



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 PM UTC

PDB ID : 1CBX / pdb_00001cbx
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN CARBOXYPEPTIDASE A AND THE BIPRODUCT ANALOG INHIBITOR L-BENZYL SUCCINATE AT 2.0 ANGSTROMS RESOLUTION
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Deposited on : 1991-10-31
Resolution : 2.00 Å(reported)

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

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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

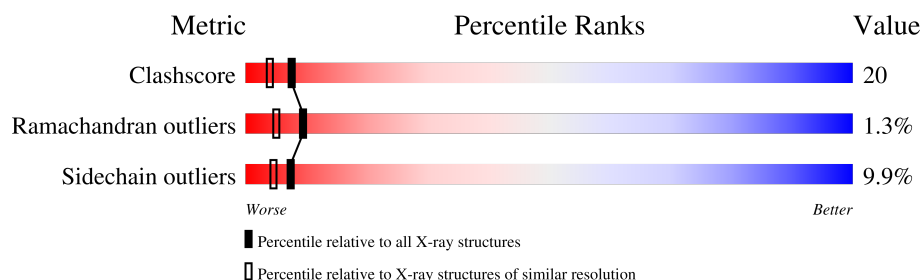
1 Overall quality at a glance

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	307	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2631 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

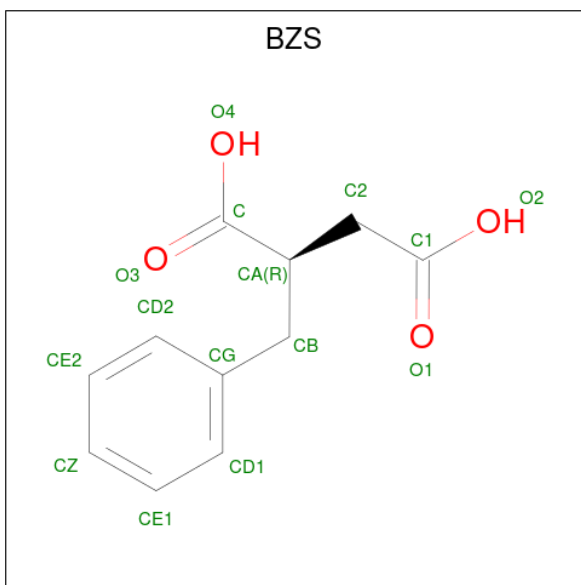
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict	UNP P00730
A	305	VAL	LEU	conflict	UNP P00730

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is L-BENZYL SUCCINIC ACID (CCD ID: BZS) (formula: C₁₁H₁₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is water.

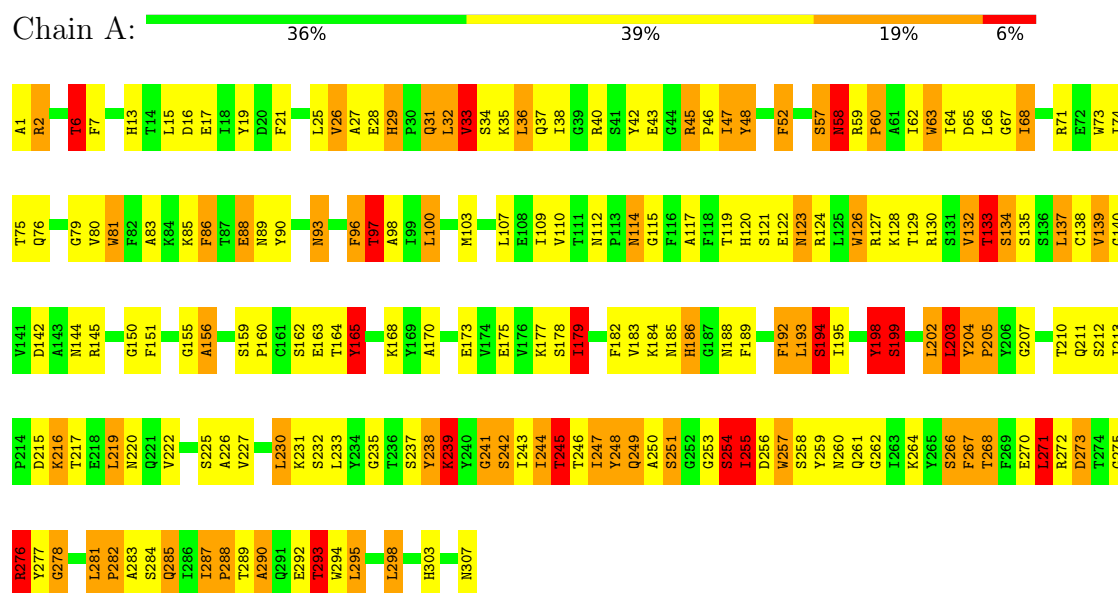
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		

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: CARBOXYPEPTIDASE A



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	51.60Å 60.27Å 47.25Å 90.00° 97.27° 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	TNT	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2631	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: BZS, ZN

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	2.27	97/2503 (3.9%)	2.44	159/3402 (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	A	0	13

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	VAL	C-N	10.24	1.46	1.33
1	A	271	LEU	C-O	9.08	1.35	1.23
1	A	178	SER	C-N	8.40	1.44	1.33
1	A	66	LEU	C-N	-8.31	1.22	1.33
1	A	184	LYS	C-N	8.27	1.44	1.33
1	A	276	ARG	C-O	8.20	1.33	1.24
1	A	183	VAL	C-O	8.10	1.33	1.24
1	A	254	SER	C-O	8.04	1.33	1.24
1	A	227	VAL	CA-C	7.63	1.62	1.52
1	A	211	GLN	CA-C	7.61	1.62	1.52
1	A	79	GLY	C-O	-7.58	1.14	1.23
1	A	75	THR	CA-CB	7.18	1.64	1.53
1	A	220	ASN	N-CA	-7.14	1.37	1.46
1	A	195	ILE	C-N	7.08	1.43	1.33
1	A	13	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	142	ASP	C-O	7.03	1.32	1.23
1	A	219	LEU	C-O	-7.01	1.15	1.24
1	A	203	LEU	C-O	-6.90	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	TYR	CA-C	6.88	1.61	1.52
1	A	173	GLU	C-N	-6.82	1.26	1.34
1	A	48	TYR	CA-C	-6.73	1.44	1.52
1	A	40	ARG	CZ-NH1	6.66	1.42	1.32
1	A	225	SER	C-O	-6.66	1.16	1.24
1	A	179	ILE	CA-CB	-6.63	1.45	1.54
1	A	37	GLN	CA-CB	-6.62	1.44	1.53
1	A	288	PRO	C-O	-6.55	1.16	1.24
1	A	119	THR	C-O	-6.53	1.16	1.24
1	A	205	PRO	CA-CB	-6.50	1.45	1.53
1	A	32	LEU	C-O	6.50	1.32	1.23
1	A	62	ILE	CA-CB	6.41	1.62	1.54
1	A	216	LYS	N-CA	-6.41	1.38	1.46
1	A	76	GLN	CA-C	6.38	1.61	1.52
1	A	80	VAL	C-O	-6.37	1.16	1.24
1	A	292	GLU	CA-C	6.35	1.60	1.52
1	A	248	TYR	C-N	6.35	1.42	1.33
1	A	110	VAL	CA-C	6.11	1.58	1.53
1	A	199	SER	C-O	6.05	1.31	1.24
1	A	90	TYR	CA-CB	6.03	1.62	1.53
1	A	237	SER	CA-C	6.02	1.60	1.52
1	A	198	TYR	C-N	-6.00	1.25	1.33
1	A	267	PHE	C-O	-6.00	1.16	1.23
1	A	47	ILE	N-CA	-6.00	1.39	1.46
1	A	193	LEU	C-N	-5.97	1.25	1.33
1	A	199	SER	N-CA	-5.96	1.38	1.46
1	A	43	GLU	CD-OE1	5.94	1.36	1.25
1	A	110	VAL	CA-CB	-5.89	1.47	1.53
1	A	47	ILE	CA-CB	5.86	1.61	1.54
1	A	130	ARG	N-CA	5.83	1.52	1.46
1	A	257	TRP	N-CA	-5.81	1.39	1.46
1	A	93	ASN	C-O	-5.76	1.16	1.24
1	A	100	LEU	C-N	-5.76	1.26	1.33
1	A	71	ARG	N-CA	-5.66	1.38	1.46
1	A	212	SER	C-O	5.66	1.30	1.23
1	A	123	ASN	CA-C	5.59	1.58	1.52
1	A	33	VAL	C-O	-5.57	1.18	1.24
1	A	226	ALA	C-O	5.56	1.30	1.24
1	A	275	GLY	C-N	5.55	1.40	1.33
1	A	63	TRP	CA-CB	5.54	1.62	1.53
1	A	249	GLN	CD-OE1	5.54	1.34	1.23
1	A	6	THR	C-O	5.54	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	PHE	CA-C	5.47	1.59	1.52
1	A	270	GLU	CA-C	5.45	1.59	1.52
1	A	36	LEU	N-CA	-5.45	1.39	1.46
1	A	170	ALA	C-O	5.45	1.30	1.23
1	A	244	ILE	CA-C	5.44	1.60	1.52
1	A	2	ARG	NE-CZ	5.42	1.39	1.33
1	A	303	HIS	ND1-CE1	5.38	1.38	1.32
1	A	140	GLY	C-O	-5.38	1.18	1.24
1	A	217	THR	CA-C	5.37	1.59	1.52
1	A	282	PRO	C-O	-5.36	1.17	1.23
1	A	293	THR	C-O	-5.36	1.17	1.24
1	A	66	LEU	C-O	-5.35	1.17	1.23
1	A	32	LEU	C-N	5.31	1.40	1.33
1	A	129	THR	C-O	5.30	1.29	1.23
1	A	139	VAL	CA-CB	-5.30	1.48	1.54
1	A	292	GLU	CA-CB	5.29	1.61	1.53
1	A	63	TRP	CA-C	5.29	1.59	1.52
1	A	29	HIS	C-O	5.25	1.29	1.23
1	A	156	ALA	CA-CB	-5.25	1.45	1.53
1	A	73	TRP	CD2-CE3	-5.23	1.31	1.40
1	A	186	HIS	CB-CG	5.21	1.57	1.50
1	A	93	ASN	C-N	-5.20	1.27	1.33
1	A	192	PHE	C-N	5.20	1.41	1.33
1	A	119	THR	C-N	5.19	1.41	1.33
1	A	60	PRO	CA-CB	-5.19	1.46	1.53
1	A	217	THR	C-O	5.17	1.30	1.24
1	A	262	GLY	C-N	5.17	1.38	1.33
1	A	273	ASP	CG-OD2	5.16	1.35	1.25
1	A	145	ARG	CZ-NH1	5.15	1.40	1.32
1	A	109	ILE	N-CA	5.14	1.52	1.46
1	A	122	GLU	CD-OE1	5.12	1.35	1.25
1	A	295	LEU	C-N	5.12	1.39	1.33
1	A	81	TRP	CA-CB	5.11	1.61	1.53
1	A	233	LEU	N-CA	-5.05	1.39	1.46
1	A	195	ILE	C-O	5.04	1.30	1.24
1	A	281	LEU	CA-C	5.02	1.58	1.53
1	A	251	SER	N-CA	5.01	1.51	1.45

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	THR	CA-C-O	-12.47	106.23	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ILE	CA-CB-CG2	10.01	127.51	110.50
1	A	124	ARG	CA-C-O	9.88	131.53	119.38
1	A	117	ALA	CA-C-O	9.81	131.19	120.10
1	A	120	HIS	N-CA-C	-9.75	100.13	112.90
1	A	48	TYR	CA-C-O	-9.49	110.44	120.70
1	A	145	ARG	NE-CZ-NH2	-9.12	111.00	119.20
1	A	163	GLU	CA-C-O	9.02	130.49	119.31
1	A	86	PHE	N-CA-C	-8.90	101.49	111.82
1	A	13	HIS	CA-CB-CG	-8.71	105.09	113.80
1	A	185	ASN	OD1-CG-ND2	-8.62	113.98	122.60
1	A	182	PHE	N-CA-C	8.33	119.99	111.07
1	A	186	HIS	CA-CB-CG	-8.25	105.55	113.80
1	A	35	LYS	CA-C-O	-8.13	111.66	120.36
1	A	109	ILE	CA-C-N	-8.10	115.27	122.96
1	A	109	ILE	C-N-CA	-8.10	115.27	122.96
1	A	163	GLU	N-CA-C	-7.83	103.17	112.89
1	A	178	SER	CA-C-O	-7.81	112.28	120.55
1	A	159	SER	O-C-N	7.57	129.44	121.42
1	A	184	LYS	O-C-N	7.53	129.83	122.07
1	A	151	PHE	CA-C-O	-7.41	113.00	121.15
1	A	48	TYR	O-C-N	7.38	132.82	123.23
1	A	43	GLU	CA-C-N	7.36	132.69	121.51
1	A	43	GLU	C-N-CA	7.36	132.69	121.51
1	A	133	THR	O-C-N	7.34	132.36	122.59
1	A	88	GLU	N-CA-C	7.29	119.31	111.36
1	A	144	ASN	CA-CB-CG	-7.20	105.40	112.60
1	A	126	TRP	CA-C-N	7.15	135.33	122.46
1	A	126	TRP	C-N-CA	7.15	135.33	122.46
1	A	122	GLU	O-C-N	-7.12	113.12	122.59
1	A	97	THR	N-CA-C	7.09	119.00	111.28
1	A	222	VAL	N-CA-C	7.08	117.21	110.42
1	A	255	ILE	CB-CA-C	7.05	121.95	112.22
1	A	162	SER	N-CA-C	7.03	120.68	110.28
1	A	211	GLN	CA-C-N	6.94	130.72	120.87
1	A	211	GLN	C-N-CA	6.94	130.72	120.87
1	A	244	ILE	CA-CB-CG2	6.86	122.16	110.50
1	A	13	HIS	ND1-CE1-NE2	6.81	115.21	108.40
1	A	210	THR	N-CA-C	-6.79	104.99	113.28
1	A	202	LEU	N-CA-CB	6.79	122.09	110.68
1	A	155	GLY	N-CA-C	-6.65	105.72	115.63
1	A	184	LYS	CA-C-O	-6.59	113.90	120.82
1	A	298	LEU	CD1-CG-CD2	-6.58	96.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	CA-C-O	-6.51	113.60	120.63
1	A	256	ASP	CA-C-O	6.51	127.45	120.55
1	A	47	ILE	N-CA-C	-6.49	99.02	108.11
1	A	287	ILE	N-CA-CB	6.46	115.49	110.45
1	A	195	ILE	O-C-N	6.42	130.16	123.03
1	A	202	LEU	CB-CA-C	-6.35	98.09	109.71
1	A	37	GLN	CG-CD-NE2	6.32	125.88	116.40
1	A	96	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	17	GLU	N-CA-C	6.29	118.14	111.28
1	A	65	ASP	N-CA-CB	6.29	121.84	111.08
1	A	46	PRO	CA-C-O	-6.28	114.01	121.67
1	A	226	ALA	O-C-N	6.27	128.86	122.09
1	A	198	TYR	CA-C-N	6.22	133.42	121.54
1	A	198	TYR	C-N-CA	6.22	133.42	121.54
1	A	83	ALA	CA-C-O	6.20	127.53	120.90
1	A	138	CYS	CA-C-O	-6.18	113.81	120.92
1	A	25	LEU	O-C-N	6.16	128.65	122.12
1	A	98	ALA	O-C-N	6.15	128.64	122.12
1	A	182	PHE	N-CA-CB	-6.14	101.11	110.01
1	A	27	ALA	N-CA-C	6.13	117.97	111.28
1	A	33	VAL	N-CA-C	6.12	117.10	108.17
1	A	195	ILE	CA-C-O	-6.10	114.04	120.57
1	A	163	GLU	O-C-N	-6.05	114.11	122.46
1	A	282	PRO	CA-C-O	-6.05	114.44	121.34
1	A	276	ARG	O-C-N	6.05	128.55	122.08
1	A	47	ILE	CA-CB-CG2	6.04	120.77	110.50
1	A	239	LYS	N-CA-CB	6.02	120.44	110.63
1	A	239	LYS	N-CA-C	-6.00	100.51	110.17
1	A	242	SER	CA-C-N	-6.00	112.91	120.77
1	A	242	SER	C-N-CA	-6.00	112.91	120.77
1	A	165	TYR	O-C-N	-5.94	115.56	122.87
1	A	247	ILE	N-CA-CB	5.94	121.03	111.23
1	A	250	ALA	N-CA-C	-5.94	97.79	108.48
1	A	123	ASN	N-CA-CB	-5.90	101.15	110.77
1	A	204	TYR	CA-C-O	5.90	128.25	120.16
1	A	186	HIS	N-CA-CB	-5.87	101.56	110.07
1	A	179	ILE	O-C-N	5.86	127.86	121.83
1	A	123	ASN	CA-C-O	5.85	127.34	120.20
1	A	248	TYR	CA-CB-CG	5.83	124.39	113.90
1	A	285	GLN	CA-C-O	-5.81	112.76	119.56
1	A	212	SER	CA-C-O	5.77	127.63	121.16
1	A	7	PHE	O-C-N	-5.76	115.81	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	SER	CA-C-O	5.76	126.84	120.80
1	A	183	VAL	CA-C-O	-5.74	114.98	120.95
1	A	254	SER	N-CA-CB	-5.74	101.39	109.94
1	A	32	LEU	CA-C-N	-5.74	114.43	122.75
1	A	32	LEU	C-N-CA	-5.74	114.43	122.75
1	A	68	ILE	CA-CB-CG2	5.73	120.25	110.50
1	A	232	SER	CA-C-O	5.72	126.42	119.38
1	A	6	THR	N-CA-CB	-5.72	102.72	110.67
1	A	293	THR	CB-CA-C	5.70	120.38	110.68
1	A	40	ARG	NE-CZ-NH2	-5.68	114.08	119.20
1	A	258	SER	CB-CA-C	5.68	120.22	110.79
1	A	194	SER	N-CA-CB	5.68	119.69	110.77
1	A	249	GLN	N-CA-CB	5.67	118.29	109.85
1	A	249	GLN	CA-CB-CG	-5.66	102.78	114.10
1	A	253	GLY	CA-C-N	5.64	128.15	120.54
1	A	253	GLY	C-N-CA	5.64	128.15	120.54
1	A	29	HIS	N-CA-CB	-5.63	102.85	110.74
1	A	37	GLN	N-CA-C	5.63	118.22	107.75
1	A	81	TRP	CD2-CE2-CZ2	-5.61	116.79	122.40
1	A	36	LEU	CA-C-O	5.61	126.65	120.71
1	A	219	LEU	N-CA-CB	-5.57	101.64	110.22
1	A	32	LEU	O-C-N	5.57	129.83	122.36
1	A	79	GLY	N-CA-C	-5.56	105.76	112.49
1	A	26	VAL	N-CA-C	-5.55	105.11	110.72
1	A	256	ASP	O-C-N	-5.55	116.24	122.12
1	A	117	ALA	O-C-N	-5.54	115.74	122.22
1	A	248	TYR	CB-CG-CD2	5.51	129.07	120.80
1	A	192	PHE	CA-C-N	-5.50	114.69	122.94
1	A	192	PHE	C-N-CA	-5.50	114.69	122.94
1	A	215	ASP	O-C-N	5.49	128.78	122.25
1	A	290	ALA	CA-C-O	5.47	126.56	120.82
1	A	59	ARG	O-C-N	5.43	127.36	121.60
1	A	164	THR	CA-C-N	-5.43	113.00	120.71
1	A	164	THR	C-N-CA	-5.43	113.00	120.71
1	A	293	THR	CA-C-O	5.43	126.49	120.63
1	A	285	GLN	O-C-N	5.42	128.85	122.34
1	A	97	THR	CA-C-O	-5.40	114.82	120.55
1	A	278	GLY	CA-C-O	-5.40	114.01	121.46
1	A	295	LEU	O-C-N	5.39	128.90	122.27
1	A	68	ILE	O-C-N	5.38	127.16	121.89
1	A	260	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	A	245	THR	OG1-CB-CG2	5.36	120.02	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	144	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	76	GLN	CA-C-O	5.34	126.11	119.97
1	A	119	THR	CA-CB-OG1	5.32	117.58	109.60
1	A	58	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	241	GLY	O-C-N	-5.28	118.66	123.78
1	A	29	HIS	CA-C-O	5.26	126.66	121.29
1	A	268	THR	CA-C-O	-5.25	115.15	120.71
1	A	29	HIS	N-CA-C	5.23	117.10	109.30
1	A	139	VAL	CA-C-O	-5.23	114.76	120.72
1	A	177	LYS	CA-C-O	5.22	126.26	120.63
1	A	114	ASN	N-CA-CB	5.20	117.56	110.01
1	A	303	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	210	THR	CA-C-O	5.19	125.35	119.18
1	A	249	GLN	CG-CD-NE2	-5.18	108.63	116.40
1	A	127	ARG	O-C-N	-5.18	115.72	122.09
1	A	173	GLU	CA-C-O	5.17	126.38	120.54
1	A	266	SER	CA-C-O	-5.17	114.64	120.32
1	A	16	ASP	CA-C-O	-5.16	114.95	120.42
1	A	45	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	185	ASN	O-C-N	-5.14	116.67	122.12
1	A	29	HIS	CA-CB-CG	-5.13	108.67	113.80
1	A	132	VAL	N-CA-CB	5.13	119.69	111.23
1	A	145	ARG	CA-C-O	5.06	124.75	119.03
1	A	38	ILE	CA-C-O	5.04	125.84	119.48
1	A	142	ASP	CB-CG-OD2	-5.04	106.82	118.40
1	A	122	GLU	CG-CD-OE1	-5.02	106.85	118.40
1	A	259	TYR	O-C-N	5.02	127.88	122.15
1	A	124	ARG	N-CA-C	-5.01	106.43	112.54
1	A	123	ASN	OD1-CG-ND2	-5.00	117.59	122.60
1	A	35	LYS	N-CA-C	5.00	116.89	108.73
1	A	193	LEU	CA-C-O	-5.00	115.30	120.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ALA	Mainchain
1	A	165	TYR	Sidechain
1	A	189	PHE	Sidechain
1	A	19	TYR	Sidechain
1	A	198	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	203	LEU	Mainchain
1	A	21	PHE	Sidechain
1	A	230	LEU	Mainchain
1	A	238	TYR	Sidechain
1	A	278	GLY	Mainchain
1	A	283	ALA	Mainchain
1	A	47	ILE	Mainchain
1	A	58	ASN	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2352	97	0
2	A	1	0	0	0	0
3	A	15	0	10	0	0
4	A	178	0	0	12	0
All	All	2631	0	2362	97	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 20.

All (97) 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:289:THR:O	1:A:293:THR:HG23	1.37	1.24
1:A:137:LEU:HD22	1:A:137:LEU:H	1.16	1.04
1:A:289:THR:O	1:A:293:THR:CG2	2.15	0.94
1:A:137:LEU:HD22	1:A:137:LEU:N	1.96	0.81
1:A:31:GLN:HB2	4:A:588:HOH:O	1.84	0.77
1:A:175:GLU:O	1:A:179:ILE:HD13	1.85	0.76
1:A:254:SER:OG	4:A:648:HOH:O	2.04	0.73
1:A:186:HIS:HD2	1:A:188:ASN:H	1.37	0.72
1:A:86:PHE:HE1	1:A:294:TRP:CZ3	2.08	0.72
1:A:85:LYS:HE3	1:A:89:ASN:ND2	2.07	0.70
1:A:207:GLY:O	1:A:249:GLN:CG	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:O	1:A:134:SER:HB3	1.91	0.69
1:A:168:LYS:HG2	4:A:547:HOH:O	1.94	0.68
1:A:45:ARG:HH11	1:A:114:ASN:ND2	1.92	0.68
1:A:179:ILE:N	1:A:179:ILE:HD12	2.10	0.67
1:A:137:LEU:H	1:A:137:LEU:CD2	2.00	0.66
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.26	0.66
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.61	0.65
1:A:242:SER:OG	1:A:245:THR:HB	1.97	0.64
1:A:134:SER:OG	1:A:135:SER:N	2.29	0.64
1:A:207:GLY:O	1:A:249:GLN:HG3	1.96	0.64
1:A:45:ARG:HH11	1:A:114:ASN:HD22	1.44	0.63
1:A:45:ARG:HD2	1:A:114:ASN:HD22	1.62	0.63
1:A:42:TYR:OH	1:A:132:VAL:HG22	1.99	0.61
1:A:245:THR:HG21	4:A:539:HOH:O	2.02	0.60
1:A:26:VAL:HG22	1:A:33:VAL:HG22	1.83	0.59
1:A:207:GLY:O	1:A:249:GLN:HG2	2.03	0.59
1:A:179:ILE:N	1:A:179:ILE:CD1	2.64	0.58
1:A:58:ASN:ND2	1:A:188:ASN:HB2	2.18	0.57
1:A:60:PRO:HB2	1:A:103:MET:HE3	1.85	0.57
1:A:230:LEU:C	1:A:230:LEU:HD23	2.30	0.57
1:A:239:LYS:HE3	4:A:668:HOH:O	2.05	0.56
1:A:244:ILE:HD12	1:A:249:GLN:HG3	1.88	0.55
1:A:93:ASN:O	1:A:97:THR:CG2	2.54	0.55
1:A:93:ASN:O	1:A:97:THR:HG23	2.08	0.53
1:A:175:GLU:O	1:A:179:ILE:CD1	2.55	0.53
1:A:186:HIS:HE1	4:A:612:HOH:O	1.92	0.52
1:A:230:LEU:HD23	1:A:230:LEU:O	2.09	0.52
1:A:241:GLY:HA3	1:A:246:THR:OG1	2.10	0.52
1:A:287:ILE:N	1:A:288:PRO:HD2	2.26	0.51
1:A:112:ASN:ND2	1:A:115:GLY:H	2.08	0.51
1:A:276:ARG:HD3	1:A:276:ARG:C	2.35	0.51
1:A:254:SER:CB	4:A:661:HOH:O	2.58	0.51
1:A:257:TRP:O	1:A:261:GLN:HG2	2.10	0.51
1:A:32:LEU:HD11	1:A:100:LEU:HD13	1.92	0.50
1:A:254:SER:HB2	4:A:661:HOH:O	2.12	0.50
1:A:204:TYR:HB2	1:A:205:PRO:HD2	1.92	0.50
1:A:28:GLU:C	1:A:29:HIS:CG	2.91	0.48
1:A:239:LYS:CE	4:A:668:HOH:O	2.60	0.48
1:A:186:HIS:HD2	1:A:188:ASN:N	2.10	0.47
1:A:192:PHE:O	1:A:193:LEU:HD12	2.14	0.47
1:A:88:GLU:OE1	4:A:584:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:CD1	1:A:179:ILE:H	2.28	0.47
1:A:32:LEU:O	1:A:52:PHE:HA	2.15	0.46
1:A:272:ARG:HB3	1:A:273:ASP:HA	1.97	0.46
1:A:123:ASN:OD1	1:A:123:ASN:C	2.56	0.46
1:A:1:ALA:N	1:A:6:THR:HG22	2.30	0.46
1:A:238:TYR:OH	1:A:271:LEU:HA	2.15	0.46
1:A:6:THR:HG21	4:A:600:HOH:O	2.15	0.46
1:A:272:ARG:HH11	1:A:285:GLN:HE21	1.62	0.46
1:A:45:ARG:HD2	1:A:114:ASN:ND2	2.29	0.46
1:A:231:LYS:O	1:A:235:GLY:HA2	2.16	0.46
1:A:132:VAL:HG23	1:A:133:THR:OG1	2.16	0.45
1:A:204:TYR:O	1:A:242:SER:HA	2.17	0.45
1:A:133:THR:O	1:A:134:SER:CB	2.63	0.45
1:A:282:PRO:C	1:A:284:SER:N	2.74	0.44
1:A:255:ILE:HD12	1:A:266:SER:HB3	1.98	0.44
1:A:160:PRO:HA	1:A:165:TYR:CD2	2.52	0.44
1:A:276:ARG:HD2	1:A:277:TYR:CE2	2.52	0.44
1:A:68:ILE:HD13	1:A:68:ILE:HG21	1.74	0.43
1:A:264:LYS:O	1:A:264:LYS:HG2	2.17	0.43
1:A:126:TRP:NE1	1:A:128:LYS:O	2.51	0.43
1:A:93:ASN:ND2	1:A:96:PHE:H	2.17	0.43
1:A:194:SER:O	1:A:268:THR:HG23	2.18	0.43
1:A:247:ILE:HG12	1:A:248:TYR:CD2	2.54	0.43
1:A:93:ASN:O	1:A:97:THR:HG22	2.18	0.43
1:A:204:TYR:CB	1:A:205:PRO:CD	2.94	0.43
1:A:2:ARG:H	1:A:6:THR:HG21	1.83	0.43
1:A:36:LEU:O	1:A:48:TYR:HA	2.19	0.43
1:A:150:GLY:O	1:A:251:SER:HB2	2.19	0.42
1:A:276:ARG:HD3	1:A:276:ARG:O	2.19	0.42
1:A:103:MET:HE2	1:A:103:MET:HB3	1.93	0.42
1:A:219:LEU:HG	1:A:267:PHE:CZ	2.55	0.42
1:A:63:TRP:C	1:A:64:ILE:HG13	2.45	0.42
1:A:192:PHE:HD1	1:A:255:ILE:CD1	2.33	0.42
1:A:213:ILE:HD12	1:A:219:LEU:HD22	2.02	0.42
1:A:282:PRO:C	1:A:284:SER:H	2.28	0.42
1:A:192:PHE:C	1:A:193:LEU:HD12	2.45	0.41
1:A:198:TYR:O	1:A:199:SER:CB	2.67	0.41
1:A:15:LEU:C	1:A:15:LEU:HD13	2.45	0.41
1:A:64:ILE:HB	1:A:107:LEU:HD12	2.01	0.41
1:A:186:HIS:CD2	1:A:188:ASN:H	2.26	0.41
1:A:207:GLY:HA2	1:A:243:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLY:O	4:A:529:HOH:O	2.21	0.40
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.75	0.40
1:A:81:TRP:CE3	1:A:290:ALA:HB1	2.57	0.40
1:A:60:PRO:HA	1:A:188:ASN:O	2.21	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	305/307 (99%)	287 (94%)	14 (5%)	4 (1%)	9 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	A	134	SER
1	A	199	SER
1	A	57	SER

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	263/263 (100%)	237 (90%)	26 (10%)	7 4

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

Mol	Chain	Res	Type
1	A	6	THR
1	A	31	GLN
1	A	33	VAL
1	A	34	SER
1	A	57	SER
1	A	58	ASN
1	A	74	ILE
1	A	97	THR
1	A	137	LEU
1	A	139	VAL
1	A	179	ILE
1	A	194	SER
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	239	LYS
1	A	245	THR
1	A	254	SER
1	A	255	ILE
1	A	271	LEU
1	A	276	ARG
1	A	281	LEU
1	A	293	THR
1	A	295	LEU
1	A	298	LEU
1	A	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	31	GLN
1	A	37	GLN
1	A	58	ASN
1	A	93	ASN
1	A	112	ASN
1	A	114	ASN
1	A	171	ASN
1	A	186	HIS
1	A	220	ASN
1	A	285	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
3	BZS	A	500	2	15,15,15	2.24	6 (40%)	19,19,19	2.36	6 (31%)

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
3	BZS	A	500	2	-	2/12/12/12	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	BZS	CA-C	5.34	1.61	1.51
3	A	500	BZS	O3-C	3.48	1.32	1.22
3	A	500	BZS	O2-C1	-2.72	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	BZS	CB-CG	2.66	1.57	1.51
3	A	500	BZS	CE2-CD2	-2.57	1.34	1.38
3	A	500	BZS	CE1-CD1	2.12	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	BZS	CG-CB-CA	-7.34	99.77	113.74
3	A	500	BZS	O2-C1-C2	3.63	125.29	114.00
3	A	500	BZS	O1-C1-C2	-3.31	112.69	122.84
3	A	500	BZS	CA-C2-C1	-3.14	106.84	113.92
3	A	500	BZS	CB-CA-C	-2.11	105.94	110.91
3	A	500	BZS	CE1-CD1-CG	-2.01	117.79	120.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	BZS	O1-C1-C2-CA
3	A	500	BZS	O2-C1-C2-CA

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.