



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:02 PM UTC

PDB ID : 1MPP / pdb_00001mpp
Title : X-RAY ANALYSES OF ASPARTIC PROTEINASES. V. STRUCTURE AND REFINEMENT AT 2.0 ANGSTROMS RESOLUTION OF THE ASPARTIC PROTEINASE FROM MUCOR PUSILLUS
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Deposited on : 1992-02-19
Resolution : 2.00 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

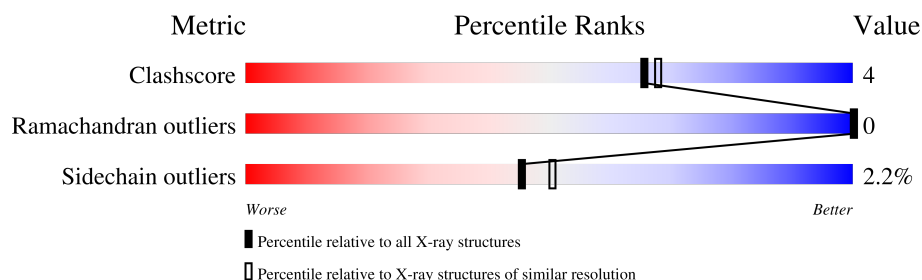
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	361	48% 45% 6% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2864 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.

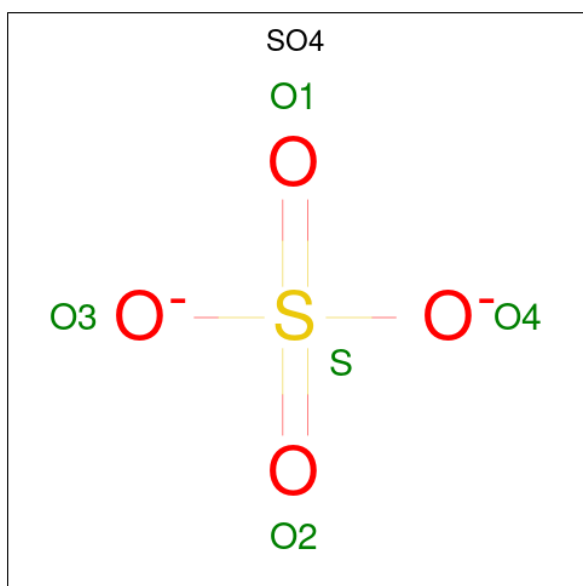
- Molecule 1 is a protein called PEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2638	1686	414	530	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ILE	MET	conflict	UNP P09177
A	170	VAL	ALA	conflict	UNP P09177
A	202	SER	ALA	conflict	UNP P09177

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

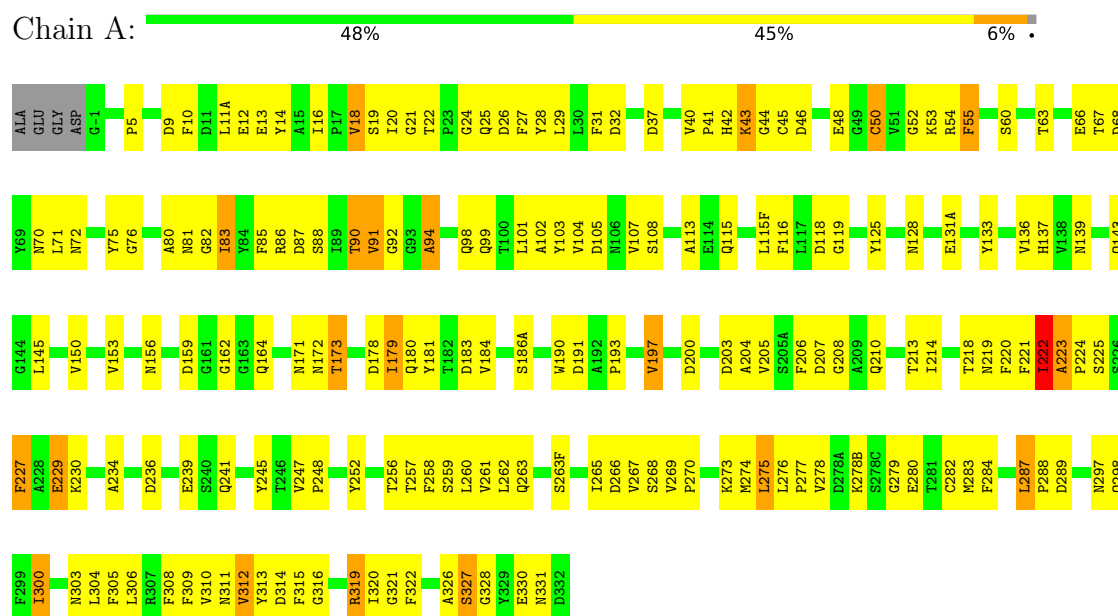
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total 221	O 221	0	0

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: PEPSIN



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	70.00Å 104.00Å 46.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2864	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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	1.91	61/2704 (2.3%)	2.75	266/3693 (7.2%)

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	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	HIS	ND1-CE1	10.80	1.43	1.32
1	A	45	CYS	N-CA	7.83	1.55	1.46
1	A	267	VAL	N-CA	7.48	1.57	1.46
1	A	68	ASP	N-CA	7.28	1.54	1.46
1	A	310	VAL	N-CA	7.12	1.54	1.46
1	A	280	GLU	N-CA	7.09	1.55	1.46
1	A	28	TYR	N-CA	7.01	1.54	1.46
1	A	115	GLN	CA-CB	6.96	1.64	1.53
1	A	42	HIS	ND1-CE1	6.93	1.39	1.32
1	A	90	THR	CB-OG1	6.88	1.54	1.43
1	A	210	GLN	CA-C	6.72	1.60	1.52
1	A	320	ILE	C-N	-6.72	1.26	1.33
1	A	80	ALA	N-CA	6.54	1.54	1.46
1	A	21	GLY	N-CA	6.51	1.53	1.45
1	A	54	ARG	N-CA	6.37	1.53	1.46
1	A	90	THR	N-CA	6.20	1.53	1.46
1	A	241	GLN	CD-OE1	6.20	1.35	1.23
1	A	98	GLN	CD-OE1	6.16	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLN	CD-OE1	6.09	1.35	1.23
1	A	210	GLN	CD-OE1	6.04	1.35	1.23
1	A	27	PHE	CA-C	6.03	1.59	1.52
1	A	284	PHE	N-CA	6.00	1.53	1.46
1	A	190	TRP	CA-C	5.88	1.60	1.53
1	A	172	ASN	CG-OD1	5.87	1.34	1.23
1	A	268	SER	C-N	5.85	1.38	1.33
1	A	72	ASN	N-CA	5.84	1.55	1.47
1	A	171	ASN	CG-OD1	5.84	1.34	1.23
1	A	71	LEU	N-CA	5.82	1.53	1.46
1	A	88	SER	CA-CB	5.82	1.62	1.53
1	A	28	TYR	CA-C	5.80	1.59	1.52
1	A	273	LYS	N-CA	5.80	1.53	1.46
1	A	13	GLU	N-CA	5.77	1.53	1.45
1	A	214	ILE	N-CA	5.73	1.53	1.46
1	A	270	PRO	N-CA	5.70	1.54	1.47
1	A	115(F)	LEU	N-CA	5.68	1.52	1.46
1	A	261	VAL	CA-CB	5.67	1.60	1.53
1	A	20	ILE	CA-C	5.67	1.59	1.52
1	A	213	THR	C-N	-5.67	1.28	1.33
1	A	76	GLY	N-CA	5.67	1.52	1.45
1	A	128	ASN	CG-OD1	5.64	1.34	1.23
1	A	222	ILE	CA-C	-5.62	1.45	1.52
1	A	218	THR	N-CA	5.60	1.52	1.45
1	A	119	GLY	N-CA	5.59	1.50	1.45
1	A	311	ASN	N-CA	5.57	1.52	1.46
1	A	313	TYR	N-CA	5.54	1.53	1.46
1	A	328	GLY	N-CA	5.51	1.53	1.45
1	A	164	GLN	N-CA	5.51	1.53	1.46
1	A	227	PHE	CA-CB	5.51	1.62	1.53
1	A	54	ARG	NE-CZ	5.49	1.39	1.33
1	A	19	SER	N-CA	5.47	1.52	1.46
1	A	18	VAL	CA-C	5.42	1.58	1.52
1	A	303	ASN	CG-OD1	5.31	1.33	1.23
1	A	263	GLN	N-CA	5.28	1.52	1.45
1	A	219	ASN	CG-OD1	5.25	1.33	1.23
1	A	41	PRO	C-O	-5.25	1.18	1.23
1	A	205	VAL	CA-CB	-5.21	1.47	1.54
1	A	14	TYR	N-CA	5.20	1.52	1.46
1	A	99	GLN	C-O	5.12	1.30	1.24
1	A	16	ILE	N-CA	-5.10	1.40	1.46
1	A	102	ALA	N-CA	5.10	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	VAL	N-CA	5.04	1.52	1.46

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLN	CG-CD-NE2	11.21	133.22	116.40
1	A	308	PHE	CA-CB-CG	-10.81	102.99	113.80
1	A	320	ILE	CA-C-N	10.67	132.71	122.36
1	A	320	ILE	C-N-CA	10.67	132.71	122.36
1	A	20	ILE	O-C-N	10.54	134.56	123.18
1	A	191	ASP	CA-CB-CG	-10.36	102.24	112.60
1	A	278(B)	LYS	CA-C-O	10.36	132.46	121.07
1	A	164	GLN	O-C-N	-10.32	112.62	123.56
1	A	115	GLN	OE1-CD-NE2	10.02	132.62	122.60
1	A	315	PHE	CA-C-O	9.91	131.42	119.43
1	A	98	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	105	ASP	CA-CB-CG	-9.74	102.86	112.60
1	A	164	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	A	164	GLN	CA-C-O	9.64	131.54	120.75
1	A	186(A)	SER	CA-C-O	-9.51	109.19	120.60
1	A	241	GLN	O-C-N	9.44	133.26	122.22
1	A	229	GLU	CA-C-O	9.37	130.48	120.55
1	A	86	ARG	CA-CB-CG	-9.27	95.56	114.10
1	A	54	ARG	NE-CZ-NH2	9.26	127.54	119.20
1	A	26	ASP	CA-C-O	-8.79	110.81	120.92
1	A	322	PHE	CA-C-O	-8.57	110.80	120.66
1	A	28	TYR	CA-C-O	-8.44	111.18	120.38
1	A	315	PHE	O-C-N	-8.44	111.50	122.39
1	A	208	GLY	CA-C-O	8.40	129.55	122.24
1	A	252	TYR	CA-C-O	-8.31	109.42	119.32
1	A	245	TYR	CA-C-O	-8.13	111.92	120.70
1	A	266	ASP	CA-C-N	-7.89	112.56	123.13
1	A	266	ASP	C-N-CA	-7.89	112.56	123.13
1	A	265	ILE	CA-C-N	-7.73	111.72	122.93
1	A	265	ILE	C-N-CA	-7.73	111.72	122.93
1	A	22	THR	CA-C-O	-7.72	112.52	120.09
1	A	319	ARG	CA-C-N	-7.64	112.52	123.06
1	A	319	ARG	C-N-CA	-7.64	112.52	123.06
1	A	143	GLN	CA-C-O	7.56	128.58	119.43
1	A	220	PHE	CA-C-O	7.46	130.51	121.94
1	A	116	PHE	CA-C-N	7.45	134.25	122.17
1	A	116	PHE	C-N-CA	7.45	134.25	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ILE	CA-C-O	-7.42	112.77	120.27
1	A	230	LYS	CA-C-O	7.42	128.41	120.55
1	A	24	GLY	N-CA-C	7.41	120.03	111.36
1	A	191	ASP	CA-C-O	-7.38	112.17	120.43
1	A	274	MET	O-C-N	-7.29	113.60	122.34
1	A	115	GLN	CA-CB-CG	-7.27	99.55	114.10
1	A	37	ASP	CA-C-N	7.27	132.29	122.84
1	A	37	ASP	C-N-CA	7.27	132.29	122.84
1	A	297	ASN	CA-C-O	7.20	127.00	119.51
1	A	197	VAL	CA-CB-CG2	7.17	122.58	110.40
1	A	143	GLN	O-C-N	-7.09	113.24	122.39
1	A	66	GLU	O-C-N	-7.08	114.26	122.89
1	A	260	LEU	CA-C-O	-7.07	112.55	120.54
1	A	44	GLY	N-CA-C	-7.03	105.56	113.79
1	A	223	ALA	CA-C-O	-7.03	113.58	120.26
1	A	316	GLY	CA-C-N	-7.01	111.62	122.49
1	A	316	GLY	C-N-CA	-7.01	111.62	122.49
1	A	322	PHE	O-C-N	7.01	131.83	123.27
1	A	88	SER	CA-CB-OG	-7.00	97.10	111.10
1	A	330	GLU	CA-CB-CG	-6.98	100.14	114.10
1	A	101	LEU	CA-C-O	-6.96	113.67	121.40
1	A	164	GLN	N-CA-CB	-6.93	100.22	111.24
1	A	257	THR	CA-C-O	6.93	128.99	121.16
1	A	306	LEU	CA-C-O	-6.86	110.95	119.38
1	A	225	SER	O-C-N	-6.85	114.40	122.20
1	A	180	GLN	CA-C-O	-6.83	112.94	120.38
1	A	208	GLY	N-CA-C	-6.82	104.23	112.48
1	A	274	MET	CA-C-O	6.81	127.52	119.56
1	A	204	ALA	CA-C-O	6.79	126.61	119.14
1	A	263(F)	SER	CA-C-O	-6.78	111.87	119.67
1	A	16	ILE	N-CA-CB	6.77	120.69	111.21
1	A	26	ASP	O-C-N	6.76	131.00	123.16
1	A	86	ARG	CA-C-O	-6.75	113.42	120.70
1	A	27	PHE	CA-C-N	-6.73	113.71	123.00
1	A	27	PHE	C-N-CA	-6.73	113.71	123.00
1	A	113	ALA	CA-C-N	-6.73	111.88	122.65
1	A	113	ALA	C-N-CA	-6.73	111.88	122.65
1	A	45	CYS	CA-C-N	6.71	135.56	122.07
1	A	45	CYS	C-N-CA	6.71	135.56	122.07
1	A	229	GLU	CB-CG-CD	6.68	123.95	112.60
1	A	80	ALA	O-C-N	6.67	130.56	123.42
1	A	236	ASP	CA-CB-CG	6.65	119.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLU	O-C-N	-6.64	115.45	123.16
1	A	277	PRO	CA-C-O	6.62	128.31	121.23
1	A	326	ALA	CA-C-O	6.61	129.54	121.87
1	A	150	VAL	O-C-N	6.61	130.02	122.82
1	A	139	ASN	CB-CG-ND2	6.60	126.30	116.40
1	A	205	VAL	CA-CB-CG2	6.59	121.61	110.40
1	A	67	THR	CA-C-N	-6.58	112.13	122.73
1	A	67	THR	C-N-CA	-6.58	112.13	122.73
1	A	145	LEU	O-C-N	-6.57	114.19	122.27
1	A	145	LEU	CA-C-O	6.57	127.52	119.97
1	A	270	PRO	N-CA-CB	-6.56	97.24	103.34
1	A	247	VAL	CA-C-N	-6.55	113.21	119.76
1	A	247	VAL	C-N-CA	-6.55	113.21	119.76
1	A	179	ILE	CA-C-O	-6.52	113.42	120.85
1	A	310	VAL	N-CA-C	-6.52	98.26	108.23
1	A	83	ILE	N-CA-CB	-6.51	100.77	111.45
1	A	22	THR	CB-CA-C	6.49	118.78	110.34
1	A	70	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	20	ILE	CA-C-O	-6.48	113.08	120.67
1	A	11(A)	LEU	CA-C-O	-6.47	111.77	119.35
1	A	85	PHE	CA-CB-CG	6.47	120.27	113.80
1	A	55	PHE	CA-C-N	-6.47	113.02	122.65
1	A	55	PHE	C-N-CA	-6.47	113.02	122.65
1	A	206	PHE	O-C-N	6.45	130.17	122.94
1	A	298	GLN	CA-C-O	6.45	127.46	120.43
1	A	262	LEU	CD1-CG-CD2	-6.41	96.69	110.80
1	A	14	TYR	CA-C-O	-6.40	113.79	120.70
1	A	261	VAL	CG1-CB-CG2	-6.35	96.82	110.80
1	A	46	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	55	PHE	CA-C-O	-6.32	113.72	121.11
1	A	32	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	234	ALA	CA-C-O	-6.28	112.37	119.79
1	A	52	GLY	CA-C-N	-6.25	112.41	121.98
1	A	52	GLY	C-N-CA	-6.25	112.41	121.98
1	A	180	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	181	TYR	CA-C-O	6.24	128.21	121.16
1	A	18	VAL	O-C-N	6.19	129.82	122.95
1	A	303	ASN	CA-C-N	6.18	130.49	120.60
1	A	303	ASN	C-N-CA	6.18	130.49	120.60
1	A	28	TYR	O-C-N	6.17	130.57	123.29
1	A	25	GLN	O-C-N	-6.17	116.01	123.29
1	A	298	GLN	O-C-N	-6.15	116.32	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ALA	N-CA-CB	-6.15	102.03	111.56
1	A	53	LYS	N-CA-CB	-6.12	102.90	110.98
1	A	327	SER	CA-C-N	-6.11	109.44	121.41
1	A	327	SER	C-N-CA	-6.11	109.44	121.41
1	A	115	GLN	CB-CG-CD	-6.10	102.22	112.60
1	A	104	VAL	CA-CB-CG2	6.10	120.76	110.40
1	A	314	ASP	O-C-N	-6.10	115.37	122.87
1	A	37	ASP	CA-CB-CG	-6.08	106.52	112.60
1	A	81	ASN	O-C-N	6.06	130.66	123.27
1	A	102	ALA	O-C-N	-6.03	116.37	123.25
1	A	259	SER	O-C-N	6.03	130.33	123.27
1	A	10	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	12	GLU	CA-CB-CG	-6.01	102.09	114.10
1	A	173	THR	CA-C-N	-5.99	111.53	122.38
1	A	173	THR	C-N-CA	-5.99	111.53	122.38
1	A	248	PRO	CA-C-N	-5.99	111.65	120.28
1	A	248	PRO	C-N-CA	-5.99	111.65	120.28
1	A	275	LEU	CA-C-O	-5.98	113.90	120.36
1	A	273	LYS	CA-CB-CG	-5.95	102.20	114.10
1	A	55	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	321	GLY	CA-C-N	-5.93	113.12	122.73
1	A	321	GLY	C-N-CA	-5.93	113.12	122.73
1	A	310	VAL	CG1-CB-CG2	-5.93	97.76	110.80
1	A	86	ARG	CD-NE-CZ	5.92	132.68	124.40
1	A	43	LYS	CA-C-N	-5.88	116.44	123.44
1	A	43	LYS	C-N-CA	-5.88	116.44	123.44
1	A	28	TYR	CA-C-N	-5.88	113.59	122.81
1	A	28	TYR	C-N-CA	-5.88	113.59	122.81
1	A	162	GLY	CA-C-O	5.86	130.76	120.57
1	A	256	THR	CA-C-O	5.85	127.53	120.81
1	A	305	PHE	CG-CD2-CE2	5.84	130.63	120.70
1	A	42	HIS	O-C-N	-5.84	116.56	123.22
1	A	303	ASN	N-CA-C	5.84	119.50	112.38
1	A	258	PHE	O-C-N	5.83	130.17	123.29
1	A	269	VAL	CG1-CB-CG2	-5.82	97.99	110.80
1	A	115	GLN	CB-CA-C	-5.82	97.75	109.68
1	A	284	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	26	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	92	GLY	O-C-N	-5.79	117.82	122.51
1	A	178	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	289	ASP	CA-CB-CG	-5.77	106.83	112.60
1	A	203	ASP	CA-CB-CG	-5.76	106.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ALA	O-C-N	5.73	126.92	121.71
1	A	43	LYS	CA-CB-CG	-5.72	102.66	114.10
1	A	44	GLY	CA-C-O	-5.70	114.60	119.56
1	A	94	ALA	CA-C-N	-5.70	115.08	123.05
1	A	94	ALA	C-N-CA	-5.70	115.08	123.05
1	A	331	ASN	CA-CB-CG	-5.69	106.91	112.60
1	A	309	PHE	CA-C-N	-5.68	115.27	122.37
1	A	309	PHE	C-N-CA	-5.68	115.27	122.37
1	A	28	TYR	N-CA-C	-5.66	99.96	109.07
1	A	241	GLN	CA-C-O	-5.64	113.73	120.10
1	A	60	SER	O-C-N	-5.63	115.30	122.34
1	A	29	LEU	CD1-CG-CD2	5.62	123.17	110.80
1	A	24	GLY	O-C-N	-5.62	117.37	122.93
1	A	18	VAL	CA-C-N	-5.62	113.63	122.73
1	A	18	VAL	C-N-CA	-5.62	113.63	122.73
1	A	31	PHE	CD1-CE1-CZ	5.58	130.04	120.00
1	A	13	GLU	CG-CD-OE1	5.56	131.19	118.40
1	A	91	VAL	CG1-CB-CG2	-5.56	98.56	110.80
1	A	207	ASP	CA-C-N	-5.56	103.74	120.92
1	A	207	ASP	C-N-CA	-5.56	103.74	120.92
1	A	45	CYS	N-CA-C	-5.54	101.65	109.96
1	A	221	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	101	LEU	O-C-N	5.53	130.14	122.78
1	A	162	GLY	O-C-N	-5.53	115.51	122.70
1	A	86	ARG	CB-CG-CD	-5.53	98.58	111.30
1	A	68	ASP	N-CA-C	-5.51	106.44	112.72
1	A	24	GLY	CA-C-O	5.49	126.24	121.41
1	A	279	GLY	O-C-N	-5.49	116.03	122.45
1	A	37	ASP	O-C-N	-5.46	116.80	123.19
1	A	31	PHE	CG-CD1-CE1	-5.44	111.45	120.70
1	A	101	LEU	CA-C-N	-5.43	112.35	121.75
1	A	101	LEU	C-N-CA	-5.43	112.35	121.75
1	A	267	VAL	N-CA-CB	-5.43	105.06	111.90
1	A	172	ASN	CA-C-N	-5.42	111.68	120.72
1	A	172	ASN	C-N-CA	-5.42	111.68	120.72
1	A	190	TRP	O-C-N	5.42	128.91	122.46
1	A	159	ASP	O-C-N	-5.40	115.66	122.19
1	A	222	ILE	CB-CG1-CD1	5.39	125.13	113.80
1	A	311	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	331	ASN	O-C-N	-5.38	117.09	123.22
1	A	214	ILE	N-CA-CB	-5.38	106.09	111.90
1	A	85	PHE	CA-C-O	-5.37	115.49	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	143	GLN	CA-CB-CG	-5.34	103.42	114.10
1	A	184	VAL	O-C-N	5.34	129.15	122.59
1	A	200	ASP	CA-C-O	-5.33	114.94	121.28
1	A	48	GLU	OE1-CD-OE2	-5.33	110.12	122.90
1	A	55	PHE	CD1-CG-CD2	5.32	126.59	118.60
1	A	133	TYR	CA-C-N	-5.32	114.21	122.09
1	A	133	TYR	C-N-CA	-5.32	114.21	122.09
1	A	208	GLY	O-C-N	-5.30	116.47	122.56
1	A	9	ASP	CA-C-O	-5.30	115.41	120.92
1	A	328	GLY	CA-C-N	5.29	130.69	122.49
1	A	328	GLY	C-N-CA	5.29	130.69	122.49
1	A	305	PHE	CD1-CE1-CZ	5.28	129.50	120.00
1	A	118	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	83	ILE	CA-C-N	-5.26	114.30	122.09
1	A	83	ILE	C-N-CA	-5.26	114.30	122.09
1	A	70	ASN	CB-CG-ND2	5.26	124.29	116.40
1	A	262	LEU	CA-C-N	-5.26	112.69	120.94
1	A	262	LEU	C-N-CA	-5.26	112.69	120.94
1	A	31	PHE	O-C-N	-5.24	116.01	122.82
1	A	128	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	159	ASP	CA-C-N	5.22	130.50	122.20
1	A	159	ASP	C-N-CA	5.22	130.50	122.20
1	A	193	PRO	CA-C-N	-5.20	116.38	122.93
1	A	193	PRO	C-N-CA	-5.20	116.38	122.93
1	A	153	VAL	N-CA-CB	-5.19	102.93	111.44
1	A	26	ASP	CA-C-N	-5.17	112.80	121.75
1	A	26	ASP	C-N-CA	-5.17	112.80	121.75
1	A	298	GLN	CA-C-N	5.17	130.62	123.07
1	A	298	GLN	C-N-CA	5.17	130.62	123.07
1	A	13	GLU	OE1-CD-OE2	-5.16	110.51	122.90
1	A	81	ASN	CB-CG-ND2	5.16	124.14	116.40
1	A	282	CYS	CA-C-N	-5.16	114.56	122.87
1	A	282	CYS	C-N-CA	-5.16	114.56	122.87
1	A	252	TYR	CA-CB-CG	-5.15	104.62	113.90
1	A	125	TYR	CA-C-N	5.15	124.94	119.28
1	A	125	TYR	C-N-CA	5.15	124.94	119.28
1	A	136	VAL	CA-CB-CG2	5.15	119.15	110.40
1	A	83	ILE	O-C-N	5.14	128.76	123.05
1	A	261	VAL	CA-CB-CG1	-5.14	101.66	110.40
1	A	229	GLU	O-C-N	-5.13	116.69	122.12
1	A	225	SER	CA-C-O	5.13	125.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	N-CA-C	-5.12	104.81	112.54
1	A	309	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	241	GLN	CG-CD-NE2	5.12	124.08	116.40
1	A	87	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	206	PHE	CA-C-O	-5.09	115.71	121.72
1	A	50	CYS	O-C-N	-5.07	115.84	122.43
1	A	14	TYR	CA-CB-CG	5.06	123.00	113.90
1	A	312	VAL	CA-CB-CG1	-5.05	101.81	110.40
1	A	28	TYR	CA-CB-CG	-5.05	104.81	113.90
1	A	108	SER	CA-C-N	-5.05	113.95	121.87
1	A	108	SER	C-N-CA	-5.05	113.95	121.87
1	A	11(A)	LEU	N-CA-C	-5.04	106.83	113.17
1	A	90	THR	OG1-CB-CG2	-5.03	99.24	109.30
1	A	5	PRO	CA-N-CD	5.03	119.04	112.00
1	A	70	ASN	O-C-N	5.02	128.88	123.10
1	A	75	TYR	CZ-CE2-CD2	5.02	128.64	119.60
1	A	53	LYS	N-CA-C	-5.01	107.13	114.39
1	A	183	ASP	CA-C-N	-5.00	113.61	121.62
1	A	183	ASP	C-N-CA	-5.00	113.61	121.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	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	A	2638	0	2415	19	0
2	A	5	0	0	0	0
3	A	221	0	0	0	0
All	All	2864	0	2415	19	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 4.

All (19) 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:278:VAL:HG11	1:A:283:MET:HB2	1.57	0.86
1:A:275:LEU:C	1:A:276:LEU:HD23	2.01	0.85
1:A:276:LEU:HD23	1:A:276:LEU:N	2.07	0.68
1:A:131(A):GLU:HG3	1:A:131(A):GLU:O	2.00	0.60
1:A:278:VAL:CG1	1:A:283:MET:HB2	2.34	0.54
1:A:222:ILE:HB	1:A:300:ILE:HB	1.91	0.51
1:A:40:VAL:O	1:A:103:TYR:HA	2.12	0.50
1:A:197:VAL:HG21	1:A:227:PHE:CZ	2.48	0.49
1:A:50:CYS:HB3	1:A:55:PHE:HE1	1.80	0.47
1:A:43:LYS:HA	1:A:55:PHE:HB3	1.97	0.46
1:A:90:THR:HA	1:A:94:ALA:O	2.15	0.46
1:A:173:THR:O	1:A:173:THR:HG22	2.16	0.45
1:A:275:LEU:O	1:A:276:LEU:HD23	2.17	0.43
1:A:82:GLY:C	1:A:83:ILE:HG13	2.44	0.43
1:A:223:ALA:HB1	1:A:224:PRO:HD2	2.01	0.42
1:A:18:VAL:HG12	1:A:91:VAL:HG12	2.01	0.42
1:A:179:ILE:HD13	1:A:312:VAL:HG21	2.03	0.41
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.82	0.40
1:A:287:LEU:HA	1:A:288:PRO:HD3	1.91	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	355/361 (98%)	349 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	272/298 (91%)	266 (98%)	6 (2%)	45 50

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	107	VAL
1	A	222	ILE
1	A	229	GLU
1	A	287	LEU
1	A	327	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	70	ASN
1	A	72	ASN
1	A	81	ASN
1	A	106	ASN
1	A	128	ASN
1	A	311	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.37	0

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

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.