Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:09 am BST

PDB ID	:	3ZXA
Title	:	Structure and Assembly of Turnip Crinkle Virus I. X-ray Crystallographic Structure Analysis at 3.2 A 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 following versions of software and data (see references ⓘ) were used in the production of this report:

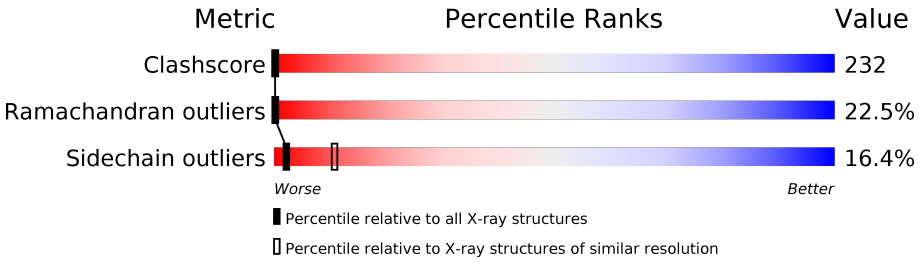
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	347	5% 40% 27% 13% 15%

2 Entry composition (i)

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

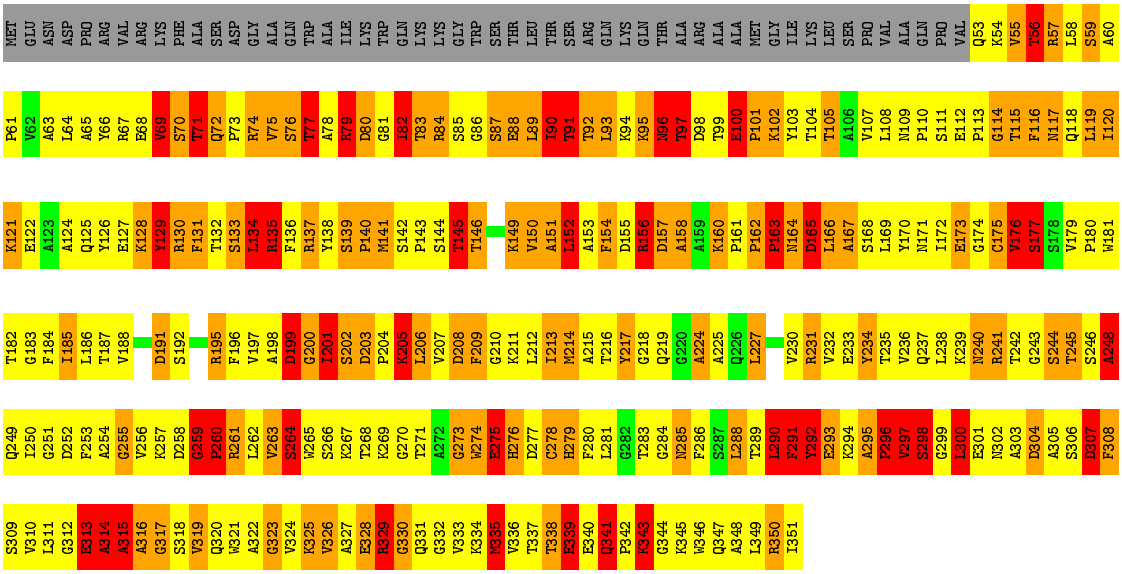
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: 5% 40% 27% 13% 15%



4 Data and refinement statistics (i)

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	2.51	55/2285 (2.4%)	2.62	148/3102 (4.8%)

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 (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	ILE	C-N	-42.34	0.36	1.34
1	C	93	LEU	N-CA	-41.10	0.64	1.46
1	C	259	GLY	C-N	33.08	1.97	1.34
1	C	133	SER	CB-OG	29.83	1.81	1.42
1	C	82	ILE	C-N	20.46	1.81	1.34
1	C	149	LYS	CD-CE	19.45	1.99	1.51
1	C	279	HIS	C-N	17.60	1.74	1.34
1	C	288	LEU	C-N	-17.30	0.94	1.34
1	C	291	PHE	C-N	16.17	1.71	1.34
1	C	264	SER	C-N	15.10	1.68	1.34
1	C	339	GLU	C-N	14.96	1.68	1.34
1	C	76	SER	N-CA	14.83	1.76	1.46
1	C	297	VAL	C-N	-14.46	1.00	1.34
1	C	53	GLN	C-N	14.34	1.67	1.34
1	C	177	SER	C-N	-12.80	1.04	1.34
1	C	121	LYS	CE-NZ	12.05	1.79	1.49
1	C	319	VAL	C-N	12.00	1.61	1.34
1	C	139	SER	C-N	-11.53	1.12	1.34
1	C	75	VAL	C-N	11.47	1.60	1.34
1	C	140	PRO	N-CD	-10.95	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	VAL	N-CA	10.88	1.68	1.46
1	C	308	PHE	C-N	-9.60	1.11	1.34
1	C	200	GLY	C-N	-9.37	1.12	1.34
1	C	91	THR	N-CA	9.26	1.64	1.46
1	C	298	SER	C-N	-9.14	1.16	1.33
1	C	299	GLY	N-CA	-8.99	1.32	1.46
1	C	75	VAL	CA-C	8.91	1.76	1.52
1	C	77	THR	N-CA	8.68	1.63	1.46
1	C	315	ALA	C-N	-8.62	1.14	1.34
1	C	76	SER	CA-C	8.60	1.75	1.52
1	C	299	GLY	CA-C	-8.48	1.38	1.51
1	C	260	PRO	C-N	-8.06	1.15	1.34
1	C	74	ARG	C-N	8.00	1.52	1.34
1	C	323	GLY	C-N	-7.70	1.16	1.34
1	C	290	LEU	C-N	7.63	1.51	1.34
1	C	300	LEU	N-CA	-7.54	1.31	1.46
1	C	330	GLY	C-N	7.12	1.50	1.34
1	C	303	ALA	C-N	7.05	1.50	1.34
1	C	299	GLY	C-N	-6.94	1.18	1.34
1	C	72	GLN	C-N	6.88	1.47	1.34
1	C	74	ARG	N-CA	6.68	1.59	1.46
1	C	76	SER	C-N	6.65	1.49	1.34
1	C	74	ARG	CA-C	6.48	1.69	1.52
1	C	259	GLY	CA-C	6.43	1.62	1.51
1	C	175	CYS	C-N	-6.36	1.19	1.34
1	C	90	ILE	CA-C	6.25	1.69	1.52
1	C	140	PRO	CA-CB	-6.11	1.41	1.53
1	C	163	PRO	N-CA	-6.04	1.36	1.47
1	C	224	ALA	C-N	5.86	1.47	1.34
1	C	175	CYS	CA-C	-5.71	1.38	1.52
1	C	70	SER	C-N	-5.52	1.21	1.34
1	C	88	GLU	C-N	-5.46	1.21	1.34
1	C	284	GLY	N-CA	5.30	1.53	1.46
1	C	176	VAL	N-CA	-5.22	1.35	1.46
1	C	203	ASP	C-N	5.18	1.44	1.34

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	201	ILE	O-C-N	-59.04	28.24	122.70
1	C	248	ALA	CA-C-N	-40.26	28.63	117.20
1	C	248	ALA	C-N-CA	-28.57	50.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ILE	O-C-N	-16.83	95.77	122.70
1	C	338	THR	O-C-N	15.61	147.67	122.70
1	C	300	LEU	O-C-N	14.53	145.95	122.70
1	C	307	ASP	C-N-CA	14.01	156.73	121.70
1	C	248	ALA	O-C-N	13.23	143.87	122.70
1	C	129	TYR	O-C-N	12.90	143.35	122.70
1	C	307	ASP	O-C-N	-12.82	102.18	122.70
1	C	93	LEU	N-CA-C	-12.63	76.89	111.00
1	C	201	ILE	CA-C-N	12.46	144.62	117.20
1	C	200	GLY	O-C-N	12.46	142.63	122.70
1	C	264	SER	O-C-N	12.38	142.51	122.70
1	C	290	LEU	O-C-N	12.38	142.50	122.70
1	C	339	GLU	C-N-CA	-12.34	90.85	121.70
1	C	330	GLY	O-C-N	-12.12	103.31	122.70
1	C	299	GLY	O-C-N	11.95	141.81	122.70
1	C	297	VAL	C-N-CA	-11.74	92.35	121.70
1	C	338	THR	CA-C-N	-11.52	91.85	117.20
1	C	264	SER	CA-C-N	-10.43	94.25	117.20
1	C	300	LEU	CA-C-N	-10.21	94.74	117.20
1	C	200	GLY	CA-C-N	-9.79	95.66	117.20
1	C	313	GLU	O-C-N	9.71	138.24	122.70
1	C	200	GLY	C-N-CA	9.68	145.91	121.70
1	C	279	HIS	O-C-N	-9.60	107.34	122.70
1	C	129	TYR	CA-C-N	-9.57	96.14	117.20
1	C	140	PRO	N-CD-CG	-9.39	89.12	103.20
1	C	299	GLY	CA-C-N	-9.35	96.63	117.20
1	C	100	GLU	O-C-N	-9.33	103.36	121.10
1	C	335	MET	CA-C-N	-9.31	96.71	117.20
1	C	140	PRO	CA-N-CD	9.26	124.66	111.70
1	C	202	SER	CB-CA-C	-9.24	92.54	110.10
1	C	264	SER	C-N-CA	-9.12	98.90	121.70
1	C	278	CYS	CA-CB-SG	-8.77	98.21	114.00
1	C	328	GLU	O-C-N	8.67	136.58	122.70
1	C	279	HIS	CA-C-N	-8.58	98.33	117.20
1	C	275	GLU	N-CA-C	-8.48	88.09	111.00
1	C	325	LYS	C-N-CA	-8.48	100.51	121.70
1	C	90	ILE	O-C-N	-8.46	109.17	122.70
1	C	314	ALA	N-CA-C	-8.43	88.25	111.00
1	C	175	CYS	CA-CB-SG	-8.29	99.08	114.00
1	C	175	CYS	C-N-CA	-8.28	101.00	121.70
1	C	307	ASP	CA-C-N	8.14	135.12	117.20
1	C	163	PRO	O-C-N	8.12	135.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	296	PRO	O-C-N	8.11	135.68	122.70
1	C	76	SER	CB-CA-C	-7.98	94.94	110.10
1	C	291	PHE	CB-CG-CD2	-7.95	115.23	120.80
1	C	350	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	C	203	ASP	O-C-N	-7.92	106.06	121.10
1	C	74	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	C	291	PHE	N-CA-CB	-7.89	96.39	110.60
1	C	330	GLY	CA-C-N	7.84	134.44	117.20
1	C	140	PRO	N-CA-CB	-7.75	94.00	103.30
1	C	273	GLY	O-C-N	7.67	134.98	122.70
1	C	273	GLY	C-N-CA	-7.51	102.91	121.70
1	C	135	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	C	84	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	57	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	63	ALA	O-C-N	7.46	134.63	122.70
1	C	195	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	C	261	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	C	241	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	130	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	C	329	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	C	156	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	290	LEU	CA-C-N	-7.32	101.11	117.20
1	C	79	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	C	57	ARG	O-C-N	7.31	134.39	122.70
1	C	313	GLU	CA-C-N	-7.29	101.17	117.20
1	C	274	TRP	O-C-N	7.23	134.27	122.70
1	C	176	VAL	O-C-N	7.18	134.19	122.70
1	C	290	LEU	CB-CA-C	-7.13	96.64	110.20
1	C	191	ASP	O-C-N	7.08	134.03	122.70
1	C	328	GLU	CA-C-N	-7.00	101.79	117.20
1	C	91	THR	N-CA-CB	6.99	123.57	110.30
1	C	202	SER	O-C-N	6.93	133.79	122.70
1	C	165	ASP	O-C-N	6.91	133.75	122.70
1	C	341	GLN	O-C-N	-6.86	108.06	121.10
1	C	338	THR	C-N-CA	6.81	138.72	121.70
1	C	69	VAL	O-C-N	-6.78	111.85	122.70
1	C	82	ILE	C-N-CA	6.78	138.65	121.70
1	C	137	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	C	273	GLY	CA-C-N	-6.60	102.67	117.20
1	C	313	GLU	C-N-CA	6.55	138.07	121.70
1	C	274	TRP	C-N-CA	6.55	138.07	121.70
1	C	202	SER	N-CA-C	6.52	128.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	102	LYS	CB-CA-C	6.45	123.29	110.40
1	C	199	ASP	O-C-N	6.41	134.09	123.20
1	C	329	ARG	O-C-N	6.41	134.09	123.20
1	C	175	CYS	CB-CA-C	-6.31	97.78	110.40
1	C	326	VAL	O-C-N	6.29	132.77	122.70
1	C	288	LEU	O-C-N	6.24	132.69	122.70
1	C	71	THR	N-CA-CB	-6.17	98.58	110.30
1	C	67	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	C	335	MET	CG-SD-CE	6.13	110.01	100.20
1	C	141	MET	CG-SD-CE	6.08	109.94	100.20
1	C	214	MET	CG-SD-CE	6.05	109.88	100.20
1	C	298	SER	C-N-CA	-6.00	109.70	122.30
1	C	339	GLU	O-C-N	5.96	132.24	122.70
1	C	288	LEU	CA-C-N	-5.96	104.10	117.20
1	C	76	SER	N-CA-C	5.95	127.06	111.00
1	C	53	GLN	O-C-N	-5.94	113.20	122.70
1	C	274	TRP	CA-C-N	-5.91	104.20	117.20
1	C	325	LYS	O-C-N	5.88	132.11	122.70
1	C	317	GLY	O-C-N	-5.86	113.32	122.70
1	C	314	ALA	CB-CA-C	5.85	118.87	110.10
1	C	202	SER	CA-C-N	-5.83	104.38	117.20
1	C	315	ALA	O-C-N	-5.82	113.38	122.70
1	C	162	PRO	O-C-N	-5.81	110.05	121.10
1	C	63	ALA	CA-C-N	-5.80	104.44	117.20
1	C	130	ARG	CB-CA-C	-5.73	98.94	110.40
1	C	231	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	C	177	SER	CA-C-N	-5.69	104.69	117.20
1	C	56	THR	CB-CA-C	-5.65	96.34	111.60
1	C	305	ALA	O-C-N	5.58	131.62	122.70
1	C	300	LEU	CA-CB-CG	-5.54	102.56	115.30
1	C	191	ASP	CA-C-N	-5.53	105.04	117.20
1	C	57	ARG	CA-C-N	-5.50	105.09	117.20
1	C	199	ASP	CA-C-N	-5.50	105.20	116.20
1	C	163	PRO	CA-C-N	-5.46	105.18	117.20
1	C	93	LEU	N-CA-CB	-5.45	99.49	110.40
1	C	273	GLY	N-CA-C	-5.45	99.48	113.10
1	C	176	VAL	CA-C-N	-5.45	105.22	117.20
1	C	72	GLN	C-N-CD	-5.39	108.73	120.60
1	C	90	ILE	CA-C-N	5.38	129.04	117.20
1	C	203	ASP	CA-C-N	5.33	132.01	117.10
1	C	264	SER	CB-CA-C	-5.32	99.99	110.10
1	C	296	PRO	CA-C-N	-5.32	105.50	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	248	ALA	CB-CA-C	-5.30	102.15	110.10
1	C	165	ASP	CA-C-N	-5.29	105.56	117.20
1	C	176	VAL	N-CA-CB	-5.28	99.88	111.50
1	C	291	PHE	CB-CA-C	5.23	120.87	110.40
1	C	338	THR	CB-CA-C	-5.23	97.48	111.60
1	C	100	GLU	CA-C-N	5.22	131.73	117.10
1	C	175	CYS	O-C-N	-5.18	114.40	122.70
1	C	129	TYR	C-N-CA	5.18	134.64	121.70
1	C	304	ASP	O-C-N	5.17	130.97	122.70
1	C	290	LEU	C-N-CA	5.14	134.55	121.70
1	C	323	GLY	C-N-CA	5.13	134.53	121.70
1	C	176	VAL	CB-CA-C	5.12	121.13	111.40
1	C	329	ARG	CA-C-N	-5.12	105.96	116.20
1	C	343	LYS	CB-CA-C	-5.06	100.28	110.40
1	C	326	VAL	CA-C-N	-5.05	106.09	117.20
1	C	339	GLU	CA-C-N	-5.04	106.11	117.20
1	C	325	LYS	CA-C-N	-5.04	106.11	117.20
1	C	130	ARG	N-CA-C	5.02	124.56	111.00
1	C	290	LEU	N-CA-C	5.00	124.51	111.00

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	Mainchain,Peptide
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 (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	C	2237	0	2184	1024	7
All	All	2237	0	2184	1024	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 232.

All (1024) 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:101:PRO:CD	1:C:166:LEU:CD1	1.75	1.56
1:C:75:VAL:CA	1:C:75:VAL:C	1.76	1.54
1:C:130:ARG:CD	1:C:237:GLN:CB	1.82	1.53
1:C:75:VAL:N	1:C:75:VAL:CA	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:C	1.75	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: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:264:SER:C	1:C:265:TRP:N	1.68	1.42
1:C:339:GLU:C	1:C:340:GLU:N	1.68	1.41
1:C:203:ASP:OD1	1:C:205:LYS:CD	1.68	1.41
1:C:291:PHE:C	1:C:292:TYR:N	1.71	1.41
1:C:296:PRO:CG	1:C:337:THR:HG22	0.96	1.40
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:269:LYS:O	1:C:277:ASP:CB	1.67	1.38
1:C:115:THR:O	1:C:116:PHE:CD1	1.76	1.38
1:C:279:HIS:C	1:C:280:PHE:N	1.74	1.37
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:ILE:C	1:C:83:THR:N	1.81	1.34
1:C:278:CYS:N	1:C:334:LYS:CD	1.87	1.34
1:C:138:TYR:CB	1:C:184:PHE:CZ	1.96	1.34
1:C:130:ARG:HD3	1:C:237:GLN:CB	1.46	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: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:291:PHE:HA	1:C:345:LYS:O	1.23	1.28
1:C:198:ALA:HB1	1:C:200:GLY:O	1.17	1.28
1:C:327:ALA:HB3	1:C:331:GLN:CD	1.53	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:133:SER:O	1:C:234:TYR:HA	1.28	1.25
1:C:80:ASP:CA	1:C:241:ARG:HH22	1.49	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:328:GLU:O	1:C:329:ARG:O	1.55	1.24
1:C:138:TYR:HB3	1:C:184:PHE:CE1	1.51	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:GLY:C	1:C:260:PRO:N	1.97	1.17
1:C:90:ILE:C	1:C:329:ARG:NH2	1.99	1.16
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:313:GLU:HG3	1:C:318:SER:HB2	1.28	1.12
1:C:277:ASP:CA	1:C:334:LYS:HD2	1.77	1.12
1:C:101:PRO:C	1:C:102:LYS:HG3	1.57	1.12
1:C:265:TRP:HZ3	1:C:348:ALA:O	1.20	1.12
1:C:164:ASN:N	1:C:164:ASN:ND2	1.88	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:101:PRO:O	1:C:102:LYS:HG3	0.95	1.11
1:C:90:ILE:CA	1:C:329:ARG:HH22	1.62	1.11
1:C:126:TYR:CA	1:C:242:THR:HG22	1.80	1.11
1:C:295:ALA:H	1:C:316:ALA:CA	1.63	1.10
1:C:151:ALA:HA	1:C:177:SER:HB2	1.28	1.10
1:C:164:ASN:N	1:C:164:ASN:HD22	1.19	1.10
1:C:119:LEU:HD22	1:C:234:TYR:CZ	1.85	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:80:ASP:CA	1:C:241:ARG:NH2	2.10	1.10
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: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: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:160:LYS:HG3	1:C:161:PRO:HD2	1.11	1.09
1:C:149:LYS:HD2	1:C:170:TYR:OH	1.44	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:71:THR:HG21	1:C:87:SER:OG	0.92	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:297:VAL:HB	1:C:336:VAL:HG13	1.26	1.08
1:C:255:GLY:HA2	1:C:342:PRO:HB3	1.33	1.08
1:C:327:ALA:N	1:C:331:GLN:OE1	1.87	1.07
1:C:149:LYS:CG	1:C:177:SER:OG	2.01	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:315:ALA:HB1	1:C:318:SER:H	1.16	1.06
1:C:277:ASP:HA	1:C:334:LYS:HD2	1.34	1.05
1:C:86:GLY:HA2	1:C:234:TYR:CE1	1.90	1.05
1:C:339:GLU:C	1:C:340:GLU:CA	2.24	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: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: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
1:C:119:LEU:HD22	1:C:234:TYR:OH	0.86	1.02
1:C:89:LEU:HD23	1:C:89:LEU:C	1.78	1.02
1:C:308:PHE:CE2	1:C:310:VAL:CG2	2.42	1.02
1:C:86:GLY:CA	1:C:234:TYR:HD1	1.68	1.02
1:C:149:LYS:HD3	1:C:170:TYR:HH	0.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:CYS:H	1:C:334:LYS:HD3	1.25	1.02
1:C:149:LYS:CD	1:C:170:TYR:HH	1.59	1.02
1:C:297:VAL:HB	1:C:336:VAL:C	1.78	1.01
1:C:85:SER:HA	1:C:234:TYR:O	1.60	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: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:86:GLY:N	1:C:234:TYR:CD1	2.29	1.01
1:C:290:LEU:HD22	1:C:346:TRP:HB2	1.41	1.00
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: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:269:LYS:C	1:C:277:ASP:HB3	1.82	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:308:PHE:CE2	1:C:310:VAL:HG23	1.97	0.99
1:C:79:ARG:O	1:C:80:ASP:HB2	1.61	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:252:ASP:CG	1:C:345:LYS:HG2	1.84	0.98
1:C:134:LEU:HD21	1:C:188:VAL:CG2	1.91	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:90:ILE:HA	1:C:329:ARG:HH22	1.24	0.98
1:C:277:ASP:C	1:C:334:LYS:HD2	1.84	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:203:ASP:CG	1:C:205:LYS:HD3	1.81	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:174:GLY:C	1:C:175:CYS:SG	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PHE:CE1	1:C:155:ASP:C	2.39	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:138:TYR:HB2	1:C:184:PHE:CE2	1.99	0.95
1:C:206:LEU:O	1:C:206:LEU:HD12	1.66	0.95
1:C:130:ARG:CB	1:C:237:GLN:HB3	1.96	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:315:ALA:O	1:C:316:ALA:C	2.00	0.95
1:C:277:ASP:OD1	1:C:334:LYS:HE2	1.67	0.94
1:C:155:ASP:HB2	1:C:172:ILE:HD11	1.47	0.94
1:C:90:ILE:CA	1:C:329:ARG:NH2	2.26	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:350:ARG:C	1:C:351:ILE:HG22	1.86	0.94
1:C:89:LEU:CD2	1:C:89:LEU:C	2.37	0.93
1:C:101:PRO:CG	1:C:166:LEU:CD1	2.45	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: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:285:ASN:O	1:C:351:ILE:CG2	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PRO:C	1:C:164:ASN:HD22	1.73	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:294:LYS:C	1:C:296:PRO:HD3	1.90	0.91
1:C:113:PRO:C	1:C:115:THR:H	1.74	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:H	1:C:164:ASN:ND2	1.47	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:203:ASP:OD1	1:C:205:LYS:HD3	0.71	0.89
1:C:264:SER:C	1:C:265:TRP:CA	2.40	0.89
1:C:89:LEU:O	1:C:89:LEU:CD2	2.20	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: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: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:90:ILE:CG2	1:C:329:ARG:HH12	1.85	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
1:C:231:ARG:HG3	1:C:232:VAL:N	1.87	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:76:SER:CB	1:C:76:SER:C	2.43	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:ASN:OD1	1:C:110:PRO:HD2	1.74	0.86
1:C:56:THR:HG23	1:C:57:ARG:N	1.89	0.86
1:C:134:LEU:HA	1:C:233:GLU:C	1.94	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:198:ALA:C	1:C:200:GLY:H	1.77	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:326:VAL:CG1	1:C:327:ALA:N	2.19	0.85
1:C:296:PRO:CG	1:C:337:THR:CB	2.52	0.85
1:C:89:LEU:O	1:C:89:LEU:HD22	1.75	0.85
1:C:101:PRO:CG	1:C:166:LEU:HD11	2.06	0.85
1:C:136:PHE:CE1	1:C:232:VAL:HG22	2.12	0.85
1:C:69:VAL:CG1	1:C:70:SER:H	1.81	0.85
1:C:288:LEU:CD1	1:C:290:LEU:CD2	2.53	0.85
1:C:90:ILE:HD11	1:C:232:VAL:HG21	1.58	0.85
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.58	0.85
1:C:82:ILE:HG21	1:C:238:LEU:HB2	1.56	0.84
1:C:80:ASP:HA	1:C:241:ARG:CZ	2.07	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: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:77:THR:HG22	1:C:78:ALA:H	1.37	0.84
1:C:149:LYS:HD3	1:C:217:TYR:OH	1.78	0.84
1:C:133:SER:C	1:C:234:TYR:HA	1.99	0.84
1:C:130:ARG:HD2	1:C:237:GLN:HB2	0.85	0.84
1:C:327:ALA:CA	1:C:331:GLN:OE1	2.26	0.84
1:C:291:PHE:O	1:C:292:TYR:HB3	1.78	0.83
1:C:95:LYS:HZ2	1:C:224:ALA:HA	1.41	0.83
1:C:328:GLU:C	1:C:329:ARG:O	2.14	0.83
1:C:288:LEU:CD1	1:C:290:LEU:HD21	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:O	1:C:80:ASP:CB	2.27	0.82
1:C:149:LYS:HG2	1:C:177:SER:HG	1.41	0.82
1:C:340:GLU:O	1:C:342:PRO:HD2	1.80	0.82
1:C:78:ALA:C	1:C:80:ASP:H	1.82	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:315:ALA:HB1	1:C:318:SER:CA	2.08	0.82
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:169:LEU:O	1:C:172:ILE:HG22	1.80	0.81
1:C:90:ILE:O	1:C:90:ILE:HG22	1.78	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: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:128:LYS:HA	1:C:195:ARG:O	1.80	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:315:ALA:CB	1:C:318:SER:H	1.94	0.80
1:C:296:PRO:HG3	1:C:337:THR:CG2	2.07	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
1:C:126:TYR:N	1:C:242:THR:CG2	2.43	0.80
1:C:227:LEU:H	1:C:227:LEU:HD12	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:H	1:C:164:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TYR:C	1:C:139:SER:O	2.16	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:339:GLU:C	1:C:340:GLU:HA	2.04	0.78
1:C:133:SER:N	1:C:235:THR:HG22	1.99	0.78
1:C:326:VAL:HG12	1:C:327:ALA:C	2.02	0.78
1:C:291:PHE:HB2	1:C:345:LYS:O	1.82	0.78
1:C:179:VAL:HG11	1:C:181:TRP:HE1	1.49	0.78
1:C:71:THR:HG21	1:C:87:SER:HG	0.95	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: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:97:THR:HA	1:C:219:GLN:CA	2.14	0.78
1:C:249:GLN:O	1:C:348:ALA:N	2.17	0.77
1:C:95:LYS:HZ3	1:C:225:ALA:H	1.30	0.77
1:C:124:ALA:O	1:C:244:SER:N	2.18	0.77
1:C:90:ILE:HG22	1:C:329:ARG:HH12	1.49	0.77
1:C:313:GLU:HB2	1:C:315:ALA:N	2.00	0.77
1:C:204:PRO:C	1:C:205:LYS:HD2	2.04	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:95:LYS:HZ1	1:C:225:ALA:N	1.82	0.77
1:C:97:THR:HA	1:C:218:GLY:O	1.85	0.77
1:C:169:LEU:HD23	1:C:169:LEU:C	2.04	0.76
1:C:117:ASN:O	1:C:117:ASN:ND2	2.17	0.76
1:C:86:GLY:CA	1:C:234:TYR:CE1	2.66	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:144:SER:C	1:C:146:THR:H	1.89	0.76
1:C:175:CYS:HB2	1:C:176:VAL:HB	1.65	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
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:59:SER:C	1:C:61:PRO:HD3	2.06	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HB3	1:C:217:TYR:CD1	2.20	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: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:310:VAL:HA	1:C:321:TRP:O	1.86	0.75
1:C:154:PHE:HD1	1:C:155:ASP:H	0.75	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:327:ALA:CB	1:C:331:GLN:CD	2.39	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: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:109:ASN:HA	1:C:129:TYR:OH	1.88	0.74
1:C:185:ILE:HD12	1:C:186:LEU:CA	2.16	0.74
1:C:85:SER:CA	1:C:234:TYR:O	2.36	0.74
1:C:277:ASP:OD1	1:C:334:LYS:NZ	2.20	0.74
1:C:310:VAL:C	1:C:311:LEU:HD12	2.08	0.74
1:C:78:ALA:C	1:C:80:ASP:N	2.32	0.74
1:C:241:ARG:HD2	1:C:241:ARG:N	2.03	0.73
1:C:71:THR:OG1	1:C:87:SER:HB2	1.87	0.73
1:C:76:SER:C	1:C:76:SER:OG	2.26	0.73
1:C:154:PHE:CE1	1:C:155:ASP:O	2.41	0.73
1:C:174:GLY:O	1:C:175:CYS:SG	2.45	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:149:LYS:CB	1:C:217:TYR:CE1	2.60	0.73
1:C:133:SER:CB	1:C:235:THR:HG22	2.17	0.73
1:C:288:LEU:CD1	1:C:290:LEU:HG	2.17	0.73
1:C:90:ILE:CD1	1:C:232:VAL:HG23	2.19	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:241:ARG:H	1:C:241:ARG:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:CG1	1:C:70:SER:N	2.38	0.72
1:C:149:LYS:HD3	1:C:217:TYR:CE1	2.24	0.72
1:C:135:ARG:HB3	1:C:186:LEU:O	1.88	0.72
1:C:72:GLN:NE2	1:C:72:GLN:HA	2.04	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:90:ILE:O	1:C:329:ARG:CZ	2.37	0.72
1:C:308:PHE:HE2	1:C:310:VAL:CG2	1.92	0.72
1:C:339:GLU:CA	1:C:340:GLU:N	2.53	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:154:PHE:CD1	1:C:154:PHE:C	2.62	0.71
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:308:PHE:CD2	1:C:310:VAL:HG23	2.25	0.71
1:C:283:THR:OG1	1:C:329:ARG:HG2	1.89	0.71
1:C:55:VAL:CG2	1:C:56:THR:H	2.03	0.71
1:C:127:GLU:O	1:C:128:LYS:HB2	1.89	0.71
1:C:169:LEU:HD23	1:C:169:LEU:O	1.90	0.71
1:C:295:ALA:CB	1:C:315:ALA:N	2.53	0.71
1:C:179:VAL:CG2	1:C:181:TRP:HD1	2.03	0.71
1:C:238:LEU:N	1:C:238:LEU:HD12	2.05	0.71
1:C:242:THR:HG23	1:C:243:GLY:N	2.05	0.71
1:C:56:THR:HG23	1:C:57:ARG:H	1.56	0.71
1:C:236:VAL:HG12	1:C:237:GLN:N	2.05	0.71
1:C:252:ASP:OD1	1:C:253:PHE:N	2.24	0.71
1:C:179:VAL:HG22	1:C:180:PRO:CD	2.19	0.70
1:C:130:ARG:HD2	1:C:237:GLN:NE2	2.06	0.70
1:C:290:LEU:HD22	1:C:346:TRP:CB	2.20	0.70
1:C:90:ILE:HG23	1:C:329:ARG:HH12	1.55	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:156:ARG:O	1:C:210:GLY:N	2.25	0.70
1:C:55:VAL:CG2	1:C:56:THR:N	2.53	0.70
1:C:80:ASP:HA	1:C:241:ARG:HH22	0.70	0.70
1:C:116:PHE:O	1:C:120:ILE:HG22	1.90	0.70
1:C:101:PRO:CG	1:C:217:TYR:CD2	2.75	0.70
1:C:313:GLU:CG	1:C:318:SER:OG	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:ALA:O	1:C:171:ASN:CG	2.30	0.69
1:C:124:ALA:HB1	1:C:245:THR:CG2	2.20	0.69
1:C:66:TYR:CZ	1:C:183:GLY:HA3	2.27	0.69
1:C:297:VAL:HB	1:C:336:VAL:CG1	1.98	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:138:TYR:O	1:C:139:SER:C	2.24	0.69
1:C:173:GLU:HG3	1:C:174:GLY:N	2.08	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:103:TYR:HE1	1:C:169:LEU:HD12	1.56	0.69
1:C:75:VAL:C	1:C:75:VAL:CB	2.59	0.69
1:C:101:PRO:C	1:C:102:LYS:CG	2.42	0.69
1:C:155:ASP:CB	1:C:172:ILE:HD11	2.23	0.68
1:C:129:TYR:HA	1:C:237:GLN:O	1.92	0.68
1:C:290:LEU:O	1:C:290:LEU:HD12	1.93	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:122:GLU:HG2	1:C:122:GLU:O	1.93	0.68
1:C:289:THR:C	1:C:290:LEU:HG	2.14	0.68
1:C:297:VAL:CB	1:C:336:VAL:O	2.36	0.68
1:C:95:LYS:HZ2	1:C:224:ALA:CA	2.02	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:127:GLU:O	1:C:128:LYS:CB	2.42	0.68
1:C:83:THR:O	1:C:84:ARG:HG2	1.94	0.68
1:C:269:LYS:HE2	1:C:270:GLY:O	1.94	0.68
1:C:185:ILE:HD13	1:C:186:LEU:H	1.53	0.68
1:C:149:LYS:HD3	1:C:217:TYR:CZ	2.29	0.68
1:C:278:CYS:CA	1:C:333:VAL:O	2.41	0.67
1:C:327:ALA:HB3	1:C:331:GLN:NE2	2.07	0.67
1:C:286:PHE:CA	1:C:351:ILE:HG21	2.25	0.67
1:C:104:THR:O	1:C:105:THR:C	2.33	0.67
1:C:251:GLY:O	1:C:346:TRP:CZ2	2.47	0.67
1:C:95:LYS:O	1:C:96:ASN:HB2	1.95	0.67
1:C:169:LEU:HD22	1:C:170:TYR:HD1	1.58	0.67
1:C:340:GLU:O	1:C:342:PRO:CD	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLY:O	1:C:346:TRP:CH2	2.47	0.67
1:C:113:PRO:C	1:C:115:THR:N	2.43	0.67
1:C:130:ARG:HD2	1:C:237:GLN:HB3	1.64	0.67
1:C:138:TYR:HH	1:C:227:LEU:HB3	1.59	0.67
1:C:253:PHE:CE2	1:C:346:TRP:CZ3	2.83	0.67
1:C:163:PRO:HA	1:C:164:ASN:ND2	2.10	0.66
1:C:261:ARG:HG3	1:C:261:ARG:O	1.94	0.66
1:C:258:ASP:CG	1:C:259:GLY:H	1.95	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:136:PHE:CE1	1:C:212:LEU:HD22	2.31	0.66
1:C:64:LEU:HD12	1:C:65:ALA:H	1.60	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:124:ALA:CB	1:C:245:THR:CG2	2.74	0.66
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:66:TYR:OH	1:C:183:GLY:HA3	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: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:333:VAL:C	1:C:334:LYS:HD3	2.12	0.65
1:C:90:ILE:C	1:C:329:ARG:CZ	2.65	0.65
1:C:170:TYR:CZ	1:C:217:TYR:OH	2.45	0.65
1:C:326:VAL:HG12	1:C:327:ALA:CA	2.27	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:207:VAL:HG13	1:C:208:ASP:CG	2.18	0.64
1:C:136:PHE:HE1	1:C:232:VAL:HG22	1.59	0.64
1:C:152:LEU:CD2	1:C:186:LEU:HD13	2.25	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:253:PHE:CD2	1:C:346:TRP:CZ3	2.85	0.64
1:C:125:GLN:C	1:C:242:THR:CG2	2.66	0.64
1:C:166:LEU:O	1:C:167:ALA:C	2.36	0.64
1:C:201:ILE:CG2	1:C:261:ARG:HB2	2.28	0.64
1:C:68:GLU:OE2	1:C:139:SER:OG	2.14	0.64
1:C:201:ILE:HG22	1:C:261:ARG:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:HB2	1:C:331:GLN:OE1	1.96	0.64
1:C:196:PHE:O	1:C:207:VAL:HG23	1.97	0.64
1:C:300:LEU:C	1:C:308:PHE:HZ	2.00	0.64
1:C:76:SER:HA	1:C:76:SER:N	2.01	0.64
1:C:138:TYR:O	1:C:139:SER:O	2.15	0.64
1:C:163:PRO:HG3	1:C:168:SER:HB3	1.80	0.64
1:C:119:LEU:CD2	1:C:234:TYR:HE2	2.10	0.64
1:C:154:PHE:CZ	1:C:156:ARG:HA	2.33	0.63
1:C:172:ILE:O	1:C:173:GLU:C	2.36	0.63
1:C:309:SER:O	1:C:321:TRP:O	2.15	0.63
1:C:61:PRO:HD2	1:C:181:TRP:CZ3	2.33	0.63
1:C:154:PHE:CE1	1:C:156:ARG:N	2.66	0.63
1:C:205:LYS:N	1:C:205:LYS:HD2	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:156:ARG:O	1:C:209:PHE:C	2.37	0.63
1:C:206:LEU:CD1	1:C:206:LEU:O	2.45	0.63
1:C:68:GLU:CD	1:C:137:ARG:NH2	2.51	0.63
1:C:135:ARG:CB	1:C:186:LEU:O	2.47	0.63
1:C:170:TYR:C	1:C:171:ASN:HD22	2.02	0.63
1:C:125:GLN:C	1:C:242:THR:HG22	2.19	0.63
1:C:291:PHE:C	1:C:292:TYR:CA	2.67	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: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
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:296:PRO:HG3	1:C:337:THR:HB	1.81	0.62
1:C:166:LEU:O	1:C:168:SER:N	2.32	0.62
1:C:82:ILE:HG23	1:C:83:THR:N	2.15	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:296:PRO:HG3	1:C:337:THR:CB	2.27	0.62
1:C:112:GLU:O	1:C:114:GLY:N	2.33	0.62
1:C:157:ASP:O	1:C:157:ASP:OD1	2.18	0.62
1:C:82:ILE:O	1:C:83:THR:N	2.29	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:155:ASP:O	1:C:156:ARG:C	2.36	0.62
1:C:186:LEU:C	1:C:186:LEU:HD23	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:236:VAL:CG1	1:C:237:GLN:N	2.62	0.61
1:C:300:LEU:C	1:C:308:PHE:CZ	2.74	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:O	1:C:188:VAL:HG23	1.99	0.61
1:C:306:SER:HB3	1:C:325:LYS:CB	2.27	0.61
1:C:85:SER:C	1:C:234:TYR:CE1	2.74	0.61
1:C:311:LEU:N	1:C:311:LEU:HD12	2.16	0.61
1:C:95:LYS:NZ	1:C:224:ALA:CB	2.64	0.61
1:C:264:SER:C	1:C:265:TRP:HA	2.22	0.60
1:C:314:ALA:O	1:C:315:ALA:HB2	2.00	0.60
1:C:77:THR:CG2	1:C:78:ALA:H	2.03	0.60
1:C:134:LEU:HD23	1:C:188:VAL:CG2	2.31	0.60
1:C:237:GLN:C	1:C:238:LEU:HD12	2.21	0.60
1:C:290:LEU:CD1	1:C:290:LEU:C	2.69	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:83:THR:HG23	1:C:130:ARG:NH1	2.15	0.60
1:C:144:SER:C	1:C:146:THR:N	2.54	0.60
1:C:124:ALA:HB2	1:C:245:THR:HG21	1.82	0.60
1:C:163:PRO:HB2	1:C:165:ASP:H	1.66	0.60
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:129:TYR:CB	1:C:237:GLN:O	2.49	0.59
1:C:306:SER:O	1:C:307:ASP:C	2.40	0.59
1:C:169:LEU:CD2	1:C:169:LEU:C	2.70	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:96:ASN:C	1:C:98:ASP:N	2.55	0.59
1:C:203:ASP:O	1:C:205:LYS:N	2.34	0.59
1:C:201:ILE:CG2	1:C:261:ARG:HA	2.33	0.59
1:C:97:THR:CA	1:C:218:GLY:O	2.50	0.59
1:C:230:VAL:HG12	1:C:231:ARG:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:PRO:CB	1:C:164:ASN:HD22	2.15	0.59
1:C:130:ARG:HB3	1:C:237:GLN:H	1.66	0.59
1:C:90:ILE:O	1:C:329:ARG:NH1	2.36	0.59
1:C:277:ASP:HA	1:C:334:LYS:CE	2.32	0.59
1:C:342:PRO:C	1:C:343:LYS:HD3	2.23	0.59
1:C:130:ARG:CB	1:C:237:GLN:CB	2.68	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:213:ILE:C	1:C:214:MET:HG3	2.24	0.58
1:C:172:ILE:O	1:C:172:ILE:HG23	2.03	0.58
1:C:95:LYS:HZ1	1:C:224:ALA:CA	2.15	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:336:VAL:HG13	1:C:336:VAL:O	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:112:GLU:O	1:C:113:PRO:C	2.41	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:163:PRO:C	1:C:164:ASN:ND2	2.44	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
1:C:307:ASP:O	1:C:323:GLY:O	2.21	0.57
1:C:83:THR:HA	1:C:236:VAL:O	2.03	0.57
1:C:198:ALA:HB1	1:C:200:GLY:C	2.14	0.57
1:C:258:ASP:CG	1:C:259:GLY:N	2.58	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: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:154:PHE:CD1	1:C:155:ASP:C	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ALA:HB2	1:C:349:LEU:HA	1.87	0.56
1:C:90:ILE:HG22	1:C:329:ARG:NH1	2.18	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:124:ALA:CB	1:C:245:THR:HG21	2.35	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:O	1:C:145:THR:CG2	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:290:LEU:C	1:C:290:LEU:HD12	2.26	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:HG13	1:C:120:ILE:O	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:162:PRO:C	1:C:163:PRO:O	2.42	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:274:TRP:CD1	1:C:339:GLU:C	2.80	0.55
1:C:302:ASN:HB2	1:C:333:VAL:HG22	1.88	0.55
1:C:291:PHE:CE1	1:C:335:MET:CE	2.90	0.55
1:C:306:SER:HB2	1:C:325:LYS:H	1.72	0.55
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:197:VAL:HG22	1:C:198:ALA:N	2.23	0.54
1:C:156:ARG:O	1:C:209:PHE:O	2.26	0.54
1:C:276:HIS:CG	1:C:277:ASP:N	2.74	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:86:GLY:N	1:C:234:TYR:CE1	2.74	0.54
1:C:95:LYS:HZ2	1:C:224:ALA:CB	2.20	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:126:TYR:C	1:C:242:THR:CG2	2.75	0.54
1:C:304:ASP:CG	1:C:332:GLY:H	2.11	0.54
1:C:274:TRP:CD1	1:C:339:GLU:HA	2.42	0.54
1:C:213:ILE:O	1:C:214:MET:CG	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LYS:NZ	1:C:224:ALA:HB1	2.22	0.54
1:C:133:SER:HB3	1:C:235:THR:CG2	2.35	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:173:GLU:HG3	1:C:174:GLY:H	1.73	0.54
1:C:138:TYR:HD2	1:C:184:PHE:CE1	2.16	0.54
1:C:199:ASP:N	1:C:199:ASP:OD1	2.40	0.53
1:C:170:TYR:HE1	1:C:217:TYR:OH	1.86	0.53
1:C:85:SER:C	1:C:234:TYR:CD1	2.82	0.53
1:C:300:LEU:O	1:C:308:PHE:CZ	2.61	0.53
1:C:313:GLU:HB2	1:C:314:ALA:C	2.29	0.53
1:C:113:PRO:HG3	1:C:120:ILE:CD1	2.39	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:142:SER:HB3	1:C:227:LEU:O	2.09	0.53
1:C:82:ILE:HG12	1:C:83:THR:N	2.24	0.53
1:C:277:ASP:CG	1:C:334:LYS:HZ3	2.12	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:109:ASN:CA	1:C:129:TYR:OH	2.55	0.52
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: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
1:C:293:GLU:HA	1:C:317:GLY:HA2	1.91	0.52
1:C:78:ALA:O	1:C:81:GLY:N	2.42	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:295:ALA:HB1	1:C:314:ALA:C	2.30	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:71:THR:CG2	1:C:87:SER:CB	2.77	0.52
1:C:94:LYS:O	1:C:95:LYS:C	2.48	0.52
1:C:126:TYR:C	1:C:242:THR:HG22	2.30	0.52
1:C:300:LEU:CG	1:C:308:PHE:HZ	2.20	0.52
1:C:239:LYS:O	1:C:240:ASN:O	2.28	0.52
1:C:54:LYS:O	1:C:55:VAL:HB	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HD12	1:C:126:TYR:CE2	2.44	0.52
1:C:125:GLN:C	1:C:242:THR:HG23	2.30	0.52
1:C:149:LYS:HE2	1:C:151:ALA:CB	2.39	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:248:ALA:HB1	1:C:348:ALA:O	2.09	0.52
1:C:84:ARG:HG3	1:C:119:LEU:HD11	1.91	0.51
1:C:166:LEU:C	1:C:168:SER:N	2.61	0.51
1:C:179:VAL:HG13	1:C:182:THR:HG22	1.90	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:138:TYR:CZ	1:C:150:VAL:HG21	2.45	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:154:PHE:CD1	1:C:155:ASP:CA	2.90	0.51
1:C:91:THR:HB	1:C:329:ARG:NE	2.25	0.51
1:C:90:ILE:HD11	1:C:232:VAL:HG22	1.83	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:O	1:C:188:VAL:CG2	2.59	0.51
1:C:224:ALA:O	1:C:225:ALA:HB2	2.10	0.51
1:C:241:ARG:H	1:C:241:ARG:CD	2.22	0.51
1:C:235:THR:O	1:C:235:THR:HG23	2.09	0.51
1:C:93:LEU:HD12	1:C:138:TYR:HE1	1.75	0.51
1:C:243:GLY:O	1:C:244:SER:HB2	2.11	0.51
1:C:128:LYS:HG3	1:C:196:PHE:CD2	2.46	0.50
1:C:103:TYR:CD1	1:C:215:ALA:HB2	2.46	0.50
1:C:95:LYS:HZ1	1:C:224:ALA:HB1	1.75	0.50
1:C:85:SER:O	1:C:234:TYR:CE1	2.65	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:129:TYR:CA	1:C:237:GLN:O	2.57	0.50
1:C:144:SER:O	1:C:146:THR:N	2.44	0.50
1:C:158:ALA:C	1:C:211:LYS:H	1.93	0.50
1:C:130:ARG:CB	1:C:237:GLN:N	2.74	0.50
1:C:101:PRO:CB	1:C:217:TYR:CD2	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ALA:HB2	1:C:315:ALA:CB	2.38	0.49
1:C:86:GLY:HA2	1:C:234:TYR:HE1	1.68	0.49
1:C:153:ALA:CA	1:C:174:GLY:HA3	2.33	0.49
1:C:66:TYR:HE2	1:C:183:GLY:HA3	1.73	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: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:71:THR:OG1	1:C:87:SER:CB	2.59	0.49
1:C:296:PRO:CD	1:C:337:THR:HG21	2.39	0.49
1:C:90:ILE:C	1:C:329:ARG:HH22	1.87	0.49
1:C:150:VAL:HG23	1:C:227:LEU:HD23	1.94	0.49
1:C:85:SER:O	1:C:234:TYR:HE1	1.96	0.49
1:C:350:ARG:O	1:C:351:ILE:CB	2.53	0.49
1:C:277:ASP:HA	1:C:334:LYS:HZ2	1.76	0.49
1:C:291:PHE:C	1:C:292:TYR:HB3	2.33	0.49
1:C:157:ASP:OD1	1:C:157:ASP:C	2.50	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:100:GLU:O	1:C:101:PRO:C	2.48	0.49
1:C:133:SER:O	1:C:234:TYR:CB	2.60	0.49
1:C:241:ARG:CD	1:C:241:ARG:N	2.75	0.49
1:C:109:ASN:O	1:C:110:PRO:C	2.51	0.48
1:C:119:LEU:HD23	1:C:234:TYR:CE2	2.43	0.48
1:C:107:VAL:O	1:C:115:THR:CG2	2.56	0.48
1:C:84:ARG:HD2	1:C:119:LEU:HD13	1.94	0.48
1:C:83:THR:HG23	1:C:130:ARG:CZ	2.44	0.48
1:C:103:TYR:CE1	1:C:169:LEU:HD12	2.43	0.48
1:C:204:PRO:N	1:C:205:LYS:HD2	2.28	0.48
1:C:290:LEU:HB2	1:C:346:TRP:HA	1.96	0.48
1:C:278:CYS:CA	1:C:334:LYS:HD3	2.42	0.48
1:C:163:PRO:CG	1:C:168:SER:CB	2.92	0.48
1:C:101:PRO:CG	1:C:217:TYR:CE2	2.74	0.48
1:C:264:SER:OG	1:C:265:TRP:N	2.45	0.48
1:C:136:PHE:HD1	1:C:231:ARG:O	1.95	0.48
1:C:150:VAL:O	1:C:151:ALA:C	2.52	0.48
1:C:336:VAL:O	1:C:337:THR:CG2	2.62	0.48
1:C:111:SER:HB3	1:C:197:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLU:OE2	1:C:118:GLN:HB3	2.13	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:244:SER:OG	1:C:245:THR:N	2.46	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:89:LEU:HD23	1:C:90:ILE:N	2.28	0.47
1:C:92:THR:HG23	1:C:93:LEU:O	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: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:278:CYS:N	1:C:333:VAL:O	2.48	0.47
1:C:130:ARG:HH11	1:C:236:VAL:C	2.16	0.47
1:C:288:LEU:C	1:C:289:THR:OG1	2.49	0.47
1:C:291:PHE:CD1	1:C:292:TYR:N	2.83	0.47
1:C:273:GLY:O	1:C:274:TRP:C	2.53	0.47
1:C:289:THR:O	1:C:290:LEU:HG	2.14	0.47
1:C:162:PRO:O	1:C:163:PRO:O	2.33	0.47
1:C:144:SER:HA	1:C:181:TRP:HB3	1.96	0.47
1:C:107:VAL:HG22	1:C:211:LYS:HB3	1.97	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:174:GLY:O	1:C:175:CYS:CB	2.64	0.46
1:C:185:ILE:HD12	1:C:186:LEU:C	2.36	0.46
1:C:234:TYR:CD2	1:C:236:VAL:HG23	2.50	0.46
1:C:71:THR:O	1:C:71:THR:HG23	2.16	0.46
1:C:149:LYS:O	1:C:216:THR:HA	2.15	0.46
1:C:162:PRO:O	1:C:163:PRO:C	2.51	0.46
1:C:174:GLY:C	1:C:175:CYS:HG	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HE2	1:C:151:ALA:HB2	1.96	0.46
1:C:172:ILE:C	1:C:173:GLU:O	2.51	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:244:SER:C	1:C:245:THR:HG22	2.31	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:74:ARG:C	1:C:75:VAL:HG23	2.37	0.46
1:C:95:LYS:HZ1	1:C:224:ALA:C	2.18	0.46
1:C:127:GLU:O	1:C:128:LYS:CG	2.64	0.45
1:C:181:TRP:CE3	1:C:181:TRP:O	2.69	0.45
1:C:133:SER:CA	1:C:235:THR:HG22	2.47	0.45
1:C:126:TYR:C	1:C:242:THR:HG21	2.37	0.45
1:C:249:GLN:NE2	1:C:265:TRP:N	2.54	0.45
1:C:100:GLU:C	1:C:101:PRO:O	2.54	0.45
1:C:90:ILE:CG2	1:C:329:ARG:NH1	2.67	0.45
1:C:262:LEU:HA	1:C:262:LEU:HD23	1.71	0.45
1:C:89:LEU:HA	1:C:230:VAL:O	2.17	0.45
1:C:89:LEU:O	1:C:89:LEU:HD23	2.00	0.45
1:C:109:ASN:OD1	1:C:129:TYR:OH	2.32	0.45
1:C:84:ARG:CD	1:C:119:LEU:HD13	2.46	0.45
1:C:236:VAL:CG1	1:C:238:LEU:CD1	2.94	0.45
1:C:118:GLN:HG2	1:C:118:GLN:O	2.17	0.45
1:C:198:ALA:C	1:C:200:GLY:N	2.55	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
1:C:101:PRO:CD	1:C:217:TYR:HD2	2.30	0.45
1:C:92:THR:O	1:C:328:GLU:OE2	2.35	0.45
1:C:112:GLU:O	1:C:112:GLU:HG3	2.16	0.44
1:C:253:PHE:HZ	1:C:268:THR:HG21	1.82	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:333:VAL:C	1:C:334:LYS:CD	2.78	0.44
1:C:213:ILE:HG23	1:C:214:MET:N	2.32	0.44
1:C:95:LYS:HZ1	1:C:224:ALA:CB	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PRO:HG3	1:C:168:SER:CB	2.47	0.44
1:C:101:PRO:HD3	1:C:166:LEU:HD11	0.47	0.44
1:C:137:ARG:N	1:C:230:VAL:HG13	2.33	0.44
1:C:293:GLU:O	1:C:316:ALA:C	2.52	0.44
1:C:201:ILE:HG22	1:C:261:ARG:CA	2.46	0.44
1:C:291:PHE:C	1:C:292:TYR:CB	2.86	0.44
1:C:350:ARG:C	1:C:351:ILE:CG2	2.58	0.44
1:C:84:ARG:NE	1:C:119:LEU:CD1	2.81	0.43
1:C:72:GLN:HE21	1:C:73:PRO:HD2	1.83	0.43
1:C:101:PRO:HB3	1:C:217:TYR:CD2	2.53	0.43
1:C:336:VAL:C	1:C:337:THR:HG23	2.37	0.43
1:C:154:PHE:CZ	1:C:156:ARG:CA	3.01	0.43
1:C:56:THR:HG23	1:C:57:ARG:HB3	1.99	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:291:PHE:CE1	1:C:335:MET:HE3	2.53	0.43
1:C:325:LYS:O	1:C:325:LYS:HG2	2.18	0.43
1:C:76:SER:OG	1:C:77:THR:N	2.50	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
1:C:279:HIS:O	1:C:280:PHE:N	2.42	0.43
1:C:126:TYR:O	1:C:242:THR:CG2	2.66	0.43
1:C:306:SER:HB2	1:C:325:LYS:N	2.33	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:87:SER:HA	1:C:231:ARG:HD2	2.01	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:130:ARG:NH1	1:C:236:VAL:C	2.70	0.42
1:C:169:LEU:C	1:C:171:ASN:H	2.22	0.42
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:137:ARG:O	1:C:230:VAL:HA	2.19	0.42
1:C:95:LYS:HB3	1:C:96:ASN:H	1.60	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:252:ASP:OD2	1:C:345:LYS:HG2	2.16	0.42
1:C:96:ASN:O	1:C:96:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:CYS:O	1:C:333:VAL:N	2.34	0.42
1:C:302:ASN:HB3	1:C:308:PHE:CE1	2.55	0.42
1:C:60:ALA:HA	1:C:61:PRO:HD2	1.81	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: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:341:GLN:O	1:C:342:PRO:C	2.58	0.42
1:C:75:VAL:HG12	1:C:76:SER:N	2.35	0.42
1:C:293:GLU:CA	1:C:317:GLY:HA2	2.50	0.42
1:C:248:ALA:HB2	1:C:349:LEU:HD23	2.01	0.42
1:C:289:THR:CG2	1:C:321:TRP:CZ3	3.03	0.42
1:C:186:LEU:C	1:C:186:LEU:CD2	2.87	0.41
1:C:292:TYR:CD1	1:C:292:TYR:C	2.94	0.41
1:C:266:SER:HA	1:C:280:PHE:HA	2.02	0.41
1:C:93:LEU:CD1	1:C:138:TYR:HE1	2.33	0.41
1:C:341:GLN:HB2	1:C:341:GLN:HE21	1.72	0.41
1:C:291:PHE:CD2	1:C:345:LYS:O	2.73	0.41
1:C:231:ARG:CG	1:C:232:VAL:H	2.27	0.41
1:C:248:ALA:O	1:C:250:ILE:N	2.49	0.41
1:C:135:ARG:N	1:C:233:GLU:O	2.54	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: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:71:THR:CG2	1:C:87:SER:HG	1.90	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: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:185:ILE:HD12	1:C:186:LEU:O	2.20	0.41
1:C:136:PHE:CG	1:C:212:LEU:HD21	2.56	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:343:LYS:HB2	1:C:344:GLY:H	1.13	0.41
1:C:302:ASN:HB3	1:C:308:PHE:CD1	2.56	0.41
1:C:90:ILE:CG2	1:C:329:ARG:HH22	2.34	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:91:THR:HG23	1:C:92:THR:N	2.36	0.41
1:C:149:LYS:CD	1:C:217:TYR:HE1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HD13	1:C:120:ILE:HG21	1.87	0.40
1:C:268:THR:CG2	1:C:268:THR:O	2.66	0.40
1:C:130:ARG:HB3	1:C:131:PHE:H	1.46	0.40
1:C:176:VAL:O	1:C:176:VAL:CG1	2.69	0.40
1:C:249:GLN:HG3	1:C:263:VAL:O	2.21	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:259:GLY:C	1:C:260:PRO:CD	2.84	0.40
1:C:93:LEU:HD12	1:C:138:TYR:CE1	2.54	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	199 (84%)	39 (16%)	2 11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	LEU
1	C	79	ARG
1	C	89	LEU

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Mol	Chain	Res	Type
1	C	91	THR
1	C	96	ASN
1	C	97	THR
1	C	108	LEU
1	C	117	ASN
1	C	120	ILE
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	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	260	PRO
1	C	264	SER
1	C	275	GLU
1	C	276	HIS
1	C	285	ASN
1	C	290	LEU
1	C	292	TYR
1	C	300	LEU
1	C	313	GLU
1	C	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	GLN
1	C	96	ASN

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Mol	Chain	Res	Type
1	C	118	GLN
1	C	125	GLN
1	C	164	ASN
1	C	171	ASN
1	C	226	GLN
1	C	237	GLN
1	C	240	ASN
1	C	249	GLN
1	C	285	ASN
1	C	341	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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.