



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:24 PM UTC

PDB ID : 1QYD / pdb_00001qyd
Title : Crystal structures of pinoresinol-lariciresinol and phenylcoumaran benzylic ether reductases, and their relationship to isoflavone reductases
Authors : Min, T.; Kasahara, H.; Bedgar, D.L.; Youn, B.; Lawrence, P.K.; Gang, D.R.; Halls, S.C.; Park, H.; Hilsenbeck, J.L.; Davin, L.B.; Kang, C.
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

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

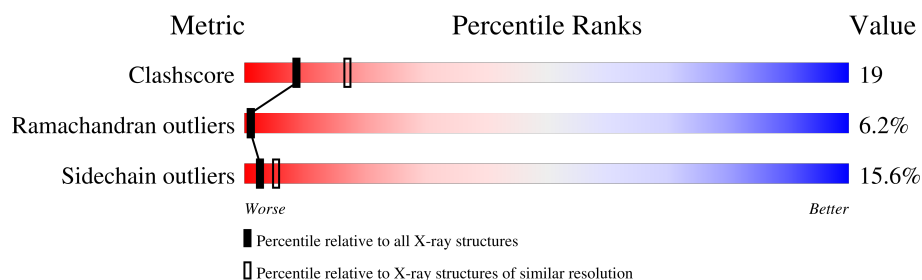
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	313	35% 45% 14% 5%
1	B	313	42% 41% 14% .
1	C	313	43% 39% 13% .
1	D	313	39% 39% 18% .

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.

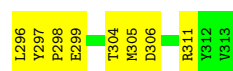
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called pinorexinol-lariciresinol reductase.

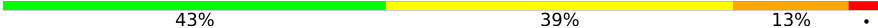
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	B	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	C	312	Total	C	N	O	S	0	0	0
			2497	1605	416	465	11			
1	D	312	Total	C	N	O	S	0	0	0
			2496	1605	416	464	11			

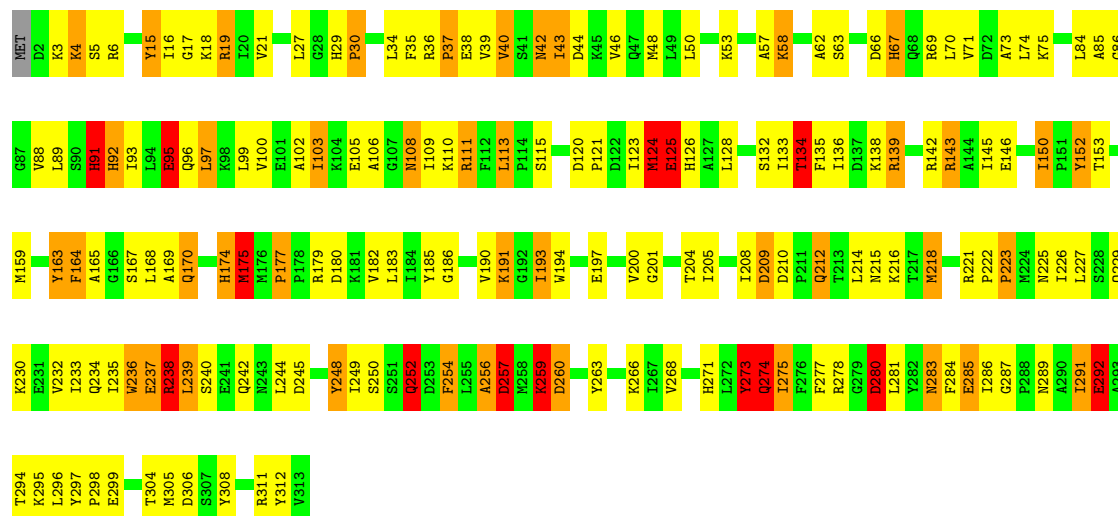
- Molecule 2 is water.

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		

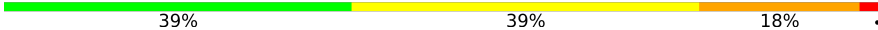


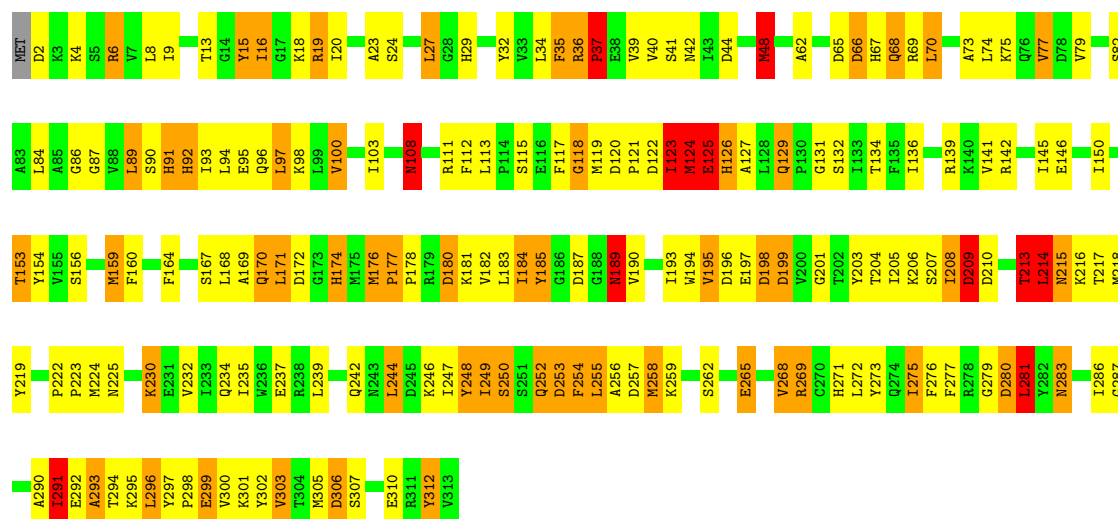
• Molecule 1: pinoresinol-lariciresinol reductase

Chain C:  43% 39% 13% .



• Molecule 1: pinoresinol-lariciresinol reductase

Chain D:  39% 39% 18% .



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 21	Depositor
Cell constants a, b, c, α , β , γ	82.57Å 125.96Å 128.58Å 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 ²)	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	1.08	11/2548 (0.4%)	2.08	91/3442 (2.6%)
1	B	1.08	11/2548 (0.4%)	2.12	108/3442 (3.1%)
1	C	1.09	13/2548 (0.5%)	2.16	108/3442 (3.1%)
1	D	1.11	13/2547 (0.5%)	2.13	114/3442 (3.3%)
All	All	1.09	48/10191 (0.5%)	2.13	421/13768 (3.1%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	VAL	CA-CB	7.75	1.61	1.53
1	D	303	VAL	CA-CB	7.70	1.64	1.54
1	C	126	HIS	CD2-NE2	-7.47	1.29	1.37
1	D	92	HIS	CD2-NE2	-7.35	1.29	1.37
1	C	29	HIS	CD2-NE2	-7.30	1.29	1.37
1	B	29	HIS	CD2-NE2	-7.14	1.29	1.37
1	C	271	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	67	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	271	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	92	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	109	ILE	CA-CB	6.72	1.61	1.54
1	C	67	HIS	CD2-NE2	-6.71	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	291	ILE	CA-CB	6.60	1.63	1.54
1	A	92	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	29	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	29	HIS	CG-ND1	-6.41	1.31	1.38
1	D	67	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	67	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	271	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	29	HIS	CG-ND1	-6.33	1.31	1.38
1	D	91	HIS	CD2-NE2	-6.33	1.30	1.37
1	C	92	HIS	CD2-NE2	-6.26	1.30	1.37
1	D	174	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	126	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	174	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	271	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	91	HIS	CD2-NE2	-6.14	1.31	1.37
1	B	177	PRO	CA-C	6.09	1.55	1.51
1	D	286	ILE	CA-CB	6.08	1.61	1.54
1	B	91	HIS	CD2-NE2	-5.97	1.31	1.37
1	D	126	HIS	CD2-NE2	-5.94	1.31	1.37
1	C	268	VAL	CA-CB	5.85	1.61	1.54
1	D	100	VAL	CA-CB	5.79	1.62	1.54
1	A	126	HIS	CD2-NE2	-5.77	1.31	1.37
1	C	174	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	91	HIS	CD2-NE2	-5.72	1.31	1.37
1	D	29	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	92	HIS	CG-ND1	-5.57	1.32	1.38
1	D	92	HIS	CG-ND1	-5.37	1.32	1.38
1	D	159	MET	CA-CB	-5.31	1.45	1.53
1	C	174	HIS	CG-ND1	-5.29	1.32	1.38
1	C	92	HIS	CG-ND1	-5.23	1.32	1.38
1	A	174	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	60	ILE	CA-CB	5.09	1.59	1.53
1	C	125	GLU	CA-CB	5.09	1.59	1.53
1	C	126	HIS	CG-ND1	-5.05	1.32	1.38
1	C	271	HIS	CG-ND1	-5.02	1.32	1.38
1	A	222	PRO	CA-CB	-5.01	1.47	1.54

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ASP	CA-CB-CG	14.08	126.68	112.60
1	A	119	MET	N-CA-C	11.92	125.42	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	HIS	CA-CB-CG	11.73	125.53	113.80
1	D	262	SER	N-CA-C	11.68	126.31	110.55
1	A	257	ASP	CA-CB-CG	11.24	123.84	112.60
1	C	42	ASN	N-CA-C	11.01	127.74	109.46
1	C	254	PHE	N-CA-C	-10.52	100.17	113.43
1	C	39	VAL	N-CA-C	-10.43	100.18	110.30
1	C	164	PHE	CA-CB-CG	-10.43	103.37	113.80
1	B	196	ASP	CA-CB-CG	10.37	122.97	112.60
1	C	209	ASP	CA-CB-CG	9.97	122.57	112.60
1	B	159	MET	CA-CB-CG	9.88	133.87	114.10
1	D	125	GLU	CA-C-O	9.80	134.53	120.51
1	C	284	PHE	CA-C-O	9.70	131.85	120.99
1	B	38	GLU	CA-C-N	9.55	139.16	121.97
1	B	38	GLU	C-N-CA	9.55	139.16	121.97
1	D	89	LEU	N-CA-C	9.53	124.59	110.30
1	B	171	LEU	N-CA-C	9.45	121.18	111.07
1	A	3	LYS	N-CA-C	9.36	124.65	110.14
1	B	126	HIS	CA-CB-CG	9.31	123.11	113.80
1	B	38	GLU	N-CA-C	-9.14	102.14	113.20
1	A	252	GLN	N-CA-C	9.08	130.13	110.80
1	D	111	ARG	N-CA-C	8.95	123.06	107.49
1	B	293	ALA	N-CA-C	8.90	122.10	111.33
1	B	152	TYR	N-CA-C	8.88	122.91	109.41
1	A	288	PRO	N-CA-C	8.87	125.86	113.53
1	C	38	GLU	CA-C-N	8.84	131.75	120.70
1	C	38	GLU	C-N-CA	8.84	131.75	120.70
1	C	57	ALA	N-CA-C	8.83	122.19	110.53
1	B	39	VAL	N-CA-C	8.75	127.53	109.34
1	D	199	ASP	CA-CB-CG	8.73	121.33	112.60
1	B	35	PHE	N-CA-C	8.60	121.59	108.52
1	A	267	ILE	N-CA-C	-8.54	103.51	111.45
1	B	36	ARG	CA-C-N	8.54	130.51	119.84
1	B	36	ARG	C-N-CA	8.54	130.51	119.84
1	C	4	LYS	N-CA-C	8.46	128.81	110.80
1	C	35	PHE	CA-CB-CG	8.31	122.11	113.80
1	D	303	VAL	CA-C-O	8.28	130.16	120.72
1	D	6	ARG	CA-CB-CG	8.27	130.65	114.10
1	C	240	SER	N-CA-C	8.23	121.81	111.69
1	A	39	VAL	N-CA-C	-8.21	101.82	113.07
1	C	260	ASP	N-CA-C	8.22	123.14	113.20
1	C	245	ASP	CA-CB-CG	8.20	120.80	112.60
1	D	206	LYS	CA-CB-CG	-8.16	97.78	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASP	CA-CB-CG	8.14	120.74	112.60
1	C	125	GLU	CA-C-N	8.06	138.07	121.94
1	C	125	GLU	C-N-CA	8.06	138.07	121.94
1	D	198	ASP	CA-CB-CG	7.98	120.58	112.60
1	D	252	GLN	OE1-CD-NE2	-7.89	114.70	122.60
1	C	252	GLN	N-CA-C	7.87	127.57	110.80
1	D	247	ILE	N-CA-C	-7.87	97.09	108.11
1	C	67	HIS	CA-CB-CG	-7.84	105.96	113.80
1	D	172	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	39	VAL	CA-C-O	7.77	130.50	120.78
1	A	289	ASN	CA-CB-CG	7.76	120.36	112.60
1	B	174	HIS	N-CA-C	7.75	120.51	108.96
1	A	125	GLU	CA-C-N	7.74	137.43	121.94
1	A	125	GLU	C-N-CA	7.74	137.43	121.94
1	B	40	VAL	N-CA-CB	-7.73	102.31	112.36
1	B	125	GLU	CA-C-N	7.73	136.30	121.54
1	B	125	GLU	C-N-CA	7.73	136.30	121.54
1	C	42	ASN	CA-C-N	7.72	130.29	120.56
1	C	42	ASN	C-N-CA	7.72	130.29	120.56
1	C	146	GLU	N-CA-C	7.71	119.68	111.28
1	A	271	HIS	N-CA-C	-7.71	94.38	110.80
1	B	177	PRO	O-C-N	-7.68	117.78	121.31
1	C	91	HIS	CA-CB-CG	7.68	121.48	113.80
1	A	172	ASP	CA-CB-CG	7.65	120.25	112.60
1	B	231	GLU	O-C-N	7.60	131.11	122.22
1	A	29	HIS	CA-CB-CG	-7.58	106.22	113.80
1	C	125	GLU	CA-C-O	7.58	129.64	120.62
1	C	66	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	39	VAL	CA-C-N	7.57	133.24	122.72
1	B	39	VAL	C-N-CA	7.57	133.24	122.72
1	D	126	HIS	N-CA-C	-7.46	104.17	113.20
1	D	164	PHE	CA-CB-CG	-7.42	106.38	113.80
1	D	90	SER	N-CA-C	-7.42	104.62	112.93
1	C	190	VAL	CA-C-N	7.39	131.36	120.87
1	C	190	VAL	C-N-CA	7.39	131.36	120.87
1	B	39	VAL	O-C-N	7.38	131.79	122.57
1	D	125	GLU	CB-CG-CD	7.32	125.04	112.60
1	B	51	TYR	CA-CB-CG	7.29	127.03	113.90
1	C	284	PHE	O-C-N	7.27	131.54	123.33
1	D	160	PHE	CA-C-O	7.27	128.98	120.69
1	B	175	MET	N-CA-C	7.26	126.26	110.80
1	A	126	HIS	CA-C-N	7.23	131.45	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	HIS	C-N-CA	7.23	131.45	120.82
1	A	127	ALA	N-CA-C	7.22	119.63	110.24
1	D	115	SER	O-C-N	7.22	131.75	122.87
1	B	255	LEU	N-CA-C	-7.20	104.30	113.23
1	B	160	PHE	CA-CB-CG	7.18	120.98	113.80
1	B	206	LYS	CA-CB-CG	-7.17	99.76	114.10
1	C	259	LYS	CB-CA-C	-7.15	99.37	110.81
1	A	91	HIS	CB-CG-CD2	-7.14	121.91	131.20
1	D	35	PHE	CA-CB-CG	7.12	120.92	113.80
1	B	62	ALA	N-CA-C	7.09	120.95	110.46
1	C	191	LYS	N-CA-C	7.09	120.78	110.28
1	C	152	TYR	N-CA-C	7.08	117.59	108.24
1	A	125	GLU	CB-CG-CD	7.08	124.63	112.60
1	C	259	LYS	CA-C-N	-7.03	107.88	121.94
1	C	259	LYS	C-N-CA	-7.03	107.88	121.94
1	A	152	TYR	N-CA-C	6.99	120.97	110.14
1	B	169	ALA	N-CA-C	6.99	121.31	111.52
1	A	198	ASP	CA-CB-CG	6.99	119.58	112.60
1	B	284	PHE	N-CA-C	6.97	120.00	109.41
1	C	257	ASP	N-CA-C	-6.94	103.65	111.07
1	A	132	SER	CA-C-N	6.93	129.96	120.46
1	A	132	SER	C-N-CA	6.93	129.96	120.46
1	B	176	MET	O-C-N	-6.93	115.84	121.80
1	D	123	ILE	N-CA-C	-6.92	95.18	106.32
1	C	245	ASP	N-CA-C	-6.88	99.48	109.59
1	D	174	HIS	CB-CG-CD2	-6.85	122.29	131.20
1	D	77	VAL	N-CA-C	6.82	118.65	108.96
1	A	283	ASN	CA-CB-CG	6.77	119.37	112.60
1	B	194	TRP	CG-CD2-CE3	6.76	140.66	133.90
1	C	108	ASN	CA-CB-CG	6.73	119.33	112.60
1	C	95	GLU	N-CA-C	-6.69	104.75	113.12
1	C	259	LYS	CA-CB-CG	6.69	127.47	114.10
1	D	65	ASP	CA-CB-CG	-6.68	105.92	112.60
1	D	185	TYR	O-C-N	6.68	130.95	122.93
1	A	287	GLY	CA-C-N	6.67	126.46	119.05
1	A	287	GLY	C-N-CA	6.67	126.46	119.05
1	B	253	ASP	CA-C-O	-6.67	114.00	121.00
1	A	250	SER	N-CA-C	6.65	118.62	109.18
1	D	122	ASP	CA-CB-CG	-6.65	105.95	112.60
1	B	37	PRO	N-CA-C	6.64	126.14	112.47
1	B	132	SER	N-CA-C	-6.64	104.05	111.28
1	A	72	ASP	O-C-N	6.63	128.90	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	VAL	N-CA-C	6.62	118.02	108.48
1	B	33	VAL	N-CA-C	6.59	117.38	107.75
1	D	253	ASP	CA-CB-CG	6.56	119.16	112.60
1	D	150	ILE	N-CA-C	6.55	114.26	108.63
1	B	90	SER	CA-C-N	6.55	129.29	120.65
1	B	90	SER	C-N-CA	6.55	129.29	120.65
1	C	259	LYS	N-CA-CB	6.55	119.69	109.94
1	D	275	ILE	N-CA-C	-6.52	105.39	111.45
1	B	262	SER	N-CA-C	6.51	124.67	110.80
1	D	48	MET	CB-CG-SD	-6.49	93.23	112.70
1	A	187	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	15	TYR	CA-C-O	-6.47	114.24	120.90
1	C	19	ARG	CG-CD-NE	-6.45	97.80	112.00
1	A	2	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	61	GLU	N-CA-C	6.43	120.70	112.34
1	A	220	ILE	N-CA-C	-6.42	98.48	107.80
1	B	233	ILE	N-CA-C	-6.42	104.25	110.42
1	C	191	LYS	CA-C-O	6.42	128.35	121.16
1	D	44	ASP	N-CA-C	6.41	118.81	111.11
1	A	18	LYS	CA-CB-CG	6.38	126.87	114.10
1	C	218	MET	CG-SD-CE	-6.38	86.87	100.90
1	C	18	LYS	CA-C-N	6.37	129.46	120.28
1	C	18	LYS	C-N-CA	6.37	129.46	120.28
1	C	271	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	291	ILE	N-CA-C	6.36	117.88	108.65
1	C	74	LEU	N-CA-CB	-6.35	100.81	110.33
1	C	215	ASN	N-CA-C	6.32	120.33	112.24
1	A	230	LYS	CA-CB-CG	6.30	126.70	114.10
1	B	146	GLU	CB-CG-CD	6.30	123.31	112.60
1	D	210	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	281	LEU	N-CA-C	-6.29	105.92	113.97
1	B	91	HIS	CB-CG-CD2	-6.27	123.04	131.20
1	A	271	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	300	VAL	CA-C-N	6.25	131.60	122.41
1	A	300	VAL	C-N-CA	6.25	131.60	122.41
1	D	167	SER	CA-C-N	6.25	131.03	122.34
1	D	167	SER	C-N-CA	6.25	131.03	122.34
1	D	174	HIS	CA-CB-CG	6.24	120.04	113.80
1	C	284	PHE	N-CA-C	6.24	118.78	108.99
1	D	265	GLU	N-CA-C	-6.23	104.38	112.23
1	C	88	VAL	N-CA-C	-6.22	103.31	111.09
1	C	93	ILE	N-CA-C	-6.22	104.98	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	LEU	CA-C-O	6.22	127.52	120.80
1	C	67	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	150	ILE	N-CA-C	-6.21	103.29	108.63
1	A	48	MET	N-CA-C	-6.20	103.84	111.40
1	C	194	TRP	CG-CD2-CE3	6.19	140.09	133.90
1	B	290	ALA	N-CA-C	6.19	118.48	109.07
1	D	249	ILE	CA-C-N	6.17	130.90	122.19
1	D	249	ILE	C-N-CA	6.17	130.90	122.19
1	B	120	ASP	CA-C-N	6.17	125.79	119.56
1	B	120	ASP	C-N-CA	6.17	125.79	119.56
1	C	278	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	D	120	ASP	CA-C-N	6.15	125.84	119.56
1	D	120	ASP	C-N-CA	6.15	125.84	119.56
1	B	117	PHE	N-CA-C	6.14	123.88	110.80
1	D	252	GLN	CA-C-N	6.14	128.79	120.44
1	D	252	GLN	C-N-CA	6.14	128.79	120.44
1	B	287	GLY	CA-C-N	6.12	127.49	119.84
1	B	287	GLY	C-N-CA	6.12	127.49	119.84
1	C	124	MET	O-C-N	6.10	130.70	122.59
1	D	73	ALA	O-C-N	6.09	128.43	122.09
1	D	111	ARG	CA-CB-CG	-6.08	101.94	114.10
1	D	171	LEU	N-CA-C	6.08	119.79	112.38
1	A	174	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	B	194	TRP	CB-CG-CD1	-6.05	117.83	126.90
1	B	43	ILE	CB-CA-C	-6.05	102.79	112.16
1	B	66	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	248	TYR	N-CA-C	-6.01	105.03	112.72
1	A	180	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	176	MET	O-C-N	-6.00	117.62	121.88
1	D	250	SER	N-CA-C	5.97	119.38	109.46
1	B	245	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	248	TYR	O-C-N	5.97	129.44	122.09
1	A	195	VAL	N-CA-C	5.97	116.72	108.12
1	D	283	ASN	CA-CB-CG	5.96	118.56	112.60
1	D	37	PRO	N-CA-C	5.96	124.75	112.47
1	B	125	GLU	O-C-N	5.96	130.60	123.33
1	A	306	ASP	N-CA-C	-5.95	103.56	111.24
1	D	306	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	222	PRO	N-CA-C	-5.94	103.45	110.70
1	D	249	ILE	N-CA-C	5.93	121.68	109.34
1	D	111	ARG	CB-CA-C	-5.93	103.35	110.94
1	D	209	ASP	N-CA-C	-5.93	97.55	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLU	CB-CG-CD	5.90	122.62	112.60
1	C	29	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	B	263	TYR	N-CA-C	5.88	123.32	110.80
1	C	274	GLN	CA-CB-CG	5.87	125.84	114.10
1	A	26	SER	N-CA-C	5.86	119.53	112.38
1	C	306	ASP	N-CA-C	-5.84	104.91	112.68
1	D	172	ASP	N-CA-C	5.83	117.50	111.03
1	C	42	ASN	CA-C-O	5.82	127.11	120.54
1	B	67	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	A	300	VAL	O-C-N	5.81	128.94	122.61
1	A	301	LYS	N-CA-C	5.81	118.21	107.99
1	B	299	GLU	CB-CG-CD	5.80	122.46	112.60
1	D	42	ASN	CA-C-N	5.80	127.95	120.70
1	D	42	ASN	C-N-CA	5.80	127.95	120.70
1	C	174	HIS	CB-CG-CD2	-5.80	123.67	131.20
1	A	245	ASP	CA-C-O	5.79	127.30	120.70
1	B	257	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	39	VAL	N-CA-CB	-5.79	104.31	110.62
1	C	180	ASP	N-CA-C	5.79	119.96	111.34
1	C	190	VAL	O-C-N	5.78	129.53	122.72
1	A	257	ASP	N-CA-C	-5.77	104.68	110.97
1	C	175	MET	N-CA-C	5.77	123.08	110.80
1	A	276	PHE	CA-CB-CG	5.76	119.56	113.80
1	D	213	THR	N-CA-C	-5.76	99.34	108.73
1	A	67	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	B	40	VAL	CA-C-O	5.75	124.38	119.38
1	D	62	ALA	N-CA-C	5.74	117.85	108.55
1	B	37	PRO	CA-N-CD	-5.74	103.97	112.00
1	B	16	ILE	CA-C-N	5.72	126.45	119.99
1	B	16	ILE	C-N-CA	5.72	126.45	119.99
1	D	93	ILE	N-CA-C	-5.71	105.28	110.82
1	D	108	ASN	N-CA-C	5.71	122.97	110.80
1	D	277	PHE	CA-CB-CG	-5.71	108.09	113.80
1	D	97	LEU	N-CA-C	-5.71	105.03	112.23
1	C	125	GLU	O-C-N	5.71	130.48	122.77
1	A	38	GLU	CA-C-O	5.70	128.66	120.51
1	D	29	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	D	187	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	85	ALA	N-CA-C	5.68	118.14	109.62
1	B	231	GLU	N-CA-C	5.67	118.23	111.71
1	A	123	ILE	O-C-N	5.67	129.46	122.32
1	A	234	GLN	N-CA-C	5.65	118.38	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	ARG	CA-CB-CG	-5.64	102.81	114.10
1	A	310	GLU	CA-CB-CG	5.64	125.38	114.10
1	B	51	TYR	N-CA-C	-5.64	104.77	111.03
1	B	140	LYS	N-CA-C	-5.63	104.53	111.40
1	B	241	GLU	N-CA-C	5.63	122.80	110.80
1	D	184	ILE	CA-CB-CG2	-5.63	100.93	110.50
1	C	212	GLN	CB-CG-CD	5.61	122.14	112.60
1	A	125	GLU	O-C-N	5.61	130.04	122.59
1	A	125	GLU	CA-C-O	5.60	128.52	120.51
1	A	168	LEU	CA-C-N	5.60	132.24	121.54
1	A	168	LEU	C-N-CA	5.60	132.24	121.54
1	D	262	SER	CA-C-N	5.60	132.24	121.54
1	D	262	SER	C-N-CA	5.60	132.24	121.54
1	A	194	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	D	180	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	256	ALA	N-CA-C	5.57	119.34	112.54
1	D	299	GLU	CA-CB-CG	5.56	125.22	114.10
1	C	139	ARG	CA-C-N	5.56	128.29	120.28
1	C	139	ARG	C-N-CA	5.56	128.29	120.28
1	A	13	THR	N-CA-C	-5.55	106.50	113.28
1	D	177	PRO	CA-C-N	5.54	125.72	119.90
1	D	177	PRO	C-N-CA	5.54	125.72	119.90
1	C	236	TRP	CE2-CD2-CG	-5.54	100.56	107.20
1	D	253	ASP	CA-C-O	5.54	126.40	120.70
1	A	113	LEU	CA-C-N	5.53	126.75	119.84
1	A	113	LEU	C-N-CA	5.53	126.75	119.84
1	A	137	ASP	CA-CB-CG	5.50	118.09	112.60
1	D	287	GLY	CA-C-N	5.49	125.16	119.56
1	D	287	GLY	C-N-CA	5.49	125.16	119.56
1	C	273	TYR	O-C-N	5.48	129.88	122.59
1	C	283	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	10	VAL	CB-CA-C	5.47	119.13	110.81
1	D	183	LEU	N-CA-C	5.46	117.64	108.73
1	B	83	ALA	CA-C-N	5.46	128.59	120.90
1	B	83	ALA	C-N-CA	5.46	128.59	120.90
1	C	91	HIS	N-CA-C	-5.46	105.44	111.71
1	D	174	HIS	CB-CG-ND1	5.45	130.88	122.70
1	D	252	GLN	CB-CG-CD	5.45	121.86	112.60
1	C	292	GLU	CB-CG-CD	5.44	121.85	112.60
1	B	33	VAL	N-CA-CB	-5.44	104.57	111.64
1	C	280	ASP	N-CA-C	5.43	122.37	110.80
1	B	90	SER	CA-C-O	5.43	127.54	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	LEU	CA-C-N	5.43	129.88	122.34
1	B	168	LEU	C-N-CA	5.43	129.88	122.34
1	B	291	ILE	CB-CA-C	-5.42	101.13	110.30
1	A	251	SER	N-CA-C	5.42	122.34	110.80
1	A	207	SER	CA-C-N	5.42	131.72	121.97
1	A	207	SER	C-N-CA	5.42	131.72	121.97
1	D	123	ILE	CA-C-N	5.41	131.88	121.54
1	D	123	ILE	C-N-CA	5.41	131.88	121.54
1	D	126	HIS	CA-C-N	5.41	128.79	121.05
1	D	126	HIS	C-N-CA	5.41	128.79	121.05
1	D	293	ALA	N-CA-C	5.40	119.04	112.23
1	B	280	ASP	N-CA-C	5.39	122.27	110.80
1	C	97	LEU	N-CA-C	-5.38	104.83	111.40
1	C	298	PRO	CA-C-N	5.37	127.73	120.38
1	C	298	PRO	C-N-CA	5.37	127.73	120.38
1	A	62	ALA	N-CA-C	5.36	122.22	110.80
1	A	254	PHE	N-CA-C	-5.35	105.01	112.45
1	B	195	VAL	CA-C-N	5.35	128.31	120.71
1	B	195	VAL	C-N-CA	5.35	128.31	120.71
1	C	259	LYS	CA-C-O	-5.35	115.17	120.90
1	C	236	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	C	284	PHE	CA-C-N	5.33	131.14	122.07
1	C	284	PHE	C-N-CA	5.33	131.14	122.07
1	B	192	GLY	O-C-N	-5.33	118.96	123.60
1	D	276	PHE	CA-C-N	-5.33	116.09	122.44
1	D	276	PHE	C-N-CA	-5.33	116.09	122.44
1	A	6	ARG	CA-C-N	-5.33	116.23	123.10
1	A	6	ARG	C-N-CA	-5.33	116.23	123.10
1	B	194	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	D	115	SER	CA-C-O	5.33	126.59	120.84
1	C	275	ILE	N-CA-C	-5.33	107.59	111.90
1	B	4	LYS	N-CA-C	5.32	120.45	112.94
1	C	39	VAL	O-C-N	5.32	127.42	121.94
1	A	91	HIS	CB-CG-ND1	5.32	130.68	122.70
1	A	77	VAL	N-CA-C	5.30	117.70	108.95
1	C	66	ASP	CA-C-O	5.29	127.24	120.57
1	B	185	TYR	O-C-N	5.29	129.40	122.68
1	B	89	LEU	CA-C-N	5.28	130.05	122.40
1	B	89	LEU	C-N-CA	5.28	130.05	122.40
1	C	5	SER	N-CA-C	-5.27	101.11	109.96
1	A	88	VAL	CA-C-N	5.26	129.60	122.19
1	A	88	VAL	C-N-CA	5.26	129.60	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	HIS	CB-CG-ND1	5.25	130.58	122.70
1	C	73	ALA	CA-C-O	5.25	125.83	119.38
1	A	120	ASP	CA-C-N	5.24	125.30	119.32
1	A	120	ASP	C-N-CA	5.24	125.30	119.32
1	B	155	VAL	N-CA-C	5.24	115.17	107.15
1	C	58	LYS	CG-CD-CE	5.24	123.36	111.30
1	B	226	ILE	N-CA-C	-5.23	99.15	107.15
1	B	179	ARG	CA-C-N	5.22	131.52	121.54
1	B	179	ARG	C-N-CA	5.22	131.52	121.54
1	A	85	ALA	N-CA-C	5.22	117.00	108.76
1	B	231	GLU	CA-C-N	5.21	129.78	121.34
1	B	231	GLU	C-N-CA	5.21	129.78	121.34
1	D	159	MET	N-CA-C	5.21	118.11	109.46
1	D	153	THR	N-CA-C	-5.21	99.71	110.80
1	A	170	GLN	N-CA-C	5.19	118.68	109.96
1	D	207	SER	N-CA-C	5.19	117.02	111.36
1	D	280	ASP	N-CA-C	5.18	121.84	110.80
1	A	194	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	B	264	GLU	CB-CG-CD	5.18	121.41	112.60
1	C	38	GLU	CA-C-O	5.18	125.41	119.35
1	D	86	GLY	CA-C-N	5.18	131.56	121.41
1	D	86	GLY	C-N-CA	5.18	131.56	121.41
1	A	236	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	C	102	ALA	N-CA-C	-5.17	107.99	114.56
1	C	256	ALA	CA-C-O	5.16	125.73	119.38
1	B	72	ASP	CA-C-N	5.16	127.45	120.44
1	B	72	ASP	C-N-CA	5.16	127.45	120.44
1	C	85	ALA	N-CA-C	5.16	117.83	109.79
1	B	91	HIS	CA-CB-CG	5.15	118.95	113.80
1	C	15	TYR	N-CA-C	5.15	117.29	111.11
1	B	210	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	150	ILE	N-CA-C	-5.15	104.20	108.63
1	B	125	GLU	N-CA-C	-5.15	104.89	110.91
1	D	299	GLU	CB-CG-CD	5.15	121.35	112.60
1	D	134	THR	CA-CB-OG1	-5.14	101.88	109.60
1	A	126	HIS	CA-CB-CG	-5.14	108.66	113.80
1	D	124	MET	CA-C-N	5.13	131.33	121.54
1	D	124	MET	C-N-CA	5.13	131.33	121.54
1	A	145	ILE	N-CA-C	-5.12	105.33	110.30
1	C	193	ILE	N-CA-C	-5.12	100.28	107.75
1	C	204	THR	CB-CA-C	-5.11	102.16	110.85
1	C	289	ASN	N-CA-C	-5.11	106.73	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ARG	O-C-N	5.11	129.32	123.29
1	B	260	ASP	N-CA-C	-5.11	104.69	112.04
1	C	108	ASN	N-CA-CB	-5.11	101.86	110.49
1	A	210	ASP	CA-C-N	5.10	124.89	119.28
1	A	210	ASP	C-N-CA	5.10	124.89	119.28
1	B	36	ARG	CB-CG-CD	5.09	123.02	111.30
1	D	189	ASN	CA-C-N	5.09	131.14	121.97
1	D	189	ASN	C-N-CA	5.09	131.14	121.97
1	B	147	ALA	N-CA-C	-5.08	105.82	111.36
1	B	311	ARG	N-CA-C	-5.08	108.83	114.62
1	C	254	PHE	CB-CA-C	5.08	118.18	109.65
1	D	177	PRO	N-CA-C	5.08	116.89	110.70
1	D	254	PHE	CA-C-N	-5.08	113.19	122.38
1	D	254	PHE	C-N-CA	-5.08	113.19	122.38
1	B	134	THR	CA-CB-OG1	-5.08	101.99	109.60
1	C	177	PRO	CA-C-N	5.07	125.07	119.89
1	C	177	PRO	C-N-CA	5.07	125.07	119.89
1	C	254	PHE	CA-CB-CG	-5.07	108.73	113.80
1	C	182	VAL	O-C-N	-5.07	117.21	123.09
1	D	160	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	196	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	210	ASP	CA-C-N	5.06	124.67	119.56
1	D	210	ASP	C-N-CA	5.06	124.67	119.56
1	A	293	ALA	N-CA-C	5.06	117.53	111.71
1	C	126	HIS	CA-C-N	5.05	128.24	120.82
1	C	126	HIS	C-N-CA	5.05	128.24	120.82
1	B	292	GLU	CA-C-O	5.04	125.86	120.32
1	B	91	HIS	CB-CG-ND1	5.04	130.26	122.70
1	D	125	GLU	CA-C-N	5.03	132.01	121.94
1	D	125	GLU	C-N-CA	5.03	132.01	121.94
1	D	268	VAL	N-CA-C	5.03	117.34	111.05
1	B	117	PHE	CA-CB-CG	-5.02	108.78	113.80
1	B	125	GLU	CA-C-O	5.02	129.06	122.44
1	C	134	THR	N-CA-C	-5.01	100.12	110.80
1	D	199	ASP	N-CA-C	-5.01	105.49	112.45
1	A	269	ARG	N-CA-C	-5.01	102.29	110.20
1	C	174	HIS	CA-C-N	5.01	131.10	121.54
1	C	174	HIS	C-N-CA	5.01	131.10	121.54
1	D	118	GLY	CA-C-N	5.00	131.10	121.54
1	D	118	GLY	C-N-CA	5.00	131.10	121.54
1	D	117	PHE	N-CA-C	5.00	121.45	110.80

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 [i](#)

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	107	0
1	B	2497	0	2525	79	0
1	C	2497	0	2525	90	0
1	D	2496	0	2525	103	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	379	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 19.

All (379) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:TYR:HA	1:C:175:MET:HE1	1.65	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:B:194:TRP:HB3	1:B:305:MET:HE2	1.75	0.69
1:C:113:LEU:HD21	1:C:208:ILE:HG22	1.75	0.69
1:C:193:ILE:HG12	1:C:226:ILE:HG12	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:96:GLN:HE22	1:A:115:SER:H	1.42	0.68
1:A:117:PHE:HE2	1:A:204:THR:HG21	1.58	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:B:274:GLN:HA	1:B:278:ARG:HB2	1.77	0.67
1:C:230:LYS:O	1:C:234:GLN:HG3	1.95	0.67
1:D:121:PRO:HB2	1:D:139:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:SER:HA	1:C:135:PHE:HD1	1.61	0.65
2:A:321:HOH:O	1:C:91:HIS:HB3	1.96	0.65
1:B:128:LEU:HD12	1:B:270:CYS:SG	2.37	0.65
1:D:254:PHE:O	1:D:257:ASP:HB2	1.96	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:B:161:ALA:HB1	1:B:305:MET:HE1	1.80	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:24:SER:HB3	1:A:31:THR:OG1	2.01	0.61
1:A:193:ILE:HD13	1:A:221:ARG:HG2	1.81	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:A:218:MET:HE1	1:A:297:TYR:HE2	1.65	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:D:129:GLN:CD	1:D:129:GLN:H	2.11	0.58
1:C:123:ILE:O	1:C:125:GLU:HG2	2.04	0.58
1:A:36:ARG:H	1:A:36:ARG:CD	2.17	0.58
1:D:170:GLN:NE2	1:D:182:VAL:HG23	2.17	0.58
1:A:3:LYS:HG3	1:A:29:HIS:CE1	2.39	0.57
1:B:296:LEU:O	1:B:298:PRO:HD3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:MET:HG3	1:D:269:ARG:HB3	1.86	0.57
1:D:305:MET:HE2	1:D:305:MET:HA	1.86	0.57
1:A:119:MET:HE1	1:A:274:GLN:HB2	1.87	0.56
1:B:138:LYS:O	1:B:142:ARG:HG3	2.04	0.56
1:A:121:PRO:HB2	1:A:139:ARG:HG3	1.87	0.56
1:A:269:ARG:O	1:A:270:CYS:SG	2.63	0.56
1:B:124:MET:HE3	1:B:127:ALA:HB2	1.86	0.56
1:C:170:GLN:NE2	1:C:183:LEU:H	2.03	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:36:ARG:C	1:B:38:GLU:H	2.13	0.56
1:B:256:ALA:HA	1:B:259:LYS:HG2	1.87	0.56
1:B:86:GLY:O	1:B:90:SER:HA	2.05	0.56
1:C:250:SER:O	1:C:254:PHE:HB2	2.06	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:A:42:ASN:ND2	1:A:44:ASP:HB2	2.20	0.55
1:C:159:MET:SD	1:C:164:PHE:CG	3.00	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:A:292:GLU:OE2	1:A:294:THR:HB	2.07	0.55
1:C:132:SER:HA	1:C:135:PHE:CD1	2.40	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:A:252:GLN:HG3	1:A:253:ASP:H	1.72	0.54
1:A:262:SER:HA	1:A:266:LYS:HZ1	1.72	0.54
1:B:17:GLY:O	1:B:21:VAL:HG23	2.06	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:A:170:GLN:HE22	1:A:182:VAL:HG12	1.73	0.54
1:C:256:ALA:O	1:C:259:LYS:HB2	2.07	0.54
1:A:212:GLN:O	1:A:216:LYS:HD2	2.07	0.54
1:A:235:ILE:O	1:A:239:LEU:HD13	2.07	0.54
1:A:258:MET:HE3	1:A:266:LYS:HB2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:15:TYR:HB3	1:C:163:TYR:OH	2.09	0.52
1:C:43:ILE:H	1:C:43:ILE:CD1	2.22	0.52
1:D:159:MET:HG3	1:D:281:LEU:HD21	1.91	0.52
1:A:70:LEU:O	1:A:74:LEU:HG	2.08	0.52
1:C:218:MET:HE1	1:C:297:TYR:HE2	1.75	0.52
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:A:218:MET:CE	1:A:297:TYR:HE2	2.23	0.52
1:D:248:TYR:O	1:D:250:SER:N	2.42	0.52
1:D:256:ALA:HA	1:D:259:LYS:HD2	1.91	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:D:189:ASN:HD22	1:D:230:LYS:HZ2	1.58	0.51
1:D:224:MET:SD	1:D:302:TYR:OH	2.68	0.51
1:D:255:LEU:HG	1:D:273:TYR:CZ	2.46	0.51
1:A:211:PRO:O	1:A:214:LEU:HB2	2.10	0.51
1:A:240:SER:OG	1:A:242:GLN:HG2	2.09	0.51
1:A:205:ILE:HA	1:A:208:ILE:HD12	1.92	0.51
1:D:219:TYR:HE2	1:D:290:ALA:HB1	1.76	0.51
1:D:223:PRO:HG2	1:D:224:MET:SD	2.50	0.51
1:D:224:MET:SD	1:D:224:MET:N	2.84	0.51
1:A:259:LYS:HA	1:A:266:LYS:HD3	1.91	0.51
1:A:263:TYR:O	1:A:264:GLU:HB2	2.11	0.51
1:A:271:HIS:H	1:A:273:TYR:H	1.59	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:C:16:ILE:O	1:C:19:ARG:HB2	2.11	0.51
1:D:208:ILE:HG23	1:D:209:ASP:N	2.22	0.51
1:C:92:HIS:HA	1:C:95:GLU:HB2	1.93	0.51
1:A:167:SER:HB3	1:A:175:MET:HE3	1.93	0.51
1:D:208:ILE:CG2	1:D:209:ASP:H	2.22	0.51
1:B:211:PRO:O	1:B:214:LEU:HB3	2.11	0.50
1:B:261:LYS:HG3	1:B:269:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:H	1:C:274:GLN:NE2	2.07	0.50
1:A:159:MET:HE2	1:A:281:LEU:HD22	1.93	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:A:161:ALA:HB1	1:A:305:MET:HE1	1.93	0.50
1:D:100:VAL:HG12	1:D:112:PHE:HE2	1.77	0.50
1:D:219:TYR:CE2	1:D:290:ALA:HB1	2.47	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:D:189:ASN:ND2	1:D:230:LYS:HZ2	2.10	0.50
1:A:75:LYS:HD2	1:A:108:ASN:ND2	2.26	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:96:GLN:O	1:C:100:VAL:HG13	2.12	0.49
1:C:163:TYR:N	1:C:163:TYR:CD1	2.80	0.49
1:A:108:ASN:HD22	1:A:108:ASN:H	1.59	0.49
1:A:179:ARG:HG3	1:A:242:GLN:NE2	2.27	0.49
1:C:67:HIS:O	1:C:71:VAL:HG23	2.13	0.49
1:D:97:LEU:HB2	1:D:98:LYS:HE3	1.95	0.49
1:D:170:GLN:NE2	1:D:178:PRO:HG2	2.27	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: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:B:2:ASP:O	1:B:4:LYS:HG3	2.13	0.48
1:C:37:PRO:HB3	1:C:40:VAL:HG23	1.95	0.48
1:B:143:ARG:HD3	1:B:146:GLU:HG2	1.94	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:A:309:LEU:C	1:A:311:ARG:H	2.21	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: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:C:252:GLN:C	1:C:254:PHE:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:O	1:A:19:ARG:HB2	2.15	0.47
1:A:69:ARG:HG3	2:A:316:HOH:O	2.14	0.47
1:B:271:HIS:O	1:B:275:ILE:HG13	2.15	0.47
1:C:183:LEU:HD12	1:C:249:ILE:HB	1.96	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:C:273:TYR:HA	1:C:277:PHE:HD1	1.80	0.47
1:D:184:ILE:HD11	1:D:246:LYS:HG3	1.96	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
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:C:285:GLU:CD	1:C:285:GLU:H	2.22	0.46
1:B:230:LYS:O	1:B:234:GLN:HG3	2.15	0.46
1:D:222:PRO:HB2	1:D:302:TYR:CE2	2.51	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:A:263:TYR:C	1:A:265:GLU:H	2.24	0.46
1:D:307:SER:O	1:D:310:GLU:HB3	2.15	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:B:217:THR:O	1:B:291:ILE:HD12	2.16	0.46
1:C:185:TYR:HD1	1:C:229:GLN:HE22	1.64	0.46
1:D:68:GLN:NE2	1:D:69:ARG:HG2	2.30	0.46
1:A:229:GLN:O	1:A:233:ILE:HG13	2.16	0.46
1:B:100:VAL:HG21	1:B:145:ILE:HG22	1.97	0.46
1:B:193:ILE:HG21	1:B:221:ARG:HA	1.98	0.46
1:D:255:LEU:O	1:D:259:LYS:HG3	2.16	0.46
1:A:130:PRO:C	1:A:132:SER:H	2.24	0.45
1:B:263:TYR:O	1:B:267:ILE:HG13	2.15	0.45
1:C:218:MET:HE1	1:C:297:TYR:CE2	2.52	0.45
1:D:201:GLY:O	1:D:205:ILE:HG12	2.17	0.45
1:D:235:ILE:HG23	1:D:306:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HB	2:A:319:HOH:O	2.15	0.45
1:A:128:LEU:HD11	1:A:278:ARG:NH2	2.31	0.45
1:C:169:ALA:HB3	1:C:229:GLN:NE2	2.32	0.45
1:D:96:GLN:O	1:D:100:VAL:HG13	2.17	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:A:125:GLU:C	1:A:127:ALA:H	2.24	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:A:202:THR:O	1:A:206:LYS:HG3	2.17	0.45
1:B:15:TYR:HB3	1:B:163:TYR:HH	1.82	0.45
1:D:159:MET:O	1:D:195:VAL:HG12	2.17	0.45
1:D:196:ASP:HB3	1:D:199:ASP:OD1	2.16	0.45
1:C:134:THR:O	1:C:138:LYS:HG3	2.17	0.45
1:C:222:PRO:HG2	1:C:225:ASN:HB2	1.99	0.45
1:B:93:ILE:HG22	1:B:94:LEU:HD13	1.97	0.45
1:C:237:GLU:HG3	1:C:238:ARG:H	1.81	0.45
1:A:120:ASP:HA	1:A:121:PRO:HD2	1.83	0.44
1:A:305:MET:O	1:A:309:LEU:HB2	2.17	0.44
1:C:75:LYS:HG3	1:C:106:ALA:HB1	1.98	0.44
1:D:219:TYR:HE2	1:D:290:ALA:CB	2.30	0.44
1:B:48:MET:O	1:B:51:TYR:HB3	2.16	0.44
1:D:217:THR:O	1:D:290:ALA:HA	2.17	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:A:210:ASP:HA	1:A:211:PRO:HD2	1.89	0.44
1:A:224:MET:HB2	1:A:302:TYR:HE2	1.82	0.44
1:B:48:MET:HE3	1:B:52:PHE:CZ	2.52	0.44
1:C:236:TRP:HD1	1:C:244:LEU:HD11	1.82	0.44
1:D:237:GLU:HG2	1:D:244:LEU:CD2	2.48	0.44
1:C:165:ALA:O	1:C:168:LEU:HD23	2.18	0.44
1:D:2:ASP:HA	1:D:27:LEU:C	2.43	0.44
1:D:237:GLU:CG	1:D:244:LEU:HD23	2.48	0.44
1:D:279:GLY:C	1:D:281:LEU:H	2.26	0.44
1:C:113:LEU:HB3	1:C:153:THR:O	2.18	0.43
1:C:177:PRO:HD3	1:C:312:TYR:CD2	2.53	0.43
1:A:159:MET:HE2	1:A:281:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:TYR:O	1:C:311:ARG:HB2	2.18	0.43
1:B:145:ILE:HG21	1:B:145:ILE:HD13	1.82	0.43
1:B:275:ILE:CG2	1:B:281:LEU:HD22	2.49	0.43
1:D:300:VAL:HG23	1:D:300:VAL:O	2.18	0.43
1:A:17:GLY:O	1:A:21:VAL:HG23	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:D:84:LEU:HG	1:D:92:HIS:HB3	1.99	0.43
1:D:255:LEU:O	1:D:258:MET:HB3	2.19	0.43
1:B:31:THR:O	1:B:58:LYS:HE3	2.18	0.43
1:C:42:ASN:O	1:C:46:VAL:HG23	2.18	0.43
1:C:111:ARG:HD2	1:C:152:TYR:O	2.18	0.43
1:C:237:GLU:O	1:C:239:LEU:N	2.47	0.43
1:D:154:TYR:HB2	1:D:217:THR:HA	2.01	0.43
1:C:292:GLU:O	1:C:296:LEU:HB2	2.19	0.43
1:B:218:MET:HE1	1:B:297:TYR:HE2	1.83	0.43
1:C:111:ARG:NH2	1:C:210:ASP:O	2.52	0.43
1:D:230:LYS:O	1:D:234:GLN:HG3	2.19	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
1:D:252:GLN:OE1	1:D:273:TYR:HB3	2.18	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:D:79:VAL:HG21	1:D:208:ILE:HG12	2.00	0.42
1:A:14:GLY:O	1:A:18:LYS:HG3	2.19	0.42
1:B:161:ALA:CB	1:B:305:MET:HE1	2.46	0.42
1:A:236:TRP:HE1	1:A:313:VAL:CG1	2.33	0.42
1:C:186:GLY:O	1:C:248:TYR:HB3	2.18	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:A:71:VAL:HA	1:A:74:LEU:HD12	2.02	0.42
1:A:208:ILE:HG22	1:A:209:ASP:CG	2.43	0.42
1:C:225:ASN:HD21	1:C:305:MET:H	1.67	0.42
1:D:123:ILE:O	1:D:125:GLU:N	2.52	0.42
1:A:186:GLY:N	1:A:249:ILE:O	2.52	0.42
1:A:308:TYR:O	1:A:311:ARG:HG2	2.20	0.42
1:B:159:MET:HE1	1:B:275:ILE:HG21	2.01	0.42
1:C:222:PRO:HA	1:C:223:PRO:HD3	1.82	0.42
1:B:16:ILE:HG22	2:B:333:HOH:O	2.20	0.42
1:C:237:GLU:C	1:C:239:LEU:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:O	1:D:145:ILE:HG13	2.19	0.42
1:A:80:VAL:HG12	1:A:109:ILE:HG12	2.01	0.42
1:B:174:HIS:HB3	1:B:175:MET:SD	2.60	0.42
1:D:18:LYS:HD3	1:D:48:MET:HE2	2.02	0.41
1:D:92:HIS:HA	1:D:95:GLU:HB3	2.03	0.41
1:D:159:MET:HE3	1:D:159:MET:HB2	1.75	0.41
1:C:201:GLY:O	1:C:205:ILE:HG12	2.21	0.41
1:A:123:ILE:O	1:A:125:GLU:HG2	2.21	0.41
1:C:138:LYS:O	1:C:142:ARG:HG3	2.21	0.41
1:C:225:ASN:HD21	1:C:304:THR:HA	1.86	0.41
1:B:42:ASN:HB3	1:B:45:LYS:HB2	2.02	0.41
1:B:43:ILE:HD12	1:B:43:ILE:H	1.85	0.41
1:C:111:ARG:NH2	1:C:210:ASP:H	2.19	0.41
1:D:125:GLU:C	1:D:127:ALA:H	2.28	0.41
1:C:121:PRO:HD2	1:C:142:ARG:NH1	2.35	0.41
1:B:53:LYS:HD3	1:B:59:LEU:HD22	2.02	0.41
1:C:133:ILE:O	1:C:133:ILE:HG22	2.21	0.41
1:A:111:ARG:HD3	1:A:151:PRO:O	2.20	0.41
1:A:170:GLN:C	1:A:172:ASP:H	2.29	0.41
1:B:64:LEU:HD11	1:B:99:LEU:HB2	2.02	0.41
1:C:170:GLN:HE22	1:C:183:LEU:H	1.68	0.41
1:D:82:SER:OG	1:D:96:GLN:NE2	2.54	0.41
1:A:129:GLN:H	1:A:129:GLN:CD	2.28	0.41
1:B:6:ARG:HB3	1:B:77:VAL:HG12	2.03	0.41
1:B:111:ARG:NH2	1:B:210:ASP:O	2.53	0.41
1:B:167:SER:HB3	1:B:175:MET:HA	2.03	0.41
1:B:179:ARG:HG2	1:B:236:TRP:HH2	1.84	0.41
1:B:283:ASN:OD1	1:B:283:ASN:N	2.54	0.41
1:C:167:SER:O	1:C:170:GLN:HB2	2.21	0.41
1:C:233:ILE:HG23	1:C:244:LEU:HD12	2.03	0.41
1:C:274:GLN:HG3	1:C:280:ASP:OD2	2.21	0.41
1:D:15:TYR:CD1	1:D:16:ILE:HG22	2.56	0.41
1:A:258:MET:HG3	1:A:269:ARG:CB	2.51	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:D:177:PRO:HA	1:D:178:PRO:HD3	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:299:GLU:H	1:A:299:GLU:HG3	1.63	0.40
1:B:207:SER:HA	1:B:297:TYR:OH	2.21	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%)	1	1
1	B	310/313 (99%)	252 (81%)	41 (13%)	17 (6%)	1	1
1	C	310/313 (99%)	258 (83%)	38 (12%)	14 (4%)	2	2
1	D	310/313 (99%)	247 (80%)	40 (13%)	23 (7%)	1	1
All	All	1240/1252 (99%)	1015 (82%)	148 (12%)	77 (6%)	1	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	231 (84%)	43 (16%)	2	5
1	B	274/275 (100%)	233 (85%)	41 (15%)	3	6
1	C	274/275 (100%)	233 (85%)	41 (15%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	274/275 (100%)	228 (83%)	46 (17%)	2	4
All	All	1096/1100 (100%)	925 (84%)	171 (16%)	2	5

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	10	VAL
1	A	15	TYR
1	A	36	ARG
1	A	38	GLU
1	A	40	VAL
1	A	42	ASN
1	A	43	ILE
1	A	50	LEU
1	A	53	LYS
1	A	78	ASP
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	123	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
1	A	174	HIS
1	A	175	MET
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	257	ASP
1	A	260	ASP

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Mol	Chain	Res	Type
1	A	261	LYS
1	A	263	TYR
1	A	271	HIS
1	A	285	GLU
1	A	291	ILE
1	A	301	LYS
1	A	312	TYR
1	B	3	LYS
1	B	4	LYS
1	B	7	VAL
1	B	8	LEU
1	B	36	ARG
1	B	37	PRO
1	B	40	VAL
1	B	43	ILE
1	B	47	GLN
1	B	50	LEU
1	B	55	LEU
1	B	59	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
1	B	134	THR
1	B	143	ARG
1	B	146	GLU
1	B	163	TYR
1	B	172	ASP
1	B	179	ARG
1	B	190	VAL
1	B	191	LYS

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Mol	Chain	Res	Type
1	B	197	GLU
1	B	208	ILE
1	B	217	THR
1	B	225	ASN
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	97	LEU
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	143	ARG
1	C	163	TYR
1	C	170	GLN
1	C	174	HIS
1	C	179	ARG
1	C	209	ASP
1	C	214	LEU
1	C	223	PRO
1	C	235	ILE
1	C	237	GLU
1	C	238	ARG
1	C	239	LEU
1	C	257	ASP
1	C	259	LYS
1	C	260	ASP
1	C	263	TYR
1	C	266	LYS
1	C	283	ASN
1	C	285	GLU

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Mol	Chain	Res	Type
1	C	286	ILE
1	C	291	ILE
1	C	292	GLU
1	C	295	LYS
1	C	299	GLU
1	D	6	ARG
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	39	VAL
1	D	48	MET
1	D	66	ASP
1	D	68	GLN
1	D	70	LEU
1	D	123	ILE
1	D	124	MET
1	D	125	GLU
1	D	129	GLN
1	D	146	GLU
1	D	170	GLN
1	D	171	LEU
1	D	174	HIS
1	D	176	MET
1	D	181	LYS
1	D	189	ASN
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	244	LEU
1	D	255	LEU
1	D	258	MET
1	D	268	VAL
1	D	269	ARG
1	D	272	LEU

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Mol	Chain	Res	Type
1	D	281	LEU
1	D	283	ASN
1	D	291	ILE
1	D	295	LYS
1	D	296	LEU
1	D	299	GLU
1	D	301	LYS
1	D	303	VAL
1	D	312	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	42	ASN
1	A	47	GLN
1	A	91	HIS
1	A	96	GLN
1	A	108	ASN
1	A	170	GLN
1	A	215	ASN
1	A	234	GLN
1	A	242	GLN
1	A	252	GLN
1	A	274	GLN
1	B	47	GLN
1	B	67	HIS
1	B	129	GLN
1	B	158	ASN
1	B	225	ASN
1	B	229	GLN
1	B	234	GLN
1	B	289	ASN
1	C	54	GLN
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	243	ASN
1	C	274	GLN

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Mol	Chain	Res	Type
1	C	283	ASN
1	C	289	ASN
1	D	68	GLN
1	D	91	HIS
1	D	96	GLN
1	D	108	ASN
1	D	129	GLN
1	D	158	ASN
1	D	170	GLN
1	D	189	ASN
1	D	215	ASN
1	D	242	GLN
1	D	271	HIS
1	D	283	ASN
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 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.