



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:27 AM UTC

PDB ID : 1BP3 / pdb_00001bp3
Title : THE XRAY STRUCTURE OF A GROWTH HORMONE-PROLACTIN RECEPTOR COMPLEX
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Deposited on : 1998-08-12
Resolution : 2.90 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
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

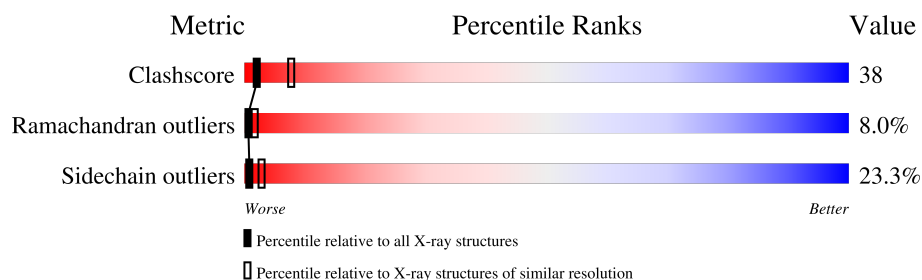
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	191	
2	B	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3123 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 PROTEIN (GROWTH HORMONE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1509	961	254	287	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ARG	GLY	engineered mutation	UNP P01241

- Molecule 2 is a protein called PROTEIN (PROLACTIN RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1613	1049	264	291	9			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

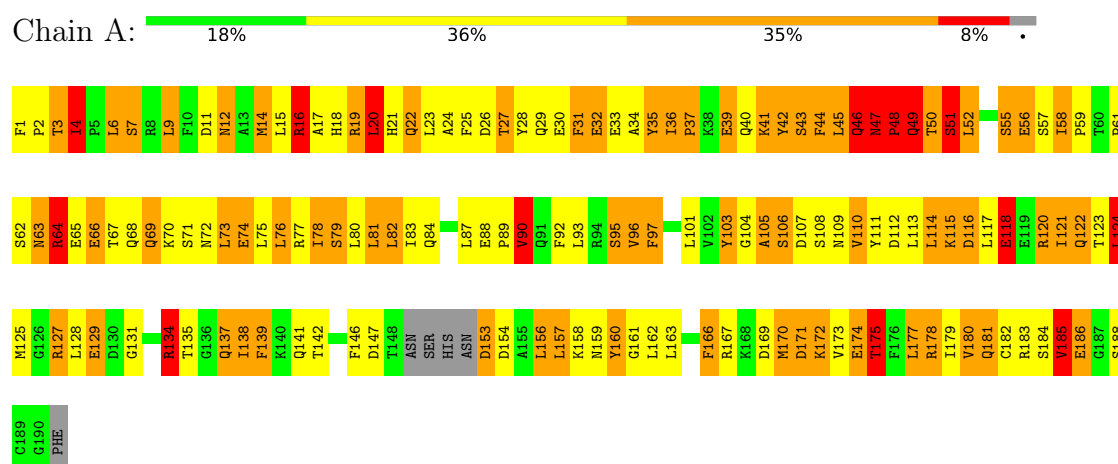
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

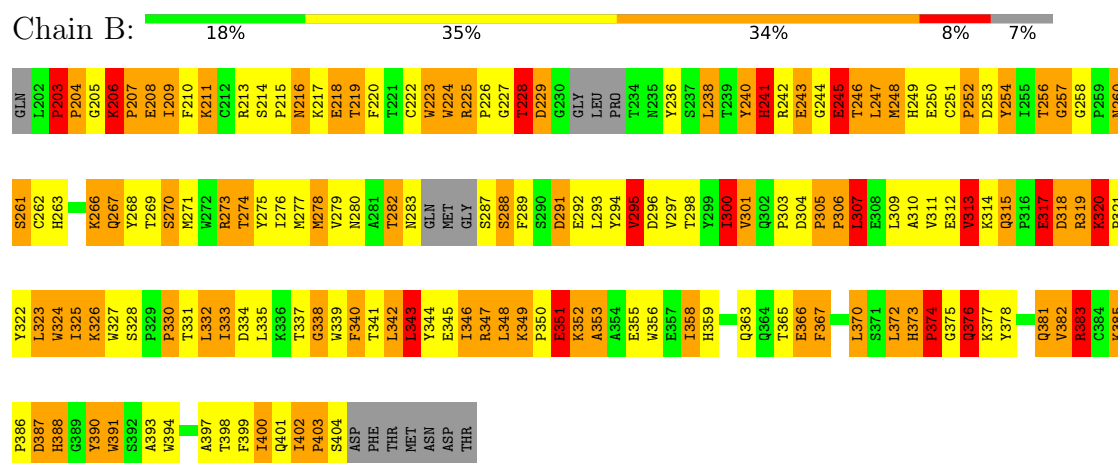
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: PROTEIN (PROLACTIN RECEPTOR)



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	154.20 Å 69.80 Å 43.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: 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	1.38	5/1539 (0.3%)	2.81	153/2079 (7.4%)
2	B	1.48	14/1672 (0.8%)	2.89	173/2283 (7.6%)
All	All	1.43	19/3211 (0.6%)	2.85	326/4362 (7.5%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	282	THR	CA-CB	7.96	1.66	1.53
2	B	338	GLY	N-CA	-7.54	1.34	1.45
1	A	37	PRO	C-O	7.32	1.33	1.24
1	A	139	PHE	N-CA	6.85	1.55	1.47
2	B	258	GLY	N-CA	6.64	1.53	1.44
2	B	246	THR	N-CA	-5.92	1.38	1.46
1	A	58	ILE	CA-C	5.84	1.59	1.52
2	B	246	THR	CA-CB	5.79	1.63	1.53
2	B	387	ASP	C-O	5.77	1.31	1.24
2	B	358	ILE	CA-CB	5.74	1.61	1.54
2	B	228	THR	CA-CB	5.46	1.61	1.53
2	B	266	LYS	C-O	5.46	1.30	1.24
2	B	205	GLY	C-O	5.41	1.30	1.23
1	A	131	GLY	N-CA	-5.35	1.37	1.45
2	B	205	GLY	N-CA	5.35	1.50	1.45
2	B	398	THR	CA-CB	5.19	1.60	1.52
1	A	50	THR	CA-CB	5.19	1.61	1.53
2	B	345	GLU	CA-CB	-5.17	1.44	1.53
2	B	337	THR	CB-OG1	5.16	1.52	1.43

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	GLU	CA-C-N	18.14	156.19	121.54
2	B	245	GLU	C-N-CA	18.14	156.19	121.54
2	B	205	GLY	CA-C-O	-15.72	111.38	122.23
2	B	337	THR	CA-C-N	15.13	151.07	121.41
2	B	337	THR	C-N-CA	15.13	151.07	121.41
2	B	296	ASP	CA-CB-CG	14.38	126.98	112.60
2	B	244	GLY	CA-C-N	14.18	148.62	121.54
2	B	244	GLY	C-N-CA	14.18	148.62	121.54
2	B	227	GLY	CA-C-N	13.90	141.38	121.50
2	B	227	GLY	C-N-CA	13.90	141.38	121.50
1	A	153	ASP	CA-CB-CG	13.26	125.86	112.60
2	B	345	GLU	CA-CB-CG	12.94	139.99	114.10
1	A	171	ASP	CA-CB-CG	12.44	125.04	112.60
1	A	157	LEU	CA-C-N	12.40	136.56	120.44
1	A	157	LEU	C-N-CA	12.40	136.56	120.44
1	A	29	GLN	OE1-CD-NE2	-12.29	110.31	122.60
2	B	282	THR	N-CA-C	12.25	128.43	108.34
1	A	16	ARG	CD-NE-CZ	12.24	141.53	124.40
1	A	127	ARG	CD-NE-CZ	12.12	141.37	124.40
1	A	33	GLU	CA-CB-CG	11.52	137.14	114.10
1	A	56	GLU	CB-CG-CD	11.45	132.06	112.60
2	B	208	GLU	CB-CG-CD	11.37	131.93	112.60
1	A	101	LEU	CA-C-N	11.17	142.07	121.97
1	A	101	LEU	C-N-CA	11.17	142.07	121.97
2	B	291	ASP	CA-C-O	-11.12	109.13	121.25
1	A	107	ASP	CA-CB-CG	10.98	123.58	112.60
1	A	39	GLU	CB-CG-CD	10.85	131.05	112.60
1	A	25	PHE	CA-CB-CG	10.65	124.45	113.80
2	B	220	PHE	CA-CB-CG	10.56	124.36	113.80
1	A	138	ILE	CA-C-N	-10.42	107.22	121.71
1	A	138	ILE	C-N-CA	-10.42	107.22	121.71
2	B	318	ASP	CB-CA-C	10.35	126.64	109.56
2	B	370	LEU	CA-C-N	10.26	138.38	122.78
2	B	370	LEU	C-N-CA	10.26	138.38	122.78
2	B	366	GLU	CA-CB-CG	10.22	134.54	114.10
1	A	182	CYS	CA-C-N	10.15	137.66	120.72
1	A	182	CYS	C-N-CA	10.15	137.66	120.72
2	B	229	ASP	CB-CA-C	10.12	127.06	112.07
2	B	385	LYS	O-C-N	9.93	132.18	122.06
2	B	337	THR	CA-C-O	9.72	134.41	120.51
1	A	138	ILE	CA-C-O	-9.69	110.00	121.04
2	B	205	GLY	N-CA-C	-9.66	101.47	112.29
1	A	182	CYS	N-CA-C	9.51	121.41	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	LEU	CA-C-N	9.27	136.18	121.17
2	B	372	LEU	C-N-CA	9.27	136.18	121.17
1	A	51	SER	N-CA-C	9.26	122.23	111.11
1	A	58	ILE	N-CA-CB	9.02	123.84	111.21
2	B	211	LYS	CA-C-O	8.87	131.20	121.26
2	B	358	ILE	N-CA-C	8.87	121.05	108.36
1	A	31	PHE	CA-CB-CG	8.78	122.58	113.80
2	B	315	GLN	OE1-CD-NE2	8.74	131.34	122.60
1	A	169	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	69	GLN	CA-C-O	-8.62	109.48	120.00
1	A	46	GLN	CB-CG-CD	8.60	127.21	112.60
1	A	92	PHE	CA-CB-CG	8.60	122.40	113.80
2	B	280	ASN	CA-CB-CG	8.49	121.09	112.60
1	A	131	GLY	N-CA-C	8.48	133.28	113.18
1	A	95	SER	CA-CB-OG	8.45	128.00	111.10
2	B	249	HIS	CA-CB-CG	8.45	122.25	113.80
1	A	64	ARG	CG-CD-NE	8.43	130.56	112.00
2	B	305	PRO	N-CA-CB	8.40	107.89	103.19
2	B	248	MET	N-CA-C	-8.39	98.42	110.59
2	B	243	GLU	CA-C-O	8.37	130.32	120.70
1	A	142	THR	CA-C-N	8.36	133.54	122.42
1	A	142	THR	C-N-CA	8.36	133.54	122.42
1	A	90	VAL	CA-C-N	8.35	134.87	120.68
1	A	90	VAL	C-N-CA	8.35	134.87	120.68
2	B	375	GLY	N-CA-C	8.33	123.65	114.40
2	B	305	PRO	O-C-N	8.32	125.14	121.31
1	A	37	PRO	N-CA-C	8.32	129.61	112.47
2	B	307	LEU	N-CA-C	8.14	122.69	109.59
1	A	33	GLU	CB-CG-CD	8.09	126.34	112.60
2	B	253	ASP	CA-C-O	-7.97	110.26	119.98
1	A	20	LEU	CA-C-O	-7.94	112.48	120.82
2	B	218	GLU	CB-CG-CD	7.92	126.07	112.60
1	A	57	SER	CA-C-N	7.86	136.68	122.13
1	A	57	SER	C-N-CA	7.86	136.68	122.13
2	B	297	VAL	N-CA-C	7.79	119.50	110.62
1	A	137	GLN	N-CA-C	7.79	120.50	108.12
1	A	139	PHE	CB-CA-C	7.72	125.82	112.00
2	B	266	LYS	CA-C-O	-7.71	112.30	120.55
1	A	39	GLU	CA-CB-CG	7.70	129.49	114.10
2	B	224	TRP	O-C-N	7.64	132.06	122.43
2	B	341	THR	N-CA-CB	7.60	122.76	110.90
2	B	224	TRP	N-CA-CB	7.58	122.72	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	VAL	CA-C-O	-7.58	113.18	121.29
2	B	253	ASP	CA-CB-CG	7.57	120.17	112.60
2	B	203	PRO	N-CA-C	7.50	119.85	110.70
2	B	373	HIS	N-CA-C	7.43	122.89	109.44
2	B	383	ARG	NE-CZ-NH2	-7.43	112.51	119.20
2	B	229	ASP	N-CA-C	-7.42	99.25	109.71
2	B	376	GLN	CB-CG-CD	7.33	125.06	112.60
1	A	19	ARG	CD-NE-CZ	7.33	134.66	124.40
2	B	267	GLN	CB-CG-CD	7.29	125.00	112.60
2	B	351	GLU	CB-CG-CD	7.25	124.93	112.60
1	A	30	GLU	CB-CG-CD	7.23	124.90	112.60
2	B	341	THR	CB-CA-C	-7.23	100.07	110.62
1	A	175	THR	CA-C-O	-7.22	113.18	120.90
2	B	317	GLU	CA-C-N	-7.21	108.68	122.53
2	B	317	GLU	C-N-CA	-7.21	108.68	122.53
2	B	317	GLU	N-CA-CB	7.21	122.67	110.49
1	A	49	GLN	CA-C-N	7.13	130.06	120.65
1	A	49	GLN	C-N-CA	7.13	130.06	120.65
2	B	292	GLU	CB-CG-CD	7.09	124.66	112.60
1	A	50	THR	CA-C-N	7.07	130.09	120.54
1	A	50	THR	C-N-CA	7.07	130.09	120.54
1	A	134	ARG	CA-C-N	7.05	132.00	120.94
1	A	134	ARG	C-N-CA	7.05	132.00	120.94
2	B	342	LEU	CB-CA-C	7.04	122.15	109.83
1	A	43	SER	N-CA-C	-7.03	104.18	112.89
1	A	29	GLN	CB-CG-CD	7.02	124.53	112.60
1	A	174	GLU	CB-CG-CD	6.95	124.42	112.60
2	B	225	ARG	O-C-N	6.95	129.31	121.32
2	B	298	THR	CA-C-O	-6.95	111.09	119.49
1	A	106	SER	CA-C-N	6.93	131.22	120.82
1	A	106	SER	C-N-CA	6.93	131.22	120.82
2	B	241	HIS	CA-CB-CG	6.92	120.72	113.80
1	A	182	CYS	CA-CB-SG	-6.90	98.53	114.40
1	A	174	GLU	CG-CD-OE2	6.89	134.25	118.40
1	A	29	GLN	CA-CB-CG	6.87	127.84	114.10
2	B	248	MET	N-CA-CB	6.87	120.85	110.42
2	B	261	SER	O-C-N	6.86	131.22	123.27
2	B	229	ASP	CA-CB-CG	6.86	119.45	112.60
2	B	252	PRO	N-CA-C	6.83	126.36	114.75
1	A	58	ILE	O-C-N	6.78	128.83	121.10
1	A	47	ASN	N-CA-C	-6.77	102.13	108.22
2	B	214	SER	CA-C-O	-6.75	114.32	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	LEU	CA-CB-CG	6.74	139.88	116.30
2	B	220	PHE	CA-C-O	-6.71	114.08	121.33
1	A	170	MET	N-CA-C	-6.71	104.05	111.36
2	B	214	SER	N-CA-CB	-6.67	101.49	110.23
1	A	167	ARG	CD-NE-CZ	-6.65	115.09	124.40
1	A	181	GLN	CA-C-N	6.64	129.47	120.44
1	A	181	GLN	C-N-CA	6.64	129.47	120.44
2	B	278	MET	CA-C-O	-6.61	112.08	120.14
1	A	58	ILE	CB-CA-C	-6.60	99.34	111.36
1	A	127	ARG	CG-CD-NE	6.59	126.50	112.00
1	A	66	GLU	CB-CG-CD	6.57	123.76	112.60
1	A	9	LEU	CA-C-O	-6.56	113.88	120.90
2	B	236	TYR	N-CA-CB	6.55	122.85	111.39
1	A	69	GLN	N-CA-CB	6.54	120.00	110.26
2	B	347	ARG	CG-CD-NE	6.53	126.37	112.00
2	B	282	THR	N-CA-CB	-6.47	100.62	110.77
1	A	159	ASN	N-CA-C	-6.45	104.17	111.07
1	A	174	GLU	O-C-N	-6.44	115.33	122.03
1	A	21	HIS	N-CA-C	6.44	118.30	111.28
2	B	330	PRO	CA-C-N	6.42	133.79	121.54
2	B	330	PRO	C-N-CA	6.42	133.79	121.54
2	B	347	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	A	170	MET	CB-CA-C	6.41	121.75	110.85
1	A	76	LEU	CA-C-N	6.38	128.74	120.44
1	A	76	LEU	C-N-CA	6.38	128.74	120.44
2	B	390	TYR	N-CA-C	6.37	120.20	109.76
2	B	372	LEU	CA-C-O	6.37	127.08	120.40
2	B	254	TYR	N-CA-CB	6.33	121.65	111.20
2	B	218	GLU	O-C-N	-6.33	114.17	122.59
1	A	26	ASP	CB-CA-C	6.33	123.01	110.42
2	B	372	LEU	N-CA-C	6.32	119.08	108.02
2	B	313	VAL	CA-C-O	-6.32	113.81	120.57
1	A	124	LEU	CA-C-N	6.31	128.65	120.44
1	A	124	LEU	C-N-CA	6.31	128.65	120.44
1	A	20	LEU	N-CA-C	-6.30	104.33	111.07
2	B	344	TYR	N-CA-C	6.25	120.11	110.42
2	B	246	THR	N-CA-C	6.24	124.08	110.80
1	A	46	GLN	CA-CB-CG	6.23	126.56	114.10
2	B	372	LEU	N-CA-CB	-6.23	100.81	110.65
2	B	340	PHE	N-CA-C	6.22	118.87	109.41
2	B	393	ALA	CA-C-O	-6.22	114.47	121.81
1	A	186	GLU	CB-CG-CD	6.21	123.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	258	GLY	N-CA-C	-6.20	99.69	112.34
2	B	268	TYR	CA-CB-CG	-6.17	102.79	113.90
2	B	209	ILE	CA-C-O	-6.17	113.62	120.97
2	B	397	ALA	CA-C-N	6.17	131.90	122.77
2	B	397	ALA	C-N-CA	6.17	131.90	122.77
1	A	37	PRO	CA-C-O	-6.16	109.38	120.60
1	A	153	ASP	CA-C-N	-6.16	114.83	122.84
1	A	153	ASP	C-N-CA	-6.16	114.83	122.84
2	B	254	TYR	CA-CB-CG	6.15	124.97	113.90
2	B	301	VAL	O-C-N	6.11	129.33	122.67
1	A	42	TYR	N-CA-C	6.11	120.16	110.70
2	B	313	VAL	CB-CA-C	6.10	119.14	110.84
1	A	95	SER	N-CA-C	-6.10	103.58	111.02
1	A	26	ASP	CA-C-N	6.09	128.76	120.54
1	A	26	ASP	C-N-CA	6.09	128.76	120.54
2	B	273	ARG	O-C-N	6.08	130.52	123.41
2	B	214	SER	CA-C-N	6.04	126.15	119.87
2	B	214	SER	C-N-CA	6.04	126.15	119.87
2	B	320	LYS	N-CA-C	6.03	118.89	110.20
2	B	345	GLU	CB-CG-CD	6.02	122.83	112.60
2	B	282	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	172	LYS	CA-C-N	6.01	128.21	120.70
1	A	172	LYS	C-N-CA	6.01	128.21	120.70
1	A	34	ALA	N-CA-C	6.00	120.69	112.04
1	A	120	ARG	CA-C-N	5.97	128.08	120.56
1	A	120	ARG	C-N-CA	5.97	128.08	120.56
1	A	173	VAL	O-C-N	5.97	128.09	121.94
2	B	300	ILE	CA-C-N	5.96	129.09	120.98
2	B	300	ILE	C-N-CA	5.96	129.09	120.98
1	A	25	PHE	O-C-N	5.95	128.45	122.03
2	B	337	THR	CB-CA-C	5.95	122.25	110.42
1	A	129	GLU	CB-CG-CD	5.94	122.70	112.60
2	B	240	TYR	O-C-N	-5.93	115.99	123.17
2	B	319	ARG	CA-C-N	5.93	130.51	121.03
2	B	319	ARG	C-N-CA	5.93	130.51	121.03
1	A	160	TYR	O-C-N	-5.89	115.96	122.09
1	A	137	GLN	CA-C-N	5.87	128.97	120.98
1	A	137	GLN	C-N-CA	5.87	128.97	120.98
2	B	260	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	277	MET	O-C-N	5.85	130.44	123.24
2	B	338	GLY	N-CA-C	5.84	127.03	113.18
1	A	45	LEU	N-CA-CB	-5.84	101.67	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	295	VAL	N-CA-C	5.84	116.28	107.75
1	A	7	SER	O-C-N	5.83	130.35	122.59
1	A	18	HIS	N-CA-C	5.79	117.60	111.28
1	A	182	CYS	N-CA-CB	-5.79	101.67	110.07
2	B	252	PRO	CA-C-N	5.79	130.97	121.58
2	B	252	PRO	C-N-CA	5.79	130.97	121.58
2	B	347	ARG	CD-NE-CZ	-5.79	116.30	124.40
2	B	367	PHE	CA-C-N	5.79	131.66	122.74
2	B	367	PHE	C-N-CA	5.79	131.66	122.74
1	A	121	ILE	N-CA-C	5.78	115.97	110.42
1	A	68	GLN	N-CA-C	-5.78	106.21	113.72
2	B	337	THR	O-C-N	-5.77	114.91	122.59
2	B	268	TYR	CA-C-N	-5.76	115.11	122.77
2	B	268	TYR	C-N-CA	-5.76	115.11	122.77
1	A	47	ASN	CB-CA-C	5.75	117.81	110.22
2	B	359	HIS	CA-CB-CG	-5.75	108.05	113.80
2	B	219	THR	N-CA-CB	-5.74	101.34	111.39
1	A	30	GLU	CA-CB-CG	5.74	125.58	114.10
2	B	341	THR	O-C-N	5.74	130.60	123.14
1	A	11	ASP	CA-CB-CG	5.73	118.33	112.60
2	B	346	ILE	CB-CA-C	-5.72	101.70	110.50
1	A	97	PHE	CA-CB-CG	5.70	119.50	113.80
2	B	315	GLN	N-CA-C	5.69	121.05	108.64
1	A	114	LEU	CA-C-O	5.68	126.78	120.82
1	A	62	SER	N-CA-C	5.67	119.39	111.56
1	A	118	GLU	CA-C-O	-5.67	114.83	120.90
2	B	307	LEU	CA-C-O	5.65	126.70	120.71
2	B	343	LEU	CB-CA-C	5.65	118.87	110.62
1	A	36	ILE	N-CA-CB	-5.64	103.31	111.21
2	B	341	THR	CA-C-O	-5.64	113.14	120.25
2	B	324	TRP	O-C-N	5.63	128.68	123.50
2	B	382	VAL	CA-C-O	-5.62	115.12	121.75
1	A	46	GLN	OE1-CD-NE2	-5.61	117.00	122.60
2	B	324	TRP	CA-CB-CG	-5.58	103.00	113.60
1	A	81	LEU	N-CA-C	-5.56	104.24	111.02
1	A	160	TYR	CA-C-O	5.55	126.84	120.90
1	A	51	SER	O-C-N	5.54	127.86	122.09
1	A	63	ASN	O-C-N	5.53	128.82	123.29
2	B	245	GLU	N-CA-C	5.53	122.57	110.80
2	B	393	ALA	O-C-N	5.52	129.14	122.85
1	A	22	GLN	CG-CD-NE2	5.51	124.67	116.40
1	A	178	ARG	N-CA-CB	5.51	118.00	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	280	ASN	CA-C-O	-5.51	114.34	121.11
2	B	333	ILE	O-C-N	5.50	130.22	122.97
1	A	14	MET	O-C-N	-5.49	116.30	122.12
1	A	20	LEU	CB-CA-C	5.49	119.50	110.88
1	A	122	GLN	OE1-CD-NE2	5.48	128.08	122.60
2	B	330	PRO	N-CA-C	-5.48	103.20	111.41
1	A	154	ASP	N-CA-C	-5.47	98.84	108.20
2	B	306	PRO	CA-C-N	5.46	130.85	122.93
2	B	306	PRO	C-N-CA	5.46	130.85	122.93
1	A	78	ILE	CA-C-N	5.46	127.91	120.54
1	A	78	ILE	C-N-CA	5.46	127.91	120.54
2	B	387	ASP	N-CA-C	5.45	122.41	110.80
2	B	269	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	22	GLN	CG-CD-OE1	-5.43	109.93	120.80
1	A	185	VAL	CA-C-N	5.43	131.91	121.54
1	A	185	VAL	C-N-CA	5.43	131.91	121.54
1	A	55	SER	CA-C-N	5.40	130.25	121.98
1	A	55	SER	C-N-CA	5.40	130.25	121.98
2	B	334	ASP	CA-C-O	5.40	126.24	120.46
1	A	66	GLU	CA-CB-CG	5.38	124.86	114.10
2	B	223	TRP	CA-C-O	-5.38	114.35	120.32
2	B	347	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	161	GLY	O-C-N	5.37	127.35	122.19
2	B	323	LEU	CA-C-N	-5.36	113.27	121.26
2	B	323	LEU	C-N-CA	-5.36	113.27	121.26
1	A	73	LEU	CB-CA-C	5.35	119.35	110.90
1	A	32	GLU	CA-C-N	5.31	127.65	120.38
1	A	32	GLU	C-N-CA	5.31	127.65	120.38
1	A	64	ARG	NE-CZ-NH1	5.30	126.81	121.50
2	B	211	LYS	N-CA-C	5.30	116.27	107.73
2	B	326	LYS	CA-C-O	-5.30	115.05	120.99
2	B	391	TRP	N-CA-C	-5.28	103.05	110.50
2	B	261	SER	CA-C-O	-5.28	114.94	121.06
2	B	387	ASP	CA-CB-CG	-5.28	107.33	112.60
2	B	393	ALA	N-CA-C	-5.27	103.43	110.55
1	A	82	LEU	N-CA-CB	-5.27	101.19	109.78
1	A	14	MET	CB-CA-C	5.26	119.62	110.68
2	B	315	GLN	N-CA-CB	-5.26	102.45	111.39
2	B	274	THR	CA-CB-OG1	-5.26	101.72	109.60
2	B	374	PRO	CA-C-N	5.25	132.24	121.17
2	B	374	PRO	C-N-CA	5.25	132.24	121.17
2	B	266	LYS	N-CA-C	5.24	117.80	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	TYR	O-C-N	5.24	129.35	123.48
2	B	385	LYS	CA-C-O	-5.24	113.95	119.50
1	A	174	GLU	CA-C-O	5.23	126.49	121.00
2	B	273	ARG	CD-NE-CZ	-5.23	117.08	124.40
2	B	216	ASN	CA-C-O	-5.22	113.05	120.51
1	A	11	ASP	N-CA-CB	5.20	117.69	109.94
2	B	236	TYR	CB-CA-C	-5.19	100.66	110.16
1	A	134	ARG	CA-CB-CG	5.19	124.48	114.10
1	A	109	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	A	109	ASN	CB-CA-C	5.17	119.15	110.88
1	A	154	ASP	CB-CA-C	5.17	119.05	110.78
2	B	388	HIS	N-CA-C	-5.17	104.58	111.87
2	B	241	HIS	N-CA-CB	5.14	119.45	110.81
1	A	112	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	372	LEU	O-C-N	-5.13	116.34	123.12
2	B	206	LYS	CG-CD-CE	5.12	123.08	111.30
2	B	340	PHE	CA-C-N	5.12	129.86	122.44
2	B	340	PHE	C-N-CA	5.12	129.86	122.44
1	A	43	SER	CA-C-O	5.12	125.65	119.31
1	A	110	VAL	CA-C-O	-5.11	114.40	120.78
2	B	280	ASN	OD1-CG-ND2	-5.11	117.49	122.60
2	B	338	GLY	O-C-N	-5.10	116.07	122.70
2	B	373	HIS	CB-CA-C	-5.09	101.42	109.82
2	B	391	TRP	O-C-N	5.09	128.87	122.86
1	A	78	ILE	CA-C-O	5.08	126.56	121.27
2	B	222	CYS	CA-C-O	-5.08	115.37	121.11
1	A	44	PHE	N-CA-C	-5.08	105.87	111.71
2	B	278	MET	N-CA-CB	-5.07	102.00	110.57
2	B	390	TYR	CA-C-O	5.03	126.38	120.80
1	A	166	PHE	CA-CB-CG	5.02	118.82	113.80
2	B	293	LEU	N-CA-C	5.00	117.56	109.06

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	1509	0	1475	116	0
2	B	1613	0	1532	123	0
3	A	1	0	0	0	0
All	All	3123	0	3007	234	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 38.

All (234) 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)
2:B:378:TYR:HE1	2:B:402:ILE:HD11	1.12	1.13
1:A:46:GLN:HE22	1:A:49:GLN:HB3	1.19	1.07
2:B:270:SER:HB3	2:B:273:ARG:HG3	1.44	0.99
2:B:378:TYR:CE1	2:B:402:ILE:HD11	2.01	0.95
1:A:36:ILE:HG12	1:A:156:LEU:HD23	1.49	0.92
1:A:19:ARG:HH22	1:A:104:GLY:HA3	1.34	0.91
2:B:247:LEU:H	2:B:247:LEU:HD12	1.34	0.91
2:B:374:PRO:HB3	2:B:404:SER:HB3	1.52	0.89
1:A:88:GLU:HB2	1:A:89:PRO:HD3	1.56	0.87
1:A:64:ARG:HD2	2:B:218:GLU:OE2	1.75	0.85
1:A:35:TYR:HB3	1:A:156:LEU:HD21	1.57	0.84
2:B:278:MET:HG3	2:B:291:ASP:O	1.81	0.80
1:A:135:THR:HA	1:A:139:PHE:HE1	1.48	0.79
1:A:77:ARG:HH21	1:A:134:ARG:HH21	1.30	0.77
1:A:108:SER:HB2	1:A:113:LEU:HD11	1.64	0.77
2:B:206:LYS:HD3	2:B:228:THR:HB	1.67	0.75
2:B:238:LEU:HB3	2:B:251:CYS:HB2	1.67	0.74
1:A:16:ARG:HB2	1:A:117:LEU:HD13	1.69	0.74
1:A:96:VAL:HG11	1:A:163:LEU:HD11	1.70	0.72
2:B:203:PRO:HB2	2:B:204:PRO:HD3	1.71	0.71
2:B:327:TRP:CZ3	2:B:346:ILE:HD11	2.25	0.71
2:B:313:VAL:HG21	2:B:403:PRO:CD	2.21	0.71
1:A:31:PHE:CE1	1:A:160:TYR:HB2	2.25	0.70
1:A:84:GLN:HA	1:A:87:LEU:HD12	1.72	0.70
2:B:311:VAL:HG12	2:B:400:ILE:HD12	1.72	0.70
1:A:79:SER:O	1:A:83:ILE:HG12	1.92	0.70
1:A:36:ILE:N	1:A:37:PRO:HD3	2.06	0.70
1:A:70:LYS:HB3	1:A:74:GLU:HB3	1.74	0.69
2:B:332:LEU:HD12	2:B:333:ILE:HG12	1.75	0.68
2:B:282:THR:HG22	2:B:288:SER:HA	1.76	0.68
1:A:146:PHE:HE2	1:A:158:LYS:HE3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:HB2	1:A:89:PRO:CD	2.24	0.66
1:A:84:GLN:HA	1:A:87:LEU:CD1	2.24	0.66
2:B:247:LEU:H	2:B:247:LEU:CD1	2.05	0.65
1:A:22:GLN:OE1	2:B:388:HIS:HE1	1.79	0.64
1:A:73:LEU:HD21	1:A:129:GLU:OE1	1.98	0.64
2:B:282:THR:HA	2:B:287:SER:O	1.97	0.63
2:B:349:LYS:HG3	2:B:353:ALA:HB3	1.80	0.63
1:A:14:MET:HE1	1:A:177:LEU:HB3	1.81	0.62
1:A:63:ASN:OD1	1:A:66:GLU:N	2.30	0.61
2:B:250:GLU:HG3	2:B:251:CYS:N	2.15	0.61
1:A:76:LEU:HD11	1:A:128:LEU:HD12	1.83	0.61
2:B:208:GLU:O	2:B:225:ARG:N	2.34	0.60
2:B:400:ILE:HG12	2:B:401:GLN:H	1.67	0.60
2:B:275:TYR:HB2	2:B:295:VAL:HG13	1.83	0.60
2:B:304:ASP:O	2:B:330:PRO:HG3	2.01	0.60
1:A:31:PHE:HE1	1:A:160:TYR:HB2	1.66	0.60
2:B:383:ARG:HD2	2:B:394:TRP:CH2	2.37	0.59
2:B:313:VAL:HG21	2:B:403:PRO:HD3	1.83	0.59
1:A:70:LYS:O	1:A:75:LEU:HG	2.02	0.59
2:B:206:LYS:CD	2:B:228:THR:HB	2.33	0.58
2:B:311:VAL:CG1	2:B:400:ILE:HD12	2.32	0.58
1:A:66:GLU:HA	1:A:69:GLN:HB2	1.85	0.58
2:B:351:GLU:N	2:B:377:LYS:O	2.34	0.57
1:A:76:LEU:HD13	1:A:125:MET:HA	1.85	0.57
2:B:366:GLU:O	2:B:367:PHE:HB2	2.04	0.57
2:B:383:ARG:HD2	2:B:394:TRP:CZ3	2.40	0.57
1:A:64:ARG:HD2	2:B:218:GLU:CD	2.29	0.57
2:B:350:PRO:HA	2:B:378:TYR:HA	1.85	0.57
1:A:181:GLN:O	1:A:185:VAL:HB	2.04	0.57
2:B:241:HIS:CD2	2:B:248:MET:SD	2.98	0.57
1:A:35:TYR:N	1:A:35:TYR:CD1	2.73	0.56
1:A:72:ASN:OD1	1:A:183:ARG:NH2	2.38	0.56
1:A:19:ARG:NH2	1:A:104:GLY:HA3	2.14	0.56
1:A:96:VAL:CG1	1:A:163:LEU:HD11	2.35	0.56
1:A:12:ASN:O	1:A:16:ARG:NH1	2.37	0.56
1:A:42:TYR:HD2	1:A:45:LEU:HD13	1.70	0.56
2:B:211:LYS:HG3	2:B:223:TRP:HE3	1.71	0.56
1:A:122:GLN:O	1:A:125:MET:HB3	2.06	0.55
2:B:209:ILE:HD11	2:B:279:VAL:HG23	1.87	0.55
2:B:374:PRO:HA	2:B:403:PRO:O	2.06	0.55
1:A:22:GLN:OE1	2:B:388:HIS:CE1	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PHE:CE1	1:A:170:MET:HE3	2.42	0.55
2:B:347:ARG:HG3	2:B:356:TRP:CE3	2.41	0.55
1:A:19:ARG:NH2	1:A:103:TYR:O	2.40	0.55
2:B:313:VAL:HG21	2:B:403:PRO:HD2	1.87	0.55
1:A:93:LEU:HA	1:A:96:VAL:HG23	1.89	0.55
2:B:240:TYR:HA	2:B:276:ILE:O	2.07	0.55
1:A:46:GLN:NE2	1:A:49:GLN:HB3	2.04	0.54
1:A:45:LEU:HA	1:A:51:SER:HB2	1.88	0.54
2:B:209:ILE:HA	2:B:224:TRP:HA	1.89	0.54
2:B:322:TYR:CD1	2:B:322:TYR:C	2.86	0.54
2:B:347:ARG:HG3	2:B:356:TRP:CZ3	2.43	0.54
1:A:79:SER:O	1:A:82:LEU:HB2	2.08	0.53
1:A:84:GLN:O	1:A:87:LEU:HB2	2.08	0.53
2:B:347:ARG:CG	2:B:381:GLN:HG3	2.39	0.53
1:A:44:PHE:CD1	1:A:44:PHE:C	2.86	0.53
1:A:20:LEU:HD21	1:A:113:LEU:HB2	1.91	0.53
1:A:35:TYR:O	1:A:36:ILE:HB	2.07	0.53
1:A:123:THR:O	1:A:124:LEU:C	2.51	0.53
1:A:36:ILE:CG1	1:A:156:LEU:HD23	2.30	0.53
1:A:63:ASN:OD1	1:A:63:ASN:C	2.52	0.53
2:B:347:ARG:HD3	2:B:394:TRP:CE2	2.44	0.52
1:A:70:LYS:HD2	1:A:137:GLN:OE1	2.09	0.52
1:A:48:PRO:O	1:A:52:LEU:HD22	2.10	0.52
2:B:252:PRO:HD2	2:B:262:CYS:SG	2.50	0.51
2:B:215:PRO:O	2:B:332:LEU:HD13	2.10	0.51
2:B:225:ARG:NH1	2:B:260:ASN:HD22	2.07	0.51
2:B:376:GLN:O	2:B:402:ILE:HD12	2.11	0.51
2:B:322:TYR:HD1	2:B:323:LEU:O	1.94	0.51
1:A:76:LEU:CD1	1:A:128:LEU:HD12	2.41	0.51
1:A:46:GLN:NE2	1:A:47:ASN:O	2.44	0.50
1:A:48:PRO:O	1:A:49:GLN:C	2.55	0.50
2:B:352:LYS:HB3	2:B:376:GLN:OE1	2.12	0.50
2:B:217:LYS:O	2:B:271:MET:HE1	2.11	0.50
1:A:40:GLN:O	1:A:41:LYS:C	2.54	0.50
2:B:217:LYS:HB3	2:B:339:TRP:HE1	1.77	0.50
2:B:273:ARG:HA	2:B:273:ARG:HH11	1.77	0.50
2:B:350:PRO:HD2	2:B:353:ALA:CB	2.42	0.50
2:B:363:GLN:O	2:B:363:GLN:HG2	2.11	0.50
2:B:402:ILE:HG22	2:B:403:PRO:HD2	1.93	0.50
2:B:215:PRO:HB2	2:B:332:LEU:HD22	1.94	0.49
2:B:273:ARG:HA	2:B:273:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:PRO:CB	2:B:204:PRO:HD3	2.38	0.49
2:B:309:LEU:HD13	2:B:382:VAL:HG11	1.94	0.49
2:B:273:ARG:CZ	2:B:273:ARG:HB3	2.42	0.49
2:B:312:GLU:HB3	2:B:324:TRP:HB3	1.95	0.49
1:A:120:ARG:O	1:A:123:THR:HB	2.13	0.49
2:B:282:THR:HG22	2:B:288:SER:CB	2.43	0.49
2:B:320:LYS:HD2	2:B:321:PRO:HD2	1.94	0.49
1:A:46:GLN:NE2	1:A:50:THR:H	2.10	0.49
2:B:251:CYS:HB3	2:B:254:TYR:CZ	2.48	0.49
1:A:72:ASN:CG	1:A:180:VAL:HG13	2.38	0.49
1:A:146:PHE:CG	1:A:147:ASP:N	2.75	0.49
1:A:63:ASN:CG	1:A:66:GLU:HG2	2.38	0.49
2:B:333:ILE:HG23	2:B:340:PHE:CD2	2.48	0.49
2:B:373:HIS:CE1	2:B:378:TYR:OH	2.65	0.49
1:A:88:GLU:CB	1:A:89:PRO:HD3	2.32	0.48
2:B:322:TYR:CB	2:B:370:LEU:HD23	2.43	0.48
1:A:44:PHE:CE1	1:A:45:LEU:HD12	2.48	0.48
1:A:47:ASN:O	1:A:48:PRO:C	2.57	0.48
2:B:206:LYS:H	2:B:207:PRO:HD2	1.79	0.48
2:B:217:LYS:HE3	2:B:339:TRP:CD1	2.49	0.48
2:B:282:THR:HG22	2:B:288:SER:HB2	1.96	0.48
1:A:6:LEU:O	1:A:7:SER:C	2.56	0.48
1:A:44:PHE:CE1	1:A:45:LEU:HB2	2.49	0.48
2:B:211:LYS:HG3	2:B:223:TRP:CE3	2.48	0.47
1:A:77:ARG:NH2	1:A:138:ILE:O	2.47	0.47
1:A:87:LEU:HD22	1:A:111:TYR:HE1	1.79	0.47
2:B:327:TRP:CE2	2:B:365:THR:HA	2.49	0.47
1:A:80:LEU:O	1:A:81:LEU:C	2.58	0.47
2:B:347:ARG:HG3	2:B:381:GLN:HG3	1.97	0.47
2:B:313:VAL:HG11	2:B:403:PRO:HD3	1.97	0.47
2:B:303:PRO:HG3	2:B:386:PRO:HG3	1.96	0.47
1:A:78:ILE:HA	1:A:81:LEU:HD12	1.96	0.46
1:A:90:VAL:HG11	1:A:114:LEU:CD1	2.45	0.46
1:A:41:LYS:HE3	2:B:294:TYR:OH	2.16	0.46
2:B:402:ILE:CG2	2:B:403:PRO:HD2	2.46	0.46
2:B:206:LYS:HD2	2:B:289:PHE:CD2	2.50	0.46
1:A:77:ARG:O	1:A:81:LEU:HG	2.16	0.45
2:B:282:THR:HG22	2:B:288:SER:CA	2.45	0.45
1:A:44:PHE:O	1:A:51:SER:HA	2.17	0.45
2:B:287:SER:OG	2:B:289:PHE:HE2	2.00	0.45
2:B:309:LEU:HD11	2:B:325:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.83	0.45
2:B:242:ARG:HH11	2:B:242:ARG:HG3	1.81	0.45
2:B:257:GLY:HA3	2:B:261:SER:OG	2.17	0.45
1:A:14:MET:HG2	1:A:181:GLN:HE22	1.82	0.45
2:B:310:ALA:HB3	2:B:326:LYS:HG3	1.99	0.45
2:B:322:TYR:CD1	2:B:322:TYR:O	2.70	0.45
2:B:238:LEU:HD23	2:B:279:VAL:HG22	1.99	0.45
2:B:251:CYS:HA	2:B:252:PRO:HD3	1.77	0.45
2:B:324:TRP:O	2:B:326:LYS:NZ	2.50	0.45
1:A:93:LEU:HB3	1:A:97:PHE:CE2	2.51	0.45
2:B:309:LEU:HD11	2:B:325:ILE:HG21	1.98	0.45
2:B:287:SER:HG	2:B:289:PHE:HE2	1.62	0.44
2:B:322:TYR:C	2:B:322:TYR:HD1	2.24	0.44
1:A:63:ASN:OD1	1:A:66:GLU:HG2	2.18	0.44
1:A:90:VAL:HA	1:A:93:LEU:HB2	1.99	0.44
2:B:347:ARG:HH11	2:B:347:ARG:HD2	1.41	0.44
1:A:171:ASP:O	1:A:172:LYS:C	2.61	0.44
1:A:118:GLU:O	1:A:122:GLN:HG3	2.17	0.44
1:A:166:PHE:O	1:A:170:MET:N	2.45	0.44
1:A:45:LEU:O	1:A:45:LEU:HD23	2.18	0.44
1:A:61:PRO:HB2	1:A:67:THR:OG1	2.17	0.44
2:B:225:ARG:HA	2:B:226:PRO:HD3	1.68	0.44
2:B:243:GLU:HB2	2:B:274:THR:H	1.83	0.44
1:A:174:GLU:O	1:A:175:THR:C	2.60	0.43
2:B:323:LEU:HA	2:B:323:LEU:HD23	1.74	0.43
1:A:19:ARG:HH22	1:A:104:GLY:CA	2.19	0.43
1:A:77:ARG:CZ	1:A:138:ILE:O	2.66	0.43
2:B:219:THR:HG23	2:B:263:HIS:CE1	2.53	0.43
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.55	0.43
2:B:352:LYS:HG3	2:B:353:ALA:N	2.33	0.43
1:A:114:LEU:O	1:A:118:GLU:HB2	2.18	0.43
1:A:23:LEU:HD12	1:A:23:LEU:O	2.18	0.43
2:B:305:PRO:HA	2:B:306:PRO:HD3	1.77	0.43
1:A:76:LEU:CD1	1:A:125:MET:HA	2.48	0.42
2:B:309:LEU:HD13	2:B:382:VAL:CG1	2.48	0.42
2:B:309:LEU:HD22	2:B:382:VAL:HG12	2.00	0.42
2:B:350:PRO:O	2:B:351:GLU:C	2.62	0.42
1:A:116:ASP:OD1	1:A:116:ASP:C	2.62	0.42
2:B:347:ARG:HD3	2:B:394:TRP:CZ2	2.55	0.42
1:A:36:ILE:N	1:A:37:PRO:CD	2.80	0.42
2:B:210:PHE:CD1	2:B:225:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:O	1:A:163:LEU:C	2.61	0.42
2:B:321:PRO:HG2	2:B:372:LEU:O	2.19	0.42
1:A:46:GLN:HE22	1:A:50:THR:H	1.66	0.42
1:A:135:THR:HA	1:A:139:PHE:CE1	2.40	0.42
2:B:347:ARG:HD3	2:B:394:TRP:CD2	2.55	0.42
1:A:178:ARG:HD2	1:A:178:ARG:HA	1.79	0.42
2:B:301:VAL:O	2:B:390:TYR:HB2	2.20	0.42
2:B:317:GLU:HG2	2:B:318:ASP:OD2	2.19	0.42
2:B:350:PRO:HB3	2:B:378:TYR:CE2	2.54	0.42
2:B:385:LYS:HB3	2:B:391:TRP:CE3	2.55	0.42
1:A:81:LEU:O	1:A:82:LEU:C	2.63	0.41
2:B:217:LYS:HG3	2:B:301:VAL:HG21	2.02	0.41
2:B:217:LYS:HE3	2:B:339:TRP:NE1	2.35	0.41
1:A:97:PHE:O	1:A:105:ALA:HB1	2.20	0.41
1:A:76:LEU:HD13	1:A:125:MET:CA	2.50	0.41
2:B:321:PRO:O	2:B:372:LEU:HB2	2.20	0.41
1:A:78:ILE:HG22	1:A:82:LEU:HD11	2.03	0.41
1:A:27:THR:HG22	1:A:28:TYR:N	2.36	0.41
1:A:20:LEU:HD21	1:A:113:LEU:CB	2.50	0.41
1:A:24:ALA:HB2	1:A:166:PHE:CD2	2.55	0.41
1:A:36:ILE:HG22	1:A:36:ILE:O	2.21	0.41
2:B:213:ARG:HA	2:B:300:ILE:O	2.20	0.41
2:B:307:LEU:O	2:B:328:SER:OG	2.36	0.41
2:B:327:TRP:CH2	2:B:346:ILE:HD11	2.55	0.41
1:A:1:PHE:HA	1:A:2:PRO:HD3	1.69	0.41
1:A:19:ARG:HD2	1:A:19:ARG:HA	1.83	0.41
1:A:42:TYR:CD2	1:A:45:LEU:HD13	2.54	0.41
2:B:322:TYR:CD1	2:B:323:LEU:O	2.72	0.41
1:A:115:LYS:NZ	1:A:118:GLU:OE1	2.38	0.41
1:A:146:PHE:H	1:A:146:PHE:HD1	1.69	0.40
1:A:59:PRO:O	1:A:137:GLN:NE2	2.54	0.40
2:B:342:LEU:O	2:B:343:LEU:HD12	2.21	0.40
2:B:383:ARG:HB3	2:B:394:TRP:CE3	2.57	0.40
1:A:16:ARG:O	1:A:17:ALA:C	2.64	0.40
1:A:51:SER:OG	1:A:52:LEU:N	2.53	0.40
2:B:327:TRP:NE1	2:B:365:THR:HA	2.36	0.40
1:A:3:THR:O	1:A:4:ILE:C	2.64	0.40
1:A:46:GLN:NE2	1:A:50:THR:HG23	2.36	0.40
2:B:374:PRO:CA	2:B:403:PRO:O	2.69	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	182/191 (95%)	134 (74%)	34 (19%)	14 (8%)	1	2
2	B	191/211 (90%)	150 (78%)	25 (13%)	16 (8%)	0	1
All	All	373/402 (93%)	284 (76%)	59 (16%)	30 (8%)	1	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	49	GLN
2	B	204	PRO
2	B	245	GLU
2	B	246	THR
2	B	317	GLU
2	B	338	GLY
2	B	353	ALA
1	A	141	GLN
1	A	186	GLU
2	B	256	THR
1	A	3	THR
1	A	46	GLN
1	A	48	PRO
1	A	105	ALA
1	A	188	SER
2	B	216	ASN
2	B	257	GLY
2	B	319	ARG
2	B	351	GLU
1	A	65	GLU
2	B	206	LYS
2	B	403	PRO
1	A	64	ARG
1	A	110	VAL

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Mol	Chain	Res	Type
2	B	332	LEU
2	B	387	ASP
2	B	203	PRO
1	A	96	VAL
1	A	4	ILE

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	A	168/177 (95%)	124 (74%)	44 (26%)	0	2
2	B	176/191 (92%)	140 (80%)	36 (20%)	1	4
All	All	344/368 (94%)	264 (77%)	80 (23%)	1	3

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LEU
1	A	9	LEU
1	A	12	ASN
1	A	15	LEU
1	A	16	ARG
1	A	20	LEU
1	A	27	THR
1	A	32	GLU
1	A	35	TYR
1	A	39	GLU
1	A	43	SER
1	A	46	GLN
1	A	47	ASN
1	A	48	PRO
1	A	49	GLN
1	A	51	SER
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	55	SER
1	A	56	GLU
1	A	58	ILE
1	A	71	SER
1	A	74	GLU
1	A	79	SER
1	A	90	VAL
1	A	95	SER
1	A	103	TYR
1	A	106	SER
1	A	115	LYS
1	A	116	ASP
1	A	118	GLU
1	A	121	ILE
1	A	124	LEU
1	A	127	ARG
1	A	134	ARG
1	A	153	ASP
1	A	156	LEU
1	A	157	LEU
1	A	175	THR
1	A	177	LEU
1	A	179	ILE
1	A	180	VAL
1	A	184	SER
1	A	185	VAL
2	B	207	PRO
2	B	228	THR
2	B	229	ASP
2	B	238	LEU
2	B	241	HIS
2	B	245	GLU
2	B	247	LEU
2	B	256	THR
2	B	266	LYS
2	B	267	GLN
2	B	270	SER
2	B	283	ASN
2	B	288	SER
2	B	295	VAL
2	B	300	ILE
2	B	307	LEU

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Mol	Chain	Res	Type
2	B	313	VAL
2	B	314	LYS
2	B	315	GLN
2	B	320	LYS
2	B	325	ILE
2	B	331	THR
2	B	335	LEU
2	B	343	LEU
2	B	348	LEU
2	B	349	LYS
2	B	352	LYS
2	B	355	GLU
2	B	358	ILE
2	B	374	PRO
2	B	376	GLN
2	B	381	GLN
2	B	383	ARG
2	B	399	PHE
2	B	400	ILE
2	B	402	ILE

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	12	ASN
1	A	46	GLN
1	A	68	GLN
1	A	122	GLN
1	A	159	ASN
1	A	181	GLN
2	B	241	HIS
2	B	260	ASN
2	B	267	GLN
2	B	283	ASN
2	B	376	GLN

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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.