



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:22 AM UTC

PDB ID : 4PEP / pdb_00004pep
Title : THE MOLECULAR AND CRYSTAL STRUCTURES OF MONOCLINIC PORCINE PEPSIN REFINED AT 1.8 ANGSTROMS RESOLUTION
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Deposited on : 1989-12-18
Resolution : 1.80 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
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

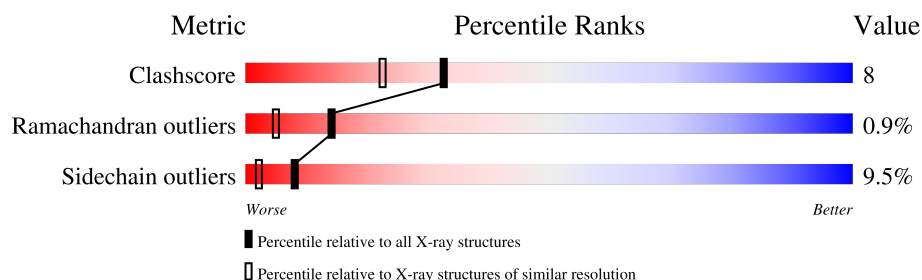
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	326	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2620 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
1	A	326	Total	C	N	O	P	S	0	0	0
			2433	1530	365	527	1	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P00791
A	263	ASP	ASN	conflict	UNP P00791

- Molecule 2 is water.

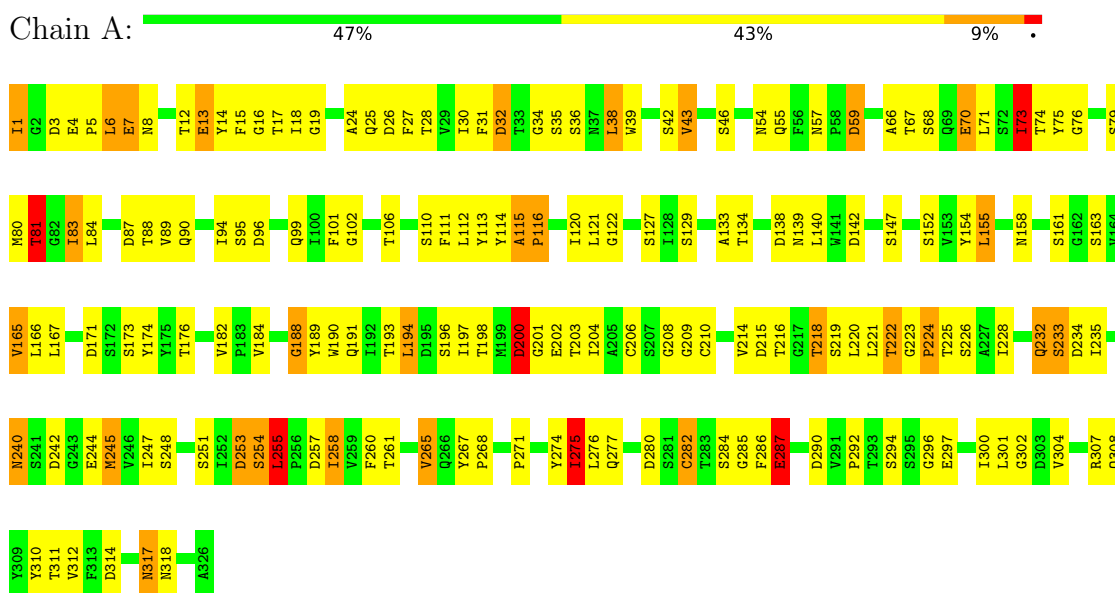
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	187	Total	O	0	0
			187	187		

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.83Å 36.44Å 73.68Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2620	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.36	8/2477 (0.3%)	2.57	194/3389 (5.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	PHE	N-CA	7.18	1.55	1.45
1	A	310	TYR	N-CA	5.96	1.53	1.46
1	A	16	GLY	N-CA	5.86	1.50	1.44
1	A	30	ILE	CA-CB	5.64	1.61	1.54
1	A	134	THR	CA-CB	5.38	1.61	1.53
1	A	203	THR	CA-CB	5.23	1.59	1.52
1	A	214	VAL	N-CA	5.22	1.52	1.46
1	A	216	THR	CA-CB	5.16	1.62	1.53

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASP	CA-CB-CG	14.31	126.91	112.60
1	A	59	ASP	CA-CB-CG	13.06	125.66	112.60
1	A	139	ASN	CA-CB-CG	11.90	124.50	112.60
1	A	138	ASP	O-C-N	11.79	134.62	122.12
1	A	73	ILE	CA-CB-CG2	11.74	130.46	110.50
1	A	26	ASP	O-C-N	11.45	136.44	123.16
1	A	253	ASP	CA-CB-CG	10.82	123.42	112.60
1	A	296	GLY	N-CA-C	10.47	125.23	111.52
1	A	39	TRP	CA-C-O	-10.43	109.42	120.89
1	A	257	ASP	CA-CB-CG	9.97	122.57	112.60
1	A	284	SER	O-C-N	9.70	134.46	123.01
1	A	184	VAL	N-CA-C	-9.33	97.54	109.58
1	A	121	LEU	CA-C-O	9.30	132.28	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLU	CA-C-O	9.28	131.82	121.06
1	A	70	GLU	CB-CG-CD	9.21	128.25	112.60
1	A	226	SER	O-C-N	9.05	131.87	122.09
1	A	35	SER	O-C-N	9.02	133.47	123.10
1	A	275	ILE	N-CA-CB	8.81	123.23	111.25
1	A	226	SER	CA-C-O	-8.74	111.70	120.70
1	A	55	GLN	OE1-CD-NE2	-8.73	113.87	122.60
1	A	102	GLY	CA-C-N	8.56	133.96	122.84
1	A	102	GLY	C-N-CA	8.56	133.96	122.84
1	A	244	GLU	CB-CG-CD	8.52	127.09	112.60
1	A	3	ASP	CB-CA-C	8.45	123.38	110.62
1	A	302	GLY	O-C-N	8.40	130.03	122.81
1	A	32	ASP	N-CA-C	8.38	122.52	108.20
1	A	90	GLN	OE1-CD-NE2	8.12	130.72	122.60
1	A	30	ILE	CA-C-N	8.07	134.72	122.77
1	A	30	ILE	C-N-CA	8.07	134.72	122.77
1	A	38	LEU	CA-C-O	-7.90	111.77	120.38
1	A	8	ASN	CB-CG-ND2	7.89	128.23	116.40
1	A	317	ASN	N-CA-C	7.81	123.10	113.50
1	A	317	ASN	CB-CA-C	-7.75	95.18	109.29
1	A	17	THR	O-C-N	7.74	132.24	123.19
1	A	81	THR	CA-CB-CG2	7.73	123.65	110.50
1	A	275	ILE	CB-CA-C	-7.59	99.52	110.83
1	A	79	SER	CB-CA-C	-7.57	96.02	110.24
1	A	198	THR	N-CA-CB	-7.55	97.47	111.52
1	A	188	GLY	N-CA-C	-7.51	95.39	113.18
1	A	87	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	133	ALA	CA-C-O	7.45	129.41	120.92
1	A	245	MET	CA-CB-CG	7.44	128.99	114.10
1	A	167	LEU	CA-C-O	-7.35	112.29	120.60
1	A	223	GLY	O-C-N	7.35	129.12	121.77
1	A	190	TRP	CB-CA-C	7.34	123.48	112.03
1	A	27	PHE	CA-CB-CG	-7.33	106.47	113.80
1	A	80	MET	O-C-N	7.33	131.69	123.48
1	A	234	ASP	CA-C-O	-7.28	110.69	119.49
1	A	90	GLN	CB-CG-CD	-7.18	100.40	112.60
1	A	32	ASP	N-CA-CB	-7.17	98.53	110.37
1	A	89	VAL	O-C-N	7.15	130.78	123.20
1	A	7	GLU	N-CA-CB	7.14	120.84	110.06
1	A	88	THR	O-C-N	7.07	131.28	123.22
1	A	176	THR	CA-CB-OG1	-7.07	99.00	109.60
1	A	261	THR	CA-CB-OG1	-7.01	99.09	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	SER	O-C-N	7.00	131.43	122.89
1	A	198	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	43	VAL	CA-CB-CG1	6.81	121.98	110.40
1	A	139	ASN	CB-CG-ND2	6.78	126.57	116.40
1	A	3	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	190	TRP	N-CA-C	-6.77	96.78	108.56
1	A	215	ASP	N-CA-C	6.71	121.18	107.69
1	A	218	THR	CA-CB-OG1	-6.66	99.61	109.60
1	A	39	TRP	O-C-N	6.61	130.88	123.48
1	A	87	ASP	O-C-N	6.59	129.89	123.04
1	A	88	THR	CA-CB-OG1	-6.58	99.73	109.60
1	A	285	GLY	N-CA-C	-6.58	104.37	115.62
1	A	287	GLU	CA-CB-CG	6.58	127.26	114.10
1	A	19	GLY	CA-C-O	-6.56	114.33	120.57
1	A	73	ILE	CB-CG1-CD1	-6.56	100.03	113.80
1	A	138	ASP	CA-C-O	-6.55	113.61	120.55
1	A	55	GLN	CG-CD-OE1	6.51	133.81	120.80
1	A	215	ASP	CB-CG-OD2	6.50	133.36	118.40
1	A	184	VAL	CA-C-O	-6.48	114.30	121.23
1	A	318	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	312	VAL	CA-C-O	6.40	127.27	120.48
1	A	15	PHE	CA-CB-CG	6.38	120.18	113.80
1	A	317	ASN	N-CA-CB	-6.36	101.17	110.53
1	A	110	SER	N-CA-C	-6.36	105.34	113.23
1	A	268	PRO	CA-C-O	6.29	128.86	121.31
1	A	139	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	224	PRO	CB-CA-C	6.29	119.07	111.46
1	A	208	GLY	N-CA-C	-6.26	107.03	115.36
1	A	113	TYR	CA-C-N	6.25	131.26	120.58
1	A	113	TYR	C-N-CA	6.25	131.26	120.58
1	A	197	ILE	N-CA-C	-6.25	99.21	108.45
1	A	99	GLN	CG-CD-NE2	-6.24	107.04	116.40
1	A	154	TYR	CA-CB-CG	-6.24	102.67	113.90
1	A	90	GLN	CA-C-O	-6.22	113.47	120.43
1	A	292	PRO	O-C-N	6.22	129.62	123.03
1	A	26	ASP	CA-C-O	-6.21	113.78	120.92
1	A	13	GLU	CA-CB-CG	6.15	126.40	114.10
1	A	142	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	134	THR	CA-CB-OG1	-6.05	100.52	109.60
1	A	129	SER	CB-CA-C	6.04	120.30	110.22
1	A	122	GLY	CA-C-N	5.98	131.88	122.49
1	A	122	GLY	C-N-CA	5.98	131.88	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	THR	N-CA-C	-5.97	99.98	109.59
1	A	198	THR	CA-CB-CG2	5.96	120.64	110.50
1	A	42	SER	CA-C-N	5.96	130.82	120.86
1	A	42	SER	C-N-CA	5.96	130.82	120.86
1	A	111	PHE	CA-C-O	-5.95	114.24	120.55
1	A	255	LEU	N-CA-C	5.92	118.24	110.08
1	A	240	ASN	CB-CA-C	5.90	124.77	111.78
1	A	310	TYR	CA-C-O	-5.88	114.05	120.81
1	A	133	ALA	CB-CA-C	5.86	119.04	109.90
1	A	121	LEU	O-C-N	-5.84	114.08	122.96
1	A	165	VAL	N-CA-CB	5.83	119.23	111.64
1	A	120	ILE	CA-C-N	5.80	131.89	123.13
1	A	120	ILE	C-N-CA	5.80	131.89	123.13
1	A	191	GLN	CA-C-O	5.80	126.75	120.43
1	A	115	ALA	O-C-N	5.76	126.86	121.27
1	A	30	ILE	O-C-N	-5.75	115.94	122.72
1	A	89	VAL	CA-C-N	-5.74	114.55	122.30
1	A	89	VAL	C-N-CA	-5.74	114.55	122.30
1	A	71	LEU	O-C-N	5.72	130.25	123.27
1	A	275	ILE	CA-C-O	-5.72	114.42	120.48
1	A	67	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	114	TYR	CA-CB-CG	-5.70	103.64	113.90
1	A	122	GLY	O-C-N	-5.69	117.15	122.96
1	A	32	ASP	O-C-N	-5.69	116.28	123.05
1	A	311	THR	N-CA-C	5.67	118.14	108.90
1	A	225	THR	O-C-N	5.64	130.10	122.59
1	A	193	THR	O-C-N	5.64	129.65	123.22
1	A	158	ASN	N-CA-C	5.63	119.33	111.90
1	A	35	SER	CA-C-N	-5.58	113.44	121.98
1	A	35	SER	C-N-CA	-5.58	113.44	121.98
1	A	42	SER	CA-C-O	5.54	127.66	121.40
1	A	191	GLN	O-C-N	-5.53	117.02	123.27
1	A	87	ASP	N-CA-CB	5.52	121.20	111.49
1	A	284	SER	CB-CA-C	-5.52	100.21	109.53
1	A	43	VAL	N-CA-CB	-5.51	99.87	110.78
1	A	277	GLN	CB-CG-CD	5.48	121.92	112.60
1	A	75	TYR	CA-CB-CG	5.47	123.75	113.90
1	A	224	PRO	N-CA-C	-5.46	102.55	110.80
1	A	161	SER	N-CA-C	-5.46	103.18	110.55
1	A	209	GLY	N-CA-C	5.46	119.56	112.68
1	A	8	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	232	GLN	CA-CB-CG	5.44	124.99	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	GLU	N-CA-C	-5.42	99.89	108.73
1	A	189	TYR	N-CA-C	-5.42	101.96	110.36
1	A	76	GLY	N-CA-C	-5.42	108.71	114.67
1	A	222	THR	CB-CA-C	5.39	119.95	109.33
1	A	36	SER	N-CA-CB	-5.36	103.91	110.98
1	A	88	THR	N-CA-CB	5.35	118.98	110.16
1	A	301	LEU	CA-C-N	5.33	129.32	121.96
1	A	301	LEU	C-N-CA	5.33	129.32	121.96
1	A	258	ILE	N-CA-C	-5.30	100.25	107.99
1	A	111	PHE	O-C-N	5.30	127.73	122.12
1	A	79	SER	N-CA-C	5.29	117.90	109.81
1	A	84	LEU	O-C-N	5.29	128.98	123.06
1	A	282	CYS	N-CA-CB	5.28	119.55	110.68
1	A	155	LEU	CA-C-O	-5.27	114.63	120.38
1	A	25	GLN	N-CA-C	-5.26	100.67	109.24
1	A	102	GLY	O-C-N	-5.26	116.90	123.21
1	A	204	ILE	N-CA-C	5.25	119.43	112.76
1	A	12	THR	CA-CB-CG2	5.25	119.42	110.50
1	A	95	SER	N-CA-CB	5.23	119.02	110.39
1	A	304	VAL	CA-C-N	5.22	127.54	120.44
1	A	304	VAL	C-N-CA	5.22	127.54	120.44
1	A	216	THR	O-C-N	-5.22	115.61	122.39
1	A	233	SER	O-C-N	5.21	127.72	122.09
1	A	152	SER	CB-CA-C	5.21	120.27	109.38
1	A	57	ASN	CA-C-N	5.19	124.86	119.56
1	A	57	ASN	C-N-CA	5.19	124.86	119.56
1	A	307	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	24	ALA	CA-C-N	5.19	129.88	122.72
1	A	24	ALA	C-N-CA	5.19	129.88	122.72
1	A	54	ASN	O-C-N	5.18	129.31	122.93
1	A	294	SER	N-CA-C	-5.18	105.08	111.40
1	A	287	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	66	ALA	CB-CA-C	-5.16	99.49	109.76
1	A	271	PRO	N-CA-CB	5.16	109.08	103.30
1	A	297	GLU	CG-CD-OE2	-5.16	106.54	118.40
1	A	96	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	81	THR	N-CA-CB	-5.13	102.03	111.37
1	A	219	SER	N-CA-C	5.12	117.99	111.69
1	A	254	SER	CA-C-O	-5.11	113.62	119.60
1	A	42	SER	O-C-N	-5.10	117.00	123.17
1	A	1	ILE	N-CA-CB	5.10	120.17	111.50
1	A	184	VAL	O-C-N	5.08	128.15	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	THR	O-C-N	5.07	129.33	123.30
1	A	81	THR	CA-C-O	-5.05	115.20	121.11
1	A	182	VAL	N-CA-CB	-5.05	107.02	112.37
1	A	5	PRO	N-CA-C	-5.04	103.25	111.68
1	A	35	SER	CA-CB-OG	5.04	121.18	111.10
1	A	18	ILE	O-C-N	-5.04	117.33	123.02
1	A	182	VAL	O-C-N	5.04	126.20	121.11
1	A	19	GLY	O-C-N	5.04	128.21	123.48
1	A	28	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	6	LEU	CA-C-O	-5.03	115.27	120.70
1	A	116	PRO	CB-CA-C	5.02	119.39	111.31
1	A	308	GLN	CG-CD-NE2	5.02	123.92	116.40
1	A	83	ILE	CA-C-O	-5.01	115.84	121.75

There are no chirality outliers.

There are no planarity outliers.

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	2433	0	2251	37	0
2	A	187	0	0	2	0
All	All	2620	0	2251	37	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 8.

All (37) 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:251:SER:HB3	1:A:255:LEU:HD22	1.76	0.68
1:A:171:ASP:HB3	1:A:174:TYR:HD1	1.59	0.67
1:A:235:ILE:O	1:A:247:ILE:HD11	1.95	0.66
1:A:275:ILE:HG21	1:A:282:CYS:HB3	1.79	0.64
1:A:265:VAL:HG13	1:A:267:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:O	2:A:362:HOH:O	2.15	0.63
1:A:6:LEU:HD11	1:A:165:VAL:HG23	1.84	0.59
1:A:194:LEU:HD21	1:A:260:PHE:HD2	1.73	0.54
1:A:81:THR:HB	1:A:106:THR:OG1	2.07	0.54
1:A:171:ASP:HB3	1:A:174:TYR:CD1	2.42	0.54
1:A:275:ILE:CG2	1:A:282:CYS:HB3	2.37	0.53
1:A:7:GLU:O	1:A:14:TYR:HA	2.08	0.53
1:A:222:THR:OG1	1:A:300:ILE:HG12	2.08	0.53
1:A:258:ILE:HD13	1:A:286:PHE:CZ	2.45	0.51
1:A:210:CYS:HB2	2:A:438:HOH:O	2.11	0.51
1:A:224:PRO:HA	1:A:290:ASP:OD1	2.12	0.50
1:A:200:ASP:O	1:A:202:GLU:N	2.48	0.47
1:A:232:GLN:HG3	1:A:245:MET:HE2	1.96	0.47
1:A:196:SER:HA	1:A:206:CYS:O	2.16	0.46
1:A:314:ASP:CG	1:A:317:ASN:HB2	2.40	0.45
1:A:275:ILE:HG22	1:A:276:LEU:N	2.30	0.45
1:A:258:ILE:HD12	1:A:274:TYR:CE2	2.52	0.45
1:A:4:GLU:HG2	1:A:31:PHE:CZ	2.52	0.44
1:A:14:TYR:CD2	1:A:155:LEU:HD22	2.52	0.44
1:A:115:ALA:HA	1:A:116:PRO:HD3	1.92	0.43
1:A:274:TYR:CD1	1:A:275:ILE:HD12	2.53	0.43
1:A:276:LEU:O	1:A:282:CYS:HA	2.19	0.43
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.89	0.43
1:A:73:ILE:HG13	1:A:74:THR:N	2.33	0.43
1:A:38:LEU:HG	1:A:101:PHE:HB2	2.01	0.42
1:A:228:ILE:HG13	1:A:287:GLU:O	2.19	0.42
1:A:32:ASP:C	1:A:34:GLY:H	2.27	0.42
1:A:258:ILE:HD12	1:A:274:TYR:CD2	2.55	0.42
1:A:200:ASP:C	1:A:202:GLU:H	2.30	0.40
1:A:94:ILE:HG21	1:A:140:LEU:HD22	2.04	0.40
1:A:218:THR:HG21	1:A:300:ILE:HG21	2.04	0.40
1:A:218:THR:HG22	1:A:220:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	323/326 (99%)	307 (95%)	13 (4%)	3 (1%)	14 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASP
1	A	201	GLY
1	A	188	GLY

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	274/274 (100%)	248 (90%)	26 (10%)	8 2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	13	GLU
1	A	43	VAL
1	A	46	SER
1	A	59	ASP
1	A	70	GLU
1	A	73	ILE
1	A	81	THR
1	A	83	ILE
1	A	112	LEU
1	A	127	SER
1	A	147	SER
1	A	166	LEU
1	A	173	SER

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	233	SER
1	A	240	ASN
1	A	242	ASP
1	A	248	SER
1	A	253	ASP
1	A	254	SER
1	A	255	LEU
1	A	265	VAL
1	A	275	ILE
1	A	280	ASP
1	A	287	GLU

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	69	GLN
1	A	98	ASN
1	A	143	GLN
1	A	240	ASN
1	A	266	GLN
1	A	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	SEP	A	68	1	8,9,10	0.99	0	7,12,14	3.15	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	68	1	-	3/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SEP	OG-P-O1P	7.41	126.47	106.44
1	A	68	SEP	O3P-P-OG	-3.50	97.54	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	SEP	CB-OG-P-O3P
1	A	68	SEP	N-CA-CB-OG
1	A	68	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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.