-5.51	115.43	122.98
1	1	302	PHE	CA-C-O	5.51	126.31	119.97
1	1	196	ARG	CB-CA-C	-5.50	101.61	110.74
1	1	151	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	1	208	ARG	CB-CA-C	5.45	122.55	111.11
1	2	501	PRO	N-CA-C	5.44	123.68	112.47
1	2	591	PRO	CA-C-N	5.44	124.96	119.19
1	2	591	PRO	C-N-CA	5.44	124.96	119.19
1	1	191	ASN	N-CA-CB	5.44	118.23	110.67
1	2	617	PHE	CA-CB-CG	5.43	119.23	113.80
1	1	143	GLY	N-CA-C	5.42	120.42	114.40
1	1	314	GLU	CB-CA-C	5.42	119.35	110.95
1	1	197	SER	CB-CA-C	5.41	120.60	110.70
1	2	474	MET	O-C-N	5.41	129.54	123.27
1	1	301	ASN	CB-CA-C	5.38	122.41	111.11
1	2	446	ILE	CA-C-N	5.37	126.56	119.84
1	2	446	ILE	C-N-CA	5.37	126.56	119.84
1	2	446	ILE	CB-CA-C	5.36	116.85	110.68
1	1	276	ARG	CD-NE-CZ	5.36	131.91	124.40
1	1	283	GLU	CA-C-N	5.36	127.40	120.44
1	1	283	GLU	C-N-CA	5.36	127.40	120.44
1	1	175	GLN	N-CA-C	-5.35	100.97	109.59
1	1	248	ASP	CA-CB-CG	5.34	117.94	112.60
1	2	544	GLU	CG-CD-OE1	5.31	130.62	118.40
1	1	293	ARG	N-CA-CB	5.29	119.43	110.49
1	1	321	GLY	CA-C-O	-5.28	109.71	120.80
1	1	235	LYS	CA-CB-CG	5.27	124.64	114.10
1	1	300	ASN	N-CA-C	5.27	116.71	111.07
1	1	167	SER	CA-C-O	-5.25	114.17	120.10
1	1	175	GLN	CA-CB-CG	5.25	124.59	114.10
1	1	262	GLU	N-CA-CB	5.25	118.08	110.47
1	2	525	ILE	N-CA-C	5.22	115.95	110.62
1	1	243	GLY	CA-C-N	5.22	128.28	120.87
1	1	243	GLY	C-N-CA	5.22	128.28	120.87
1	1	313	ARG	CD-NE-CZ	5.21	131.70	124.40
1	1	315	LYS	N-CA-CB	5.21	118.27	109.78
1	2	434	ASP	CA-CB-CG	5.21	117.81	112.60
1	1	286	THR	CA-CB-OG1	-5.21	101.79	109.60
1	2	569	ILE	CA-C-O	-5.20	114.92	120.59
1	2	434	ASP	CB-CA-C	5.19	120.35	111.68
1	2	532	ASN	CA-CB-CG	5.19	117.79	112.60
1	1	150	PHE	N-CA-CB	5.16	117.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	171	PHE	CA-CB-CG	5.15	118.95	113.80
1	1	221	GLU	CA-C-N	5.15	127.60	120.29
1	1	221	GLU	C-N-CA	5.15	127.60	120.29
1	2	450	PHE	N-CA-C	-5.14	105.85	111.82
1	1	186	PHE	O-C-N	5.14	127.57	122.12
1	1	179	GLU	CA-C-O	-5.14	115.21	121.78
1	1	225	ILE	CB-CA-C	5.11	118.73	112.04
1	1	288	ALA	O-C-N	5.09	128.87	122.86
1	2	444	SER	CB-CA-C	5.09	117.93	109.38
1	2	567	TYR	CA-CB-CG	5.06	123.02	113.90
1	2	458	SER	N-CA-CB	5.06	117.48	109.94
1	1	205	LEU	CA-C-N	5.06	131.00	123.05
1	1	205	LEU	C-N-CA	5.06	131.00	123.05
1	1	191	ASN	O-C-N	5.06	128.60	122.48
1	1	244	GLU	CB-CG-CD	5.05	121.19	112.60
1	1	287	ILE	CB-CA-C	-5.05	105.43	112.04
1	1	187	LYS	N-CA-CB	-5.04	102.54	110.46
1	1	163	GLN	OE1-CD-NE2	5.04	127.64	122.60
1	2	605	LEU	O-C-N	5.04	129.24	122.49
1	1	218	VAL	N-CA-C	-5.03	105.00	110.23
1	2	481	ARG	CA-C-O	-5.03	115.08	120.46
1	2	553	GLU	CA-CB-CG	5.01	124.13	114.10
1	1	162	GLU	N-CA-CB	5.00	118.94	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	151	ARG	Sidechain
1	1	266	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	1548	83	0
1	2	1530	0	1548	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	1	0	0	0	0
2	2	1	0	0	0	0
3	1	90	0	0	5	0
3	2	35	0	0	6	0
All	All	3187	0	3096	169	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 28.

All (169) 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)
1:1:153:MET:HE3	1:1:302:PHE:HE2	1.33	0.93
1:2:609:GLN:HB2	3:2:42:HOH:O	1.69	0.92
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.53	0.91
1:1:311:GLN:HE21	1:1:311:GLN:H	1.18	0.91
1:2:569:ILE:HD11	1:2:612:LEU:HD22	1.55	0.87
1:2:542:ASP:OD1	3:2:18:HOH:O	1.96	0.82
1:2:474:MET:HE2	1:2:482:ILE:HG12	1.63	0.81
1:1:277:SER:C	1:1:279:LYS:H	1.90	0.79
1:1:294:ASP:O	1:1:315:LYS:NZ	2.16	0.79
1:2:518:VAL:HG11	1:2:537:LEU:HD13	1.66	0.78
1:1:306:LYS:HD2	1:1:306:LYS:H	1.49	0.77
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.65	0.77
1:1:294:ASP:HB3	3:1:15:HOH:O	1.86	0.73
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.23	0.72
1:1:168:LYS:HA	1:1:168:LYS:HE2	1.72	0.71
1:1:173:LEU:HD23	1:1:174:MET:N	2.07	0.69
1:1:311:GLN:H	1:1:311:GLN:NE2	1.90	0.69
1:2:473:LEU:HG	1:2:474:MET:N	2.08	0.68
1:2:563:GLY:HA2	3:2:48:HOH:O	1.94	0.68
1:1:260:ASP:HB2	3:1:848:HOH:O	1.94	0.68
1:2:500:LYS:CG	1:2:501:PRO:HD3	2.24	0.68
1:1:288:ALA:O	3:1:858:HOH:O	2.11	0.67
1:1:153:MET:HE3	1:1:302:PHE:CE2	2.22	0.67
1:1:299:VAL:HG22	1:1:304:ALA:HB3	1.77	0.67
1:2:515:ILE:HD11	1:2:587:ILE:HG23	1.76	0.67
1:1:135:ILE:O	1:1:171:PHE:HA	1.95	0.66
1:2:439:ILE:HD11	1:2:473:LEU:HD21	1.76	0.66
1:2:459:THR:CG2	1:2:463:GLN:HE21	2.09	0.66
1:1:181:ARG:HG2	1:1:205:LEU:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:306:LYS:H	1:1:306:LYS:CD	2.09	0.65
1:1:306:LYS:HD2	1:1:306:LYS:N	2.12	0.65
1:1:178:GLU:HG3	1:1:208:ARG:H	1.62	0.65
1:2:606:LYS:N	1:2:606:LYS:HD3	2.14	0.63
1:1:218:VAL:HG11	1:1:237:LEU:HD13	1.79	0.63
1:2:483:HIS:O	1:2:484:PHE:HB3	1.98	0.63
1:2:610:ASN:HA	1:2:613:ARG:HH21	1.64	0.63
1:1:214:GLY:O	1:1:218:VAL:HG23	1.98	0.62
1:2:474:MET:CE	1:2:482:ILE:HG12	2.28	0.62
1:1:299:VAL:CG1	1:1:305:LEU:HD23	2.30	0.61
1:2:480:PHE:CZ	1:2:513:THR:HG22	2.35	0.61
1:2:552:TYR:O	1:2:556:ILE:HB	2.00	0.61
1:2:449:ASP:HB3	1:2:602:PHE:CG	2.36	0.61
1:1:277:SER:O	1:1:281:ARG:HG2	2.00	0.61
1:2:459:THR:HG22	1:2:463:GLN:HE21	1.66	0.60
1:1:178:GLU:HG2	1:1:208:ARG:HG2	1.83	0.59
1:1:271:VAL:CG2	1:1:305:LEU:HD21	2.33	0.58
1:1:164:LEU:HD21	1:1:313:ARG:HA	1.85	0.58
1:2:515:ILE:HD11	1:2:587:ILE:CG2	2.33	0.58
1:1:314:GLU:O	1:1:315:LYS:C	2.47	0.58
1:1:277:SER:C	1:1:279:LYS:N	2.60	0.57
1:1:266:ARG:NH2	3:1:858:HOH:O	2.38	0.56
1:1:299:VAL:HG11	1:1:305:LEU:HD23	1.87	0.56
1:2:492:ASN:ND2	1:2:498:LEU:HD21	2.21	0.56
1:2:515:ILE:CD1	1:2:587:ILE:HG23	2.35	0.56
1:1:161:MET:HE3	1:1:171:PHE:CB	2.36	0.55
1:2:545:LYS:HE2	1:2:548:ASP:HB3	1.88	0.55
1:1:276:ARG:H	1:1:276:ARG:CD	2.20	0.55
1:2:604:ALA:O	1:2:607:THR:OG1	2.25	0.55
1:1:162:GLU:OE2	1:1:196:ARG:HG2	2.07	0.55
1:1:281:ARG:O	1:1:284:LEU:HB2	2.07	0.54
1:2:446:ILE:HD12	1:2:448:HIS:CE1	2.43	0.54
1:1:192:ASN:O	1:1:194:ASN:N	2.35	0.54
1:1:200:LYS:HB3	1:1:201:PRO:HD3	1.88	0.53
1:1:169:THR:O	1:1:170:LEU:HD23	2.09	0.53
1:2:464:LEU:HD23	1:2:613:ARG:HG3	1.89	0.53
1:2:452:ARG:O	1:2:453:MET:C	2.50	0.53
1:2:578:GLU:O	1:2:579:LYS:HD2	2.10	0.52
1:1:245:LYS:HD2	1:1:248:ASP:HB3	1.90	0.52
1:1:279:LYS:O	1:1:282:GLN:HB3	2.10	0.52
1:1:299:VAL:HG22	1:1:304:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:443:GLY:HA2	1:2:506:LEU:HD23	1.92	0.52
1:2:552:TYR:O	1:2:556:ILE:N	2.38	0.52
1:2:461:MET:HE1	1:2:484:PHE:HZ	1.75	0.52
1:1:308:ILE:HD12	1:1:308:ILE:C	2.34	0.51
1:2:492:ASN:N	1:2:493:PRO:HD3	2.25	0.51
1:2:480:PHE:CZ	1:2:513:THR:CG2	2.93	0.51
1:1:277:SER:O	1:1:279:LYS:N	2.44	0.51
1:2:439:ILE:CD1	1:2:473:LEU:HD11	2.41	0.51
1:2:442:SER:C	1:2:444:SER:H	2.19	0.51
1:2:451:ARG:HH12	1:2:455:GLU:HB2	1.76	0.50
1:1:276:ARG:H	1:1:276:ARG:HD3	1.77	0.50
1:2:440:ASP:C	1:2:440:ASP:OD1	2.54	0.50
1:1:290:LYS:HA	1:1:291:PRO:C	2.36	0.49
1:2:610:ASN:CB	1:2:613:ARG:HH21	2.25	0.49
1:2:448:HIS:O	1:2:451:ARG:HB3	2.12	0.49
1:2:610:ASN:OD1	1:2:613:ARG:NH2	2.45	0.49
1:1:256:ILE:N	1:1:257:PRO:CD	2.76	0.49
1:1:154:LYS:HE3	1:1:199:VAL:O	2.12	0.49
1:2:506:LEU:O	1:2:507:GLY:O	2.31	0.49
1:2:545:LYS:NZ	1:2:551:GLY:HA2	2.27	0.48
1:2:442:SER:OG	3:2:18:HOH:O	2.20	0.48
1:1:178:GLU:CG	1:1:208:ARG:HG2	2.43	0.48
1:2:513:THR:OG1	1:2:550:LEU:HD13	2.13	0.48
1:2:453:MET:HE2	1:2:540:ILE:CG2	2.44	0.48
1:2:516:ARG:HB2	1:2:555:VAL:HG12	1.94	0.48
1:2:571:VAL:HG11	1:2:602:PHE:CZ	2.48	0.48
1:1:187:LYS:HA	1:1:190:GLN:HG2	1.95	0.47
1:1:303:GLU:O	1:1:306:LYS:HD3	2.14	0.47
1:1:271:VAL:HG22	1:1:305:LEU:HD21	1.95	0.47
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.95	0.47
1:1:187:LYS:HB3	1:1:228:GLY:HA3	1.97	0.47
1:1:282:GLN:HA	1:1:285:ASN:HD22	1.80	0.47
1:1:153:MET:CE	1:1:302:PHE:HE2	2.15	0.46
1:1:183:HIS:HB3	3:1:824:HOH:O	2.15	0.46
1:2:487:LYS:HD2	1:2:526:THR:O	2.16	0.46
1:1:161:MET:HE3	1:1:171:PHE:HB2	1.98	0.46
1:2:481:ARG:HD3	1:2:483:HIS:CE1	2.50	0.46
1:1:308:ILE:HA	1:1:311:GLN:CD	2.41	0.46
1:2:611:GLN:C	1:2:613:ARG:N	2.74	0.46
1:1:269:ILE:HA	1:1:297:PHE:O	2.16	0.45
1:2:569:ILE:HD12	1:2:608:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:443:GLY:HA2	1:2:506:LEU:CD2	2.46	0.45
1:2:583:GLU:O	1:2:587:ILE:HG13	2.17	0.45
1:1:139:ILE:O	1:1:139:ILE:HG13	2.17	0.45
1:2:496:ARG:O	1:2:500:LYS:HG2	2.17	0.45
1:2:453:MET:HE2	1:2:540:ILE:HG22	1.99	0.45
1:1:139:ILE:O	1:1:175:GLN:HB2	2.17	0.44
1:2:599:VAL:HG13	1:2:604:ALA:O	2.18	0.44
1:1:313:ARG:NE	1:1:314:GLU:OE2	2.51	0.44
1:2:492:ASN:H	1:2:493:PRO:HD3	1.82	0.44
1:2:556:ILE:HB	1:2:557:PRO:HD3	2.00	0.44
1:2:599:VAL:HG11	1:2:605:LEU:HD23	1.99	0.44
1:2:504:GLN:HB3	3:2:22:HOH:O	2.17	0.44
1:2:610:ASN:O	1:2:614:GLU:HG2	2.17	0.44
1:1:274:ALA:O	1:1:276:ARG:NH1	2.43	0.44
1:1:189:PHE:C	1:1:191:ASN:H	2.25	0.43
1:2:552:TYR:O	1:2:556:ILE:CB	2.65	0.43
1:1:149:ASP:HB3	1:1:302:PHE:CG	2.53	0.43
1:1:310:ASN:O	1:1:314:GLU:HG2	2.18	0.43
1:2:525:ILE:HG23	1:2:526:THR:N	2.33	0.43
1:1:192:ASN:O	1:1:198:LEU:HD11	2.19	0.43
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.48	0.43
1:2:439:ILE:HD13	1:2:473:LEU:HD11	1.99	0.43
1:2:485:THR:O	1:2:486:PHE:C	2.62	0.43
1:2:495:PRO:O	1:2:499:VAL:HG23	2.19	0.43
1:1:153:MET:HE2	1:1:240:ILE:CG2	2.49	0.42
1:1:274:ALA:C	1:1:276:ARG:HD2	2.44	0.42
1:2:448:HIS:C	1:2:451:ARG:H	2.27	0.42
1:1:278:GLU:O	1:1:278:GLU:HG2	2.18	0.42
1:1:168:LYS:HA	1:1:168:LYS:CE	2.47	0.42
1:1:256:ILE:HB	1:1:257:PRO:HD3	2.01	0.42
1:1:271:VAL:HG21	1:1:305:LEU:HD21	2.00	0.42
1:2:613:ARG:HE	1:2:613:ARG:HB3	1.53	0.42
1:1:177:SER:O	1:1:210:HIS:HB2	2.20	0.42
1:2:571:VAL:HG11	1:2:602:PHE:CE1	2.55	0.42
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.78	0.42
1:2:470:LEU:HD12	1:2:530:ARG:NE	2.34	0.42
1:2:491:ASN:O	1:2:492:ASN:HB2	2.20	0.42
1:2:556:ILE:HD13	1:2:556:ILE:HA	1.69	0.42
1:1:174:MET:CE	1:1:182:ILE:HG12	2.50	0.42
1:1:163:GLN:OE1	1:1:313:ARG:HD3	2.20	0.41
1:2:599:VAL:CG1	1:2:604:ALA:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:281:ARG:C	1:1:283:GLU:H	2.27	0.41
1:2:474:MET:HB2	1:2:481:ARG:O	2.21	0.41
1:1:194:ASN:HD22	1:1:197:SER:CB	2.34	0.41
1:1:292:PRO:O	1:1:293:ARG:C	2.62	0.41
1:2:578:GLU:C	1:2:579:LYS:HD2	2.46	0.41
1:2:610:ASN:CA	1:2:613:ARG:HH21	2.33	0.41
1:1:273:ASP:O	1:1:276:ARG:HD2	2.21	0.41
1:1:281:ARG:C	1:1:283:GLU:N	2.79	0.41
1:1:223:PHE:CD1	1:1:235:LYS:HD2	2.56	0.41
1:2:443:GLY:CA	1:2:506:LEU:CD2	2.98	0.41
1:1:210:HIS:CE1	1:1:247:GLY:O	2.75	0.40
1:2:446:ILE:HG12	3:2:35:HOH:O	2.21	0.40
1:2:465:LYS:HE2	1:2:489:PHE:HE1	1.85	0.40
1:1:161:MET:HE2	1:1:161:MET:HB3	1.90	0.40
1:1:299:VAL:CG2	1:1:304:ALA:CB	2.99	0.40
1:1:249:PRO:HB2	1:2:550:LEU:HD11	2.02	0.40
1:2:611:GLN:O	1:2:613:ARG:N	2.54	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	1	188/190 (99%)	169 (90%)	15 (8%)	4 (2%)	5	15
1	2	188/190 (99%)	161 (86%)	19 (10%)	8 (4%)	2	4
All	All	376/380 (99%)	330 (88%)	34 (9%)	12 (3%)	3	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	492	ASN

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Mol	Chain	Res	Type
1	2	507	GLY
1	2	604	ALA
1	2	620	GLU
1	1	278	GLU
1	1	177	SER
1	2	477	SER
1	2	611	GLN
1	2	447	PRO
1	2	612	LEU
1	1	193	PRO
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	151	ARG
1	1	166	LYS
1	1	168	LYS
1	1	187	LYS
1	1	311	GLN
1	2	481	ARG
1	2	590	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	300	ASN
1	1	301	ASN
1	1	309	GLN
1	1	311	GLN
1	2	463	GLN
1	2	492	ASN
1	2	510	HIS
1	2	601	ASN

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 2 ligands modelled in this entry, 2 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 ⓘ

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.