



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 3ZXA / pdb_00003zxa
Title : Structure and Assembly of Turnip Crinkle Virus I. X-ray Crystallographic
Structure Analysis at 3.2 Å Resolution
Authors : Hogle, J.M.; Maeda, A.; Harrison, S.C.
Deposited on : 2011-08-08
Resolution : 3.20 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

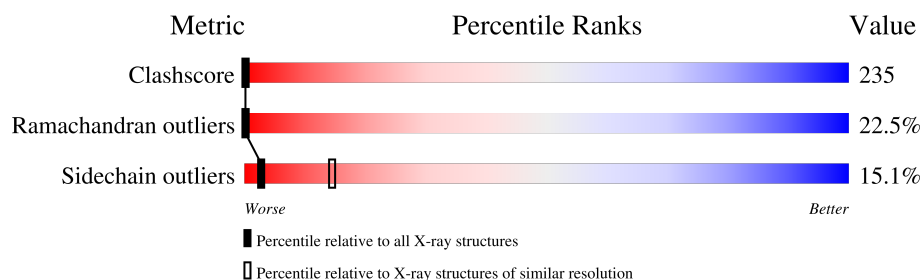
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	C	347	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2237 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	295	Total	C	N	O	S	0	0	0
			2237	1410	386	436	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP P06663
C	?	-	ASN	deletion	UNP P06663
C	?	-	ASP	deletion	UNP P06663
C	?	-	ASP	deletion	UNP P06663
C	346	TRP	LEU	variant	UNP P06663

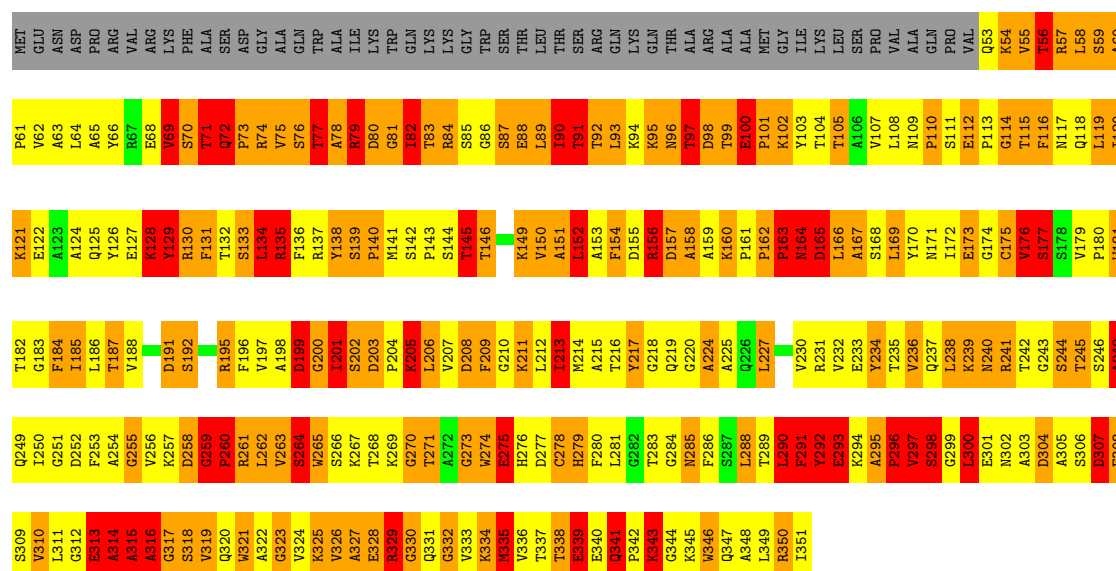
3 Residue-property plots

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: CAPSID PROTEIN

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	348.80Å 379.10Å 397.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-3.20)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BILDER	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2237	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	C	3.46	100/2285 (4.4%)	3.26	187/3102 (6.0%)

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	C	0	12

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	ILE	C-N	-69.29	0.36	1.33
1	C	93	LEU	N-CA	-50.27	0.64	1.45
1	C	82	ILE	C-N	33.86	1.81	1.33
1	C	288	LEU	C-N	-28.16	0.94	1.33
1	C	279	HIS	C-N	27.14	1.74	1.33
1	C	259	GLY	C-N	27.04	1.97	1.33
1	C	291	PHE	C-N	26.82	1.71	1.33
1	C	264	SER	C-N	25.06	1.68	1.33
1	C	297	VAL	C-N	-23.49	1.00	1.33
1	C	76	SER	N-CA	23.33	1.76	1.45
1	C	53	GLN	C-N	23.16	1.67	1.33
1	C	319	VAL	C-N	22.25	1.61	1.33
1	C	177	SER	C-N	-21.20	1.04	1.33
1	C	75	VAL	C-N	20.66	1.60	1.33
1	C	133	SER	CB-OG	19.44	1.81	1.42
1	C	339	GLU	C-N	18.95	1.68	1.34
1	C	75	VAL	CA-C	18.40	1.76	1.52
1	C	76	SER	CA-C	18.32	1.75	1.52
1	C	75	VAL	N-CA	17.41	1.68	1.46
1	C	308	PHE	C-N	-16.28	1.11	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	LYS	CD-CE	15.80	1.99	1.52
1	C	200	GLY	C-N	-15.54	1.12	1.33
1	C	91	THR	N-CA	14.48	1.64	1.46
1	C	315	ALA	C-N	-13.90	1.14	1.33
1	C	74	ARG	CA-C	13.86	1.69	1.52
1	C	74	ARG	C-N	13.83	1.52	1.33
1	C	77	THR	N-CA	13.58	1.63	1.46
1	C	260	PRO	C-N	-12.99	1.15	1.33
1	C	90	ILE	CA-C	12.95	1.69	1.52
1	C	303	ALA	C-N	12.93	1.50	1.33
1	C	290	LEU	C-N	12.79	1.51	1.33
1	C	323	GLY	C-N	-12.72	1.16	1.33
1	C	330	GLY	C-N	12.53	1.50	1.33
1	C	298	SER	C-N	-11.57	1.16	1.33
1	C	300	LEU	N-CA	-11.56	1.31	1.46
1	C	76	SER	C-N	11.18	1.49	1.33
1	C	299	GLY	C-N	-11.15	1.18	1.33
1	C	72	GLN	C-N	11.15	1.47	1.33
1	C	140	PRO	N-CD	-10.87	1.32	1.47
1	C	74	ARG	N-CA	10.70	1.59	1.45
1	C	175	CYS	C-N	-10.45	1.19	1.33
1	C	175	CYS	CA-C	-10.31	1.38	1.52
1	C	121	LYS	CE-NZ	9.94	1.79	1.49
1	C	224	ALA	C-N	9.88	1.47	1.33
1	C	299	GLY	CA-C	-9.64	1.38	1.51
1	C	139	SER	C-N	-9.19	1.12	1.33
1	C	299	GLY	N-CA	-8.83	1.32	1.45
1	C	70	SER	C-N	-8.81	1.21	1.33
1	C	284	GLY	N-CA	8.79	1.53	1.45
1	C	140	PRO	CA-CB	-8.76	1.41	1.53
1	C	332	GLY	C-N	8.61	1.45	1.33
1	C	58	LEU	C-N	-8.42	1.22	1.33
1	C	162	PRO	CA-C	-8.38	1.44	1.52
1	C	176	VAL	N-CA	-8.36	1.35	1.46
1	C	288	LEU	CA-C	-8.32	1.41	1.53
1	C	57	ARG	CA-C	-8.09	1.42	1.52
1	C	163	PRO	N-CA	-8.07	1.36	1.47
1	C	138	TYR	CA-C	-7.89	1.43	1.53
1	C	284	GLY	CA-C	7.65	1.59	1.51
1	C	99	THR	N-CA	7.56	1.54	1.46
1	C	270	GLY	C-N	-7.44	1.23	1.33
1	C	54	LYS	C-N	-7.40	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	SER	CA-C	-7.35	1.43	1.52
1	C	73	PRO	C-N	7.24	1.43	1.33
1	C	259	GLY	CA-C	7.15	1.62	1.51
1	C	187	THR	C-N	7.00	1.41	1.33
1	C	56	THR	C-N	-6.92	1.23	1.33
1	C	213	ILE	C-N	-6.83	1.24	1.33
1	C	181	TRP	N-CA	6.79	1.54	1.46
1	C	163	PRO	C-N	-6.77	1.24	1.33
1	C	300	LEU	C-N	6.64	1.42	1.33
1	C	139	SER	N-CA	-6.56	1.36	1.46
1	C	176	VAL	CA-C	-6.55	1.44	1.52
1	C	327	ALA	C-N	-6.55	1.24	1.33
1	C	335	MET	C-N	-6.43	1.24	1.33
1	C	164	ASN	N-CA	-6.32	1.38	1.46
1	C	329	ARG	N-CA	-6.00	1.38	1.46
1	C	317	GLY	N-CA	5.97	1.53	1.45
1	C	316	ALA	C-N	5.94	1.41	1.33
1	C	271	THR	C-N	5.92	1.42	1.33
1	C	285	ASN	N-CA	5.86	1.53	1.46
1	C	274	TRP	NE1-CE2	-5.79	1.31	1.37
1	C	88	GLU	C-N	-5.79	1.21	1.34
1	C	293	GLU	N-CA	5.78	1.53	1.46
1	C	181	TRP	NE1-CE2	-5.72	1.31	1.37
1	C	98	ASP	CA-C	5.68	1.59	1.52
1	C	274	TRP	C-N	-5.68	1.26	1.33
1	C	328	GLU	CA-C	-5.62	1.46	1.52
1	C	313	GLU	C-N	-5.56	1.25	1.33
1	C	184	PHE	C-N	-5.54	1.26	1.33
1	C	63	ALA	N-CA	-5.51	1.39	1.46
1	C	90	ILE	C-N	5.49	1.41	1.33
1	C	265	TRP	NE1-CE2	-5.42	1.31	1.37
1	C	328	GLU	N-CA	-5.41	1.39	1.46
1	C	346	TRP	NE1-CE2	-5.40	1.31	1.37
1	C	192	SER	N-CA	-5.34	1.38	1.46
1	C	321	TRP	NE1-CE2	-5.33	1.31	1.37
1	C	327	ALA	N-CA	-5.18	1.39	1.46
1	C	140	PRO	CA-C	5.07	1.59	1.52
1	C	191	ASP	CA-C	-5.01	1.47	1.53

All (187) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	ILE	O-C-N	-75.47	28.24	122.57
1	C	248	ALA	CA-C-N	-49.28	50.27	121.72
1	C	248	ALA	C-N-CA	-49.28	50.27	121.72
1	C	307	ASP	CA-C-N	22.07	156.73	121.86
1	C	307	ASP	C-N-CA	22.07	156.73	121.86
1	C	82	ILE	O-C-N	-21.44	95.77	122.57
1	C	129	TYR	O-C-N	21.37	143.35	123.26
1	C	338	THR	O-C-N	21.30	147.67	122.75
1	C	93	LEU	N-CA-C	-19.36	76.89	109.80
1	C	300	LEU	O-C-N	17.56	145.95	122.59
1	C	264	SER	O-C-N	17.24	142.51	123.03
1	C	248	ALA	O-C-N	16.00	143.87	122.59
1	C	100	GLU	O-C-N	-15.61	103.36	121.32
1	C	307	ASP	O-C-N	-15.35	102.18	122.59
1	C	297	VAL	CA-C-N	-15.29	92.35	121.54
1	C	297	VAL	C-N-CA	-15.29	92.35	121.54
1	C	290	LEU	O-C-N	14.97	142.50	122.59
1	C	330	GLY	O-C-N	-14.91	103.31	122.70
1	C	299	GLY	O-C-N	14.70	141.81	122.70
1	C	200	GLY	O-C-N	13.74	142.63	123.67
1	C	339	GLU	CA-C-N	-13.51	90.85	122.20
1	C	339	GLU	C-N-CA	-13.51	90.85	122.20
1	C	275	GLU	N-CA-C	-13.44	88.09	108.52
1	C	200	GLY	CA-C-N	13.30	145.91	121.97
1	C	200	GLY	C-N-CA	13.30	145.91	121.97
1	C	273	GLY	CA-C-N	-12.70	102.91	120.82
1	C	273	GLY	C-N-CA	-12.70	102.91	120.82
1	C	203	ASP	O-C-N	-12.28	106.06	121.29
1	C	325	LYS	CA-C-N	-11.92	100.51	121.97
1	C	325	LYS	C-N-CA	-11.92	100.51	121.97
1	C	264	SER	CA-C-N	-11.86	98.90	121.54
1	C	264	SER	C-N-CA	-11.86	98.90	121.54
1	C	76	SER	N-CA-C	11.80	127.06	109.24
1	C	313	GLU	O-C-N	11.76	138.24	122.59
1	C	328	GLU	O-C-N	11.69	136.58	123.13
1	C	175	CYS	CA-C-N	-11.65	101.00	121.97
1	C	175	CYS	C-N-CA	-11.65	101.00	121.97
1	C	341	GLN	O-C-N	-11.53	108.06	121.32
1	C	90	ILE	O-C-N	-10.72	109.17	122.57
1	C	279	HIS	O-C-N	-10.71	107.34	122.76
1	C	314	ALA	N-CA-C	-10.59	88.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASP	N-CA-C	-10.51	101.83	112.97
1	C	162	PRO	O-C-N	-9.67	110.05	121.46
1	C	163	PRO	O-C-N	9.66	135.69	122.64
1	C	296	PRO	O-C-N	9.66	135.68	122.64
1	C	273	GLY	O-C-N	9.45	134.98	122.70
1	C	140	PRO	N-CD-CG	-9.39	89.12	103.20
1	C	191	ASP	O-C-N	9.35	134.03	121.78
1	C	176	VAL	O-C-N	9.29	134.19	122.57
1	C	338	THR	N-CA-C	9.26	122.56	110.43
1	C	57	ARG	O-C-N	9.14	134.39	123.33
1	C	72	GLN	CA-C-N	9.14	129.57	120.52
1	C	72	GLN	C-N-CA	9.14	129.57	120.52
1	C	274	TRP	O-C-N	9.12	134.27	122.95
1	C	63	ALA	O-C-N	9.10	134.63	123.44
1	C	140	PRO	CA-N-CD	9.04	124.66	112.00
1	C	162	PRO	N-CA-C	-9.00	99.72	110.70
1	C	338	THR	CA-C-N	9.00	138.72	121.54
1	C	338	THR	C-N-CA	9.00	138.72	121.54
1	C	202	SER	CB-CA-C	-8.98	92.54	110.42
1	C	199	ASP	O-C-N	8.98	134.09	122.06
1	C	82	ILE	CA-C-N	8.96	138.65	121.54
1	C	82	ILE	C-N-CA	8.96	138.65	121.54
1	C	140	PRO	N-CA-CB	-8.81	94.00	103.25
1	C	313	GLU	CA-C-N	8.66	138.07	121.54
1	C	313	GLU	C-N-CA	8.66	138.07	121.54
1	C	329	ARG	O-C-N	8.65	134.09	122.59
1	C	288	LEU	O-C-N	8.63	132.69	122.85
1	C	165	ASP	O-C-N	8.59	133.75	123.27
1	C	69	VAL	O-C-N	-8.58	111.85	122.57
1	C	202	SER	O-C-N	8.42	133.79	122.59
1	C	202	SER	N-CA-C	8.35	128.59	110.80
1	C	291	PHE	N-CA-CB	-8.34	96.39	110.49
1	C	325	LYS	O-C-N	8.32	132.11	123.62
1	C	53	GLN	CA-C-N	-8.16	110.01	122.09
1	C	53	GLN	C-N-CA	-8.16	110.01	122.09
1	C	326	VAL	O-C-N	8.16	132.77	122.57
1	C	308	PHE	CA-C-N	-8.15	110.63	122.44
1	C	308	PHE	C-N-CA	-8.15	110.63	122.44
1	C	175	CYS	CB-CA-C	-8.12	97.78	110.04
1	C	164	ASN	N-CA-C	-7.96	103.53	113.55
1	C	62	VAL	O-C-N	7.93	129.56	121.87
1	C	317	GLY	O-C-N	-7.81	113.32	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	THR	N-CA-CB	7.74	123.57	110.49
1	C	175	CYS	O-C-N	-7.45	114.40	122.00
1	C	339	GLU	O-C-N	7.26	132.24	122.59
1	C	274	TRP	CA-C-N	7.23	138.07	121.87
1	C	274	TRP	C-N-CA	7.23	138.07	121.87
1	C	62	VAL	CB-CA-C	-7.22	102.39	112.14
1	C	90	ILE	N-CA-C	7.22	124.36	109.34
1	C	82	ILE	N-CA-CB	-7.12	99.48	111.23
1	C	56	THR	CB-CA-C	-7.08	96.34	110.42
1	C	71	THR	N-CA-CB	-7.05	98.58	110.49
1	C	278	CYS	CA-CB-SG	-7.04	98.21	114.40
1	C	305	ALA	O-C-N	6.99	131.62	123.17
1	C	323	GLY	CA-C-N	6.98	134.53	121.97
1	C	323	GLY	C-N-CA	6.98	134.53	121.97
1	C	290	LEU	CB-CA-C	-6.92	96.64	110.42
1	C	315	ALA	O-C-N	-6.92	113.38	122.59
1	C	310	VAL	O-C-N	6.92	130.53	123.20
1	C	176	VAL	N-CA-CB	-6.88	99.88	111.23
1	C	76	SER	CB-CA-C	-6.88	94.94	110.07
1	C	129	TYR	CA-C-N	6.86	134.64	121.54
1	C	129	TYR	C-N-CA	6.86	134.64	121.54
1	C	290	LEU	CA-C-N	6.81	134.55	121.54
1	C	290	LEU	C-N-CA	6.81	134.55	121.54
1	C	317	GLY	N-CA-C	-6.80	105.50	115.63
1	C	316	ALA	CA-C-N	6.80	131.94	122.29
1	C	316	ALA	C-N-CA	6.80	131.94	122.29
1	C	305	ALA	N-CA-C	6.76	119.45	109.24
1	C	220	GLY	N-CA-C	-6.73	104.19	111.93
1	C	175	CYS	CA-CB-SG	-6.66	99.08	114.40
1	C	304	ASP	O-C-N	6.61	130.97	122.71
1	C	102	LYS	CB-CA-C	6.47	123.29	110.42
1	C	130	ARG	N-CA-C	6.46	124.56	110.80
1	C	290	LEU	N-CA-C	6.44	124.51	110.80
1	C	112	GLU	O-C-N	-6.31	114.06	121.32
1	C	275	GLU	O-C-N	-6.24	116.94	123.56
1	C	318	SER	N-CA-C	6.22	124.05	110.80
1	C	53	GLN	O-C-N	-6.13	113.20	123.00
1	C	330	GLY	CA-C-N	6.05	131.44	121.39
1	C	330	GLY	C-N-CA	6.05	131.44	121.39
1	C	201	ILE	CA-C-N	-6.04	110.01	121.54
1	C	201	ILE	C-N-CA	-6.04	110.01	121.54
1	C	140	PRO	CB-CA-C	-6.01	101.64	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	VAL	CB-CA-C	6.00	121.13	111.29
1	C	298	SER	CA-C-N	-5.97	109.70	121.41
1	C	298	SER	C-N-CA	-5.97	109.70	121.41
1	C	264	SER	CB-CA-C	-5.95	99.99	109.80
1	C	81	GLY	O-C-N	5.94	130.53	123.46
1	C	75	VAL	N-CA-C	5.90	121.61	109.34
1	C	338	THR	CB-CA-C	-5.88	97.48	109.65
1	C	258	ASP	CA-C-O	5.87	121.34	117.94
1	C	99	THR	CB-CA-C	-5.84	101.30	110.94
1	C	273	GLY	N-CA-C	-5.78	99.48	113.18
1	C	130	ARG	CB-CA-C	-5.77	98.94	110.42
1	C	262	LEU	CA-C-N	5.75	132.32	121.97
1	C	262	LEU	C-N-CA	5.75	132.32	121.97
1	C	110	PRO	CB-CA-C	5.72	121.00	111.56
1	C	201	ILE	N-CA-C	5.72	121.23	109.34
1	C	271	THR	O-C-N	5.71	130.01	123.27
1	C	75	VAL	O-C-N	-5.71	115.43	122.57
1	C	327	ALA	CA-C-N	-5.66	114.66	122.30
1	C	327	ALA	C-N-CA	-5.66	114.66	122.30
1	C	350	ARG	NE-CZ-NH2	5.63	124.26	119.20
1	C	74	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	C	308	PHE	CB-CA-C	-5.61	102.05	110.24
1	C	236	VAL	O-C-N	5.60	127.90	122.69
1	C	300	LEU	CA-C-N	-5.53	113.10	122.67
1	C	300	LEU	C-N-CA	-5.53	113.10	122.67
1	C	303	ALA	O-C-N	-5.52	115.25	122.59
1	C	162	PRO	CA-C-N	-5.47	113.00	119.84
1	C	162	PRO	C-N-CA	-5.47	113.00	119.84
1	C	319	VAL	CA-C-N	-5.47	113.02	122.10
1	C	319	VAL	C-N-CA	-5.47	113.02	122.10
1	C	239	LYS	O-C-N	5.47	128.57	121.79
1	C	93	LEU	N-CA-CB	-5.43	99.49	109.10
1	C	343	LYS	O-C-N	5.40	129.77	122.59
1	C	338	THR	N-CA-CB	5.39	117.97	110.26
1	C	135	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	84	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	57	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	334	LYS	O-C-N	5.37	129.37	123.25
1	C	195	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	C	261	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	C	241	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	130	ARG	NE-CZ-NH2	5.33	124.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	THR	O-C-N	-5.32	115.51	122.59
1	C	329	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	60	ALA	O-C-N	5.32	127.43	121.32
1	C	156	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	78	ALA	O-C-N	5.30	129.63	122.59
1	C	239	LYS	N-CA-CB	5.29	118.38	110.39
1	C	79	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	C	291	PHE	CB-CA-C	5.25	120.87	110.42
1	C	341	GLN	N-CA-C	5.22	121.34	109.81
1	C	259	GLY	CA-C-O	-5.18	114.12	121.52
1	C	258	ASP	CB-CA-C	-5.16	109.64	117.07
1	C	224	ALA	O-C-N	5.16	129.10	123.27
1	C	211	LYS	N-CA-CB	5.16	117.44	110.38
1	C	202	SER	CA-C-N	5.14	131.38	122.28
1	C	202	SER	C-N-CA	5.14	131.38	122.28
1	C	343	LYS	CB-CA-C	-5.09	100.28	110.42
1	C	76	SER	CA-C-N	5.09	131.26	121.54
1	C	76	SER	C-N-CA	5.09	131.26	121.54
1	C	74	ARG	O-C-N	-5.05	117.06	123.17
1	C	334	LYS	N-CA-C	5.03	116.71	109.07

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	100	GLU	Mainchain
1	C	177	SER	Mainchain
1	C	201	ILE	Mainchain
1	C	248	ALA	Peptide,Mainchain
1	C	260	PRO	Mainchain
1	C	307	ASP	Mainchain
1	C	330	GLY	Mainchain
1	C	335	MET	Mainchain
1	C	59	SER	Mainchain
1	C	69	VAL	Mainchain
1	C	92	THR	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	C	2237	0	2191	1042	7
All	All	2237	0	2191	1042	7

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 235.

All (1042) 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:C:138:TYR:CB	1:C:184:PHE:CE1	1.75	1.66
1:C:101:PRO:CD	1:C:166:LEU:HD11	1.22	1.62
1:C:138:TYR:HB2	1:C:184:PHE:CZ	1.15	1.62
1:C:76:SER:C	1:C:76:SER:CA	1.75	1.60
1:C:75:VAL:C	1:C:75:VAL:CA	1.76	1.59
1:C:101:PRO:CD	1:C:166:LEU:CD1	1.75	1.56
1:C:130:ARG:CD	1:C:237:GLN:CB	1.82	1.53
1:C:75:VAL:CA	1:C:75:VAL:N	1.68	1.52
1:C:278:CYS:H	1:C:334:LYS:CD	1.21	1.51
1:C:101:PRO:HD3	1:C:166:LEU:CD1	1.34	1.50
1:C:76:SER:CA	1:C:76:SER:N	1.76	1.49
1:C:153:ALA:CB	1:C:174:GLY:HA3	1.43	1.48
1:C:185:ILE:HD12	1:C:186:LEU:N	1.18	1.47
1:C:80:ASP:HA	1:C:241:ARG:NH2	1.24	1.47
1:C:264:SER:C	1:C:265:TRP:N	1.68	1.46
1:C:339:GLU:C	1:C:340:GLU:N	1.68	1.46
1:C:291:PHE:C	1:C:292:TYR:N	1.71	1.46
1:C:130:ARG:CD	1:C:237:GLN:HB2	0.98	1.45
1:C:134:LEU:CA	1:C:233:GLU:O	1.66	1.43
1:C:121:LYS:NZ	1:C:121:LYS:CE	1.79	1.42
1:C:203:ASP:OD1	1:C:205:LYS:CD	1.68	1.41
1:C:279:HIS:C	1:C:280:PHE:N	1.74	1.41
1:C:296:PRO:CG	1:C:337:THR:HG22	0.96	1.40
1:C:82:ILE:C	1:C:83:THR:N	1.81	1.39
1:C:185:ILE:CD1	1:C:186:LEU:H	1.32	1.39
1:C:149:LYS:CE	1:C:149:LYS:CD	1.99	1.38
1:C:115:THR:O	1:C:116:PHE:CD1	1.76	1.38
1:C:269:LYS:O	1:C:277:ASP:CB	1.67	1.38
1:C:350:ARG:O	1:C:351:ILE:CG2	1.71	1.37
1:C:130:ARG:HD2	1:C:237:GLN:CB	1.47	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TYR:CG	1:C:184:PHE:CE1	2.12	1.36
1:C:165:ASP:O	1:C:168:SER:HB2	1.26	1.36
1:C:149:LYS:CD	1:C:170:TYR:OH	1.72	1.36
1:C:296:PRO:HG2	1:C:337:THR:CG2	0.89	1.35
1:C:153:ALA:HB1	1:C:174:GLY:CA	1.57	1.34
1:C:278:CYS:N	1:C:334:LYS:CD	1.87	1.34
1:C:130:ARG:HD3	1:C:237:GLN:CB	1.46	1.34
1:C:138:TYR:CB	1:C:184:PHE:CZ	1.96	1.34
1:C:138:TYR:CD2	1:C:184:PHE:HE1	1.46	1.33
1:C:149:LYS:HG2	1:C:177:SER:OG	1.23	1.33
1:C:327:ALA:HB3	1:C:331:GLN:CD	1.53	1.33
1:C:265:TRP:CZ3	1:C:348:ALA:O	1.82	1.33
1:C:278:CYS:H	1:C:334:LYS:CE	1.41	1.31
1:C:333:VAL:O	1:C:334:LYS:HD3	1.30	1.31
1:C:71:THR:CG2	1:C:87:SER:OG	1.78	1.31
1:C:304:ASP:O	1:C:331:GLN:HB3	1.14	1.31
1:C:309:SER:O	1:C:322:ALA:HA	1.19	1.30
1:C:291:PHE:CA	1:C:345:LYS:O	1.78	1.29
1:C:88:GLU:O	1:C:231:ARG:HB2	1.18	1.29
1:C:154:PHE:CD1	1:C:155:ASP:N	2.01	1.29
1:C:198:ALA:HB1	1:C:200:GLY:O	1.17	1.28
1:C:291:PHE:HA	1:C:345:LYS:O	1.23	1.28
1:C:105:THR:OG1	1:C:211:LYS:CD	1.82	1.27
1:C:78:ALA:O	1:C:80:ASP:N	1.63	1.27
1:C:119:LEU:CD2	1:C:234:TYR:OH	1.82	1.26
1:C:313:GLU:HG3	1:C:318:SER:CB	1.63	1.26
1:C:80:ASP:CA	1:C:241:ARG:HH22	1.49	1.25
1:C:133:SER:O	1:C:234:TYR:HA	1.28	1.25
1:C:288:LEU:HD11	1:C:290:LEU:CD2	1.66	1.25
1:C:133:SER:CB	1:C:133:SER:OG	1.81	1.25
1:C:179:VAL:HG11	1:C:181:TRP:CD1	1.71	1.25
1:C:138:TYR:HB3	1:C:184:PHE:CE1	1.51	1.24
1:C:328:GLU:O	1:C:329:ARG:O	1.55	1.24
1:C:138:TYR:OH	1:C:227:LEU:HB3	1.38	1.24
1:C:156:ARG:O	1:C:210:GLY:HA3	1.36	1.23
1:C:259:GLY:C	1:C:260:PRO:N	1.97	1.22
1:C:90:ILE:HD11	1:C:232:VAL:CG2	1.69	1.22
1:C:293:GLU:O	1:C:317:GLY:N	1.72	1.22
1:C:96:ASN:O	1:C:98:ASP:N	1.70	1.22
1:C:101:PRO:O	1:C:102:LYS:CG	1.88	1.22
1:C:154:PHE:HD1	1:C:155:ASP:N	1.32	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HB3	1:C:217:TYR:CE1	1.75	1.21
1:C:294:LYS:O	1:C:296:PRO:HD3	1.04	1.21
1:C:90:ILE:C	1:C:329:ARG:NH2	1.99	1.20
1:C:327:ALA:CB	1:C:331:GLN:OE1	1.88	1.20
1:C:138:TYR:CG	1:C:184:PHE:HE1	1.56	1.18
1:C:138:TYR:HB3	1:C:184:PHE:CD1	1.78	1.18
1:C:326:VAL:CG1	1:C:327:ALA:H	1.54	1.17
1:C:101:PRO:C	1:C:102:LYS:HG3	1.57	1.17
1:C:88:GLU:O	1:C:231:ARG:CB	1.93	1.15
1:C:179:VAL:HG11	1:C:181:TRP:NE1	1.61	1.15
1:C:105:THR:OG1	1:C:211:LYS:HD3	0.98	1.14
1:C:297:VAL:HB	1:C:336:VAL:O	1.47	1.14
1:C:309:SER:O	1:C:322:ALA:CA	1.94	1.14
1:C:138:TYR:CD2	1:C:184:PHE:CE1	2.34	1.14
1:C:249:GLN:NE2	1:C:265:TRP:CE3	2.15	1.14
1:C:116:PHE:O	1:C:120:ILE:HG21	1.46	1.13
1:C:295:ALA:N	1:C:316:ALA:HA	1.51	1.13
1:C:101:PRO:CD	1:C:166:LEU:HD12	1.73	1.13
1:C:101:PRO:HG3	1:C:217:TYR:CE2	1.83	1.13
1:C:86:GLY:HA2	1:C:234:TYR:CD1	1.83	1.12
1:C:294:LYS:O	1:C:296:PRO:CD	1.96	1.12
1:C:277:ASP:CA	1:C:334:LYS:HD2	1.77	1.12
1:C:313:GLU:HG3	1:C:318:SER:HB2	1.28	1.12
1:C:265:TRP:HZ3	1:C:348:ALA:O	1.20	1.12
1:C:326:VAL:HG12	1:C:327:ALA:N	1.60	1.12
1:C:198:ALA:CB	1:C:200:GLY:O	1.97	1.11
1:C:90:ILE:CA	1:C:329:ARG:HH22	1.62	1.11
1:C:101:PRO:O	1:C:102:LYS:HG3	0.95	1.11
1:C:126:TYR:CA	1:C:242:THR:HG22	1.80	1.11
1:C:151:ALA:HA	1:C:177:SER:HB2	1.28	1.10
1:C:295:ALA:H	1:C:316:ALA:CA	1.63	1.10
1:C:119:LEU:HD22	1:C:234:TYR:CZ	1.85	1.10
1:C:164:ASN:HD22	1:C:164:ASN:N	1.19	1.10
1:C:149:LYS:HD3	1:C:170:TYR:HH	0.97	1.10
1:C:315:ALA:CB	1:C:318:SER:HB3	1.82	1.10
1:C:116:PHE:O	1:C:120:ILE:CG2	2.00	1.10
1:C:301:GLU:O	1:C:333:VAL:HG13	1.50	1.10
1:C:339:GLU:C	1:C:340:GLU:CA	2.24	1.10
1:C:80:ASP:CA	1:C:241:ARG:NH2	2.10	1.10
1:C:69:VAL:HG12	1:C:70:SER:H	1.09	1.09
1:C:86:GLY:CA	1:C:234:TYR:CD1	2.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PRO:HD2	1:C:166:LEU:CD1	1.68	1.09
1:C:288:LEU:HD11	1:C:290:LEU:HD21	1.31	1.09
1:C:160:LYS:HG3	1:C:161:PRO:HD2	1.11	1.09
1:C:179:VAL:CG2	1:C:180:PRO:HD2	1.83	1.09
1:C:315:ALA:HB1	1:C:318:SER:N	1.67	1.09
1:C:149:LYS:HD2	1:C:170:TYR:OH	1.44	1.08
1:C:71:THR:HG21	1:C:87:SER:OG	0.92	1.08
1:C:134:LEU:HD21	1:C:188:VAL:HG21	1.08	1.08
1:C:278:CYS:N	1:C:334:LYS:HD2	1.68	1.08
1:C:130:ARG:HD3	1:C:237:GLN:CA	1.83	1.08
1:C:278:CYS:HB3	1:C:333:VAL:O	1.53	1.08
1:C:244:SER:O	1:C:245:THR:HG22	1.54	1.08
1:C:255:GLY:HA2	1:C:342:PRO:HB3	1.33	1.08
1:C:297:VAL:HB	1:C:336:VAL:HG13	1.26	1.08
1:C:149:LYS:CG	1:C:177:SER:OG	2.01	1.07
1:C:327:ALA:N	1:C:331:GLN:OE1	1.87	1.07
1:C:89:LEU:HD23	1:C:89:LEU:C	1.78	1.07
1:C:172:ILE:O	1:C:173:GLU:O	1.72	1.07
1:C:130:ARG:HB2	1:C:237:GLN:HB3	1.07	1.07
1:C:315:ALA:HB2	1:C:318:SER:HB3	1.36	1.07
1:C:69:VAL:HG12	1:C:70:SER:N	1.66	1.07
1:C:152:LEU:HD22	1:C:186:LEU:CD1	1.85	1.06
1:C:288:LEU:HD11	1:C:290:LEU:CG	1.84	1.06
1:C:297:VAL:HB	1:C:336:VAL:C	1.78	1.06
1:C:315:ALA:HB1	1:C:318:SER:H	1.16	1.06
1:C:86:GLY:HA2	1:C:234:TYR:CE1	1.90	1.05
1:C:277:ASP:HA	1:C:334:LYS:HD2	1.34	1.05
1:C:156:ARG:O	1:C:210:GLY:CA	2.03	1.05
1:C:166:LEU:O	1:C:169:LEU:N	1.88	1.05
1:C:96:ASN:OD1	1:C:216:THR:O	1.74	1.05
1:C:327:ALA:HB3	1:C:331:GLN:OE1	1.48	1.05
1:C:249:GLN:HB3	1:C:265:TRP:HZ3	1.17	1.05
1:C:291:PHE:CB	1:C:345:LYS:O	2.03	1.05
1:C:269:LYS:C	1:C:277:ASP:HB3	1.82	1.04
1:C:304:ASP:O	1:C:331:GLN:CB	2.04	1.04
1:C:252:ASP:OD2	1:C:345:LYS:HE2	1.55	1.04
1:C:278:CYS:N	1:C:334:LYS:HD3	1.71	1.04
1:C:130:ARG:HB2	1:C:237:GLN:CB	1.88	1.03
1:C:252:ASP:CG	1:C:345:LYS:HG2	1.84	1.03
1:C:179:VAL:CG1	1:C:181:TRP:CD1	2.40	1.03
1:C:254:ALA:O	1:C:256:VAL:N	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD22	1:C:234:TYR:OH	0.86	1.02
1:C:277:ASP:C	1:C:334:LYS:HD2	1.84	1.02
1:C:86:GLY:CA	1:C:234:TYR:HD1	1.68	1.02
1:C:308:PHE:CE2	1:C:310:VAL:CG2	2.42	1.02
1:C:203:ASP:CG	1:C:205:LYS:HD3	1.81	1.02
1:C:278:CYS:H	1:C:334:LYS:HD3	1.25	1.02
1:C:174:GLY:C	1:C:175:CYS:SG	2.42	1.01
1:C:85:SER:HA	1:C:234:TYR:O	1.60	1.01
1:C:154:PHE:CE1	1:C:155:ASP:C	2.39	1.01
1:C:68:GLU:OE2	1:C:137:ARG:NH2	1.94	1.01
1:C:135:ARG:HG3	1:C:233:GLU:HB3	1.43	1.01
1:C:165:ASP:O	1:C:168:SER:CB	2.07	1.01
1:C:286:PHE:HA	1:C:351:ILE:CG2	1.89	1.01
1:C:86:GLY:N	1:C:234:TYR:CD1	2.29	1.01
1:C:90:ILE:HA	1:C:329:ARG:NH2	1.76	1.00
1:C:249:GLN:HB3	1:C:265:TRP:CZ3	1.97	1.00
1:C:290:LEU:HD22	1:C:346:TRP:HB2	1.41	1.00
1:C:133:SER:O	1:C:234:TYR:CA	2.09	1.00
1:C:125:GLN:HA	1:C:243:GLY:HA2	1.37	1.00
1:C:278:CYS:N	1:C:334:LYS:CE	2.20	1.00
1:C:278:CYS:H	1:C:334:LYS:HE2	1.27	1.00
1:C:315:ALA:O	1:C:316:ALA:C	2.00	0.99
1:C:79:ARG:O	1:C:80:ASP:HB2	1.61	0.99
1:C:308:PHE:CE2	1:C:310:VAL:HG23	1.97	0.99
1:C:338:THR:OG1	1:C:339:GLU:HB2	1.60	0.99
1:C:152:LEU:HD22	1:C:186:LEU:HD13	1.45	0.99
1:C:134:LEU:CD2	1:C:188:VAL:HG21	1.91	0.99
1:C:296:PRO:CG	1:C:337:THR:CG2	1.76	0.98
1:C:350:ARG:C	1:C:351:ILE:HG22	1.86	0.98
1:C:134:LEU:HD21	1:C:188:VAL:CG2	1.91	0.98
1:C:90:ILE:HA	1:C:329:ARG:HH22	1.24	0.98
1:C:160:LYS:HG3	1:C:161:PRO:CD	1.93	0.98
1:C:278:CYS:CB	1:C:333:VAL:O	2.12	0.98
1:C:89:LEU:C	1:C:89:LEU:CD2	2.37	0.98
1:C:297:VAL:CB	1:C:336:VAL:HG13	1.41	0.98
1:C:185:ILE:CD1	1:C:186:LEU:N	2.05	0.98
1:C:143:PRO:O	1:C:146:THR:CG2	2.13	0.97
1:C:290:LEU:CD2	1:C:346:TRP:HB2	1.94	0.97
1:C:77:THR:HG22	1:C:78:ALA:N	1.78	0.97
1:C:274:TRP:NE1	1:C:339:GLU:O	1.98	0.97
1:C:149:LYS:HD3	1:C:170:TYR:OH	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LYS:HG2	1:C:270:GLY:N	1.75	0.97
1:C:95:LYS:NZ	1:C:224:ALA:HA	1.80	0.97
1:C:101:PRO:HD2	1:C:166:LEU:HD12	1.38	0.96
1:C:253:PHE:HA	1:C:258:ASP:HA	1.44	0.96
1:C:150:VAL:HG12	1:C:150:VAL:O	1.65	0.96
1:C:113:PRO:O	1:C:115:THR:N	1.99	0.96
1:C:296:PRO:HG2	1:C:337:THR:CB	1.95	0.96
1:C:163:PRO:C	1:C:164:ASN:HD22	1.73	0.96
1:C:138:TYR:HB2	1:C:184:PHE:CE2	1.99	0.95
1:C:294:LYS:C	1:C:296:PRO:HD3	1.90	0.95
1:C:113:PRO:C	1:C:115:THR:H	1.74	0.95
1:C:206:LEU:HD12	1:C:206:LEU:O	1.66	0.95
1:C:130:ARG:CB	1:C:237:GLN:HB3	1.96	0.95
1:C:164:ASN:N	1:C:164:ASN:ND2	1.88	0.95
1:C:350:ARG:O	1:C:351:ILE:HG22	0.78	0.95
1:C:149:LYS:CB	1:C:217:TYR:HE1	1.79	0.95
1:C:278:CYS:N	1:C:334:LYS:HE2	1.78	0.95
1:C:285:ASN:O	1:C:351:ILE:HG23	1.66	0.95
1:C:179:VAL:HG23	1:C:180:PRO:HD2	1.46	0.95
1:C:277:ASP:OD1	1:C:334:LYS:HE2	1.67	0.94
1:C:90:ILE:CA	1:C:329:ARG:NH2	2.26	0.94
1:C:155:ASP:HB2	1:C:172:ILE:HD11	1.47	0.94
1:C:101:PRO:HG3	1:C:217:TYR:HE2	1.28	0.94
1:C:291:PHE:HB2	1:C:346:TRP:HB3	1.48	0.94
1:C:326:VAL:HG12	1:C:327:ALA:O	1.65	0.94
1:C:130:ARG:NH1	1:C:236:VAL:O	2.00	0.94
1:C:269:LYS:O	1:C:277:ASP:HB3	0.76	0.94
1:C:101:PRO:CG	1:C:166:LEU:CD1	2.45	0.93
1:C:264:SER:C	1:C:265:TRP:CA	2.40	0.93
1:C:291:PHE:CE1	1:C:335:MET:HE1	2.02	0.93
1:C:265:TRP:O	1:C:281:LEU:N	2.02	0.93
1:C:141:MET:O	1:C:141:MET:HG3	1.66	0.93
1:C:315:ALA:CB	1:C:318:SER:CB	2.46	0.93
1:C:308:PHE:HE2	1:C:310:VAL:HG21	1.34	0.93
1:C:154:PHE:HB2	1:C:212:LEU:CD1	1.99	0.93
1:C:285:ASN:O	1:C:351:ILE:CG2	2.17	0.93
1:C:289:THR:HG23	1:C:321:TRP:CE3	2.03	0.93
1:C:338:THR:OG1	1:C:339:GLU:N	1.94	0.93
1:C:86:GLY:N	1:C:234:TYR:HD1	1.63	0.92
1:C:82:ILE:HD11	1:C:122:GLU:OE2	1.69	0.92
1:C:149:LYS:HB3	1:C:217:TYR:HE1	1.11	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:SER:C	1:C:76:SER:CB	2.43	0.91
1:C:126:TYR:HA	1:C:242:THR:HG22	1.50	0.91
1:C:286:PHE:HA	1:C:351:ILE:HG22	1.52	0.91
1:C:163:PRO:CA	1:C:164:ASN:HD22	1.82	0.91
1:C:333:VAL:O	1:C:334:LYS:CD	2.18	0.91
1:C:83:THR:HG22	1:C:84:ARG:H	1.34	0.91
1:C:134:LEU:HA	1:C:233:GLU:C	1.94	0.91
1:C:327:ALA:CB	1:C:331:GLN:CD	2.39	0.91
1:C:124:ALA:HB1	1:C:245:THR:HG22	1.51	0.91
1:C:143:PRO:O	1:C:146:THR:HG23	1.71	0.91
1:C:134:LEU:HA	1:C:233:GLU:O	0.73	0.91
1:C:119:LEU:HD22	1:C:234:TYR:HH	1.29	0.90
1:C:130:ARG:HD3	1:C:237:GLN:N	1.84	0.90
1:C:342:PRO:O	1:C:343:LYS:HD3	1.70	0.90
1:C:277:ASP:HA	1:C:334:LYS:CD	2.02	0.90
1:C:130:ARG:HH11	1:C:237:GLN:HA	1.36	0.90
1:C:296:PRO:CB	1:C:337:THR:HG22	2.00	0.90
1:C:296:PRO:CD	1:C:337:THR:HG22	2.01	0.90
1:C:134:LEU:CD2	1:C:188:VAL:CG2	2.49	0.90
1:C:126:TYR:N	1:C:242:THR:HG22	1.86	0.90
1:C:164:ASN:ND2	1:C:164:ASN:H	1.47	0.90
1:C:198:ALA:C	1:C:200:GLY:H	1.77	0.90
1:C:300:LEU:HG	1:C:308:PHE:CZ	2.06	0.89
1:C:313:GLU:CG	1:C:318:SER:CB	2.49	0.89
1:C:150:VAL:O	1:C:150:VAL:CG1	2.18	0.89
1:C:89:LEU:CD2	1:C:89:LEU:O	2.20	0.89
1:C:203:ASP:OD1	1:C:205:LYS:HD3	0.71	0.89
1:C:105:THR:HG1	1:C:211:LYS:CD	1.72	0.89
1:C:95:LYS:NZ	1:C:224:ALA:CA	2.35	0.89
1:C:130:ARG:HD3	1:C:237:GLN:HB2	0.97	0.89
1:C:244:SER:O	1:C:245:THR:CG2	2.21	0.89
1:C:133:SER:C	1:C:234:TYR:HA	1.99	0.88
1:C:274:TRP:CD1	1:C:339:GLU:O	2.25	0.88
1:C:249:GLN:CB	1:C:265:TRP:CZ3	2.56	0.88
1:C:90:ILE:CG2	1:C:329:ARG:HH12	1.85	0.88
1:C:186:LEU:HD23	1:C:187:THR:N	1.87	0.88
1:C:304:ASP:OD2	1:C:331:GLN:HA	1.73	0.88
1:C:328:GLU:C	1:C:329:ARG:O	2.14	0.88
1:C:71:THR:HG21	1:C:87:SER:CB	2.04	0.87
1:C:152:LEU:O	1:C:186:LEU:HD12	1.74	0.87
1:C:154:PHE:HB2	1:C:212:LEU:HD12	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:HG3	1:C:232:VAL:N	1.87	0.87
1:C:78:ALA:C	1:C:80:ASP:H	1.82	0.87
1:C:90:ILE:HD11	1:C:232:VAL:HG23	1.53	0.87
1:C:115:THR:O	1:C:116:PHE:HD1	1.48	0.87
1:C:199:ASP:O	1:C:262:LEU:HD23	1.74	0.87
1:C:130:ARG:HH11	1:C:237:GLN:CA	1.88	0.87
1:C:326:VAL:HG12	1:C:327:ALA:H	1.18	0.87
1:C:68:GLU:HG2	1:C:137:ARG:HH22	1.38	0.87
1:C:264:SER:CA	1:C:265:TRP:N	2.38	0.86
1:C:56:THR:HG23	1:C:57:ARG:N	1.89	0.86
1:C:109:ASN:OD1	1:C:110:PRO:HD2	1.74	0.86
1:C:130:ARG:NE	1:C:237:GLN:HB2	1.90	0.86
1:C:251:GLY:O	1:C:346:TRP:CD2	2.28	0.86
1:C:154:PHE:HE1	1:C:155:ASP:O	1.59	0.86
1:C:308:PHE:CE2	1:C:310:VAL:HG21	2.07	0.86
1:C:125:GLN:HA	1:C:243:GLY:CA	2.06	0.86
1:C:59:SER:O	1:C:61:PRO:HD3	1.74	0.85
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.38	0.85
1:C:89:LEU:O	1:C:89:LEU:HD22	1.75	0.85
1:C:296:PRO:CG	1:C:337:THR:CB	2.52	0.85
1:C:101:PRO:CG	1:C:166:LEU:HD11	2.06	0.85
1:C:69:VAL:CG1	1:C:70:SER:H	1.81	0.85
1:C:136:PHE:CE1	1:C:232:VAL:HG22	2.12	0.85
1:C:90:ILE:HD11	1:C:232:VAL:HG21	1.58	0.85
1:C:288:LEU:CD1	1:C:290:LEU:CD2	2.53	0.85
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.58	0.85
1:C:80:ASP:HA	1:C:241:ARG:CZ	2.07	0.84
1:C:82:ILE:HG21	1:C:238:LEU:HB2	1.56	0.84
1:C:95:LYS:HZ2	1:C:224:ALA:HA	1.41	0.84
1:C:269:LYS:HG2	1:C:270:GLY:H	1.42	0.84
1:C:318:SER:OG	1:C:319:VAL:N	2.07	0.84
1:C:288:LEU:HD11	1:C:290:LEU:HG	1.58	0.84
1:C:91:THR:OG1	1:C:328:GLU:HG3	1.77	0.84
1:C:77:THR:HG22	1:C:78:ALA:H	1.37	0.84
1:C:119:LEU:CD2	1:C:234:TYR:CE2	2.60	0.84
1:C:251:GLY:O	1:C:346:TRP:CE3	2.31	0.84
1:C:130:ARG:HD2	1:C:237:GLN:HB2	0.85	0.84
1:C:149:LYS:HD3	1:C:217:TYR:OH	1.78	0.84
1:C:327:ALA:CA	1:C:331:GLN:OE1	2.26	0.84
1:C:138:TYR:C	1:C:139:SER:O	2.16	0.83
1:C:291:PHE:O	1:C:292:TYR:HB3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:GLU:C	1:C:340:GLU:HA	2.04	0.83
1:C:288:LEU:CD1	1:C:290:LEU:HD21	2.08	0.83
1:C:326:VAL:HG12	1:C:327:ALA:C	2.02	0.83
1:C:288:LEU:HD21	1:C:290:LEU:HD11	1.60	0.83
1:C:55:VAL:HG22	1:C:56:THR:N	1.93	0.82
1:C:79:ARG:O	1:C:80:ASP:CB	2.27	0.82
1:C:340:GLU:O	1:C:342:PRO:HD2	1.80	0.82
1:C:249:GLN:HE22	1:C:265:TRP:N	1.77	0.82
1:C:66:TYR:CE2	1:C:183:GLY:HA3	2.14	0.82
1:C:286:PHE:HA	1:C:351:ILE:HG21	1.61	0.82
1:C:277:ASP:OD1	1:C:334:LYS:CE	2.27	0.82
1:C:300:LEU:HD11	1:C:333:VAL:CG1	2.09	0.82
1:C:277:ASP:OD1	1:C:279:HIS:ND1	2.10	0.82
1:C:95:LYS:HZ3	1:C:225:ALA:H	1.26	0.82
1:C:204:PRO:C	1:C:205:LYS:HD2	2.04	0.82
1:C:315:ALA:HB1	1:C:318:SER:CA	2.08	0.82
1:C:149:LYS:HG2	1:C:177:SER:HG	1.41	0.81
1:C:170:TYR:CE1	1:C:217:TYR:OH	2.32	0.81
1:C:315:ALA:HB1	1:C:318:SER:CB	2.07	0.81
1:C:90:ILE:O	1:C:90:ILE:HG22	1.78	0.81
1:C:169:LEU:C	1:C:169:LEU:HD23	2.04	0.81
1:C:169:LEU:O	1:C:172:ILE:HG22	1.80	0.81
1:C:285:ASN:ND2	1:C:324:VAL:O	2.13	0.81
1:C:251:GLY:O	1:C:346:TRP:CE2	2.34	0.81
1:C:101:PRO:CG	1:C:166:LEU:HD12	2.10	0.81
1:C:113:PRO:HG2	1:C:265:TRP:CD1	2.14	0.81
1:C:295:ALA:HB1	1:C:315:ALA:N	1.93	0.81
1:C:152:LEU:HD22	1:C:186:LEU:HD12	1.61	0.81
1:C:144:SER:C	1:C:146:THR:H	1.89	0.81
1:C:128:LYS:HA	1:C:195:ARG:O	1.80	0.81
1:C:130:ARG:CD	1:C:237:GLN:HB3	2.02	0.81
1:C:130:ARG:HD2	1:C:237:GLN:HE21	1.46	0.81
1:C:288:LEU:HG	1:C:289:THR:N	1.94	0.80
1:C:107:VAL:O	1:C:115:THR:HG21	1.81	0.80
1:C:296:PRO:HG3	1:C:337:THR:CG2	2.07	0.80
1:C:315:ALA:CB	1:C:318:SER:H	1.94	0.80
1:C:59:SER:C	1:C:61:PRO:HD3	2.06	0.80
1:C:95:LYS:NZ	1:C:225:ALA:N	2.28	0.80
1:C:153:ALA:CB	1:C:174:GLY:CA	2.35	0.80
1:C:96:ASN:HD21	1:C:102:LYS:HD3	1.45	0.80
1:C:119:LEU:CD2	1:C:234:TYR:CZ	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:N	1:C:242:THR:CG2	2.43	0.80
1:C:227:LEU:HD12	1:C:227:LEU:H	1.47	0.80
1:C:112:GLU:O	1:C:115:THR:HG22	1.81	0.79
1:C:101:PRO:HG3	1:C:217:TYR:CD2	2.17	0.79
1:C:249:GLN:HB3	1:C:348:ALA:O	1.83	0.79
1:C:293:GLU:O	1:C:317:GLY:CA	2.31	0.79
1:C:164:ASN:HD22	1:C:164:ASN:H	0.82	0.79
1:C:296:PRO:CD	1:C:337:THR:CG2	2.60	0.79
1:C:300:LEU:CD1	1:C:333:VAL:HG12	2.13	0.79
1:C:249:GLN:NE2	1:C:265:TRP:HE3	1.77	0.79
1:C:95:LYS:NZ	1:C:225:ALA:H	1.80	0.78
1:C:133:SER:HB3	1:C:235:THR:HG22	1.64	0.78
1:C:78:ALA:C	1:C:80:ASP:N	2.32	0.78
1:C:310:VAL:C	1:C:311:LEU:HD12	2.08	0.78
1:C:133:SER:N	1:C:235:THR:HG22	1.99	0.78
1:C:291:PHE:HB2	1:C:345:LYS:O	1.82	0.78
1:C:71:THR:HG21	1:C:87:SER:HG	0.95	0.78
1:C:179:VAL:HG11	1:C:181:TRP:HE1	1.49	0.78
1:C:296:PRO:CG	1:C:337:THR:HG21	2.06	0.78
1:C:300:LEU:HD11	1:C:333:VAL:HG12	1.63	0.78
1:C:90:ILE:CD1	1:C:232:VAL:CG2	2.58	0.78
1:C:97:THR:HA	1:C:219:GLN:CA	2.14	0.78
1:C:179:VAL:CG2	1:C:180:PRO:CD	2.62	0.78
1:C:249:GLN:HE22	1:C:265:TRP:H	1.29	0.78
1:C:249:GLN:O	1:C:348:ALA:N	2.17	0.77
1:C:149:LYS:CD	1:C:170:TYR:HH	1.71	0.77
1:C:76:SER:C	1:C:76:SER:OG	2.26	0.77
1:C:90:ILE:HG22	1:C:329:ARG:HH12	1.49	0.77
1:C:124:ALA:O	1:C:244:SER:N	2.18	0.77
1:C:163:PRO:CA	1:C:164:ASN:ND2	2.47	0.77
1:C:236:VAL:HG12	1:C:238:LEU:HD12	1.66	0.77
1:C:97:THR:HA	1:C:218:GLY:O	1.85	0.77
1:C:86:GLY:CA	1:C:234:TYR:CE1	2.66	0.76
1:C:117:ASN:ND2	1:C:117:ASN:O	2.17	0.76
1:C:154:PHE:CD1	1:C:154:PHE:C	2.62	0.76
1:C:134:LEU:O	1:C:134:LEU:HG	1.83	0.76
1:C:289:THR:O	1:C:290:LEU:HB3	1.83	0.76
1:C:175:CYS:HB2	1:C:176:VAL:HB	1.65	0.76
1:C:313:GLU:HB2	1:C:315:ALA:N	2.00	0.76
1:C:109:ASN:HD21	1:C:197:VAL:HG23	1.50	0.76
1:C:156:ARG:O	1:C:158:ALA:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HB2	1:C:185:ILE:HD11	1.67	0.76
1:C:83:THR:HG22	1:C:84:ARG:N	2.01	0.75
1:C:149:LYS:HE2	1:C:151:ALA:HA	1.66	0.75
1:C:251:GLY:O	1:C:346:TRP:CZ3	2.38	0.75
1:C:292:TYR:HB2	1:C:318:SER:O	1.86	0.75
1:C:149:LYS:HB3	1:C:217:TYR:CD1	2.20	0.75
1:C:174:GLY:C	1:C:175:CYS:HG	1.92	0.75
1:C:300:LEU:CD1	1:C:333:VAL:CG1	2.64	0.75
1:C:115:THR:O	1:C:116:PHE:CG	2.40	0.75
1:C:136:PHE:CZ	1:C:212:LEU:HD22	2.22	0.75
1:C:310:VAL:HA	1:C:321:TRP:O	1.86	0.75
1:C:314:ALA:O	1:C:315:ALA:CB	2.34	0.75
1:C:315:ALA:O	1:C:317:GLY:N	2.18	0.75
1:C:154:PHE:HD1	1:C:155:ASP:H	0.75	0.75
1:C:333:VAL:C	1:C:334:LYS:HD3	2.12	0.75
1:C:68:GLU:HG2	1:C:137:ARG:NH2	2.02	0.75
1:C:326:VAL:CG1	1:C:331:GLN:HG3	2.17	0.75
1:C:306:SER:HB3	1:C:325:LYS:HB3	1.69	0.74
1:C:301:GLU:O	1:C:333:VAL:CG1	2.34	0.74
1:C:289:THR:O	1:C:290:LEU:CB	2.35	0.74
1:C:136:PHE:CD1	1:C:232:VAL:HG22	2.23	0.74
1:C:279:HIS:CA	1:C:280:PHE:N	2.50	0.74
1:C:167:ALA:O	1:C:171:ASN:CG	2.30	0.74
1:C:271:THR:HG21	1:C:275:GLU:OE2	1.87	0.74
1:C:276:HIS:CG	1:C:277:ASP:H	2.03	0.74
1:C:75:VAL:N	1:C:75:VAL:CB	2.51	0.74
1:C:138:TYR:O	1:C:139:SER:C	2.24	0.74
1:C:109:ASN:HA	1:C:129:TYR:OH	1.88	0.74
1:C:85:SER:CA	1:C:234:TYR:O	2.36	0.74
1:C:95:LYS:HZ1	1:C:225:ALA:N	1.85	0.74
1:C:185:ILE:HD12	1:C:186:LEU:CA	2.16	0.74
1:C:277:ASP:OD1	1:C:334:LYS:NZ	2.20	0.74
1:C:71:THR:OG1	1:C:87:SER:HB2	1.87	0.73
1:C:241:ARG:HD2	1:C:241:ARG:N	2.03	0.73
1:C:75:VAL:C	1:C:75:VAL:CB	2.59	0.73
1:C:94:LYS:O	1:C:95:LYS:O	2.07	0.73
1:C:149:LYS:HE2	1:C:151:ALA:CA	2.19	0.73
1:C:297:VAL:O	1:C:298:SER:OG	2.07	0.73
1:C:252:ASP:OD2	1:C:345:LYS:CE	2.37	0.73
1:C:289:THR:C	1:C:290:LEU:HG	2.14	0.73
1:C:90:ILE:CD1	1:C:232:VAL:HG23	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:SER:CB	1:C:235:THR:HG22	2.17	0.73
1:C:149:LYS:CB	1:C:217:TYR:CE1	2.60	0.73
1:C:288:LEU:CD1	1:C:290:LEU:HG	2.17	0.73
1:C:253:PHE:CD2	1:C:346:TRP:HZ3	2.07	0.73
1:C:338:THR:OG1	1:C:339:GLU:CB	2.37	0.72
1:C:69:VAL:CG1	1:C:70:SER:N	2.38	0.72
1:C:241:ARG:HD2	1:C:241:ARG:H	1.54	0.72
1:C:149:LYS:HD3	1:C:217:TYR:CE1	2.24	0.72
1:C:174:GLY:O	1:C:175:CYS:SG	2.45	0.72
1:C:135:ARG:HB3	1:C:186:LEU:O	1.88	0.72
1:C:90:ILE:O	1:C:329:ARG:CZ	2.37	0.72
1:C:126:TYR:CA	1:C:242:THR:CG2	2.64	0.72
1:C:267:LYS:O	1:C:279:HIS:HB2	1.90	0.72
1:C:308:PHE:HE2	1:C:310:VAL:CG2	1.92	0.72
1:C:104:THR:O	1:C:105:THR:C	2.33	0.72
1:C:258:ASP:CG	1:C:259:GLY:H	1.95	0.72
1:C:276:HIS:ND1	1:C:277:ASP:N	2.38	0.72
1:C:288:LEU:CG	1:C:289:THR:N	2.50	0.72
1:C:326:VAL:HG13	1:C:331:GLN:CG	2.20	0.72
1:C:313:GLU:HG3	1:C:318:SER:HB3	1.69	0.71
1:C:132:THR:HG22	1:C:235:THR:O	1.89	0.71
1:C:55:VAL:CG2	1:C:56:THR:H	2.03	0.71
1:C:283:THR:OG1	1:C:329:ARG:HG2	1.89	0.71
1:C:308:PHE:CD2	1:C:310:VAL:HG23	2.25	0.71
1:C:127:GLU:O	1:C:128:LYS:HB2	1.89	0.71
1:C:295:ALA:CB	1:C:315:ALA:N	2.53	0.71
1:C:56:THR:HG23	1:C:57:ARG:H	1.56	0.71
1:C:179:VAL:CG2	1:C:181:TRP:HD1	2.03	0.71
1:C:238:LEU:HD12	1:C:238:LEU:N	2.05	0.71
1:C:242:THR:HG23	1:C:243:GLY:N	2.05	0.71
1:C:252:ASP:OD1	1:C:253:PHE:N	2.24	0.71
1:C:90:ILE:HG23	1:C:329:ARG:HH12	1.55	0.70
1:C:130:ARG:HD2	1:C:237:GLN:NE2	2.06	0.70
1:C:179:VAL:HG22	1:C:180:PRO:CD	2.19	0.70
1:C:290:LEU:HD22	1:C:346:TRP:CB	2.20	0.70
1:C:242:THR:HG23	1:C:243:GLY:H	1.56	0.70
1:C:201:ILE:HG21	1:C:261:ARG:CB	2.21	0.70
1:C:286:PHE:HA	1:C:350:ARG:O	1.91	0.70
1:C:137:ARG:O	1:C:230:VAL:HG13	1.91	0.70
1:C:55:VAL:CG2	1:C:56:THR:N	2.53	0.70
1:C:156:ARG:O	1:C:210:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASP:HA	1:C:241:ARG:HH22	0.70	0.70
1:C:101:PRO:CG	1:C:217:TYR:CD2	2.75	0.70
1:C:116:PHE:O	1:C:120:ILE:HG22	1.90	0.70
1:C:313:GLU:CG	1:C:318:SER:OG	2.40	0.70
1:C:169:LEU:HD23	1:C:169:LEU:O	1.90	0.70
1:C:179:VAL:HG21	1:C:181:TRP:HD1	1.56	0.70
1:C:326:VAL:HG13	1:C:331:GLN:HG3	1.74	0.70
1:C:72:GLN:HA	1:C:72:GLN:NE2	2.04	0.69
1:C:90:ILE:C	1:C:329:ARG:CZ	2.65	0.69
1:C:66:TYR:CZ	1:C:183:GLY:HA3	2.27	0.69
1:C:124:ALA:HB1	1:C:245:THR:CG2	2.20	0.69
1:C:236:VAL:HG12	1:C:237:GLN:N	2.05	0.69
1:C:149:LYS:NZ	1:C:170:TYR:CE1	2.52	0.69
1:C:326:VAL:HG13	1:C:327:ALA:H	1.54	0.69
1:C:138:TYR:CG	1:C:184:PHE:CZ	2.62	0.69
1:C:173:GLU:HG3	1:C:174:GLY:N	2.08	0.69
1:C:207:VAL:HG13	1:C:208:ASP:CG	2.18	0.69
1:C:244:SER:O	1:C:245:THR:CB	2.41	0.69
1:C:201:ILE:HD12	1:C:260:PRO:HD2	1.75	0.69
1:C:339:GLU:CA	1:C:340:GLU:N	2.53	0.69
1:C:103:TYR:HE1	1:C:169:LEU:HD12	1.56	0.69
1:C:125:GLN:C	1:C:242:THR:CG2	2.66	0.69
1:C:166:LEU:O	1:C:167:ALA:C	2.36	0.69
1:C:129:TYR:HA	1:C:237:GLN:O	1.92	0.68
1:C:155:ASP:CB	1:C:172:ILE:HD11	2.23	0.68
1:C:290:LEU:HD12	1:C:290:LEU:O	1.93	0.68
1:C:300:LEU:C	1:C:308:PHE:HZ	2.00	0.68
1:C:151:ALA:CA	1:C:177:SER:HB2	2.17	0.68
1:C:170:TYR:OH	1:C:217:TYR:OH	2.11	0.68
1:C:230:VAL:HG12	1:C:231:ARG:N	2.09	0.68
1:C:172:ILE:O	1:C:173:GLU:C	2.36	0.68
1:C:297:VAL:CB	1:C:336:VAL:O	2.36	0.68
1:C:124:ALA:O	1:C:243:GLY:HA2	1.93	0.68
1:C:143:PRO:O	1:C:146:THR:HG22	1.92	0.68
1:C:83:THR:O	1:C:84:ARG:HG2	1.94	0.68
1:C:127:GLU:O	1:C:128:LYS:CB	2.42	0.68
1:C:269:LYS:HE2	1:C:270:GLY:O	1.94	0.68
1:C:149:LYS:HD3	1:C:217:TYR:CZ	2.29	0.68
1:C:156:ARG:O	1:C:209:PHE:C	2.37	0.68
1:C:185:ILE:HD13	1:C:186:LEU:H	1.53	0.68
1:C:68:GLU:CD	1:C:137:ARG:NH2	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLN:C	1:C:242:THR:HG22	2.19	0.67
1:C:170:TYR:C	1:C:171:ASN:HD22	2.02	0.67
1:C:278:CYS:CA	1:C:333:VAL:O	2.41	0.67
1:C:291:PHE:C	1:C:292:TYR:CA	2.67	0.67
1:C:286:PHE:CA	1:C:351:ILE:HG21	2.25	0.67
1:C:95:LYS:O	1:C:96:ASN:HB2	1.95	0.67
1:C:251:GLY:O	1:C:346:TRP:CZ2	2.47	0.67
1:C:95:LYS:HZ2	1:C:224:ALA:CA	2.04	0.67
1:C:122:GLU:O	1:C:122:GLU:HG2	1.93	0.67
1:C:169:LEU:HD22	1:C:170:TYR:HD1	1.58	0.67
1:C:198:ALA:HB1	1:C:200:GLY:C	2.14	0.67
1:C:340:GLU:O	1:C:342:PRO:CD	2.43	0.67
1:C:251:GLY:O	1:C:346:TRP:CH2	2.47	0.67
1:C:130:ARG:HD2	1:C:237:GLN:HB3	1.64	0.67
1:C:253:PHE:CE2	1:C:346:TRP:CZ3	2.83	0.67
1:C:155:ASP:O	1:C:156:ARG:C	2.36	0.66
1:C:163:PRO:HA	1:C:164:ASN:ND2	2.10	0.66
1:C:186:LEU:HD23	1:C:186:LEU:C	2.20	0.66
1:C:261:ARG:O	1:C:261:ARG:HG3	1.94	0.66
1:C:297:VAL:HB	1:C:336:VAL:CG1	1.98	0.66
1:C:327:ALA:HB3	1:C:331:GLN:NE2	2.07	0.66
1:C:135:ARG:HG3	1:C:233:GLU:CB	2.23	0.66
1:C:254:ALA:N	1:C:257:LYS:O	2.27	0.66
1:C:300:LEU:CG	1:C:308:PHE:CZ	2.78	0.66
1:C:113:PRO:HG2	1:C:265:TRP:HD1	1.60	0.66
1:C:64:LEU:HD12	1:C:65:ALA:H	1.60	0.66
1:C:136:PHE:CE1	1:C:212:LEU:HD22	2.31	0.66
1:C:300:LEU:C	1:C:308:PHE:CZ	2.74	0.66
1:C:126:TYR:O	1:C:242:THR:HG21	1.95	0.66
1:C:236:VAL:HG12	1:C:238:LEU:CD1	2.26	0.66
1:C:101:PRO:C	1:C:102:LYS:CG	2.42	0.66
1:C:124:ALA:CB	1:C:245:THR:CG2	2.74	0.66
1:C:170:TYR:CZ	1:C:217:TYR:OH	2.45	0.66
1:C:291:PHE:CZ	1:C:335:MET:HE1	2.30	0.66
1:C:85:SER:C	1:C:234:TYR:CE1	2.74	0.65
1:C:66:TYR:OH	1:C:183:GLY:HA3	1.97	0.65
1:C:96:ASN:ND2	1:C:102:LYS:HD3	2.10	0.65
1:C:118:GLN:O	1:C:119:LEU:HB2	1.97	0.65
1:C:68:GLU:CG	1:C:137:ARG:NH2	2.59	0.65
1:C:153:ALA:HA	1:C:186:LEU:HD11	1.78	0.65
1:C:237:GLN:C	1:C:238:LEU:HD12	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASN:HB2	1:C:208:ASP:HB3	1.77	0.65
1:C:249:GLN:HB2	1:C:265:TRP:CZ3	2.30	0.65
1:C:264:SER:C	1:C:265:TRP:HA	2.22	0.65
1:C:169:LEU:C	1:C:169:LEU:CD2	2.70	0.65
1:C:326:VAL:HG12	1:C:327:ALA:CA	2.27	0.65
1:C:144:SER:C	1:C:146:THR:N	2.54	0.65
1:C:306:SER:O	1:C:307:ASP:O	2.14	0.65
1:C:312:GLY:HA3	1:C:320:GLN:HG2	1.78	0.65
1:C:136:PHE:HE1	1:C:232:VAL:HG22	1.59	0.64
1:C:290:LEU:CD1	1:C:290:LEU:C	2.69	0.64
1:C:152:LEU:CD2	1:C:186:LEU:HD13	2.25	0.64
1:C:253:PHE:CD2	1:C:346:TRP:CZ3	2.85	0.64
1:C:268:THR:HG23	1:C:268:THR:O	1.96	0.64
1:C:274:TRP:NE1	1:C:340:GLU:OE1	2.31	0.64
1:C:306:SER:O	1:C:307:ASP:C	2.40	0.64
1:C:68:GLU:OE2	1:C:139:SER:OG	2.14	0.64
1:C:96:ASN:C	1:C:98:ASP:N	2.55	0.64
1:C:201:ILE:CG2	1:C:261:ARG:HB2	2.28	0.64
1:C:201:ILE:HG22	1:C:261:ARG:HA	1.80	0.64
1:C:327:ALA:HB2	1:C:331:GLN:OE1	1.96	0.64
1:C:76:SER:N	1:C:76:SER:HA	2.01	0.64
1:C:196:PHE:O	1:C:207:VAL:HG23	1.97	0.64
1:C:138:TYR:O	1:C:139:SER:O	2.15	0.64
1:C:119:LEU:CD2	1:C:234:TYR:HE2	2.10	0.64
1:C:163:PRO:HG3	1:C:168:SER:HB3	1.80	0.64
1:C:154:PHE:CZ	1:C:156:ARG:HA	2.33	0.63
1:C:342:PRO:C	1:C:343:LYS:HD3	2.23	0.63
1:C:61:PRO:HD2	1:C:181:TRP:CZ3	2.33	0.63
1:C:309:SER:O	1:C:321:TRP:O	2.15	0.63
1:C:154:PHE:CE1	1:C:156:ARG:N	2.66	0.63
1:C:205:LYS:HD2	1:C:205:LYS:N	2.12	0.63
1:C:249:GLN:O	1:C:347:GLN:HA	1.98	0.63
1:C:292:TYR:CB	1:C:318:SER:O	2.47	0.63
1:C:206:LEU:O	1:C:206:LEU:CD1	2.45	0.63
1:C:135:ARG:CB	1:C:186:LEU:O	2.47	0.63
1:C:231:ARG:HG3	1:C:232:VAL:H	1.63	0.63
1:C:68:GLU:CG	1:C:137:ARG:HH22	2.12	0.62
1:C:83:THR:CG2	1:C:84:ARG:H	2.08	0.62
1:C:86:GLY:N	1:C:234:TYR:O	2.31	0.62
1:C:295:ALA:H	1:C:316:ALA:HA	0.69	0.62
1:C:309:SER:O	1:C:322:ALA:CB	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:C	1:C:214:MET:HG3	2.24	0.62
1:C:296:PRO:HG3	1:C:337:THR:HB	1.81	0.62
1:C:82:ILE:HG23	1:C:83:THR:N	2.15	0.62
1:C:166:LEU:O	1:C:168:SER:N	2.32	0.62
1:C:137:ARG:O	1:C:230:VAL:HG22	1.98	0.62
1:C:130:ARG:NH1	1:C:237:GLN:HA	2.10	0.62
1:C:163:PRO:C	1:C:164:ASN:ND2	2.44	0.62
1:C:296:PRO:HG3	1:C:337:THR:CB	2.27	0.62
1:C:82:ILE:O	1:C:83:THR:N	2.29	0.62
1:C:112:GLU:O	1:C:114:GLY:N	2.33	0.62
1:C:157:ASP:OD1	1:C:157:ASP:O	2.18	0.62
1:C:109:ASN:ND2	1:C:197:VAL:HG23	2.14	0.62
1:C:124:ALA:HB1	1:C:244:SER:O	2.00	0.62
1:C:136:PHE:CE2	1:C:212:LEU:HD11	2.35	0.62
1:C:83:THR:HG23	1:C:236:VAL:O	2.00	0.62
1:C:55:VAL:HG22	1:C:56:THR:H	1.60	0.61
1:C:98:ASP:OD1	1:C:99:THR:N	2.33	0.61
1:C:286:PHE:CD2	1:C:350:ARG:HA	2.35	0.61
1:C:154:PHE:CD1	1:C:155:ASP:C	2.78	0.61
1:C:236:VAL:CG1	1:C:237:GLN:N	2.62	0.61
1:C:277:ASP:CG	1:C:334:LYS:HZ3	2.08	0.61
1:C:136:PHE:CE2	1:C:212:LEU:CD1	2.84	0.61
1:C:90:ILE:O	1:C:329:ARG:NH2	2.33	0.61
1:C:213:ILE:O	1:C:214:MET:HG3	2.00	0.61
1:C:130:ARG:HD2	1:C:237:GLN:CG	2.27	0.61
1:C:201:ILE:HG21	1:C:261:ARG:HB2	1.81	0.61
1:C:188:VAL:HG23	1:C:188:VAL:O	1.99	0.61
1:C:306:SER:HB3	1:C:325:LYS:CB	2.27	0.61
1:C:311:LEU:HD12	1:C:311:LEU:N	2.16	0.61
1:C:95:LYS:NZ	1:C:224:ALA:CB	2.64	0.61
1:C:77:THR:CG2	1:C:78:ALA:H	2.03	0.60
1:C:314:ALA:O	1:C:315:ALA:HB2	2.00	0.60
1:C:134:LEU:HD23	1:C:188:VAL:CG2	2.31	0.60
1:C:83:THR:HG23	1:C:130:ARG:NH1	2.15	0.60
1:C:156:ARG:NH1	1:C:173:GLU:OE1	2.34	0.60
1:C:200:GLY:HA3	1:C:201:ILE:HG22	1.84	0.60
1:C:113:PRO:C	1:C:115:THR:N	2.43	0.60
1:C:124:ALA:HB2	1:C:245:THR:HG21	1.82	0.60
1:C:290:LEU:HD12	1:C:290:LEU:C	2.26	0.60
1:C:154:PHE:HE1	1:C:155:ASP:C	1.95	0.60
1:C:163:PRO:HB2	1:C:165:ASP:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD22	1:C:170:TYR:CD1	2.35	0.60
1:C:136:PHE:CD2	1:C:212:LEU:HD21	2.37	0.59
1:C:112:GLU:O	1:C:113:PRO:C	2.41	0.59
1:C:129:TYR:CB	1:C:237:GLN:O	2.49	0.59
1:C:162:PRO:C	1:C:163:PRO:O	2.42	0.59
1:C:274:TRP:CD1	1:C:339:GLU:C	2.80	0.59
1:C:105:THR:HG1	1:C:211:LYS:HD3	0.77	0.59
1:C:300:LEU:HB3	1:C:310:VAL:HG21	1.84	0.59
1:C:203:ASP:O	1:C:205:LYS:N	2.34	0.59
1:C:97:THR:CA	1:C:218:GLY:O	2.50	0.59
1:C:201:ILE:CG2	1:C:261:ARG:HA	2.33	0.59
1:C:126:TYR:C	1:C:242:THR:CG2	2.75	0.59
1:C:230:VAL:HG12	1:C:231:ARG:H	1.68	0.59
1:C:95:LYS:HZ1	1:C:224:ALA:CA	2.13	0.59
1:C:120:ILE:CG1	1:C:120:ILE:O	2.50	0.59
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.85	0.59
1:C:90:ILE:O	1:C:329:ARG:NH1	2.36	0.59
1:C:130:ARG:HB3	1:C:237:GLN:H	1.66	0.59
1:C:163:PRO:CB	1:C:164:ASN:HD22	2.15	0.59
1:C:277:ASP:HA	1:C:334:LYS:CE	2.32	0.59
1:C:130:ARG:CB	1:C:237:GLN:CB	2.68	0.59
1:C:304:ASP:CG	1:C:332:GLY:H	2.11	0.59
1:C:315:ALA:HA	1:C:318:SER:HB2	1.84	0.58
1:C:207:VAL:HG13	1:C:208:ASP:OD2	2.03	0.58
1:C:340:GLU:HA	1:C:340:GLU:OE1	2.04	0.58
1:C:85:SER:C	1:C:234:TYR:CD1	2.82	0.58
1:C:172:ILE:O	1:C:172:ILE:HG23	2.03	0.58
1:C:291:PHE:HB2	1:C:346:TRP:CB	2.29	0.58
1:C:138:TYR:HE2	1:C:180:PRO:HA	1.68	0.58
1:C:313:GLU:HB2	1:C:314:ALA:C	2.29	0.58
1:C:336:VAL:O	1:C:336:VAL:HG13	2.03	0.58
1:C:179:VAL:HG21	1:C:181:TRP:CD1	2.37	0.58
1:C:326:VAL:CG1	1:C:327:ALA:O	2.48	0.58
1:C:280:PHE:HD2	1:C:331:GLN:O	1.87	0.57
1:C:338:THR:HG1	1:C:339:GLU:HB2	1.68	0.57
1:C:217:TYR:CD1	1:C:217:TYR:N	2.69	0.57
1:C:185:ILE:HD12	1:C:186:LEU:H	0.65	0.57
1:C:302:ASN:CB	1:C:333:VAL:HG22	2.34	0.57
1:C:238:LEU:N	1:C:238:LEU:CD1	2.67	0.57
1:C:136:PHE:HB3	1:C:230:VAL:HG11	1.87	0.57
1:C:265:TRP:CH2	1:C:348:ALA:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:HA	1:C:236:VAL:O	2.03	0.57
1:C:94:LYS:O	1:C:95:LYS:C	2.48	0.57
1:C:307:ASP:O	1:C:323:GLY:O	2.21	0.57
1:C:61:PRO:HD2	1:C:181:TRP:HZ3	1.67	0.57
1:C:78:ALA:O	1:C:80:ASP:CA	2.52	0.57
1:C:258:ASP:CG	1:C:259:GLY:N	2.58	0.57
1:C:295:ALA:HB1	1:C:314:ALA:C	2.30	0.57
1:C:126:TYR:C	1:C:242:THR:HG22	2.30	0.57
1:C:152:LEU:CD1	1:C:184:PHE:HE2	2.18	0.57
1:C:201:ILE:CG2	1:C:261:ARG:CB	2.82	0.57
1:C:138:TYR:HA	1:C:230:VAL:HG22	1.86	0.56
1:C:250:ILE:HA	1:C:347:GLN:HA	1.87	0.56
1:C:179:VAL:CG1	1:C:181:TRP:HD1	2.14	0.56
1:C:90:ILE:HG22	1:C:329:ARG:NH1	2.18	0.56
1:C:125:GLN:C	1:C:242:THR:HG23	2.30	0.56
1:C:248:ALA:HB2	1:C:349:LEU:HA	1.87	0.56
1:C:166:LEU:C	1:C:168:SER:N	2.61	0.56
1:C:198:ALA:CA	1:C:200:GLY:O	2.54	0.56
1:C:82:ILE:CG2	1:C:238:LEU:HB2	2.32	0.56
1:C:285:ASN:HD22	1:C:286:PHE:N	2.03	0.56
1:C:154:PHE:CE1	1:C:155:ASP:O	2.41	0.56
1:C:124:ALA:CB	1:C:245:THR:HG21	2.35	0.56
1:C:138:TYR:HH	1:C:227:LEU:HB3	1.66	0.56
1:C:152:LEU:HD12	1:C:184:PHE:HE2	1.70	0.56
1:C:153:ALA:HB1	1:C:174:GLY:HA3	0.62	0.56
1:C:149:LYS:CE	1:C:151:ALA:HA	2.35	0.56
1:C:145:THR:CG2	1:C:145:THR:O	2.54	0.55
1:C:300:LEU:CA	1:C:308:PHE:HZ	2.19	0.55
1:C:313:GLU:CG	1:C:318:SER:HB2	2.19	0.55
1:C:201:ILE:CD1	1:C:260:PRO:HD2	2.36	0.55
1:C:104:THR:O	1:C:105:THR:O	2.24	0.55
1:C:120:ILE:O	1:C:120:ILE:HG13	2.05	0.55
1:C:227:LEU:H	1:C:227:LEU:CD1	2.17	0.55
1:C:277:ASP:HA	1:C:334:LYS:NZ	2.21	0.55
1:C:77:THR:CG2	1:C:78:ALA:N	2.49	0.55
1:C:116:PHE:HE2	1:C:234:TYR:CE2	2.24	0.55
1:C:300:LEU:HD12	1:C:333:VAL:CG1	2.36	0.55
1:C:95:LYS:HZ1	1:C:224:ALA:HB1	1.71	0.55
1:C:302:ASN:HB2	1:C:333:VAL:HG22	1.88	0.55
1:C:306:SER:HB2	1:C:325:LYS:H	1.72	0.55
1:C:309:SER:C	1:C:322:ALA:HA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLU:O	1:C:101:PRO:O	2.25	0.54
1:C:197:VAL:HG22	1:C:198:ALA:H	1.72	0.54
1:C:156:ARG:O	1:C:209:PHE:O	2.26	0.54
1:C:197:VAL:HG22	1:C:198:ALA:N	2.23	0.54
1:C:300:LEU:CB	1:C:308:PHE:HZ	2.20	0.54
1:C:341:GLN:O	1:C:343:LYS:HG2	2.07	0.54
1:C:289:THR:HG23	1:C:321:TRP:CZ3	2.41	0.54
1:C:191:ASP:OD1	1:C:209:PHE:CZ	2.61	0.54
1:C:276:HIS:CG	1:C:277:ASP:N	2.74	0.54
1:C:274:TRP:CD1	1:C:339:GLU:HA	2.42	0.54
1:C:90:ILE:C	1:C:329:ARG:HH22	1.87	0.54
1:C:95:LYS:NZ	1:C:224:ALA:HB1	2.22	0.54
1:C:213:ILE:O	1:C:214:MET:CG	2.56	0.54
1:C:90:ILE:CG2	1:C:90:ILE:O	2.54	0.54
1:C:97:THR:O	1:C:97:THR:OG1	2.25	0.54
1:C:133:SER:HB3	1:C:235:THR:CG2	2.35	0.54
1:C:138:TYR:HD2	1:C:184:PHE:CE1	2.16	0.54
1:C:173:GLU:HG3	1:C:174:GLY:H	1.73	0.54
1:C:291:PHE:C	1:C:292:TYR:HB3	2.33	0.54
1:C:170:TYR:HE1	1:C:217:TYR:OH	1.86	0.53
1:C:199:ASP:OD1	1:C:199:ASP:N	2.40	0.53
1:C:157:ASP:OD1	1:C:157:ASP:C	2.50	0.53
1:C:300:LEU:O	1:C:308:PHE:CZ	2.61	0.53
1:C:100:GLU:O	1:C:101:PRO:C	2.48	0.53
1:C:109:ASN:O	1:C:110:PRO:C	2.51	0.53
1:C:113:PRO:HG3	1:C:120:ILE:CD1	2.39	0.53
1:C:244:SER:C	1:C:245:THR:HG22	2.31	0.53
1:C:130:ARG:O	1:C:131:PHE:HB2	2.08	0.53
1:C:179:VAL:HG22	1:C:180:PRO:N	2.23	0.53
1:C:179:VAL:HG13	1:C:181:TRP:CD1	2.38	0.53
1:C:82:ILE:HG12	1:C:83:THR:N	2.24	0.53
1:C:142:SER:HB3	1:C:227:LEU:O	2.09	0.53
1:C:150:VAL:O	1:C:151:ALA:C	2.52	0.53
1:C:136:PHE:CZ	1:C:212:LEU:CD2	2.91	0.53
1:C:269:LYS:HB3	1:C:277:ASP:OD2	2.09	0.53
1:C:179:VAL:CG1	1:C:182:THR:HG22	2.39	0.52
1:C:339:GLU:O	1:C:340:GLU:HA	2.08	0.52
1:C:109:ASN:CA	1:C:129:TYR:OH	2.55	0.52
1:C:112:GLU:HB3	1:C:115:THR:CG2	2.39	0.52
1:C:135:ARG:CB	1:C:185:ILE:HD11	2.38	0.52
1:C:293:GLU:O	1:C:317:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ALA:O	1:C:81:GLY:N	2.42	0.52
1:C:293:GLU:HA	1:C:317:GLY:HA2	1.91	0.52
1:C:71:THR:CG2	1:C:87:SER:CB	2.77	0.52
1:C:115:THR:C	1:C:116:PHE:CD1	2.78	0.52
1:C:128:LYS:O	1:C:129:TYR:HB3	2.10	0.52
1:C:149:LYS:CD	1:C:177:SER:OG	2.50	0.52
1:C:152:LEU:HD12	1:C:184:PHE:CE2	2.45	0.52
1:C:154:PHE:CB	1:C:212:LEU:HD12	2.35	0.52
1:C:158:ALA:C	1:C:211:LYS:H	1.93	0.52
1:C:304:ASP:OD2	1:C:332:GLY:N	2.43	0.52
1:C:339:GLU:O	1:C:340:GLU:OE1	2.27	0.52
1:C:300:LEU:CG	1:C:308:PHE:HZ	2.20	0.52
1:C:54:LYS:O	1:C:55:VAL:HB	2.08	0.52
1:C:239:LYS:O	1:C:240:ASN:O	2.28	0.52
1:C:82:ILE:HD12	1:C:126:TYR:CE2	2.44	0.52
1:C:149:LYS:HE2	1:C:151:ALA:CB	2.39	0.52
1:C:248:ALA:HB1	1:C:348:ALA:O	2.09	0.52
1:C:271:THR:CG2	1:C:275:GLU:OE2	2.56	0.52
1:C:295:ALA:N	1:C:316:ALA:CA	2.40	0.52
1:C:130:ARG:HH11	1:C:236:VAL:C	2.16	0.52
1:C:333:VAL:C	1:C:334:LYS:CD	2.78	0.52
1:C:84:ARG:HG3	1:C:119:LEU:HD11	1.91	0.51
1:C:179:VAL:HG13	1:C:182:THR:HG22	1.90	0.51
1:C:273:GLY:O	1:C:274:TRP:C	2.53	0.51
1:C:185:ILE:CD1	1:C:186:LEU:O	2.58	0.51
1:C:236:VAL:CG1	1:C:237:GLN:H	2.23	0.51
1:C:244:SER:O	1:C:245:THR:HB	2.08	0.51
1:C:300:LEU:O	1:C:308:PHE:CE2	2.63	0.51
1:C:56:THR:CG2	1:C:57:ARG:N	2.58	0.51
1:C:83:THR:CB	1:C:130:ARG:HH12	2.24	0.51
1:C:138:TYR:CZ	1:C:150:VAL:HG21	2.45	0.51
1:C:90:ILE:HD11	1:C:232:VAL:HG22	1.83	0.51
1:C:91:THR:HB	1:C:329:ARG:NE	2.25	0.51
1:C:154:PHE:CD1	1:C:155:ASP:CA	2.90	0.51
1:C:185:ILE:HD12	1:C:186:LEU:C	2.36	0.51
1:C:288:LEU:C	1:C:289:THR:OG1	2.49	0.51
1:C:136:PHE:HB3	1:C:230:VAL:CG1	2.40	0.51
1:C:230:VAL:CG1	1:C:231:ARG:N	2.74	0.51
1:C:149:LYS:HD3	1:C:217:TYR:HE1	1.73	0.51
1:C:188:VAL:CG2	1:C:188:VAL:O	2.59	0.51
1:C:224:ALA:O	1:C:225:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:H	1:C:241:ARG:CD	2.22	0.51
1:C:93:LEU:HD12	1:C:138:TYR:HE1	1.75	0.51
1:C:235:THR:O	1:C:235:THR:HG23	2.09	0.51
1:C:172:ILE:C	1:C:173:GLU:O	2.51	0.51
1:C:243:GLY:O	1:C:244:SER:HB2	2.11	0.51
1:C:103:TYR:CD1	1:C:215:ALA:HB2	2.46	0.50
1:C:128:LYS:HG3	1:C:196:PHE:CD2	2.46	0.50
1:C:85:SER:O	1:C:234:TYR:CE1	2.65	0.50
1:C:95:LYS:HZ2	1:C:224:ALA:CB	2.24	0.50
1:C:125:GLN:CA	1:C:243:GLY:HA2	2.27	0.50
1:C:314:ALA:O	1:C:315:ALA:HB3	2.11	0.50
1:C:74:ARG:C	1:C:75:VAL:HG23	2.37	0.50
1:C:126:TYR:C	1:C:242:THR:HG21	2.37	0.50
1:C:129:TYR:CA	1:C:237:GLN:O	2.57	0.50
1:C:95:LYS:HZ1	1:C:224:ALA:C	2.19	0.50
1:C:100:GLU:C	1:C:101:PRO:O	2.54	0.50
1:C:144:SER:O	1:C:146:THR:N	2.44	0.50
1:C:101:PRO:CB	1:C:217:TYR:CD2	2.94	0.50
1:C:130:ARG:CB	1:C:237:GLN:N	2.74	0.50
1:C:167:ALA:O	1:C:171:ASN:ND2	2.45	0.49
1:C:300:LEU:CB	1:C:308:PHE:CZ	2.95	0.49
1:C:86:GLY:HA2	1:C:234:TYR:HE1	1.68	0.49
1:C:295:ALA:HB2	1:C:315:ALA:CB	2.38	0.49
1:C:66:TYR:HE2	1:C:183:GLY:HA3	1.73	0.49
1:C:153:ALA:CA	1:C:174:GLY:HA3	2.33	0.49
1:C:279:HIS:HB3	1:C:280:PHE:N	2.27	0.49
1:C:285:ASN:HD22	1:C:286:PHE:H	1.58	0.49
1:C:150:VAL:CG2	1:C:227:LEU:HD23	2.43	0.49
1:C:71:THR:OG1	1:C:87:SER:CB	2.59	0.49
1:C:107:VAL:HA	1:C:211:LYS:HA	1.93	0.49
1:C:130:ARG:CB	1:C:237:GLN:H	2.25	0.49
1:C:151:ALA:HA	1:C:177:SER:CB	2.21	0.49
1:C:296:PRO:CD	1:C:337:THR:HG21	2.39	0.49
1:C:85:SER:O	1:C:234:TYR:HE1	1.96	0.49
1:C:150:VAL:HG23	1:C:227:LEU:HD23	1.94	0.49
1:C:350:ARG:O	1:C:351:ILE:CB	2.53	0.49
1:C:185:ILE:HD12	1:C:185:ILE:C	2.14	0.49
1:C:116:PHE:CE2	1:C:234:TYR:CE2	3.00	0.49
1:C:249:GLN:O	1:C:347:GLN:CA	2.61	0.49
1:C:291:PHE:CG	1:C:345:LYS:O	2.64	0.49
1:C:133:SER:O	1:C:234:TYR:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:N	1:C:241:ARG:CD	2.75	0.49
1:C:119:LEU:HD23	1:C:234:TYR:CE2	2.43	0.48
1:C:293:GLU:O	1:C:316:ALA:C	2.52	0.48
1:C:198:ALA:C	1:C:200:GLY:N	2.55	0.48
1:C:291:PHE:C	1:C:292:TYR:CB	2.86	0.48
1:C:350:ARG:C	1:C:351:ILE:CG2	2.58	0.48
1:C:86:GLY:N	1:C:234:TYR:CE1	2.74	0.48
1:C:83:THR:HG23	1:C:130:ARG:CZ	2.44	0.48
1:C:84:ARG:HD2	1:C:119:LEU:HD13	1.94	0.48
1:C:103:TYR:CE1	1:C:169:LEU:HD12	2.43	0.48
1:C:107:VAL:O	1:C:115:THR:CG2	2.56	0.48
1:C:204:PRO:N	1:C:205:LYS:HD2	2.28	0.48
1:C:278:CYS:CA	1:C:334:LYS:HD3	2.42	0.48
1:C:290:LEU:HB2	1:C:346:TRP:HA	1.96	0.48
1:C:336:VAL:C	1:C:337:THR:HG23	2.37	0.48
1:C:101:PRO:CG	1:C:217:TYR:CE2	2.74	0.48
1:C:163:PRO:CG	1:C:168:SER:CB	2.92	0.48
1:C:264:SER:OG	1:C:265:TRP:N	2.45	0.48
1:C:95:LYS:HZ1	1:C:224:ALA:CB	2.26	0.48
1:C:136:PHE:HD1	1:C:231:ARG:O	1.95	0.48
1:C:336:VAL:O	1:C:337:THR:CG2	2.62	0.48
1:C:88:GLU:OE2	1:C:118:GLN:HB3	2.13	0.48
1:C:111:SER:HB3	1:C:197:VAL:CG2	2.44	0.48
1:C:163:PRO:HB2	1:C:165:ASP:N	2.28	0.48
1:C:269:LYS:CG	1:C:270:GLY:N	2.58	0.48
1:C:92:THR:HG23	1:C:93:LEU:O	2.14	0.47
1:C:114:GLY:HA3	1:C:281:LEU:O	2.13	0.47
1:C:336:VAL:O	1:C:337:THR:HG23	2.14	0.47
1:C:130:ARG:HB3	1:C:237:GLN:N	2.30	0.47
1:C:101:PRO:CG	1:C:217:TYR:HD2	2.26	0.47
1:C:170:TYR:C	1:C:171:ASN:ND2	2.72	0.47
1:C:130:ARG:NH1	1:C:236:VAL:C	2.70	0.47
1:C:185:ILE:HD11	1:C:186:LEU:O	2.15	0.47
1:C:269:LYS:HG2	1:C:270:GLY:O	2.14	0.47
1:C:105:THR:O	1:C:105:THR:HG23	2.14	0.47
1:C:136:PHE:CE2	1:C:212:LEU:CD2	2.98	0.47
1:C:134:LEU:CD2	1:C:188:VAL:HG22	2.41	0.47
1:C:150:VAL:O	1:C:151:ALA:O	2.32	0.47
1:C:244:SER:OG	1:C:245:THR:N	2.46	0.47
1:C:278:CYS:N	1:C:333:VAL:O	2.48	0.47
1:C:291:PHE:CD1	1:C:292:TYR:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:THR:O	1:C:290:LEU:HG	2.14	0.47
1:C:107:VAL:HG22	1:C:211:LYS:HB3	1.97	0.47
1:C:144:SER:HA	1:C:181:TRP:HB3	1.96	0.47
1:C:162:PRO:O	1:C:163:PRO:O	2.33	0.47
1:C:179:VAL:CG2	1:C:181:TRP:CD1	2.93	0.47
1:C:290:LEU:HD23	1:C:346:TRP:HB2	1.90	0.47
1:C:152:LEU:O	1:C:186:LEU:CD1	2.55	0.46
1:C:271:THR:HG23	1:C:275:GLU:HG2	1.97	0.46
1:C:313:GLU:HG3	1:C:315:ALA:HA	1.97	0.46
1:C:71:THR:HG23	1:C:71:THR:O	2.16	0.46
1:C:174:GLY:O	1:C:175:CYS:CB	2.64	0.46
1:C:186:LEU:C	1:C:186:LEU:CD2	2.87	0.46
1:C:234:TYR:CD2	1:C:236:VAL:HG23	2.50	0.46
1:C:149:LYS:O	1:C:216:THR:HA	2.15	0.46
1:C:169:LEU:C	1:C:171:ASN:H	2.22	0.46
1:C:292:TYR:CD1	1:C:292:TYR:C	2.94	0.46
1:C:338:THR:OG1	1:C:339:GLU:CA	2.63	0.46
1:C:133:SER:N	1:C:235:THR:CG2	2.74	0.46
1:C:291:PHE:HD2	1:C:346:TRP:HE3	1.63	0.46
1:C:136:PHE:CE2	1:C:212:LEU:HD21	2.51	0.46
1:C:149:LYS:HE2	1:C:151:ALA:HB2	1.96	0.46
1:C:290:LEU:HD13	1:C:291:PHE:HB3	1.98	0.46
1:C:163:PRO:CG	1:C:168:SER:HB3	2.44	0.46
1:C:230:VAL:CG1	1:C:231:ARG:H	2.28	0.46
1:C:249:GLN:CG	1:C:263:VAL:O	2.64	0.46
1:C:279:HIS:CB	1:C:280:PHE:N	2.78	0.46
1:C:280:PHE:HZ	1:C:324:VAL:HG21	1.81	0.46
1:C:127:GLU:O	1:C:128:LYS:CG	2.64	0.45
1:C:133:SER:CA	1:C:235:THR:HG22	2.47	0.45
1:C:181:TRP:CE3	1:C:181:TRP:O	2.69	0.45
1:C:249:GLN:NE2	1:C:265:TRP:N	2.54	0.45
1:C:90:ILE:CG2	1:C:329:ARG:NH1	2.67	0.45
1:C:89:LEU:HA	1:C:230:VAL:O	2.17	0.45
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.71	0.45
1:C:84:ARG:CD	1:C:119:LEU:HD13	2.46	0.45
1:C:109:ASN:OD1	1:C:129:TYR:OH	2.32	0.45
1:C:236:VAL:CG1	1:C:238:LEU:CD1	2.94	0.45
1:C:118:GLN:O	1:C:118:GLN:HG2	2.17	0.45
1:C:153:ALA:HB2	1:C:175:CYS:N	2.32	0.45
1:C:254:ALA:O	1:C:257:LYS:N	2.38	0.45
1:C:315:ALA:O	1:C:318:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:O	1:C:328:GLU:OE2	2.35	0.45
1:C:101:PRO:CD	1:C:217:TYR:HD2	2.30	0.45
1:C:68:GLU:CD	1:C:139:SER:OG	2.59	0.44
1:C:112:GLU:O	1:C:112:GLU:HG3	2.16	0.44
1:C:203:ASP:CG	1:C:205:LYS:CD	2.64	0.44
1:C:253:PHE:HZ	1:C:268:THR:HG21	1.82	0.44
1:C:277:ASP:CG	1:C:279:HIS:HD1	2.18	0.44
1:C:326:VAL:HG13	1:C:331:GLN:OE1	2.17	0.44
1:C:105:THR:HA	1:C:212:LEU:O	2.18	0.44
1:C:271:THR:CG2	1:C:275:GLU:HG2	2.47	0.44
1:C:213:ILE:HG23	1:C:214:MET:N	2.32	0.44
1:C:259:GLY:C	1:C:260:PRO:CD	2.84	0.44
1:C:95:LYS:NZ	1:C:224:ALA:C	2.76	0.44
1:C:109:ASN:O	1:C:111:SER:N	2.50	0.44
1:C:295:ALA:HB2	1:C:315:ALA:HB3	1.99	0.44
1:C:119:LEU:C	1:C:121:LYS:H	2.25	0.44
1:C:101:PRO:HD3	1:C:166:LEU:HD11	0.47	0.44
1:C:163:PRO:HG3	1:C:168:SER:CB	2.47	0.44
1:C:137:ARG:N	1:C:230:VAL:HG13	2.33	0.44
1:C:201:ILE:HG22	1:C:261:ARG:CA	2.46	0.44
1:C:341:GLN:O	1:C:342:PRO:C	2.58	0.44
1:C:72:GLN:HE21	1:C:73:PRO:HD2	1.83	0.43
1:C:84:ARG:NE	1:C:119:LEU:CD1	2.81	0.43
1:C:101:PRO:HB3	1:C:217:TYR:CD2	2.53	0.43
1:C:152:LEU:C	1:C:186:LEU:HD12	2.40	0.43
1:C:56:THR:HG23	1:C:57:ARG:HB3	1.99	0.43
1:C:130:ARG:HD2	1:C:237:GLN:CD	2.43	0.43
1:C:130:ARG:HD3	1:C:236:VAL:C	2.40	0.43
1:C:154:PHE:CZ	1:C:156:ARG:CA	3.01	0.43
1:C:277:ASP:HA	1:C:334:LYS:HZ2	1.83	0.43
1:C:333:VAL:C	1:C:334:LYS:CG	2.91	0.43
1:C:336:VAL:O	1:C:336:VAL:CG1	2.66	0.43
1:C:149:LYS:CG	1:C:217:TYR:HE1	2.29	0.43
1:C:243:GLY:O	1:C:244:SER:CB	2.67	0.43
1:C:269:LYS:O	1:C:277:ASP:CA	2.57	0.43
1:C:70:SER:O	1:C:71:THR:C	2.62	0.43
1:C:76:SER:OG	1:C:77:THR:N	2.50	0.43
1:C:109:ASN:CG	1:C:110:PRO:HD2	2.40	0.43
1:C:325:LYS:O	1:C:325:LYS:HG2	2.18	0.43
1:C:121:LYS:HG3	1:C:121:LYS:O	2.19	0.43
1:C:201:ILE:CG2	1:C:261:ARG:CA	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:SER:HA	1:C:231:ARG:HD2	2.01	0.43
1:C:125:GLN:HA	1:C:243:GLY:N	2.34	0.43
1:C:278:CYS:O	1:C:333:VAL:O	2.37	0.43
1:C:154:PHE:CE1	1:C:156:ARG:CA	3.02	0.43
1:C:216:THR:OG1	1:C:227:LEU:HD21	2.18	0.43
1:C:242:THR:CG2	1:C:243:GLY:N	2.73	0.43
1:C:269:LYS:C	1:C:277:ASP:CB	2.63	0.43
1:C:236:VAL:CG1	1:C:238:LEU:HD11	2.49	0.42
1:C:258:ASP:OD1	1:C:259:GLY:N	2.52	0.42
1:C:95:LYS:HB3	1:C:96:ASN:H	1.60	0.42
1:C:137:ARG:O	1:C:230:VAL:HA	2.19	0.42
1:C:96:ASN:O	1:C:96:ASN:ND2	2.51	0.42
1:C:111:SER:HB3	1:C:197:VAL:HG21	2.02	0.42
1:C:315:ALA:CA	1:C:318:SER:CB	2.97	0.42
1:C:278:CYS:O	1:C:333:VAL:N	2.34	0.42
1:C:60:ALA:HA	1:C:61:PRO:HD2	1.81	0.42
1:C:302:ASN:HB3	1:C:308:PHE:CE1	2.55	0.42
1:C:94:LYS:C	1:C:95:LYS:O	2.63	0.42
1:C:269:LYS:CE	1:C:270:GLY:O	2.63	0.42
1:C:273:GLY:O	1:C:275:GLU:HB3	2.19	0.42
1:C:75:VAL:HG12	1:C:76:SER:N	2.35	0.42
1:C:163:PRO:CG	1:C:168:SER:HB2	2.50	0.42
1:C:315:ALA:CA	1:C:318:SER:HB2	2.49	0.42
1:C:150:VAL:C	1:C:151:ALA:O	2.62	0.42
1:C:248:ALA:HB2	1:C:349:LEU:HD23	2.01	0.42
1:C:293:GLU:CA	1:C:317:GLY:HA2	2.50	0.42
1:C:315:ALA:C	1:C:318:SER:H	2.28	0.42
1:C:288:LEU:O	1:C:289:THR:OG1	2.37	0.42
1:C:289:THR:CG2	1:C:321:TRP:CZ3	3.03	0.42
1:C:157:ASP:C	1:C:159:ALA:H	2.27	0.41
1:C:266:SER:HA	1:C:280:PHE:HA	2.02	0.41
1:C:309:SER:O	1:C:321:TRP:C	2.63	0.41
1:C:93:LEU:CD1	1:C:138:TYR:HE1	2.33	0.41
1:C:291:PHE:CD2	1:C:345:LYS:O	2.73	0.41
1:C:341:GLN:HE21	1:C:341:GLN:HB2	1.72	0.41
1:C:231:ARG:CG	1:C:232:VAL:H	2.27	0.41
1:C:55:VAL:O	1:C:57:ARG:N	2.52	0.41
1:C:66:TYR:HE2	1:C:183:GLY:CA	2.32	0.41
1:C:135:ARG:N	1:C:233:GLU:O	2.54	0.41
1:C:71:THR:CG2	1:C:87:SER:HG	1.90	0.41
1:C:252:ASP:OD2	1:C:345:LYS:HG2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:HG12	1:C:336:VAL:HG11	0.98	0.41
1:C:313:GLU:HB2	1:C:315:ALA:CA	2.50	0.41
1:C:128:LYS:O	1:C:238:LEU:HA	2.21	0.41
1:C:264:SER:OG	1:C:265:TRP:CA	2.69	0.41
1:C:95:LYS:HZ3	1:C:225:ALA:N	1.97	0.41
1:C:101:PRO:HG2	1:C:166:LEU:HD12	1.94	0.41
1:C:339:GLU:O	1:C:340:GLU:CA	2.60	0.41
1:C:93:LEU:CD1	1:C:138:TYR:CE1	3.03	0.41
1:C:130:ARG:HB2	1:C:237:GLN:CA	2.49	0.41
1:C:136:PHE:CG	1:C:212:LEU:HD21	2.56	0.41
1:C:185:ILE:HD12	1:C:186:LEU:O	2.20	0.41
1:C:291:PHE:CE1	1:C:335:MET:CE	2.90	0.41
1:C:343:LYS:HB2	1:C:344:GLY:H	1.13	0.41
1:C:86:GLY:O	1:C:87:SER:CB	2.69	0.41
1:C:88:GLU:O	1:C:231:ARG:HB3	2.05	0.41
1:C:90:ILE:CG2	1:C:329:ARG:HH22	2.34	0.41
1:C:91:THR:HG23	1:C:92:THR:N	2.36	0.41
1:C:302:ASN:HB3	1:C:308:PHE:CD1	2.56	0.41
1:C:149:LYS:CD	1:C:217:TYR:HE1	2.33	0.40
1:C:120:ILE:HG21	1:C:120:ILE:HD13	1.87	0.40
1:C:268:THR:O	1:C:268:THR:CG2	2.66	0.40
1:C:75:VAL:N	1:C:75:VAL:CG2	2.84	0.40
1:C:82:ILE:HD13	1:C:238:LEU:HD22	2.03	0.40
1:C:130:ARG:HB3	1:C:131:PHE:H	1.46	0.40
1:C:249:GLN:HG3	1:C:263:VAL:O	2.21	0.40
1:C:326:VAL:HG13	1:C:331:GLN:CD	2.46	0.40
1:C:93:LEU:HD12	1:C:138:TYR:CE1	2.54	0.40
1:C:252:ASP:O	1:C:258:ASP:C	2.64	0.40

All (7) 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:C:319:VAL:CG1	1:C:319:VAL:CG1[2_555]	0.84	1.36
1:C:349:LEU:CD1	1:C:349:LEU:CD1[2_555]	0.89	1.31
1:C:319:VAL:CG2	1:C:319:VAL:CG2[2_555]	1.90	0.30
1:C:349:LEU:CG	1:C:349:LEU:CD1[2_555]	1.99	0.21
1:C:319:VAL:CB	1:C:319:VAL:CG1[2_555]	2.05	0.15
1:C:292:TYR:OH	1:C:311:LEU:CD2[2_555]	2.07	0.13
1:C:72:GLN:NE2	1:C:241:ARG:CG[2_555]	2.12	0.08

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	C	293/347 (84%)	162 (55%)	65 (22%)	66 (22%)	0 0

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	VAL
1	C	56	THR
1	C	77	THR
1	C	79	ARG
1	C	80	ASP
1	C	83	THR
1	C	87	SER
1	C	90	ILE
1	C	95	LYS
1	C	96	ASN
1	C	97	THR
1	C	119	LEU
1	C	128	LYS
1	C	140	PRO
1	C	157	ASP
1	C	160	LYS
1	C	166	LEU
1	C	173	GLU
1	C	202	SER
1	C	209	PHE
1	C	227	LEU
1	C	240	ASN
1	C	244	SER
1	C	245	THR
1	C	246	SER
1	C	255	GLY
1	C	290	LEU
1	C	293	GLU

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Mol	Chain	Res	Type
1	C	295	ALA
1	C	307	ASP
1	C	316	ALA
1	C	329	ARG
1	C	339	GLU
1	C	341	GLN
1	C	69	VAL
1	C	101	PRO
1	C	105	THR
1	C	114	GLY
1	C	115	THR
1	C	116	PHE
1	C	151	ALA
1	C	156	ARG
1	C	158	ALA
1	C	167	ALA
1	C	291	PHE
1	C	292	TYR
1	C	296	PRO
1	C	315	ALA
1	C	145	THR
1	C	152	LEU
1	C	263	VAL
1	C	131	PHE
1	C	205	LYS
1	C	298	SER
1	C	343	LYS
1	C	134	LEU
1	C	163	PRO
1	C	201	ILE
1	C	260	PRO
1	C	300	LEU
1	C	314	ALA
1	C	71	THR
1	C	82	ILE
1	C	313	GLU
1	C	297	VAL
1	C	259	GLY

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	C	238/282 (84%)	202 (85%)	36 (15%)	3 14

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	LEU
1	C	72	GLN
1	C	89	LEU
1	C	91	THR
1	C	97	THR
1	C	108	LEU
1	C	120	ILE
1	C	128	LYS
1	C	129	TYR
1	C	134	LEU
1	C	135	ARG
1	C	145	THR
1	C	146	THR
1	C	150	VAL
1	C	152	LEU
1	C	154	PHE
1	C	164	ASN
1	C	165	ASP
1	C	169	LEU
1	C	176	VAL
1	C	185	ILE
1	C	192	SER
1	C	199	ASP
1	C	205	LYS
1	C	206	LEU
1	C	208	ASP
1	C	213	ILE
1	C	217	TYR
1	C	234	TYR
1	C	238	LEU

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Mol	Chain	Res	Type
1	C	264	SER
1	C	275	GLU
1	C	292	TYR
1	C	300	LEU
1	C	313	GLU
1	C	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	GLN
1	C	96	ASN
1	C	125	GLN
1	C	164	ASN
1	C	171	ASN
1	C	237	GLN
1	C	240	ASN
1	C	249	GLN
1	C	285	ASN
1	C	341	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	21

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	259:GLY	C	260:PRO	N	1.97
1	C	82:ILE	C	83:THR	N	1.81
1	C	279:HIS	C	280:PHE	N	1.74
1	C	291:PHE	C	292:TYR	N	1.71
1	C	264:SER	C	265:TRP	N	1.68
1	C	339:GLU	C	340:GLU	N	1.68
1	C	53:GLN	C	54:LYS	N	1.67
1	C	319:VAL	C	320:GLN	N	1.61
1	C	175:CYS	C	176:VAL	N	1.19
1	C	299:GLY	C	300:LEU	N	1.18
1	C	298:SER	C	299:GLY	N	1.16
1	C	323:GLY	C	324:VAL	N	1.16
1	C	260:PRO	C	261:ARG	N	1.15
1	C	315:ALA	C	316:ALA	N	1.14
1	C	139:SER	C	140:PRO	N	1.12
1	C	200:GLY	C	201:ILE	N	1.12
1	C	308:PHE	C	309:SER	N	1.12
1	C	177:SER	C	178:SER	N	1.04
1	C	297:VAL	C	298:SER	N	1.00
1	C	288:LEU	C	289:THR	N	0.94
1	C	201:ILE	C	202:SER	N	0.36

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.