



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 AM UTC

PDB ID : 1BBS / pdb_00001bbs
Title : X-RAY ANALYSES OF PEPTIDE INHIBITOR COMPLEXES DEFINE
THE STRUCTURAL BASIS OF SPECIFICITY FOR HUMAN AND MOUSE
RENINS
Authors : Dhanaraj, V.; Blundell, T.L.
Deposited on : 1992-05-21
Resolution : 2.80 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
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

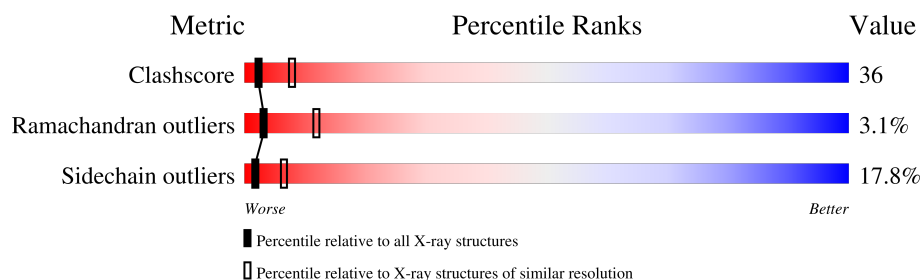
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	340	34% 42% 17% . .
1	B	340	33% 42% 18% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5018 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 RENIN.

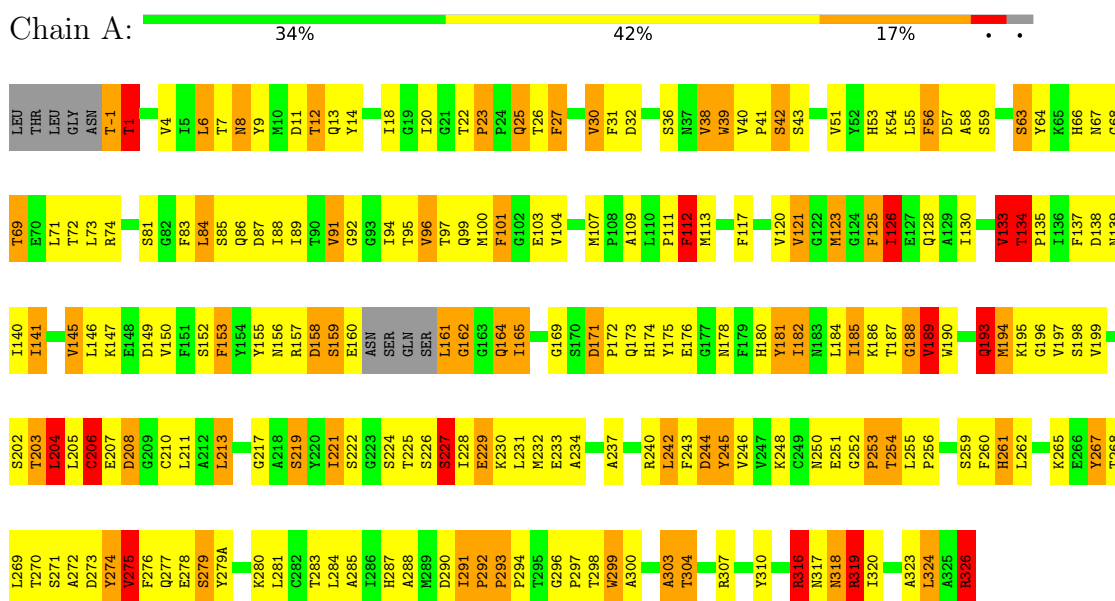
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			
1	B	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			

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: RENIN



T268	L269	T270	S271	A272	D273	Y274	Y276	F276	Q277	E278	S279	Y279A		K280	L281	C282	T283	L284	A285	T286	H287	A288	N289	D290	T291	P292	P293	P294	T295	G296	P297	T298	W299	A300		A303	T304		R307		Y310		R316	N317	N318	R319	I320		A323	L324	A325	R326
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	143.10Å 143.10Å 143.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.33	26/2568 (1.0%)	2.15	123/3493 (3.5%)
1	B	1.33	26/2568 (1.0%)	2.15	124/3493 (3.5%)
All	All	1.33	52/5136 (1.0%)	2.15	247/6986 (3.5%)

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	1	4
1	B	1	4
All	All	2	8

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	TYR	C-N	12.76	1.50	1.33
1	B	245	TYR	C-N	12.69	1.50	1.33
1	B	204	LEU	C-N	9.12	1.45	1.33
1	A	204	LEU	C-N	9.10	1.45	1.33
1	B	206	CYS	CA-C	-8.82	1.41	1.52
1	A	206	CYS	CA-C	-8.78	1.41	1.52
1	B	180	HIS	CE1-NE2	7.45	1.40	1.32
1	A	180	HIS	CE1-NE2	7.41	1.40	1.32
1	A	261	HIS	CE1-NE2	7.35	1.40	1.32
1	A	180	HIS	ND1-CE1	7.34	1.39	1.32
1	B	180	HIS	ND1-CE1	7.34	1.39	1.32
1	B	261	HIS	CE1-NE2	7.32	1.39	1.32
1	A	53	HIS	ND1-CE1	7.29	1.39	1.32
1	B	53	HIS	ND1-CE1	7.27	1.39	1.32
1	A	66	HIS	CE1-NE2	7.16	1.39	1.32
1	B	174	HIS	CE1-NE2	7.10	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	HIS	CE1-NE2	7.09	1.39	1.32
1	B	66	HIS	CE1-NE2	7.08	1.39	1.32
1	B	174	HIS	ND1-CE1	6.85	1.39	1.32
1	A	174	HIS	ND1-CE1	6.83	1.39	1.32
1	B	66	HIS	ND1-CE1	6.75	1.39	1.32
1	B	158	ASP	N-CA	6.69	1.54	1.46
1	A	66	HIS	ND1-CE1	6.68	1.39	1.32
1	A	158	ASP	N-CA	6.68	1.54	1.46
1	B	261	HIS	ND1-CE1	6.38	1.39	1.32
1	A	261	HIS	ND1-CE1	6.34	1.38	1.32
1	A	53	HIS	CE1-NE2	6.08	1.38	1.32
1	B	53	HIS	CE1-NE2	6.00	1.38	1.32
1	B	190	TRP	NE1-CE2	-5.82	1.31	1.37
1	A	190	TRP	NE1-CE2	-5.78	1.31	1.37
1	A	39	TRP	NE1-CE2	-5.50	1.31	1.37
1	B	39	TRP	NE1-CE2	-5.45	1.31	1.37
1	B	299	TRP	NE1-CE2	-5.45	1.31	1.37
1	A	299	TRP	NE1-CE2	-5.43	1.31	1.37
1	A	157	ARG	CA-C	5.42	1.59	1.53
1	B	157	ARG	CA-C	5.40	1.59	1.53
1	A	25	GLN	CD-OE1	5.27	1.33	1.23
1	B	25	GLN	CD-OE1	5.27	1.33	1.23
1	A	193	GLN	CD-OE1	5.25	1.33	1.23
1	A	161	LEU	N-CA	5.24	1.56	1.46
1	B	193	GLN	CD-OE1	5.23	1.33	1.23
1	B	161	LEU	N-CA	5.22	1.56	1.46
1	B	128	GLN	CD-OE1	5.17	1.33	1.23
1	A	128	GLN	CD-OE1	5.16	1.33	1.23
1	A	164	GLN	CD-OE1	5.08	1.33	1.23
1	A	280	LYS	C-N	5.05	1.40	1.33
1	B	164	GLN	CD-OE1	5.05	1.33	1.23
1	B	86	GLN	CD-OE1	5.04	1.33	1.23
1	A	318	ASN	CG-OD1	5.03	1.33	1.23
1	B	318	ASN	CG-OD1	5.03	1.33	1.23
1	A	86	GLN	CD-OE1	5.02	1.33	1.23
1	B	280	LYS	C-N	5.01	1.40	1.33

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PHE	CA-C-N	13.53	144.09	122.17
1	A	31	PHE	C-N-CA	13.53	144.09	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	PHE	CA-C-N	13.53	144.09	122.17
1	B	31	PHE	C-N-CA	13.53	144.09	122.17
1	B	162	GLY	O-C-N	-12.48	110.20	122.18
1	A	162	GLY	O-C-N	-12.46	110.22	122.18
1	A	101	PHE	CA-C-N	-11.80	113.72	122.33
1	A	101	PHE	C-N-CA	-11.80	113.72	122.33
1	B	101	PHE	CA-C-N	-11.75	113.75	122.33
1	B	101	PHE	C-N-CA	-11.75	113.75	122.33
1	A	291	ILE	CA-C-N	10.20	127.00	119.66
1	A	291	ILE	C-N-CA	10.20	127.00	119.66
1	B	292	PRO	O-C-N	10.19	125.94	121.15
1	B	291	ILE	CA-C-N	10.17	126.98	119.66
1	B	291	ILE	C-N-CA	10.17	126.98	119.66
1	A	292	PRO	O-C-N	10.14	125.92	121.15
1	A	134	THR	CA-C-N	9.56	129.63	119.78
1	A	134	THR	C-N-CA	9.56	129.63	119.78
1	B	134	THR	CA-C-N	9.55	129.62	119.78
1	B	134	THR	C-N-CA	9.55	129.62	119.78
1	B	204	LEU	CA-C-N	-9.14	107.42	121.86
1	B	204	LEU	C-N-CA	-9.14	107.42	121.86
1	A	204	LEU	CA-C-N	-9.11	107.47	121.86
1	A	204	LEU	C-N-CA	-9.11	107.47	121.86
1	B	18	ILE	CA-C-N	-8.98	115.78	122.33
1	B	18	ILE	C-N-CA	-8.98	115.78	122.33
1	A	18	ILE	CA-C-N	-8.92	115.82	122.33
1	A	18	ILE	C-N-CA	-8.92	115.82	122.33
1	A	292	PRO	N-CA-CB	-8.84	98.62	103.22
1	B	292	PRO	N-CA-CB	-8.84	98.62	103.22
1	A	53	HIS	CA-CB-CG	-8.71	105.09	113.80
1	B	53	HIS	CA-CB-CG	-8.65	105.15	113.80
1	A	153	PHE	CA-CB-CG	-8.35	105.45	113.80
1	B	153	PHE	CA-CB-CG	-8.32	105.48	113.80
1	B	291	ILE	O-C-N	-8.12	116.26	121.37
1	A	291	ILE	O-C-N	-8.09	116.27	121.37
1	A	174	HIS	CA-CB-CG	-8.06	105.74	113.80
1	B	174	HIS	CA-CB-CG	-8.04	105.76	113.80
1	B	96	VAL	CA-CB-CG2	7.99	123.98	110.40
1	A	96	VAL	CA-CB-CG2	7.98	123.96	110.40
1	B	274	TYR	CA-C-N	-7.87	112.95	123.10
1	B	274	TYR	C-N-CA	-7.87	112.95	123.10
1	A	274	TYR	CA-C-N	-7.82	113.02	123.10
1	A	274	TYR	C-N-CA	-7.82	113.02	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLN	N-CA-C	-7.69	103.63	113.16
1	B	128	GLN	N-CA-C	-7.69	103.63	113.16
1	B	217	GLY	CA-C-N	7.36	133.36	122.99
1	B	217	GLY	C-N-CA	7.36	133.36	122.99
1	A	217	GLY	CA-C-N	7.33	133.32	122.99
1	A	217	GLY	C-N-CA	7.33	133.32	122.99
1	B	290	ASP	O-C-N	7.31	131.71	122.93
1	A	227	SER	O-C-N	7.31	129.90	122.08
1	A	290	ASP	O-C-N	7.28	131.67	122.93
1	B	227	SER	O-C-N	7.26	129.85	122.08
1	A	63	SER	CA-C-N	7.25	131.76	121.02
1	A	63	SER	C-N-CA	7.25	131.76	121.02
1	B	63	SER	CA-C-N	7.24	131.74	121.02
1	B	63	SER	C-N-CA	7.24	131.74	121.02
1	A	171	ASP	CA-CB-CG	-6.99	105.61	112.60
1	B	310	TYR	CA-C-O	-6.97	113.48	121.15
1	B	171	ASP	CA-CB-CG	-6.97	105.63	112.60
1	A	310	TYR	CA-C-O	-6.95	113.50	121.15
1	A	326	ARG	CD-NE-CZ	-6.89	114.75	124.40
1	B	326	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	A	206	CYS	N-CA-C	6.84	125.37	110.80
1	B	4	VAL	CA-CB-CG2	6.83	122.01	110.40
1	B	206	CYS	N-CA-C	6.83	125.34	110.80
1	B	265	LYS	CA-C-N	-6.81	113.16	122.77
1	B	265	LYS	C-N-CA	-6.81	113.16	122.77
1	A	4	VAL	CA-CB-CG2	6.81	121.97	110.40
1	A	265	LYS	CA-C-N	-6.79	113.19	122.77
1	A	265	LYS	C-N-CA	-6.79	113.19	122.77
1	A	38	VAL	CA-CB-CG2	6.75	121.87	110.40
1	B	38	VAL	CA-CB-CG2	6.74	121.86	110.40
1	B	300	ALA	CA-C-N	-6.67	113.55	122.42
1	B	300	ALA	C-N-CA	-6.67	113.55	122.42
1	A	300	ALA	CA-C-N	-6.67	113.55	122.42
1	A	300	ALA	C-N-CA	-6.67	113.55	122.42
1	A	304	THR	CA-C-N	6.61	131.75	120.71
1	A	304	THR	C-N-CA	6.61	131.75	120.71
1	B	112	PHE	CA-CB-CG	-6.60	107.20	113.80
1	B	304	THR	CA-C-N	6.59	131.72	120.71
1	B	304	THR	C-N-CA	6.59	131.72	120.71
1	A	112	PHE	CA-CB-CG	-6.55	107.25	113.80
1	B	126	ILE	CA-C-N	-6.50	111.45	122.11
1	B	126	ILE	C-N-CA	-6.50	111.45	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ILE	CA-C-N	-6.48	111.48	122.11
1	A	126	ILE	C-N-CA	-6.48	111.48	122.11
1	A	320	ILE	O-C-N	-6.46	116.40	123.18
1	A	319	ARG	CD-NE-CZ	-6.45	115.38	124.40
1	B	319	ARG	CD-NE-CZ	-6.44	115.38	124.40
1	B	320	ILE	O-C-N	-6.44	116.42	123.18
1	A	32	ASP	N-CA-C	6.42	119.28	108.23
1	B	137	PHE	CA-CB-CG	-6.41	107.39	113.80
1	B	32	ASP	N-CA-C	6.40	119.23	108.23
1	A	137	PHE	CA-CB-CG	-6.39	107.41	113.80
1	A	178	ASN	CA-CB-CG	-6.38	106.22	112.60
1	B	178	ASN	CA-CB-CG	-6.34	106.26	112.60
1	B	175	TYR	CA-C-N	-6.28	111.94	122.29
1	B	175	TYR	C-N-CA	-6.28	111.94	122.29
1	A	175	TYR	CA-C-N	-6.27	111.94	122.29
1	A	175	TYR	C-N-CA	-6.27	111.94	122.29
1	A	182	ILE	CA-C-O	-6.23	113.98	120.27
1	B	319	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	B	293	PRO	O-C-N	6.22	128.80	121.46
1	A	221	ILE	CA-C-N	-6.20	112.16	122.21
1	A	221	ILE	C-N-CA	-6.20	112.16	122.21
1	A	293	PRO	O-C-N	6.20	128.78	121.46
1	B	1	THR	O-C-N	-6.20	115.80	123.36
1	B	221	ILE	CA-C-N	-6.20	112.17	122.21
1	B	221	ILE	C-N-CA	-6.20	112.17	122.21
1	A	319	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	A	1	THR	O-C-N	-6.18	115.82	123.36
1	B	182	ILE	CA-C-O	-6.18	114.03	120.27
1	A	245	TYR	O-C-N	-6.15	115.20	123.19
1	A	74	ARG	O-C-N	-6.12	115.50	122.84
1	B	74	ARG	O-C-N	-6.11	115.51	122.84
1	B	245	TYR	O-C-N	-6.11	115.24	123.19
1	B	95	THR	CA-C-N	-6.07	114.51	122.94
1	B	95	THR	C-N-CA	-6.07	114.51	122.94
1	A	95	THR	CA-C-N	-6.07	114.51	122.94
1	A	95	THR	C-N-CA	-6.07	114.51	122.94
1	B	193	GLN	O-C-N	6.05	129.84	123.06
1	A	193	GLN	O-C-N	6.04	129.83	123.06
1	B	72	THR	CA-C-N	-5.96	112.98	121.50
1	B	72	THR	C-N-CA	-5.96	112.98	121.50
1	A	72	THR	CA-C-N	-5.95	112.99	121.50
1	A	72	THR	C-N-CA	-5.95	112.99	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASN	O-C-N	5.95	128.44	122.08
1	B	250	ASN	O-C-N	5.94	128.43	122.08
1	A	12	THR	O-C-N	5.93	128.30	122.19
1	B	12	THR	O-C-N	5.92	128.29	122.19
1	A	188	GLY	N-CA-C	-5.91	106.83	115.63
1	A	206	CYS	N-CA-CB	5.90	120.46	110.49
1	B	188	GLY	N-CA-C	-5.90	106.84	115.63
1	B	206	CYS	N-CA-CB	5.88	120.44	110.49
1	B	51	VAL	CA-CB-CG2	5.88	120.39	110.40
1	A	51	VAL	CA-CB-CG2	5.87	120.37	110.40
1	B	125	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	275	VAL	CA-CB-CG2	5.85	120.35	110.40
1	A	125	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	206	CYS	O-C-N	5.84	130.35	122.59
1	B	275	VAL	CA-CB-CG2	5.84	120.32	110.40
1	A	30	VAL	CA-CB-CG2	5.83	120.31	110.40
1	B	30	VAL	CA-CB-CG2	5.83	120.31	110.40
1	B	121	VAL	CA-CB-CG2	5.82	120.29	110.40
1	A	121	VAL	CA-CB-CG2	5.80	120.26	110.40
1	B	206	CYS	O-C-N	5.79	130.29	122.59
1	B	6	LEU	O-C-N	5.79	129.57	123.03
1	A	323	ALA	CA-C-O	-5.75	114.56	120.89
1	A	6	LEU	O-C-N	5.75	129.52	123.03
1	A	245	TYR	CA-C-N	-5.72	115.33	123.17
1	A	245	TYR	C-N-CA	-5.72	115.33	123.17
1	B	323	ALA	CA-C-O	-5.72	114.60	120.89
1	B	245	TYR	CA-C-N	-5.71	115.34	123.17
1	B	245	TYR	C-N-CA	-5.71	115.34	123.17
1	A	172	PRO	CA-C-N	-5.69	111.64	121.66
1	A	172	PRO	C-N-CA	-5.69	111.64	121.66
1	B	172	PRO	CA-C-N	-5.69	111.65	121.66
1	B	172	PRO	C-N-CA	-5.69	111.65	121.66
1	B	91	VAL	CA-CB-CG2	5.68	120.06	110.40
1	B	53	HIS	CA-C-O	5.68	128.10	121.46
1	A	91	VAL	CA-CB-CG2	5.67	120.03	110.40
1	A	273	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	53	HIS	CA-C-O	5.66	128.08	121.46
1	B	273	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	66	HIS	CA-C-N	5.65	132.34	121.54
1	A	66	HIS	C-N-CA	5.65	132.34	121.54
1	B	66	HIS	CA-C-N	5.65	132.33	121.54
1	B	66	HIS	C-N-CA	5.65	132.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	VAL	CA-CB-CG1	5.64	119.98	110.40
1	B	133	VAL	CA-CB-CG1	5.64	119.98	110.40
1	B	86	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	184	LEU	CA-C-O	-5.60	114.53	120.92
1	A	86	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	181	TYR	CA-C-O	5.59	127.90	121.47
1	B	184	LEU	CA-C-O	-5.59	114.55	120.92
1	B	27	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	280	LYS	O-C-N	5.58	130.19	123.16
1	A	280	LYS	O-C-N	5.58	130.19	123.16
1	A	181	TYR	CA-C-O	5.58	127.88	121.47
1	A	27	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	303	ALA	CA-C-N	5.56	128.00	120.38
1	A	303	ALA	C-N-CA	5.56	128.00	120.38
1	B	303	ALA	CA-C-N	5.55	127.98	120.38
1	B	303	ALA	C-N-CA	5.55	127.98	120.38
1	A	120	VAL	CA-CB-CG2	5.53	119.80	110.40
1	B	120	VAL	CA-CB-CG2	5.52	119.78	110.40
1	B	237	ALA	O-C-N	-5.50	116.04	123.19
1	B	87	ASP	CA-C-O	-5.49	115.26	121.25
1	A	87	ASP	CA-C-O	-5.48	115.28	121.25
1	A	237	ALA	O-C-N	-5.48	116.07	123.19
1	B	56	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	36	SER	CA-C-O	5.46	124.52	118.52
1	A	56	PHE	CA-CB-CG	-5.46	108.34	113.80
1	B	36	SER	CA-C-O	5.44	124.50	118.52
1	B	189	VAL	CA-CB-CG2	5.43	119.64	110.40
1	B	157	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	A	189	VAL	CA-CB-CG2	5.42	119.62	110.40
1	B	23	PRO	CA-C-N	5.41	125.33	119.76
1	B	23	PRO	C-N-CA	5.41	125.33	119.76
1	A	157	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	317	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	23	PRO	CA-C-N	5.39	125.31	119.76
1	A	23	PRO	C-N-CA	5.39	125.31	119.76
1	B	317	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	101	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	13	GLN	CA-C-N	5.25	130.74	123.07
1	B	13	GLN	C-N-CA	5.25	130.74	123.07
1	A	13	GLN	CA-C-N	5.24	130.72	123.07
1	A	13	GLN	C-N-CA	5.24	130.72	123.07
1	B	101	PHE	CA-CB-CG	-5.23	108.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	N-CA-CB	-5.22	105.15	111.31
1	B	291	ILE	N-CA-CB	-5.21	105.16	111.31
1	A	123	MET	CG-SD-CE	5.20	112.35	100.90
1	B	169	GLY	N-CA-C	5.20	117.21	110.45
1	B	123	MET	CG-SD-CE	5.20	112.33	100.90
1	B	316	ARG	CD-NE-CZ	-5.18	117.14	124.40
1	A	316	ARG	CD-NE-CZ	-5.18	117.14	124.40
1	A	169	GLY	N-CA-C	5.17	117.18	110.45
1	A	173	GLN	CB-CG-CD	-5.16	103.82	112.60
1	B	173	GLN	CB-CG-CD	-5.16	103.83	112.60
1	B	307	ARG	CA-C-O	-5.16	114.04	119.97
1	A	307	ARG	CA-C-O	-5.14	114.06	119.97
1	B	176	GLU	CB-CG-CD	-5.14	103.86	112.60
1	A	176	GLU	CB-CG-CD	-5.13	103.87	112.60
1	B	12	THR	CA-C-N	5.12	129.97	122.39
1	B	12	THR	C-N-CA	5.12	129.97	122.39
1	A	32	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	12	THR	CA-C-N	5.11	129.95	122.39
1	A	12	THR	C-N-CA	5.11	129.95	122.39
1	A	145	VAL	CA-CB-CG2	5.11	119.08	110.40
1	B	32	ASP	CA-CB-CG	-5.10	107.50	112.60
1	B	145	VAL	CA-CB-CG2	5.09	119.05	110.40
1	A	73	LEU	CA-C-N	-5.06	115.29	123.23
1	A	73	LEU	C-N-CA	-5.06	115.29	123.23
1	B	13	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	40	VAL	CA-CB-CG2	5.05	118.99	110.40
1	B	73	LEU	CA-C-N	-5.05	115.30	123.23
1	B	73	LEU	C-N-CA	-5.05	115.30	123.23
1	B	304	THR	O-C-N	5.04	127.47	122.12
1	A	13	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	40	VAL	CA-CB-CG2	5.04	118.97	110.40
1	B	139	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	267	TYR	CA-CB-CG	-5.03	104.86	113.90
1	A	139	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	267	TYR	CA-CB-CG	-5.01	104.88	113.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	303	ALA	CA
1	B	303	ALA	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Mainchain
1	A	195	LYS	Mainchain
1	A	316	ARG	Sidechain
1	A	326	ARG	Sidechain
1	B	162	GLY	Mainchain
1	B	195	LYS	Mainchain
1	B	316	ARG	Sidechain
1	B	326	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	2509	0	2398	175	1
1	B	2509	0	2398	176	2
All	All	5018	0	4796	351	2

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 36.

All (351) 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:196:GLY:HA2	1:A:206:CYS:CB	1.77	1.15
1:B:196:GLY:HA2	1:B:206:CYS:CB	1.77	1.15
1:B:196:GLY:CA	1:B:206:CYS:HB3	1.76	1.15
1:A:196:GLY:CA	1:A:206:CYS:HB3	1.76	1.13
1:B:199:VAL:HG21	1:B:204:LEU:HD21	1.28	1.08
1:A:199:VAL:HG21	1:A:204:LEU:HD21	1.28	1.04
1:A:194:MET:HE1	1:A:197:VAL:HG22	1.43	1.00
1:B:199:VAL:HB	1:B:204:LEU:HD23	1.39	1.00
1:A:270:THR:HG22	1:A:272:ALA:H	1.26	0.99
1:B:194:MET:HE1	1:B:197:VAL:HG22	1.43	0.99
1:A:199:VAL:HB	1:A:204:LEU:HD23	1.39	0.99
1:B:270:THR:HG22	1:B:272:ALA:H	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD2	1:A:283:THR:HG23	1.64	0.97
1:B:89:ILE:HD12	1:B:99:GLN:HB3	1.46	0.95
1:B:244:ASP:OD2	1:B:283:THR:HG23	1.64	0.95
1:A:199:VAL:HG21	1:A:204:LEU:CD2	1.95	0.95
1:A:89:ILE:HD12	1:A:99:GLN:HB3	1.46	0.95
1:B:199:VAL:HG21	1:B:204:LEU:CD2	1.95	0.95
1:A:199:VAL:CG2	1:A:204:LEU:CD2	2.46	0.94
1:B:8:ASN:HD21	1:B:11:ASP:H	1.11	0.94
1:B:199:VAL:CG2	1:B:204:LEU:CD2	2.46	0.93
1:A:197:VAL:N	1:A:205:LEU:O	2.02	0.92
1:B:197:VAL:N	1:B:205:LEU:O	2.02	0.92
1:A:8:ASN:HD21	1:A:11:ASP:H	1.11	0.92
1:B:199:VAL:CG2	1:B:204:LEU:HD21	2.01	0.90
1:A:199:VAL:CG2	1:A:204:LEU:HD21	2.01	0.90
1:B:41:PRO:HB3	1:B:107:MET:HE3	1.54	0.90
1:B:8:ASN:C	1:B:8:ASN:HD22	1.80	0.88
1:B:8:ASN:HD22	1:B:9:TYR:N	1.71	0.88
1:A:41:PRO:HB3	1:A:107:MET:HE3	1.54	0.87
1:A:8:ASN:HD22	1:A:9:TYR:N	1.71	0.87
1:A:204:LEU:O	1:A:205:LEU:HD23	1.75	0.86
1:B:109:ALA:HB1	1:B:113:MET:HG3	1.56	0.86
1:B:204:LEU:O	1:B:205:LEU:HD23	1.75	0.86
1:A:8:ASN:HD22	1:A:8:ASN:C	1.80	0.86
1:A:109:ALA:HB1	1:A:113:MET:HG3	1.56	0.86
1:B:186:LYS:HG3	1:B:187:THR:N	1.91	0.85
1:A:186:LYS:HG3	1:A:187:THR:N	1.91	0.84
1:A:199:VAL:CB	1:A:204:LEU:HD23	2.09	0.82
1:B:199:VAL:CB	1:B:204:LEU:HD23	2.09	0.82
1:B:25:GLN:HE22	1:B:57:ASP:H	1.28	0.82
1:A:244:ASP:OD2	1:A:283:THR:CG2	2.27	0.81
1:B:244:ASP:OD2	1:B:283:THR:CG2	2.27	0.81
1:A:25:GLN:HE22	1:A:57:ASP:H	1.28	0.81
1:A:181:TYR:HB3	1:A:319:ARG:HD3	1.65	0.79
1:A:84:LEU:HD11	1:A:133:VAL:HG11	1.66	0.77
1:A:84:LEU:HD13	1:A:100:MET:HE2	1.66	0.77
1:B:181:TYR:HB3	1:B:319:ARG:HD3	1.65	0.77
1:B:84:LEU:HD13	1:B:100:MET:HE2	1.66	0.77
1:A:8:ASN:HD21	1:A:11:ASP:N	1.83	0.76
1:B:84:LEU:HD11	1:B:133:VAL:HG11	1.66	0.76
1:A:199:VAL:CB	1:A:204:LEU:CD2	2.64	0.76
1:B:244:ASP:OD1	1:B:287:HIS:CE1	2.39	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD1	1:A:287:HIS:CE1	2.39	0.75
1:B:199:VAL:CB	1:B:204:LEU:CD2	2.64	0.75
1:A:252:GLY:N	1:A:253:PRO:HD2	2.01	0.74
1:B:252:GLY:N	1:B:253:PRO:HD2	2.00	0.74
1:B:207:GLU:O	1:B:208:ASP:HB2	1.86	0.74
1:B:8:ASN:HD21	1:B:11:ASP:N	1.83	0.74
1:A:207:GLU:O	1:A:208:ASP:HB2	1.86	0.73
1:A:27:PHE:CE1	1:A:54:LYS:HG2	2.23	0.73
1:B:27:PHE:CE1	1:B:54:LYS:HG2	2.23	0.73
1:A:298:THR:HG22	1:A:299:TRP:O	1.90	0.72
1:A:8:ASN:ND2	1:A:11:ASP:H	1.88	0.71
1:B:298:THR:HG22	1:B:299:TRP:O	1.90	0.71
1:B:89:ILE:HD12	1:B:99:GLN:CB	2.20	0.71
1:B:246:VAL:CG2	1:B:281:LEU:HD23	2.21	0.71
1:A:246:VAL:CG2	1:A:281:LEU:HD23	2.21	0.71
1:A:224:SER:OG	1:A:227:SER:HB2	1.91	0.71
1:B:224:SER:OG	1:B:227:SER:HB2	1.91	0.71
1:B:8:ASN:ND2	1:B:11:ASP:H	1.88	0.70
1:B:199:VAL:HB	1:B:204:LEU:CD2	2.18	0.70
1:A:275:VAL:HG22	1:A:284:LEU:CD2	2.22	0.70
1:B:275:VAL:HG22	1:B:284:LEU:CD2	2.22	0.70
1:A:89:ILE:HD12	1:A:99:GLN:CB	2.20	0.69
1:A:246:VAL:HG21	1:A:281:LEU:HD23	1.76	0.68
1:B:246:VAL:HG21	1:B:281:LEU:HD23	1.76	0.68
1:A:270:THR:HG22	1:A:271:SER:N	2.09	0.68
1:A:204:LEU:O	1:A:205:LEU:CD2	2.41	0.67
1:B:204:LEU:O	1:B:205:LEU:CD2	2.41	0.67
1:A:194:MET:HE1	1:A:260:PHE:HD1	1.59	0.67
1:A:185:ILE:HD13	1:A:193:GLN:HG3	1.75	0.67
1:A:199:VAL:HB	1:A:204:LEU:CD2	2.18	0.67
1:B:84:LEU:CD1	1:B:100:MET:HE2	2.24	0.67
1:A:84:LEU:CD1	1:A:100:MET:HE2	2.24	0.67
1:B:270:THR:HG22	1:B:271:SER:N	2.09	0.67
1:B:194:MET:HE1	1:B:260:PHE:HD1	1.59	0.67
1:A:194:MET:CE	1:A:260:PHE:HD1	2.08	0.66
1:B:185:ILE:HD13	1:B:193:GLN:CG	2.26	0.66
1:B:185:ILE:HD13	1:B:193:GLN:HG3	1.75	0.66
1:B:194:MET:CE	1:B:260:PHE:HD1	2.09	0.66
1:A:185:ILE:HD13	1:A:193:GLN:CG	2.26	0.65
1:B:262:LEU:HD12	1:B:267:TYR:CD2	2.32	0.64
1:A:270:THR:HG22	1:A:272:ALA:N	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD22	1:B:101:PHE:O	1.97	0.64
1:A:84:LEU:HD22	1:A:101:PHE:O	1.97	0.64
1:B:38:VAL:HG22	1:B:121:VAL:HG13	1.79	0.64
1:A:262:LEU:HD12	1:A:267:TYR:CD2	2.32	0.63
1:B:225:THR:O	1:B:229:GLU:HB2	1.99	0.63
1:A:38:VAL:HG22	1:A:121:VAL:HG13	1.79	0.62
1:B:270:THR:HG22	1:B:272:ALA:N	2.06	0.62
1:A:204:LEU:O	1:A:204:LEU:HD12	2.00	0.62
1:B:204:LEU:O	1:B:204:LEU:HD12	2.00	0.62
1:B:41:PRO:HG3	1:B:107:MET:HE1	1.81	0.62
1:A:270:THR:CG2	1:A:271:SER:N	2.63	0.61
1:A:225:THR:O	1:A:229:GLU:HB2	1.99	0.61
1:B:232:MET:HG3	1:B:245:TYR:CD1	2.36	0.61
1:A:41:PRO:HG3	1:A:107:MET:HE1	1.81	0.61
1:B:270:THR:CG2	1:B:271:SER:N	2.63	0.61
1:B:159:SER:O	1:B:160:GLU:CB	2.49	0.61
1:A:248:LYS:O	1:A:251:GLU:HG3	2.01	0.60
1:A:232:MET:HG3	1:A:245:TYR:CD1	2.35	0.60
1:B:244:ASP:OD1	1:B:287:HIS:HE1	1.82	0.60
1:B:278:GLU:O	1:B:279:SER:HB3	2.01	0.60
1:B:248:LYS:O	1:B:251:GLU:HG3	2.00	0.60
1:A:198:SER:OG	1:A:261:HIS:HE1	1.85	0.60
1:B:196:GLY:HA2	1:B:206:CYS:HB3	0.83	0.60
1:B:228:ILE:HG21	1:B:288:ALA:HB2	1.84	0.60
1:B:8:ASN:C	1:B:8:ASN:ND2	2.51	0.59
1:A:196:GLY:HA2	1:A:206:CYS:HB3	0.83	0.59
1:A:228:ILE:HG21	1:A:288:ALA:HB2	1.84	0.59
1:A:251:GLU:O	1:A:252:GLY:C	2.42	0.59
1:A:159:SER:O	1:A:160:GLU:CB	2.49	0.59
1:A:278:GLU:O	1:A:279:SER:HB3	2.01	0.59
1:B:293:PRO:HA	1:B:294:PRO:C	2.28	0.59
1:A:39:TRP:HZ3	1:A:107:MET:HE2	1.68	0.59
1:B:-1:THR:HG23	1:B:1:THR:N	2.18	0.59
1:B:39:TRP:HZ3	1:B:107:MET:HE2	1.68	0.58
1:B:251:GLU:O	1:B:252:GLY:C	2.42	0.58
1:A:244:ASP:OD1	1:A:287:HIS:HE1	1.82	0.58
1:A:293:PRO:HA	1:A:294:PRO:C	2.28	0.58
1:A:41:PRO:HB2	1:A:55:LEU:HD23	1.86	0.58
1:B:198:SER:OG	1:B:261:HIS:HE1	1.85	0.58
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.86	0.58
1:B:207:GLU:O	1:B:208:ASP:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:THR:HG23	1:A:1:THR:N	2.18	0.57
1:A:101:PHE:N	1:A:101:PHE:CD1	2.71	0.57
1:A:126:ILE:HD12	1:A:135:PRO:HD2	1.86	0.57
1:A:207:GLU:O	1:A:208:ASP:CB	2.52	0.57
1:B:101:PHE:N	1:B:101:PHE:CD1	2.71	0.57
1:A:109:ALA:CB	1:A:113:MET:HG3	2.34	0.56
1:B:126:ILE:HD12	1:B:135:PRO:HD2	1.86	0.56
1:A:155:TYR:CD2	1:A:303:ALA:HB2	2.41	0.56
1:B:155:TYR:CD2	1:B:303:ALA:HB2	2.41	0.56
1:B:194:MET:CE	1:B:197:VAL:HG22	2.28	0.56
1:A:206:CYS:SG	1:A:210:CYS:N	2.79	0.56
1:A:94:ILE:HD13	1:A:140:ILE:CG2	2.35	0.56
1:B:94:ILE:HD13	1:B:140:ILE:CG2	2.35	0.56
1:B:206:CYS:SG	1:B:210:CYS:N	2.79	0.55
1:A:41:PRO:HB3	1:A:107:MET:CE	2.34	0.55
1:A:68:GLY:O	1:A:83:PHE:HB2	2.07	0.55
1:B:194:MET:HE1	1:B:197:VAL:CG2	2.29	0.55
1:B:68:GLY:O	1:B:83:PHE:HB2	2.07	0.55
1:A:41:PRO:CB	1:A:107:MET:HE3	2.34	0.55
1:A:242:LEU:HG	1:A:243:PHE:HD2	1.72	0.54
1:A:171:ASP:C	1:A:171:ASP:OD1	2.48	0.54
1:B:41:PRO:HB3	1:B:107:MET:CE	2.34	0.54
1:B:41:PRO:CB	1:B:107:MET:HE3	2.34	0.54
1:A:202:SER:C	1:A:204:LEU:H	2.16	0.54
1:A:8:ASN:C	1:A:8:ASN:ND2	2.51	0.54
1:A:58:ALA:HB1	1:A:64:TYR:CG	2.44	0.53
1:B:58:ALA:HB1	1:B:64:TYR:CG	2.44	0.53
1:A:88:ILE:HG13	1:A:88:ILE:O	2.09	0.53
1:A:-1:THR:HB	1:A:145:VAL:O	2.09	0.53
1:B:202:SER:C	1:B:204:LEU:H	2.16	0.53
1:A:199:VAL:CB	1:A:204:LEU:HD21	2.37	0.53
1:A:221:ILE:HG13	1:A:304:THR:HB	1.91	0.53
1:B:182:ILE:HD13	1:B:262:LEU:HB3	1.91	0.53
1:B:242:LEU:HG	1:B:243:PHE:HD2	1.72	0.52
1:B:271:SER:HA	1:B:274:TYR:CE2	2.44	0.52
1:B:-1:THR:HB	1:B:145:VAL:O	2.09	0.52
1:B:204:LEU:O	1:B:205:LEU:CG	2.58	0.52
1:A:94:ILE:HD13	1:A:140:ILE:HG21	1.90	0.52
1:B:94:ILE:HD13	1:B:140:ILE:HG21	1.90	0.52
1:A:109:ALA:HB1	1:A:113:MET:CG	2.36	0.52
1:B:109:ALA:CB	1:B:113:MET:HG3	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:O	1:A:205:LEU:CG	2.57	0.52
1:B:109:ALA:HB1	1:B:113:MET:CG	2.36	0.52
1:B:199:VAL:HG23	1:B:204:LEU:HG	1.92	0.52
1:A:199:VAL:HG23	1:A:204:LEU:HG	1.92	0.52
1:B:194:MET:HE1	1:B:260:PHE:CD1	2.42	0.52
1:A:271:SER:HA	1:A:274:TYR:CE2	2.44	0.51
1:A:58:ALA:HB1	1:A:64:TYR:CD2	2.45	0.51
1:B:58:ALA:HB1	1:B:64:TYR:CD2	2.45	0.51
1:A:199:VAL:HG11	1:A:234:ALA:CB	2.40	0.51
1:B:126:ILE:HD12	1:B:134:THR:HA	1.93	0.51
1:A:181:TYR:CB	1:A:319:ARG:HD3	2.38	0.51
1:A:182:ILE:HD13	1:A:262:LEU:HB3	1.92	0.51
1:B:221:ILE:HG13	1:B:304:THR:HB	1.92	0.51
1:A:186:LYS:HG3	1:A:187:THR:H	1.74	0.51
1:A:6:LEU:HD21	1:A:165:ILE:HG13	1.94	0.50
1:A:246:VAL:HG23	1:A:281:LEU:HD23	1.93	0.50
1:B:88:ILE:HG13	1:B:88:ILE:O	2.09	0.50
1:B:199:VAL:HG11	1:B:234:ALA:CB	2.40	0.50
1:A:194:MET:HE1	1:A:260:PHE:CD1	2.42	0.50
1:B:6:LEU:HD21	1:B:165:ILE:HG13	1.93	0.50
1:A:194:MET:CE	1:A:197:VAL:HG22	2.28	0.50
1:A:298:THR:HG22	1:A:299:TRP:N	2.27	0.50
1:B:30:VAL:HG23	1:B:117:PHE:CD2	2.47	0.50
1:B:275:VAL:HG22	1:B:284:LEU:HD22	1.94	0.50
1:B:240:ARG:O	1:B:242:LEU:C	2.55	0.50
1:A:126:ILE:HD12	1:A:134:THR:HA	1.93	0.50
1:A:30:VAL:HG23	1:A:117:PHE:CD2	2.47	0.49
1:A:64:TYR:CD1	1:A:64:TYR:C	2.90	0.49
1:A:199:VAL:HG21	1:A:204:LEU:CG	2.42	0.49
1:B:181:TYR:CB	1:B:319:ARG:HD3	2.38	0.49
1:B:171:ASP:OD1	1:B:171:ASP:C	2.48	0.49
1:B:298:THR:HG22	1:B:299:TRP:N	2.27	0.49
1:A:194:MET:HE1	1:A:197:VAL:CG2	2.29	0.49
1:A:255:LEU:HB3	1:A:256:PRO:HD2	1.94	0.49
1:B:199:VAL:CG2	1:B:204:LEU:CG	2.90	0.49
1:B:199:VAL:HG21	1:B:204:LEU:CG	2.42	0.49
1:A:199:VAL:CG2	1:A:204:LEU:CG	2.90	0.49
1:A:240:ARG:O	1:A:242:LEU:C	2.55	0.48
1:B:64:TYR:CD1	1:B:64:TYR:C	2.90	0.48
1:A:125:PHE:CB	1:A:188:GLY:HA2	2.43	0.48
1:B:125:PHE:CB	1:B:188:GLY:HA2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:O	1:B:133:VAL:CG2	2.62	0.48
1:B:246:VAL:HG23	1:B:281:LEU:HD23	1.93	0.48
1:B:255:LEU:HD12	1:B:275:VAL:HG21	1.95	0.48
1:B:199:VAL:CB	1:B:204:LEU:HD21	2.37	0.48
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.94	0.48
1:B:185:ILE:HD12	1:B:211:LEU:CD2	2.43	0.48
1:B:202:SER:C	1:B:204:LEU:N	2.71	0.48
1:B:42:SER:HB2	1:B:103:GLU:HG2	1.96	0.47
1:A:12:THR:O	1:A:219:SER:HB3	2.14	0.47
1:A:232:MET:HG3	1:A:245:TYR:CE1	2.49	0.47
1:A:255:LEU:HD12	1:A:275:VAL:HG21	1.95	0.47
1:A:153:PHE:CZ	1:A:165:ILE:HD13	2.50	0.47
1:A:185:ILE:HD12	1:A:211:LEU:CD2	2.43	0.47
1:B:291:ILE:O	1:B:296:GLY:HA3	2.15	0.47
1:A:202:SER:C	1:A:204:LEU:N	2.71	0.47
1:B:22:THR:HA	1:B:23:PRO:C	2.40	0.47
1:A:291:ILE:O	1:A:296:GLY:HA3	2.15	0.47
1:B:153:PHE:CZ	1:B:165:ILE:HD13	2.50	0.47
1:A:42:SER:HB2	1:A:103:GLU:HG2	1.96	0.47
1:A:275:VAL:HG22	1:A:284:LEU:HD22	1.94	0.47
1:B:205:LEU:HD11	1:B:227:SER:O	2.15	0.47
1:B:296:GLY:HA2	1:B:298:THR:OG1	2.15	0.47
1:A:205:LEU:HD11	1:A:227:SER:O	2.15	0.47
1:A:252:GLY:C	1:A:254:THR:H	2.23	0.47
1:A:296:GLY:HA2	1:A:298:THR:OG1	2.15	0.47
1:A:155:TYR:HD2	1:A:303:ALA:HB2	1.80	0.46
1:B:252:GLY:C	1:B:254:THR:H	2.23	0.46
1:B:12:THR:O	1:B:219:SER:HB3	2.14	0.46
1:A:133:VAL:O	1:A:133:VAL:CG2	2.62	0.46
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.79	0.46
1:B:232:MET:HG3	1:B:245:TYR:CE1	2.49	0.46
1:A:41:PRO:HG2	1:A:54:LYS:O	2.16	0.46
1:A:231:LEU:O	1:A:231:LEU:HD12	2.16	0.46
1:B:271:SER:O	1:B:275:VAL:HB	2.15	0.46
1:B:155:TYR:HD2	1:B:303:ALA:HB2	1.80	0.46
1:B:186:LYS:HG3	1:B:187:THR:H	1.74	0.46
1:A:22:THR:HA	1:A:23:PRO:C	2.40	0.46
1:B:231:LEU:HD12	1:B:231:LEU:O	2.16	0.46
1:A:271:SER:O	1:A:275:VAL:HB	2.15	0.45
1:B:41:PRO:HG2	1:B:54:LYS:O	2.16	0.45
1:A:22:THR:CA	1:A:23:PRO:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HB2	1:B:267:TYR:CE2	2.52	0.45
1:A:262:LEU:HB2	1:A:267:TYR:CE2	2.52	0.45
1:B:111:PRO:HD2	1:B:112:PHE:H	1.82	0.45
1:A:276:PHE:HB2	1:A:283:THR:O	2.17	0.45
1:B:91:VAL:O	1:B:92:GLY:C	2.60	0.45
1:A:94:ILE:CD1	1:A:140:ILE:HG21	2.47	0.45
1:B:230:LYS:O	1:B:233:GLU:HB3	2.17	0.45
1:B:194:MET:HG2	1:B:262:LEU:HD23	1.99	0.45
1:A:99:GLN:HG3	1:A:100:MET:N	2.32	0.45
1:A:194:MET:HG2	1:A:262:LEU:HD23	1.99	0.45
1:A:198:SER:HA	1:A:203:THR:HA	1.99	0.45
1:B:94:ILE:CD1	1:B:140:ILE:HG21	2.47	0.44
1:B:99:GLN:HG3	1:B:100:MET:N	2.32	0.44
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.62	0.44
1:B:199:VAL:CG2	1:B:204:LEU:HG	2.47	0.44
1:B:268:THR:HG22	1:B:269:LEU:N	2.32	0.44
1:A:111:PRO:HD2	1:A:112:PHE:H	1.82	0.44
1:B:22:THR:CA	1:B:23:PRO:C	2.90	0.44
1:B:135:PRO:HG2	1:B:138:ASP:OD1	2.17	0.44
1:B:255:LEU:HD12	1:B:275:VAL:CG2	2.47	0.44
1:B:276:PHE:HB2	1:B:283:THR:O	2.17	0.44
1:A:135:PRO:HG2	1:A:138:ASP:OD1	2.18	0.44
1:A:268:THR:HG22	1:A:269:LEU:N	2.32	0.44
1:B:133:VAL:O	1:B:133:VAL:HG22	2.18	0.44
1:A:204:LEU:O	1:A:205:LEU:HG	2.18	0.44
1:A:255:LEU:HD12	1:A:275:VAL:CG2	2.47	0.44
1:A:198:SER:OG	1:A:261:HIS:CE1	2.70	0.43
1:A:56:PHE:CD1	1:A:56:PHE:C	2.96	0.43
1:B:56:PHE:CD1	1:B:56:PHE:C	2.96	0.43
1:B:292:PRO:HA	1:B:293:PRO:HD3	1.71	0.43
1:A:225:THR:HA	1:A:288:ALA:HB1	2.01	0.43
1:A:230:LYS:O	1:A:233:GLU:HB3	2.17	0.43
1:A:133:VAL:O	1:A:133:VAL:HG22	2.18	0.43
1:A:199:VAL:CG2	1:A:204:LEU:HG	2.47	0.43
1:A:185:ILE:CD1	1:A:211:LEU:HD23	2.48	0.43
1:B:141:ILE:HD13	1:B:146:LEU:HD12	2.01	0.43
1:B:199:VAL:CG2	1:B:204:LEU:HD23	2.35	0.43
1:B:225:THR:HA	1:B:288:ALA:HB1	2.01	0.43
1:A:279:SER:C	1:A:279(A):TYR:CD1	2.97	0.43
1:B:198:SER:HA	1:B:203:THR:HA	1.99	0.43
1:A:42:SER:HB2	1:A:103:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:SER:OG	1:B:261:HIS:CE1	2.70	0.43
1:B:204:LEU:O	1:B:205:LEU:HG	2.18	0.42
1:B:242:LEU:HG	1:B:243:PHE:CD2	2.53	0.42
1:A:41:PRO:CG	1:A:107:MET:HE1	2.49	0.42
1:A:242:LEU:HG	1:A:243:PHE:CD2	2.53	0.42
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.87	0.42
1:B:185:ILE:CD1	1:B:211:LEU:HD23	2.48	0.42
1:A:125:PHE:CG	1:A:188:GLY:HA2	2.54	0.42
1:B:125:PHE:CG	1:B:188:GLY:HA2	2.54	0.42
1:B:279:SER:C	1:B:279(A):TYR:CD1	2.97	0.42
1:A:141:ILE:HD13	1:A:146:LEU:HD12	2.01	0.42
1:B:213:LEU:HB2	1:B:298:THR:HG21	2.01	0.42
1:A:7:THR:O	1:A:14:TYR:HA	2.20	0.42
1:B:180:HIS:CE1	1:B:265:LYS:HZ3	2.38	0.42
1:A:41:PRO:CG	1:A:107:MET:CE	2.98	0.42
1:A:231:LEU:HD12	1:A:231:LEU:C	2.44	0.42
1:B:42:SER:HB2	1:B:103:GLU:CG	2.49	0.42
1:B:231:LEU:HD12	1:B:231:LEU:C	2.44	0.42
1:A:71:LEU:CD2	1:A:130:ILE:HG22	2.50	0.42
1:A:134:THR:HA	1:A:135:PRO:HD2	1.55	0.42
1:A:213:LEU:HB2	1:A:298:THR:HG21	2.00	0.42
1:B:319:ARG:HH11	1:B:319:ARG:HD2	1.59	0.42
1:A:141:ILE:CD1	1:A:146:LEU:HD12	2.50	0.41
1:A:147:LYS:O	1:A:147:LYS:HG3	2.19	0.41
1:A:185:ILE:HD13	1:A:193:GLN:HG2	2.00	0.41
1:B:41:PRO:CB	1:B:107:MET:CE	2.97	0.41
1:B:149:ASP:C	1:B:150:VAL:HG13	2.45	0.41
1:A:285:ALA:HB1	1:A:304:THR:OG1	2.21	0.41
1:B:7:THR:O	1:B:14:TYR:HA	2.20	0.41
1:B:185:ILE:HD13	1:B:193:GLN:HG2	2.00	0.41
1:A:30:VAL:HG23	1:A:117:PHE:CG	2.56	0.41
1:B:30:VAL:HG23	1:B:117:PHE:CG	2.55	0.41
1:B:41:PRO:CG	1:B:107:MET:HE1	2.49	0.41
1:B:41:PRO:CG	1:B:107:MET:CE	2.97	0.41
1:B:188:GLY:O	1:B:189:VAL:HG22	2.21	0.41
1:B:285:ALA:HB1	1:B:304:THR:OG1	2.21	0.41
1:B:141:ILE:CD1	1:B:146:LEU:HD12	2.50	0.41
1:A:91:VAL:O	1:A:92:GLY:C	2.60	0.41
1:A:188:GLY:O	1:A:189:VAL:HG22	2.21	0.41
1:B:71:LEU:CD2	1:B:130:ILE:HG22	2.50	0.41
1:B:147:LYS:O	1:B:147:LYS:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:C	1:B:173:GLN:H	2.29	0.41
1:B:96:VAL:O	1:B:96:VAL:CG1	2.69	0.41
1:A:41:PRO:CB	1:A:107:MET:CE	2.97	0.40
1:A:96:VAL:O	1:A:96:VAL:CG1	2.69	0.40
1:B:292:PRO:HD2	1:B:292:PRO:O	2.21	0.40
1:A:203:THR:O	1:A:203:THR:OG1	2.33	0.40
1:B:292:PRO:C	1:B:293:PRO:O	2.64	0.40
1:A:149:ASP:C	1:A:150:VAL:HG13	2.46	0.40
1:A:155:TYR:CE2	1:A:303:ALA:HB2	2.56	0.40
1:A:292:PRO:HD2	1:A:292:PRO:O	2.21	0.40
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.92	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:CD2	1:B:254:THR:CG2[5_555]	1.86	0.34
1:A:270:THR:OG1	1:B:17:GLU:OE2[5_555]	1.93	0.27

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	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	3	12
1	B	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	3	12
All	All	654/680 (96%)	580 (89%)	54 (8%)	20 (3%)	3	12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP

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Mol	Chain	Res	Type
1	A	206	CYS
1	B	158	ASP
1	B	206	CYS
1	A	242	LEU
1	B	242	LEU
1	A	69	THR
1	A	112	PHE
1	A	208	ASP
1	A	279	SER
1	B	69	THR
1	B	112	PHE
1	B	208	ASP
1	B	279	SER
1	A	67	ASN
1	A	126	ILE
1	B	67	ASN
1	B	126	ILE
1	A	253	PRO
1	B	253	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/290 (93%)	222 (82%)	48 (18%)	2	6
1	B	270/290 (93%)	222 (82%)	48 (18%)	2	6
All	All	540/580 (93%)	444 (82%)	96 (18%)	2	6

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	THR
1	A	1	THR
1	A	8	ASN
1	A	20	ILE

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Mol	Chain	Res	Type
1	A	26	THR
1	A	42	SER
1	A	43	SER
1	A	59	SER
1	A	63	SER
1	A	69	THR
1	A	81	SER
1	A	84	LEU
1	A	85	SER
1	A	97	THR
1	A	104	VAL
1	A	123	MET
1	A	133	VAL
1	A	134	THR
1	A	141	ILE
1	A	152	SER
1	A	156	ASN
1	A	159	SER
1	A	161	LEU
1	A	164	GLN
1	A	165	ILE
1	A	185	ILE
1	A	189	VAL
1	A	193	GLN
1	A	194	MET
1	A	203	THR
1	A	204	LEU
1	A	213	LEU
1	A	219	SER
1	A	222	SER
1	A	226	SER
1	A	227	SER
1	A	229	GLU
1	A	244	ASP
1	A	254	THR
1	A	259	SER
1	A	275	VAL
1	A	277	GLN
1	A	297	PRO
1	A	316	ARG
1	A	318	ASN
1	A	319	ARG

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	326	ARG
1	B	-1	THR
1	B	1	THR
1	B	8	ASN
1	B	20	ILE
1	B	26	THR
1	B	42	SER
1	B	43	SER
1	B	59	SER
1	B	63	SER
1	B	69	THR
1	B	81	SER
1	B	84	LEU
1	B	85	SER
1	B	97	THR
1	B	104	VAL
1	B	123	MET
1	B	133	VAL
1	B	134	THR
1	B	141	ILE
1	B	152	SER
1	B	156	ASN
1	B	159	SER
1	B	161	LEU
1	B	164	GLN
1	B	165	ILE
1	B	185	ILE
1	B	189	VAL
1	B	193	GLN
1	B	194	MET
1	B	203	THR
1	B	204	LEU
1	B	213	LEU
1	B	219	SER
1	B	222	SER
1	B	226	SER
1	B	227	SER
1	B	229	GLU
1	B	244	ASP
1	B	254	THR
1	B	259	SER

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Mol	Chain	Res	Type
1	B	275	VAL
1	B	277	GLN
1	B	297	PRO
1	B	316	ARG
1	B	318	ASN
1	B	319	ARG
1	B	324	LEU
1	B	326	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	25	GLN
1	A	99	GLN
1	A	128	GLN
1	A	156	ASN
1	A	174	HIS
1	A	178	ASN
1	A	191	GLN
1	A	261	HIS
1	B	8	ASN
1	B	25	GLN
1	B	99	GLN
1	B	128	GLN
1	B	156	ASN
1	B	174	HIS
1	B	178	ASN
1	B	191	GLN
1	B	261	HIS

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 [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.