



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1QYD  
Title : Crystal structures of pinoresinol-lariciresinol and phenylcoumaran benzylic ether reductases, and their relationship to isoflavone reductases  
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Deposited on : 2003-09-10  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

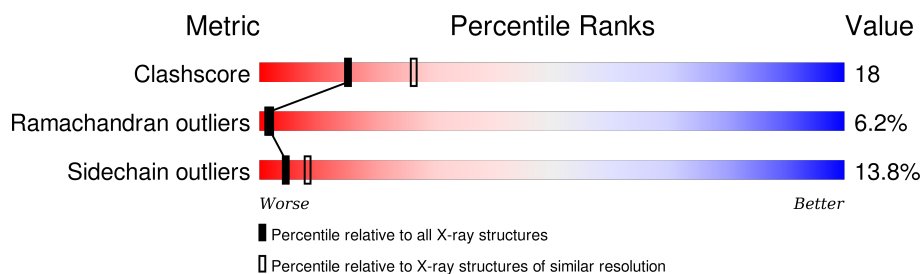
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	313	 45% 39% 12% •
1	B	313	 53% 33% 11% •
1	C	313	 52% 35% 11% •
1	D	313	 48% 39% 11% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10072 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 pinorexinol-laricresinol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	B	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	C	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	D	312	Total	C	N	O	S	0	0	0
			2496	1605	416	464	11			

- Molecule 2 is water.

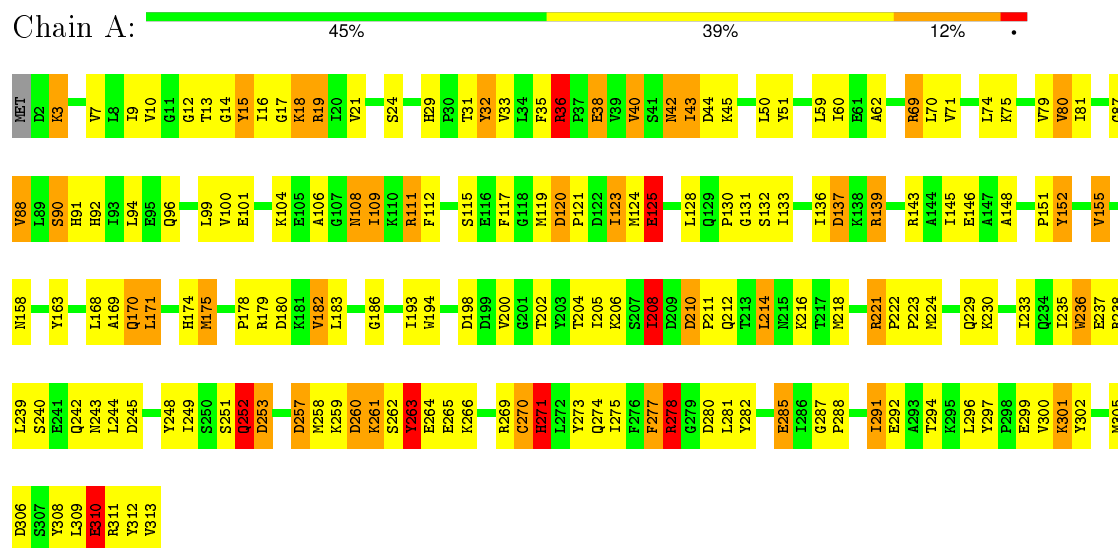
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	24	Total	O	0	0
			24	24		
2	C	18	Total	O	0	0
			18	18		
2	D	23	Total	O	0	0
			23	23		

### 3 Residue-property plots

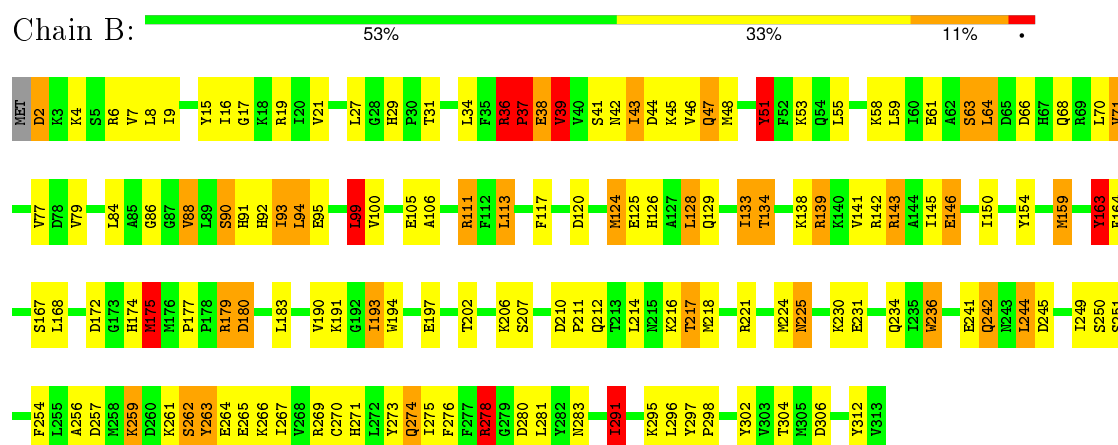
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: pinoresinol-lariciresinol reductase

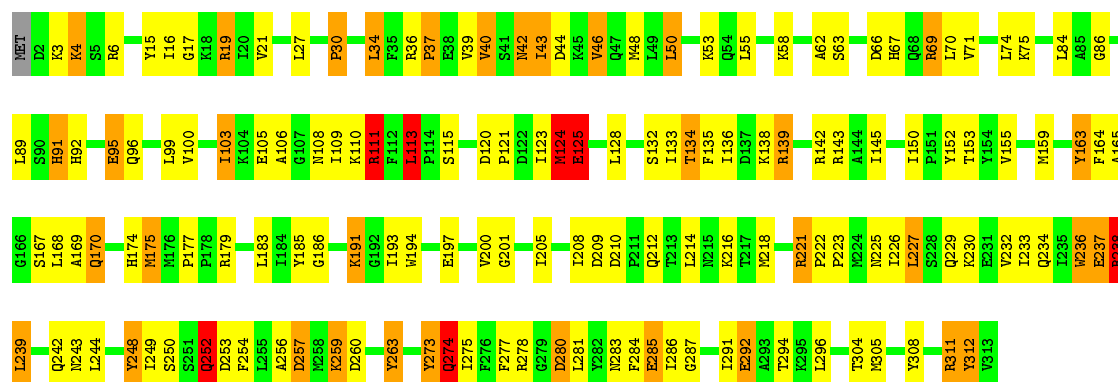


- Molecule 1: pinoresinol-lariciresinol reductase



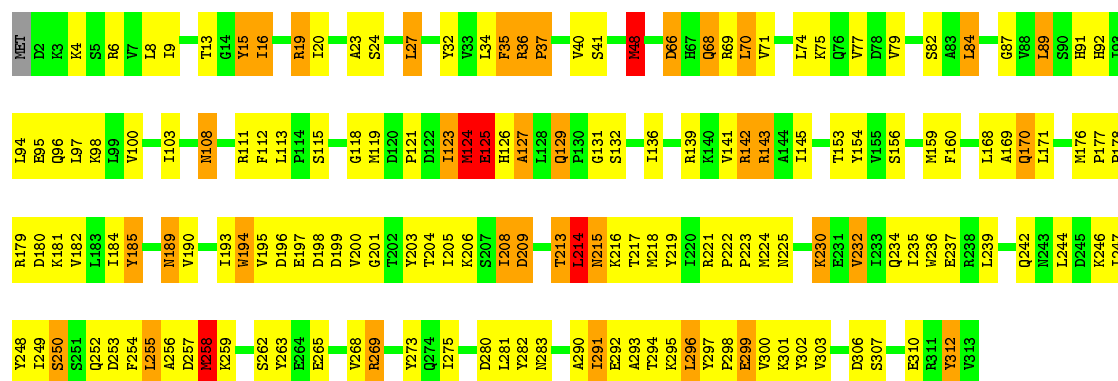
- Molecule 1: pinoresinol-lariciresinol reductase





- Molecule 1: pinorensinol-lariciresinol reductase

Chain D: 48% 39% 11% •



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.57 Å   125.96 Å   128.58 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.193 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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	0.82	0/2548	1.62	42/3442 (1.2%)
1	B	0.83	1/2548 (0.0%)	1.69	49/3442 (1.4%)
1	C	0.84	0/2548	1.73	51/3442 (1.5%)
1	D	0.84	0/2547	1.66	34/3442 (1.0%)
All	All	0.83	1/10191 (0.0%)	1.68	176/13768 (1.3%)

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	3
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	TRP	CG-CD2	-5.16	1.34	1.43

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	GLU	CA-C-N	-15.50	83.10	117.20
1	C	125	GLU	CA-C-N	-12.52	89.66	117.20
1	B	159	MET	CA-CB-CG	12.10	133.87	113.30
1	C	111	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	B	51	TYR	CB-CG-CD1	-9.88	115.07	121.00
1	C	263	TYR	CB-CG-CD2	-9.54	115.28	121.00
1	C	284	PHE	CA-C-N	-9.41	96.50	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	VAL	CA-C-N	-9.30	96.74	117.20
1	C	278	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	C	236	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	C	111	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	236	TRP	CE2-CD2-CG	-8.43	100.56	107.30
1	C	218	MET	CG-SD-CE	-8.33	86.87	100.20
1	B	236	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	C	19	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	125	GLU	CA-C-N	-8.15	99.27	117.20
1	C	139	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	B	194	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	C	113	LEU	CA-CB-CG	7.98	133.66	115.30
1	A	194	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	D	6	ARG	CA-CB-CG	7.84	130.65	113.40
1	B	194	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	125	GLU	CA-C-N	-7.61	100.47	117.20
1	B	194	TRP	CG-CD2-CE3	7.51	140.66	133.90
1	B	236	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	221	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	C	194	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	D	194	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	137	ASP	CB-CG-OD1	7.19	124.78	118.30
1	B	51	TYR	CA-CB-CG	7.17	127.03	113.40
1	D	115	SER	CA-C-N	-7.17	101.42	117.20
1	D	206	LYS	CA-CB-CG	-7.10	97.78	113.40
1	A	252	GLN	N-CA-C	7.09	130.13	111.00
1	A	32	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	B	194	TRP	CB-CG-CD1	-7.06	117.83	127.00
1	A	91	HIS	CA-CB-CG	7.02	125.53	113.60
1	D	236	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	B	38	GLU	C-N-CA	6.98	139.16	121.70
1	A	278	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	214	LEU	CA-CB-CG	6.95	131.27	115.30
1	D	236	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	C	194	TRP	CG-CD2-CE3	6.88	140.09	133.90
1	D	125	GLU	CA-C-O	6.87	134.53	120.10
1	A	236	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	B	139	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	19	ARG	CG-CD-NE	-6.67	97.80	111.80
1	B	139	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	4	LYS	N-CA-C	6.60	128.81	111.00
1	C	55	LEU	CA-CB-CG	6.60	130.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	LYS	CA-C-N	-6.59	103.03	116.20
1	C	125	GLU	C-N-CA	6.55	138.07	121.70
1	D	303	VAL	CA-C-N	-6.54	102.82	117.20
1	C	259	LYS	CA-CB-CG	6.40	127.47	113.40
1	D	48	MET	CB-CG-SD	-6.39	93.23	112.40
1	C	312	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	194	TRP	CD1-CG-CD2	6.31	111.35	106.30
1	A	125	GLU	C-N-CA	6.29	137.43	121.70
1	A	123	ILE	CA-C-N	-6.26	103.43	117.20
1	B	8	LEU	CA-CB-CG	6.26	129.69	115.30
1	C	74	LEU	CA-CB-CG	6.25	129.69	115.30
1	C	263	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	194	TRP	CG-CD2-CE3	6.21	139.49	133.90
1	C	42	ASN	N-CA-C	6.20	127.74	111.00
1	B	206	LYS	CA-CB-CG	-6.20	99.76	113.40
1	D	143	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	271	HIS	N-CA-C	-6.16	94.38	111.00
1	C	252	GLN	N-CA-C	6.14	127.57	111.00
1	B	278	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	39	VAL	N-CA-C	6.12	127.53	111.00
1	A	18	LYS	CA-CB-CG	6.12	126.87	113.40
1	D	179	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	19	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	278	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	194	TRP	CD1-CG-CD2	6.07	111.15	106.30
1	B	36	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	230	LYS	CA-CB-CG	6.05	126.70	113.40
1	B	306	ASP	CA-CB-CG	6.04	126.68	113.40
1	A	19	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	33	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	B	193	ILE	CG1-CB-CG2	-6.00	98.19	111.40
1	D	221	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	88	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	A	221	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	236	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	D	200	VAL	CG1-CB-CG2	-5.92	101.42	110.90
1	B	99	LEU	CA-CB-CG	5.92	128.92	115.30
1	C	42	ASN	CA-C-N	-5.86	104.31	117.20
1	D	123	ILE	N-CA-C	-5.86	95.18	111.00
1	B	125	GLU	C-N-CA	5.84	136.30	121.70
1	D	142	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	137	ASP	CB-CG-OD2	-5.81	113.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	LEU	CA-CB-CG	5.79	128.61	115.30
1	C	66	ASP	CA-C-N	-5.78	104.47	117.20
1	B	19	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	236	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	C	124	MET	CA-C-N	-5.75	104.55	117.20
1	B	46	VAL	CA-CB-CG2	-5.75	102.28	110.90
1	D	232	VAL	CG1-CB-CG2	-5.74	101.71	110.90
1	C	46	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	D	71	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	C	39	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	D	189	ASN	CA-C-N	-5.70	104.66	117.20
1	B	39	VAL	O-C-N	5.68	131.79	122.70
1	D	262	SER	N-CA-C	5.67	126.31	111.00
1	D	160	PHE	CA-C-N	-5.66	104.75	117.20
1	D	115	SER	O-C-N	5.66	131.75	122.70
1	C	274	GLN	CA-CB-CG	5.65	125.84	113.40
1	B	175	MET	N-CA-C	5.65	126.26	111.00
1	A	111	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	113	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	163	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	A	236	TRP	CD1-CG-CD2	5.60	110.78	106.30
1	C	155	VAL	CG1-CB-CG2	-5.60	101.95	110.90
1	C	284	PHE	CA-C-O	5.60	131.85	120.10
1	A	15	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	126	HIS	CA-CB-CG	5.59	123.11	113.60
1	D	194	TRP	CD1-CG-CD2	5.59	110.77	106.30
1	A	99	LEU	CA-CB-CG	5.58	128.15	115.30
1	C	238	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	34	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	34	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	302	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	C	259	LYS	C-N-CA	-5.53	107.88	121.70
1	C	284	PHE	O-C-N	5.53	131.54	122.70
1	C	214	LEU	CA-CB-CG	5.53	128.01	115.30
1	C	259	LYS	CB-CA-C	-5.52	99.37	110.40
1	A	245	ASP	CA-C-N	-5.52	105.06	117.20
1	C	50	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	71	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	B	39	VAL	CA-CB-CG2	-5.48	102.68	110.90
1	A	139	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	152	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	69	ARG	NE-CZ-NH2	-5.45	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	GLU	CA-CB-CG	5.45	125.38	113.40
1	C	311	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	218	MET	CG-SD-CE	-5.41	91.55	100.20
1	B	37	PRO	N-CA-C	5.40	126.14	112.10
1	B	224	MET	CA-CB-CG	5.39	122.46	113.30
1	B	37	PRO	CA-N-CD	-5.38	103.97	111.50
1	D	299	GLU	CA-CB-CG	5.37	125.22	113.40
1	B	312	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	119	MET	N-CA-C	5.34	125.42	111.00
1	C	69	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	243	ASN	CA-C-N	-5.30	105.54	117.20
1	A	288	PRO	N-CA-C	5.29	125.86	112.10
1	A	38	GLU	CA-C-N	-5.28	105.59	117.20
1	C	227	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	231	GLU	O-C-N	5.26	131.11	122.70
1	B	90	SER	CA-C-N	-5.24	105.68	117.20
1	B	291	ILE	CB-CA-C	-5.23	101.13	111.60
1	B	250	SER	CA-C-N	-5.22	105.73	117.20
1	D	250	SER	CA-C-N	-5.22	105.72	117.20
1	D	111	ARG	CA-CB-CG	-5.21	101.94	113.40
1	A	171	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	236	TRP	CB-CG-CD1	-5.19	120.25	127.00
1	A	175	MET	CA-CB-CG	-5.19	104.48	113.30
1	A	238	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	163	TYR	CB-CG-CD2	5.17	124.10	121.00
1	D	185	TYR	CA-C-N	-5.16	105.89	116.20
1	D	247	ILE	N-CA-C	-5.15	97.09	111.00
1	A	40	VAL	CA-C-N	-5.12	105.93	117.20
1	B	159	MET	CG-SD-CE	-5.10	92.04	100.20
1	C	125	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	111	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	258	MET	CB-CG-SD	5.08	127.65	112.40
1	C	221	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	262	SER	N-CA-C	5.06	124.67	111.00
1	A	3	LYS	N-CA-C	5.05	124.65	111.00
1	C	259	LYS	N-CA-CB	5.05	119.69	110.60
1	D	89	LEU	N-CA-C	5.03	124.59	111.00
1	D	127	ALA	CA-C-N	-5.03	106.14	117.20
1	B	124	MET	CA-CB-CG	5.03	121.85	113.30
1	D	35	PHE	CB-CG-CD2	-5.01	117.29	120.80
1	A	270	CYS	CA-C-N	-5.01	106.18	117.20
1	A	198	ASP	CB-CG-OD2	5.01	122.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	MET	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	GLY	Peptide
1	A	36	ARG	Peptide
1	A	51	TYR	Sidechain
1	B	36	ARG	Peptide
1	C	125	GLU	Mainchain
1	C	248	TYR	Sidechain
1	C	287	GLY	Peptide
1	C	36	ARG	Peptide
1	D	125	GLU	Mainchain
1	D	185	TYR	Sidechain
1	D	297	TYR	Sidechain
1	D	36	ARG	Peptide

## 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	2497	0	2525	96	0
1	B	2497	0	2525	71	0
1	C	2497	0	2525	87	0
1	D	2496	0	2525	98	0
2	A	20	0	0	4	0
2	B	24	0	0	1	0
2	C	18	0	0	0	0
2	D	23	0	0	0	0
All	All	10072	0	10100	352	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 18.

All (352) 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:D:275:ILE:HG23	1:D:281:LEU:HD22	1.48	0.95
1:C:86:GLY:HA3	1:C:89:LEU:HB2	1.49	0.93
1:C:170:GLN:HE22	1:C:183:LEU:HB2	1.35	0.89
1:D:113:LEU:HD22	1:D:153:THR:HB	1.53	0.89
1:A:155:VAL:HG11	1:A:204:THR:HG22	1.58	0.85
1:A:81:ILE:HD11	1:A:208:ILE:HD11	1.59	0.83
1:A:270:CYS:HA	1:A:273:TYR:HB2	1.60	0.81
1:C:71:VAL:HG13	1:C:106:ALA:HB2	1.64	0.80
1:D:208:ILE:HG23	1:D:209:ASP:H	1.47	0.79
1:A:193:ILE:HD11	1:A:282:TYR:HD1	1.48	0.79
1:B:254:PHE:HA	1:B:257:ASP:HB2	1.65	0.77
1:D:170:GLN:HE22	1:D:182:VAL:HG23	1.49	0.77
1:C:128:LEU:H	1:C:274:GLN:HE22	1.34	0.75
1:C:256:ALA:HA	1:C:259:LYS:HG3	1.69	0.75
1:C:96:GLN:HE22	1:C:115:SER:H	1.34	0.74
1:B:143:ARG:HH11	1:B:146:GLU:HG2	1.53	0.73
1:B:183:LEU:HD22	1:B:249:ILE:HD11	1.69	0.73
1:A:301:LYS:HE2	1:A:301:LYS:H	1.53	0.73
1:C:227:LEU:HD23	1:C:232:VAL:HG12	1.70	0.72
1:D:125:GLU:HG3	1:D:127:ALA:HB2	1.72	0.70
1:A:32:TYR:HD2	1:A:60:ILE:HD11	1.56	0.69
1:A:128:LEU:H	1:A:274:GLN:HE22	1.41	0.69
1:C:193:ILE:HG12	1:C:226:ILE:HG12	1.75	0.69
1:C:113:LEU:HD21	1:C:208:ILE:HG22	1.75	0.69
1:A:43:ILE:HD12	1:A:43:ILE:H	1.59	0.68
1:C:99:LEU:HG	1:C:103:ILE:HD11	1.74	0.68
1:D:24:SER:HA	1:D:205:ILE:HG21	1.74	0.68
1:D:258:MET:HG3	1:D:273:TYR:HE1	1.57	0.68
1:A:117:PHE:HE2	1:A:204:THR:HG21	1.58	0.68
1:A:96:GLN:HE22	1:A:115:SER:H	1.42	0.68
1:C:43:ILE:H	1:C:43:ILE:HD12	1.58	0.67
1:C:170:GLN:NE2	1:C:183:LEU:HB2	2.08	0.67
1:D:246:LYS:HB3	1:D:248:TYR:CE1	2.29	0.67
1:D:121:PRO:HB2	1:D:139:ARG:HG3	1.77	0.67
1:C:230:LYS:O	1:C:234:GLN:HG3	1.95	0.67
1:B:274:GLN:HA	1:B:278:ARG:HB2	1.77	0.67
1:B:15:TYR:HB3	1:B:163:TYR:OH	1.95	0.66
1:C:275:ILE:HG23	1:C:281:LEU:HG	1.77	0.65
1:C:254:PHE:HA	1:C:257:ASP:HB2	1.77	0.65
1:A:300:VAL:HA	1:A:301:LYS:HE2	1.78	0.65
1:A:179:ARG:HG3	1:A:242:GLN:HE22	1.61	0.65
1:C:132:SER:HA	1:C:135:PHE:HD1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:321:HOH:O	1:C:91:HIS:HB3	1.96	0.65
1:D:254:PHE:O	1:D:257:ASP:HB2	1.96	0.65
1:B:128:LEU:HD12	1:B:270:CYS:SG	2.37	0.65
1:D:193:ILE:H	1:D:281:LEU:HD23	1.61	0.65
1:B:71:VAL:HG13	1:B:106:ALA:HB2	1.80	0.64
1:B:216:LYS:HD3	1:B:291:ILE:HG13	1.79	0.64
1:D:170:GLN:HE21	1:D:178:PRO:HG2	1.63	0.64
1:D:142:ARG:HA	1:D:145:ILE:HD12	1.80	0.64
1:A:136:ILE:HD13	1:A:139:ARG:HH12	1.63	0.64
1:D:91:HIS:HA	1:D:94:LEU:HD12	1.80	0.63
1:D:79:VAL:HG11	1:D:208:ILE:HG13	1.79	0.63
1:D:75:LYS:HA	1:D:108:ASN:HD21	1.63	0.62
1:C:193:ILE:HG21	1:C:221:ARG:HA	1.82	0.62
1:D:215:ASN:N	1:D:215:ASN:HD22	1.97	0.62
1:A:266:LYS:O	1:A:270:CYS:SG	2.57	0.62
1:A:193:ILE:HD13	1:A:221:ARG:HG2	1.81	0.61
1:A:24:SER:HB3	1:A:31:THR:OG1	2.01	0.61
1:D:124:MET:HB2	1:D:126:HIS:ND1	2.15	0.61
1:A:90:SER:HA	1:A:137:ASP:OD2	2.01	0.60
1:C:100:VAL:HA	1:C:103:ILE:HG13	1.83	0.60
1:B:7:VAL:HG23	1:B:29:HIS:HB3	1.82	0.60
1:B:154:TYR:HD1	1:B:217:THR:HG22	1.67	0.60
1:D:170:GLN:HE22	1:D:182:VAL:CG2	2.15	0.59
1:A:291:ILE:HG13	1:A:296:LEU:HD11	1.85	0.59
1:C:191:LYS:HD2	1:C:226:ILE:HG22	1.84	0.59
1:B:264:GLU:HA	1:B:267:ILE:HD12	1.85	0.59
1:A:104:LYS:HD3	1:A:148:ALA:HB1	1.85	0.59
1:D:237:GLU:HG2	1:D:244:LEU:HD23	1.84	0.58
1:A:36:ARG:H	1:A:36:ARG:HD2	1.68	0.58
1:C:123:ILE:O	1:C:125:GLU:HG2	2.04	0.58
1:D:170:GLN:NE2	1:D:182:VAL:HG23	2.17	0.58
1:A:36:ARG:H	1:A:36:ARG:CD	2.17	0.58
1:B:296:LEU:O	1:B:298:PRO:HD3	2.03	0.57
1:A:3:LYS:HG3	1:A:29:HIS:CE1	2.39	0.57
1:B:291:ILE:HG21	1:B:296:LEU:HD21	1.85	0.57
1:D:23:ALA:O	1:D:27:LEU:HB2	2.04	0.57
1:B:120:ASP:O	1:B:124:MET:HG2	2.04	0.57
1:D:258:MET:HG3	1:D:269:ARG:HB3	1.86	0.57
1:B:138:LYS:O	1:B:142:ARG:HG3	2.04	0.56
1:C:170:GLN:NE2	1:C:183:LEU:H	2.03	0.56
1:A:269:ARG:O	1:A:270:CYS:SG	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HB2	1:A:139:ARG:HG3	1.87	0.56
1:D:13:THR:HG22	1:D:48:MET:SD	2.45	0.56
1:A:79:VAL:HG21	1:A:208:ILE:HG23	1.86	0.56
1:B:256:ALA:HA	1:B:259:LYS:HG2	1.87	0.56
1:C:250:SER:O	1:C:254:PHE:HB2	2.06	0.56
1:B:86:GLY:O	1:B:90:SER:HA	2.05	0.56
1:D:66:ASP:O	1:D:70:LEU:HB2	2.06	0.56
1:D:223:PRO:HD2	1:D:294:THR:HG21	1.88	0.55
1:C:159:MET:SD	1:C:164:PHE:CG	3.00	0.55
1:A:42:ASN:ND2	1:A:44:ASP:HB2	2.20	0.55
1:C:139:ARG:O	1:C:143:ARG:HG2	2.05	0.55
1:A:193:ILE:HD11	1:A:282:TYR:CD1	2.37	0.55
1:C:132:SER:HA	1:C:135:PHE:CD1	2.40	0.55
1:A:292:GLU:OE2	1:A:294:THR:HB	2.07	0.55
1:D:132:SER:O	1:D:136:ILE:HG13	2.06	0.55
1:C:34:LEU:HD21	1:C:62:ALA:HB3	1.89	0.55
1:A:96:GLN:O	1:A:100:VAL:HG23	2.06	0.54
1:B:39:VAL:HG13	1:B:41:SER:H	1.72	0.54
1:B:17:GLY:O	1:B:21:VAL:HG23	2.06	0.54
1:A:252:GLN:HG3	1:A:253:ASP:H	1.72	0.54
1:D:89:LEU:HB2	1:D:91:HIS:HB2	1.88	0.54
1:A:13:THR:HG21	1:A:45:LYS:HG2	1.90	0.54
1:A:42:ASN:HD22	1:A:45:LYS:H	1.55	0.54
1:A:79:VAL:HG13	1:A:111:ARG:HB3	1.90	0.54
1:B:159:MET:HB2	1:B:164:PHE:CD1	2.43	0.54
1:C:256:ALA:O	1:C:259:LYS:HB2	2.07	0.54
1:A:170:GLN:HE22	1:A:182:VAL:HG12	1.73	0.54
1:A:235:ILE:O	1:A:239:LEU:HD13	2.07	0.54
1:A:212:GLN:O	1:A:216:LYS:HD2	2.07	0.54
1:C:46:VAL:O	1:C:50:LEU:HG	2.08	0.53
1:D:189:ASN:HD22	1:D:230:LYS:NZ	2.06	0.53
1:A:32:TYR:CD2	1:A:60:ILE:HD11	2.40	0.53
1:B:259:LYS:HA	1:B:266:LYS:HE2	1.91	0.53
1:D:129:GLN:CD	1:D:129:GLN:H	2.11	0.53
1:B:254:PHE:HB3	1:B:273:TYR:OH	2.08	0.53
1:D:296:LEU:O	1:D:298:PRO:HD3	2.08	0.53
1:C:6:ARG:HG2	1:C:30:PRO:HB2	1.90	0.53
1:D:159:MET:HG3	1:D:281:LEU:HD21	1.91	0.52
1:C:43:ILE:CD1	1:C:43:ILE:H	2.22	0.52
1:C:15:TYR:HB3	1:C:163:TYR:OH	2.09	0.52
1:A:70:LEU:O	1:A:74:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:HD23	1:D:89:LEU:H	1.75	0.52
1:C:99:LEU:O	1:C:103:ILE:HG12	2.10	0.52
1:D:256:ALA:HA	1:D:259:LYS:HD2	1.91	0.52
1:D:248:TYR:O	1:D:250:SER:N	2.42	0.52
1:A:218:MET:CE	1:A:297:TYR:HE2	2.23	0.52
1:A:200:VAL:O	1:A:204:THR:HG23	2.10	0.52
1:B:242:GLN:HG2	1:B:244:LEU:HD12	1.91	0.52
1:C:120:ASP:HB3	1:C:123:ILE:HG12	1.93	0.52
1:A:193:ILE:CD1	1:A:221:ARG:HG2	2.40	0.51
1:D:20:ILE:HD12	1:D:204:THR:HG21	1.90	0.51
1:B:36:ARG:C	1:B:38:GLU:H	2.13	0.51
1:D:255:LEU:HG	1:D:273:TYR:CZ	2.46	0.51
1:A:240:SER:OG	1:A:242:GLN:HG2	2.09	0.51
1:A:211:PRO:O	1:A:214:LEU:HB2	2.10	0.51
1:A:205:ILE:HA	1:A:208:ILE:HD12	1.92	0.51
1:D:223:PRO:HG2	1:D:224:MET:SD	2.50	0.51
1:D:224:MET:N	1:D:224:MET:SD	2.84	0.51
1:D:219:TYR:HE2	1:D:290:ALA:HB1	1.76	0.51
1:A:259:LYS:HA	1:A:266:LYS:HD3	1.91	0.51
1:A:271:HIS:H	1:A:273:TYR:H	1.59	0.51
1:D:208:ILE:HG23	1:D:209:ASP:N	2.22	0.51
1:C:16:ILE:O	1:C:19:ARG:HB2	2.11	0.51
1:B:190:VAL:HG11	1:B:276:PHE:O	2.11	0.51
1:B:225:ASN:HD21	1:B:304:THR:HA	1.75	0.51
1:A:263:TYR:O	1:A:264:GLU:HB2	2.11	0.51
1:C:92:HIS:HA	1:C:95:GLU:HB2	1.93	0.51
1:D:208:ILE:CG2	1:D:209:ASP:H	2.22	0.51
1:C:128:LEU:H	1:C:274:GLN:NE2	2.07	0.50
1:B:261:LYS:HG3	1:B:269:ARG:HH12	1.76	0.50
1:B:211:PRO:O	1:B:214:LEU:HB3	2.11	0.50
1:D:156:SER:O	1:D:219:TYR:HA	2.11	0.50
1:A:237:GLU:HG2	1:A:242:GLN:O	2.11	0.50
1:B:47:GLN:O	1:B:51:TYR:HB2	2.11	0.50
1:C:84:LEU:HD12	1:C:96:GLN:HG2	1.93	0.50
1:D:219:TYR:CE2	1:D:290:ALA:HB1	2.47	0.50
1:D:100:VAL:HG12	1:D:112:PHE:HE2	1.77	0.50
1:B:159:MET:HG2	1:B:193:ILE:O	2.12	0.50
1:B:36:ARG:HD2	1:B:63:SER:HB2	1.94	0.50
1:C:133:ILE:HA	1:C:136:ILE:HG12	1.94	0.50
1:A:75:LYS:HD2	1:A:108:ASN:ND2	2.26	0.49
1:C:96:GLN:O	1:C:100:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TYR:N	1:C:163:TYR:CD1	2.80	0.49
1:B:262:SER:O	1:B:265:GLU:HB2	2.12	0.49
1:B:275:ILE:HG23	1:B:281:LEU:HD22	1.93	0.49
1:C:67:HIS:O	1:C:71:VAL:HG23	2.13	0.49
1:A:179:ARG:HG3	1:A:242:GLN:NE2	2.27	0.49
1:A:108:ASN:H	1:A:108:ASN:HD22	1.59	0.49
1:D:170:GLN:NE2	1:D:178:PRO:HG2	2.27	0.49
1:D:97:LEU:HB2	1:D:98:LYS:HE3	1.95	0.49
1:A:128:LEU:HB2	1:A:270:CYS:HB2	1.95	0.49
1:C:145:ILE:HA	1:C:150:ILE:HD12	1.95	0.49
1:D:189:ASN:HD22	1:D:230:LYS:HZ2	1.60	0.49
1:B:179:ARG:HG2	1:B:236:TRP:CH2	2.48	0.49
1:A:146:GLU:HG2	1:A:152:TYR:CZ	2.48	0.49
1:C:37:PRO:HB3	1:C:40:VAL:HG23	1.95	0.48
1:B:2:ASP:O	1:B:4:LYS:HG3	2.13	0.48
1:B:143:ARG:HD3	1:B:146:GLU:HG2	1.94	0.48
1:D:189:ASN:ND2	1:D:230:LYS:HZ2	2.11	0.48
1:D:214:LEU:O	1:D:216:LYS:HG3	2.13	0.48
1:A:35:PHE:HE2	1:A:59:LEU:HB3	1.77	0.48
1:D:74:LEU:HA	1:D:77:VAL:HG22	1.94	0.48
1:B:84:LEU:HG	1:B:92:HIS:HB3	1.95	0.48
1:A:218:MET:HE1	1:A:297:TYR:HE2	1.78	0.48
1:D:20:ILE:HG22	1:D:205:ILE:HD11	1.96	0.48
1:D:292:GLU:O	1:D:296:LEU:HB2	2.13	0.48
1:A:306:ASP:O	1:A:310:GLU:HB2	2.14	0.48
1:D:189:ASN:ND2	1:D:230:LYS:NZ	2.62	0.48
1:D:19:ARG:HG2	1:D:197:GLU:HB3	1.94	0.47
1:A:69:ARG:HG3	2:A:316:HOH:O	2.14	0.47
1:A:16:ILE:O	1:A:19:ARG:HB2	2.15	0.47
1:C:183:LEU:HD12	1:C:249:ILE:HB	1.96	0.47
1:B:271:HIS:O	1:B:275:ILE:HG13	2.15	0.47
1:D:194:TRP:HD1	1:D:225:ASN:O	1.96	0.47
1:C:17:GLY:O	1:C:21:VAL:HG23	2.14	0.47
1:D:184:ILE:HD11	1:D:246:LYS:HG3	1.96	0.47
1:C:273:TYR:HA	1:C:277:PHE:HD1	1.80	0.47
1:A:42:ASN:ND2	1:A:45:LYS:H	2.12	0.47
1:A:253:ASP:O	1:A:257:ASP:HB3	2.15	0.47
1:A:285:GLU:HA	2:A:325:HOH:O	2.15	0.47
1:C:292:GLU:OE1	1:C:294:THR:HB	2.14	0.47
1:A:42:ASN:HD21	1:A:44:ASP:HB2	1.79	0.47
1:A:71:VAL:HG13	1:A:106:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HD13	1:C:221:ARG:HG2	1.96	0.46
1:D:97:LEU:HA	1:D:100:VAL:HG22	1.97	0.46
1:D:213:THR:HG23	1:D:291:ILE:HD11	1.95	0.46
1:A:132:SER:O	1:A:136:ILE:HG12	2.15	0.46
1:B:139:ARG:HA	1:B:142:ARG:HB2	1.97	0.46
1:D:222:PRO:HB2	1:D:302:TYR:CE2	2.51	0.46
1:B:230:LYS:O	1:B:234:GLN:HG3	2.15	0.46
1:D:265:GLU:O	1:D:269:ARG:HD2	2.16	0.46
1:A:301:LYS:HE2	1:A:301:LYS:N	2.27	0.46
1:B:9:ILE:HD13	1:B:21:VAL:HG22	1.97	0.46
1:D:307:SER:O	1:D:310:GLU:HB3	2.15	0.46
1:B:217:THR:O	1:B:291:ILE:HD12	2.16	0.46
1:B:42:ASN:OD1	1:B:44:ASP:HB2	2.16	0.46
1:B:141:VAL:O	1:B:145:ILE:HG23	2.16	0.46
1:D:68:GLN:NE2	1:D:69:ARG:HG2	2.30	0.46
1:C:185:TYR:HD1	1:C:229:GLN:HE22	1.64	0.46
1:D:255:LEU:O	1:D:259:LYS:HG3	2.16	0.46
1:B:193:ILE:HG21	1:B:221:ARG:HA	1.98	0.46
1:B:100:VAL:HG21	1:B:145:ILE:HG22	1.97	0.46
1:A:229:GLN:O	1:A:233:ILE:HG13	2.16	0.46
1:D:201:GLY:O	1:D:205:ILE:HG12	2.17	0.45
1:B:263:TYR:O	1:B:267:ILE:HG13	2.15	0.45
1:D:235:ILE:HG23	1:D:306:ASP:HB3	1.98	0.45
1:A:128:LEU:HD11	1:A:278:ARG:NH2	2.31	0.45
1:A:88:VAL:HB	2:A:319:HOH:O	2.15	0.45
1:D:96:GLN:O	1:D:100:VAL:HG13	2.17	0.45
1:C:169:ALA:HB3	1:C:229:GLN:NE2	2.32	0.45
1:D:203:TYR:CE2	1:D:300:VAL:HG11	2.52	0.45
1:D:100:VAL:HG12	1:D:112:PHE:CE2	2.51	0.45
1:A:260:ASP:HB3	1:A:261:LYS:NZ	2.31	0.45
1:A:7:VAL:HG21	1:A:24:SER:OG	2.17	0.45
1:D:224:MET:SD	1:D:302:TYR:OH	2.68	0.45
1:C:212:GLN:O	1:C:216:LYS:HD2	2.17	0.45
1:C:225:ASN:HD21	1:C:305:MET:N	2.14	0.45
1:D:159:MET:O	1:D:195:VAL:HG12	2.17	0.45
1:A:202:THR:O	1:A:206:LYS:HG3	2.17	0.45
1:D:196:ASP:HB3	1:D:199:ASP:OD1	2.16	0.45
1:C:222:PRO:HG2	1:C:225:ASN:HB2	1.99	0.45
1:C:134:THR:O	1:C:138:LYS:HG3	2.17	0.45
1:C:237:GLU:HG3	1:C:238:ARG:H	1.81	0.45
1:B:93:ILE:HG22	1:B:94:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:HG3	1:C:106:ALA:HB1	1.98	0.44
1:A:120:ASP:HA	1:A:121:PRO:HD2	1.83	0.44
1:D:219:TYR:HE2	1:D:290:ALA:CB	2.30	0.44
1:A:305:MET:O	1:A:309:LEU:HB2	2.17	0.44
1:C:252:GLN:C	1:C:254:PHE:H	2.20	0.44
1:D:217:THR:O	1:D:290:ALA:HA	2.17	0.44
1:B:48:MET:O	1:B:51:TYR:HB3	2.16	0.44
1:B:202:THR:HG22	1:B:202:THR:O	2.18	0.44
1:D:203:TYR:CE2	1:D:300:VAL:HG21	2.52	0.44
1:B:27:LEU:HD11	1:B:202:THR:HG23	1.98	0.44
1:C:44:ASP:O	1:C:48:MET:HB2	2.18	0.44
1:D:237:GLU:HG2	1:D:244:LEU:CD2	2.48	0.44
1:A:210:ASP:HA	1:A:211:PRO:HD2	1.89	0.44
1:C:236:TRP:HD1	1:C:244:LEU:HD11	1.82	0.44
1:A:224:MET:HB2	1:A:302:TYR:HE2	1.82	0.44
1:C:165:ALA:O	1:C:168:LEU:HD23	2.18	0.44
1:D:237:GLU:CG	1:D:244:LEU:HD23	2.48	0.44
1:C:113:LEU:HB3	1:C:153:THR:O	2.18	0.43
1:A:309:LEU:C	1:A:311:ARG:H	2.21	0.43
1:C:177:PRO:HD3	1:C:312:TYR:CD2	2.53	0.43
1:C:308:TYR:O	1:C:311:ARG:HB2	2.18	0.43
1:D:215:ASN:N	1:D:215:ASN:ND2	2.65	0.43
1:B:275:ILE:CG2	1:B:281:LEU:HD22	2.49	0.43
1:B:145:ILE:HD13	1:B:145:ILE:HG21	1.82	0.43
1:C:163:TYR:HA	1:C:175:MET:HE1	2.00	0.43
1:D:300:VAL:HG23	1:D:300:VAL:O	2.18	0.43
1:D:255:LEU:O	1:D:258:MET:HB3	2.19	0.43
1:A:29:HIS:ND1	1:A:29:HIS:N	2.66	0.43
1:B:100:VAL:HG13	1:B:150:ILE:HD12	2.01	0.43
1:A:17:GLY:O	1:A:21:VAL:HG23	2.19	0.43
1:D:84:LEU:HG	1:D:92:HIS:HB3	1.99	0.43
1:C:42:ASN:O	1:C:46:VAL:HG23	2.18	0.43
1:D:154:TYR:HB2	1:D:217:THR:HA	2.01	0.43
1:C:237:GLU:O	1:C:239:LEU:N	2.47	0.43
1:B:31:THR:O	1:B:58:LYS:HE3	2.18	0.43
1:C:111:ARG:HD2	1:C:152:TYR:O	2.18	0.43
1:C:292:GLU:O	1:C:296:LEU:HB2	2.19	0.43
1:D:230:LYS:O	1:D:234:GLN:HG3	2.19	0.43
1:C:111:ARG:NH2	1:C:210:ASP:O	2.52	0.43
1:A:273:TYR:O	1:A:277:PHE:HB2	2.19	0.42
1:C:143:ARG:HH11	1:C:143:ARG:HD2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:GLN:OE1	1:D:273:TYR:HB3	2.18	0.42
1:D:79:VAL:HG21	1:D:208:ILE:HG12	2.00	0.42
1:A:170:GLN:HE21	1:A:178:PRO:HG3	1.84	0.42
1:B:210:ASP:HA	1:B:211:PRO:HD2	1.88	0.42
1:D:74:LEU:HD13	1:D:103:ILE:HG12	2.02	0.42
1:A:14:GLY:O	1:A:18:LYS:HG3	2.19	0.42
1:D:113:LEU:CD2	1:D:153:THR:HB	2.37	0.42
1:D:253:ASP:O	1:D:256:ALA:N	2.52	0.42
1:C:186:GLY:O	1:C:248:TYR:HB3	2.18	0.42
1:C:285:GLU:H	1:C:285:GLU:CD	2.22	0.42
1:A:236:TRP:HE1	1:A:313:VAL:CG1	2.33	0.42
1:D:123:ILE:O	1:D:125:GLU:N	2.52	0.42
1:A:71:VAL:HA	1:A:74:LEU:HD12	2.02	0.42
1:C:225:ASN:HD21	1:C:305:MET:H	1.67	0.42
1:C:222:PRO:HA	1:C:223:PRO:HD3	1.82	0.42
1:A:308:TYR:O	1:A:311:ARG:HG2	2.20	0.42
1:A:186:GLY:N	1:A:249:ILE:O	2.52	0.42
1:D:141:VAL:O	1:D:145:ILE:HG13	2.19	0.42
1:B:16:ILE:HG22	2:B:333:HOH:O	2.20	0.42
1:B:174:HIS:HB3	1:B:175:MET:SD	2.60	0.42
1:A:80:VAL:HG12	1:A:109:ILE:HG12	2.01	0.42
1:D:92:HIS:HA	1:D:95:GLU:HB3	2.03	0.41
1:C:201:GLY:O	1:C:205:ILE:HG12	2.21	0.41
1:C:225:ASN:HD21	1:C:304:THR:HA	1.86	0.41
1:C:138:LYS:O	1:C:142:ARG:HG3	2.21	0.41
1:A:123:ILE:O	1:A:125:GLU:HG2	2.21	0.41
1:A:263:TYR:C	1:A:265:GLU:H	2.24	0.41
1:B:42:ASN:HB3	1:B:45:LYS:HB2	2.02	0.41
1:C:111:ARG:NH2	1:C:210:ASP:H	2.19	0.41
1:B:43:ILE:H	1:B:43:ILE:HD12	1.85	0.41
1:C:121:PRO:HD2	1:C:142:ARG:NH1	2.35	0.41
1:C:133:ILE:HG22	1:C:133:ILE:O	2.21	0.41
1:B:53:LYS:HD3	1:B:59:LEU:HD22	2.02	0.41
1:C:170:GLN:HE22	1:C:183:LEU:H	1.68	0.41
1:A:111:ARG:HD3	1:A:151:PRO:O	2.20	0.41
1:D:82:SER:OG	1:D:96:GLN:NE2	2.54	0.41
1:B:64:LEU:HD11	1:B:99:LEU:HB2	2.02	0.41
1:C:167:SER:O	1:C:170:GLN:HB2	2.21	0.41
1:C:274:GLN:HG3	1:C:280:ASP:OD2	2.21	0.41
1:B:111:ARG:NH2	1:B:210:ASP:O	2.53	0.41
1:B:179:ARG:HG2	1:B:236:TRP:HH2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:HG23	1:C:244:LEU:HD12	2.03	0.41
1:B:167:SER:HB3	1:B:175:MET:HA	2.03	0.41
1:D:15:TYR:CD1	1:D:16:ILE:HG22	2.56	0.41
1:B:6:ARG:HB3	1:B:77:VAL:HG12	2.03	0.41
1:B:283:ASN:N	1:B:283:ASN:OD1	2.54	0.41
1:A:258:MET:HG3	1:A:269:ARG:CB	2.51	0.41
1:D:177:PRO:HA	1:D:178:PRO:HD3	1.97	0.41
1:B:177:PRO:HB2	1:B:236:TRP:CH2	2.56	0.41
1:D:168:LEU:CD2	1:D:232:VAL:HG12	2.51	0.41
1:A:112:PHE:CE2	1:A:145:ILE:HD11	2.56	0.40
1:C:197:GLU:HA	1:C:200:VAL:HG23	2.02	0.40
1:A:130:PRO:C	1:A:132:SER:H	2.24	0.40
1:A:222:PRO:HA	1:A:223:PRO:HD3	1.85	0.40
1:B:133:ILE:HG22	1:B:134:THR:N	2.36	0.40
1:C:109:ILE:HG22	1:C:111:ARG:H	1.85	0.40
1:B:212:GLN:O	1:B:216:LYS:HD2	2.21	0.40
1:D:8:LEU:HB2	1:D:77:VAL:HG21	2.03	0.40
1:D:203:TYR:HE2	1:D:300:VAL:HG21	1.86	0.40
1:A:9:ILE:HD13	1:A:21:VAL:HG22	2.03	0.40
1:A:275:ILE:HG12	1:A:281:LEU:HD11	2.02	0.40
1:B:207:SER:HA	1:B:297:TYR:OH	2.21	0.40
1:A:299:GLU:HG3	1:A:299:GLU:H	1.63	0.40
1:D:218:MET:SD	1:D:293:ALA:HB2	2.62	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	310/313 (99%)	258 (83%)	29 (9%)	23 (7%)	<a href="#">1</a> <a href="#">1</a>
1	B	310/313 (99%)	252 (81%)	41 (13%)	17 (6%)	<a href="#">2</a> <a href="#">2</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	310/313 (99%)	258 (83%)	38 (12%)	14 (4%)	3	3
1	D	310/313 (99%)	247 (80%)	40 (13%)	23 (7%)	1	1
All	All	1240/1252 (99%)	1015 (82%)	148 (12%)	77 (6%)	2	1

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	262	SER
1	A	263	TYR
1	B	37	PRO
1	B	39	VAL
1	B	133	ILE
1	B	175	MET
1	B	180	ASP
1	B	251	SER
1	C	4	LYS
1	C	37	PRO
1	C	124	MET
1	C	175	MET
1	C	238	ARG
1	C	252	GLN
1	C	274	GLN
1	D	34	LEU
1	D	35	PHE
1	D	108	ASN
1	D	124	MET
1	D	208	ILE
1	D	249	ILE
1	D	280	ASP
1	D	312	TYR
1	A	62	ALA
1	A	87	GLY
1	A	124	MET
1	A	131	GLY
1	A	171	LEU
1	A	208	ILE
1	A	271	HIS
1	A	280	ASP
1	B	117	PHE
1	B	168	LEU

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Mol	Chain	Res	Type
1	B	241	GLU
1	B	244	LEU
1	C	108	ASN
1	D	40	VAL
1	D	41	SER
1	D	87	GLY
1	D	131	GLY
1	D	180	ASP
1	A	277	PHE
1	A	310	GLU
1	B	245	ASP
1	B	280	ASP
1	C	280	ASP
1	D	4	LYS
1	D	15	TYR
1	D	37	PRO
1	D	125	GLU
1	D	169	ALA
1	D	239	LEU
1	A	38	GLU
1	A	125	GLU
1	A	158	ASN
1	A	169	ALA
1	B	66	ASP
1	B	263	TYR
1	C	242	GLN
1	C	273	TYR
1	D	118	GLY
1	D	119	MET
1	D	214	LEU
1	A	12	GLY
1	A	36	ARG
1	A	120	ASP
1	A	248	TYR
1	A	251	SER
1	B	88	VAL
1	B	274	GLN
1	B	259	LYS
1	C	3	LYS
1	C	40	VAL
1	A	88	VAL
1	D	36	ARG

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Mol	Chain	Res	Type
1	C	30	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	274/275 (100%)	233 (85%)	41 (15%)	3	6
1	B	274/275 (100%)	237 (86%)	37 (14%)	5	9
1	C	274/275 (100%)	240 (88%)	34 (12%)	6	11
1	D	274/275 (100%)	235 (86%)	39 (14%)	4	7
All	All	1096/1100 (100%)	945 (86%)	151 (14%)	4	8

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	15	TYR
1	A	36	ARG
1	A	40	VAL
1	A	42	ASN
1	A	43	ILE
1	A	50	LEU
1	A	80	VAL
1	A	90	SER
1	A	92	HIS
1	A	94	LEU
1	A	101	GLU
1	A	108	ASN
1	A	109	ILE
1	A	133	ILE
1	A	143	ARG
1	A	155	VAL
1	A	163	TYR
1	A	168	LEU
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	174	HIS
1	A	175	MET
1	A	180	ASP
1	A	182	VAL
1	A	183	LEU
1	A	208	ILE
1	A	210	ASP
1	A	214	LEU
1	A	243	ASN
1	A	244	LEU
1	A	253	ASP
1	A	257	ASP
1	A	260	ASP
1	A	261	LYS
1	A	263	TYR
1	A	271	HIS
1	A	278	ARG
1	A	285	GLU
1	A	291	ILE
1	A	301	LYS
1	A	312	TYR
1	B	2	ASP
1	B	37	PRO
1	B	43	ILE
1	B	47	GLN
1	B	51	TYR
1	B	55	LEU
1	B	61	GLU
1	B	63	SER
1	B	64	LEU
1	B	68	GLN
1	B	70	LEU
1	B	79	VAL
1	B	91	HIS
1	B	93	ILE
1	B	94	LEU
1	B	95	GLU
1	B	99	LEU
1	B	105	GLU
1	B	113	LEU
1	B	128	LEU
1	B	129	GLN

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Mol	Chain	Res	Type
1	B	134	THR
1	B	143	ARG
1	B	146	GLU
1	B	163	TYR
1	B	172	ASP
1	B	175	MET
1	B	179	ARG
1	B	180	ASP
1	B	191	LYS
1	B	197	GLU
1	B	217	THR
1	B	225	ASN
1	B	242	GLN
1	B	278	ARG
1	B	291	ILE
1	B	295	LYS
1	C	27	LEU
1	C	43	ILE
1	C	53	LYS
1	C	58	LYS
1	C	63	SER
1	C	69	ARG
1	C	70	LEU
1	C	91	HIS
1	C	95	GLU
1	C	103	ILE
1	C	105	GLU
1	C	110	LYS
1	C	111	ARG
1	C	113	LEU
1	C	124	MET
1	C	134	THR
1	C	163	TYR
1	C	170	GLN
1	C	174	HIS
1	C	179	ARG
1	C	209	ASP
1	C	237	GLU
1	C	238	ARG
1	C	239	LEU
1	C	253	ASP
1	C	257	ASP

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Mol	Chain	Res	Type
1	C	260	ASP
1	C	263	TYR
1	C	274	GLN
1	C	283	ASN
1	C	285	GLU
1	C	286	ILE
1	C	291	ILE
1	C	292	GLU
1	D	9	ILE
1	D	16	ILE
1	D	19	ARG
1	D	27	LEU
1	D	32	TYR
1	D	37	PRO
1	D	48	MET
1	D	66	ASP
1	D	68	GLN
1	D	70	LEU
1	D	124	MET
1	D	125	GLU
1	D	129	GLN
1	D	143	ARG
1	D	170	GLN
1	D	171	LEU
1	D	176	MET
1	D	181	LYS
1	D	190	VAL
1	D	198	ASP
1	D	209	ASP
1	D	213	THR
1	D	214	LEU
1	D	215	ASN
1	D	230	LYS
1	D	242	GLN
1	D	255	LEU
1	D	258	MET
1	D	263	TYR
1	D	268	VAL
1	D	269	ARG
1	D	282	TYR
1	D	283	ASN
1	D	291	ILE

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Mol	Chain	Res	Type
1	D	295	LYS
1	D	296	LEU
1	D	299	GLU
1	D	301	LYS
1	D	312	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	42	ASN
1	A	47	GLN
1	A	96	GLN
1	A	108	ASN
1	A	170	GLN
1	A	242	GLN
1	A	274	GLN
1	B	47	GLN
1	B	158	ASN
1	B	215	ASN
1	B	225	ASN
1	B	229	GLN
1	B	234	GLN
1	B	289	ASN
1	C	22	ASN
1	C	96	GLN
1	C	126	HIS
1	C	158	ASN
1	C	170	GLN
1	C	189	ASN
1	C	225	ASN
1	C	274	GLN
1	C	283	ASN
1	D	68	GLN
1	D	96	GLN
1	D	108	ASN
1	D	158	ASN
1	D	170	GLN
1	D	189	ASN
1	D	215	ASN
1	D	271	HIS
1	D	283	ASN

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Mol	Chain	Res	Type
1	D	289	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.