



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 AM UTC

PDB ID : 2HWE / pdb_00002hwe
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING
POCKET IN HRV14 AND HRV1A
Authors : Kim, K.H.; Rossmann, M.G.
Deposited on : 1994-01-25
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

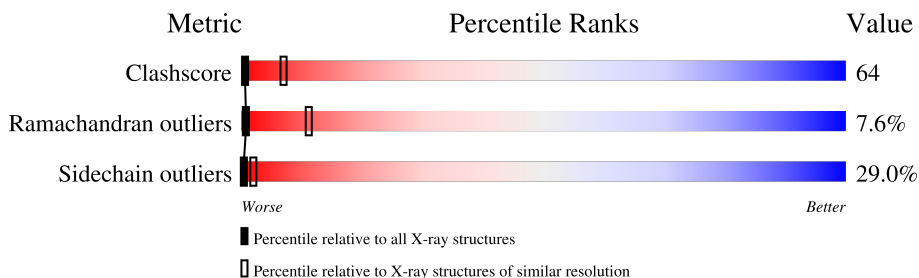
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)

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	1	287	
2	2	263	
3	3	238	
4	4	44	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6248 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 HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2262	1431	389	430	12			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	253	Total	C	N	O	S	0	0	0
			1979	1249	349	371	10			

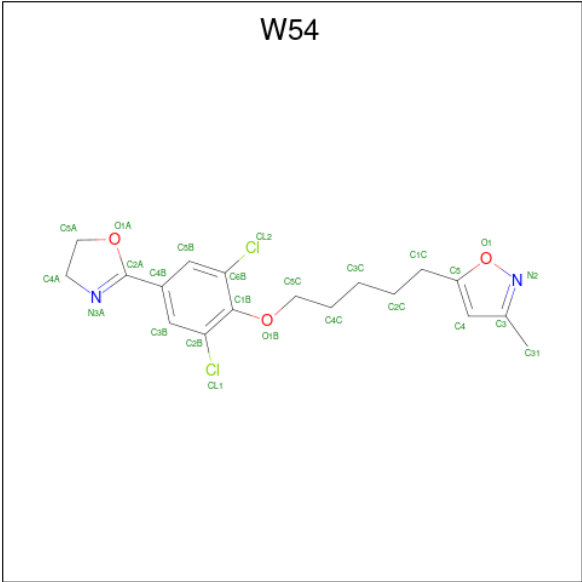
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1831	1169	297	348	17			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	19	Total	C	N	O	0	0	0
			151	96	25	30			

- Molecule 5 is 5-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYL ISOXAZOLE (CCD ID: W54) (formula: C₁₈H₂₀Cl₂N₂O₃).



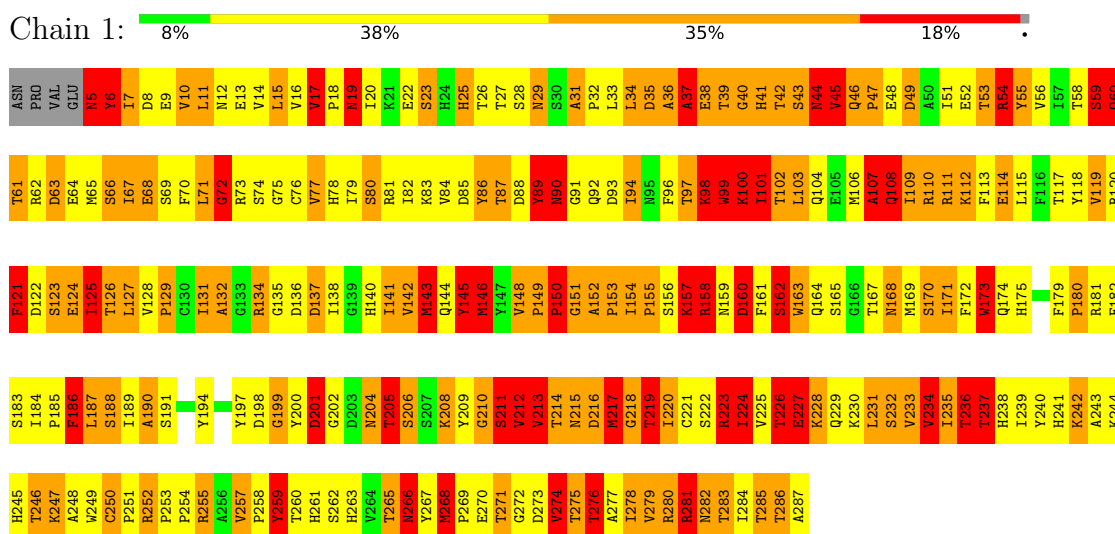
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

3 Residue-property plots

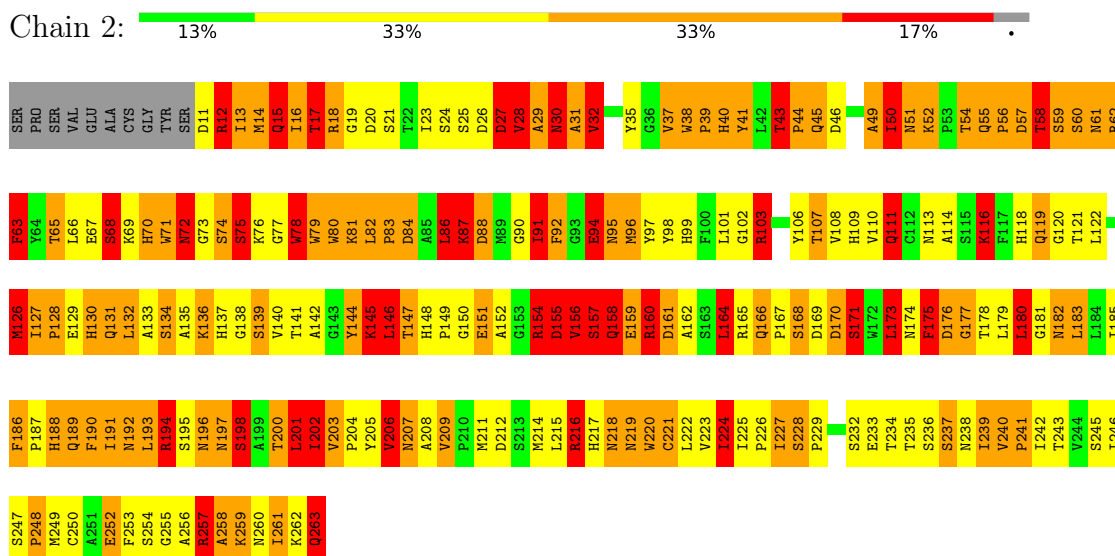
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)

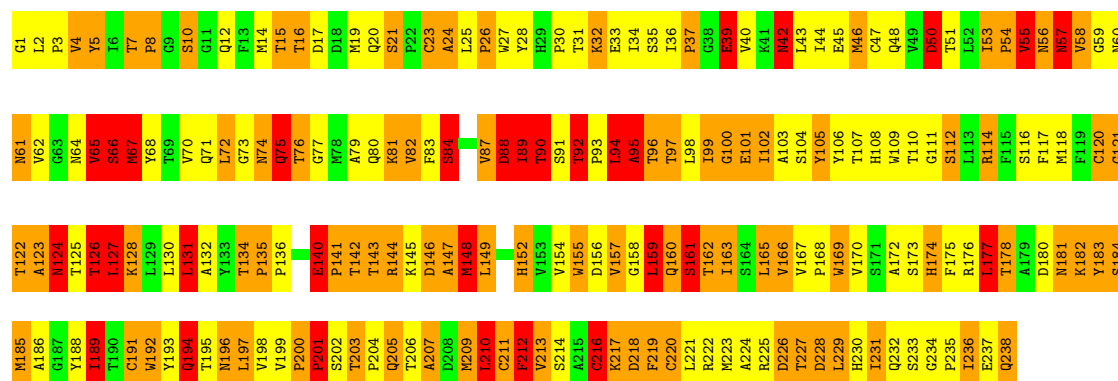


• Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)



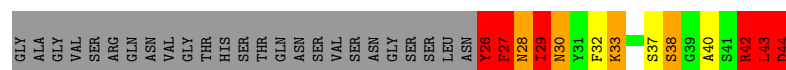
• Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)

Chain 3: 



• Molecule 4: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4)

Chain 4: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	1	1.62	21/2322 (0.9%)	3.22	304/3162 (9.6%)
2	2	1.23	2/2033 (0.1%)	3.12	291/2770 (10.5%)
3	3	1.22	0/1878	3.03	227/2570 (8.8%)
4	4	1.46	0/154	3.74	35/206 (17.0%)
All	All	1.39	23/6387 (0.4%)	3.14	857/8708 (9.8%)

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	1	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	MET	C-N	-25.02	0.98	1.33
1	1	213	VAL	C-N	19.63	1.61	1.33
1	1	98	LYS	C-N	-13.09	1.15	1.33
1	1	145	TYR	C-N	12.39	1.48	1.33
1	1	118	TYR	C-N	-12.01	1.19	1.33
1	1	223	ARG	C-N	11.77	1.49	1.33
1	1	150	PRO	C-N	-9.45	1.25	1.33
1	1	218	GLY	CA-C	-7.87	1.40	1.51
1	1	144	GLN	C-N	7.80	1.44	1.33
1	1	149	PRO	CA-C	-7.69	1.45	1.52
1	1	219	THR	N-CA	-7.08	1.37	1.46
1	1	148	VAL	CA-C	-7.04	1.45	1.52
1	1	107	ALA	N-CA	6.52	1.54	1.46
1	1	217	MET	N-CA	-6.35	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	106	MET	CA-C	6.07	1.59	1.53
1	1	214	THR	CA-C	-6.02	1.45	1.53
1	1	211	SER	C-N	-5.75	1.25	1.33
1	1	217	MET	CA-C	-5.70	1.45	1.53
1	1	90	ASN	N-CA	5.50	1.53	1.46
1	1	99	TRP	NE1-CE2	-5.41	1.31	1.37
2	2	58	THR	CA-CB	5.38	1.62	1.53
1	1	108	GLN	N-CA	5.12	1.52	1.46
2	2	127	ILE	CA-CB	5.04	1.60	1.54

All (857) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-39.13	77.88	123.27
1	1	150	PRO	CA-C-N	-30.99	87.58	120.43
1	1	150	PRO	C-N-CA	-30.99	87.58	120.43
2	2	62	ARG	CD-NE-CZ	24.23	158.32	124.40
1	1	98	LYS	CA-C-N	18.44	156.75	121.54
1	1	98	LYS	C-N-CA	18.44	156.75	121.54
1	1	218	GLY	O-C-N	16.52	144.18	122.70
1	1	164	GLN	OE1-CD-NE2	-16.42	106.18	122.60
1	1	187	LEU	CA-C-O	-15.47	102.67	122.63
3	3	222	ARG	CD-NE-CZ	15.30	145.82	124.40
2	2	72	ASN	OD1-CG-ND2	15.02	137.62	122.60
1	1	211	SER	CA-C-N	-14.87	95.21	121.97
1	1	211	SER	C-N-CA	-14.87	95.21	121.97
1	1	151	GLY	N-CA-C	-14.55	90.66	111.03
3	3	235	PRO	CA-C-N	14.35	141.02	122.93
3	3	235	PRO	C-N-CA	14.35	141.02	122.93
1	1	68	GLU	CB-CG-CD	14.23	136.79	112.60
3	3	218	ASP	CA-CB-CG	-13.89	98.70	112.60
1	1	213	VAL	CA-C-N	-13.80	102.61	123.17
1	1	213	VAL	C-N-CA	-13.80	102.61	123.17
2	2	196	ASN	OD1-CG-ND2	13.77	136.37	122.60
3	3	212	PHE	CA-CB-CG	13.55	127.35	113.80
1	1	146	MET	O-C-N	13.53	136.85	123.46
2	2	218	ASN	CA-CB-CG	13.39	125.99	112.60
1	1	214	THR	CB-CA-C	-13.33	88.58	111.23
1	1	281	ARG	CA-CB-CG	13.09	140.27	114.10
2	2	187	PRO	CB-CA-C	13.09	128.13	111.64
3	3	203	THR	O-C-N	13.09	131.17	121.88
1	1	274	VAL	N-CA-CB	13.08	125.34	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	111	ARG	CA-C-N	12.92	140.20	120.82
1	1	111	ARG	C-N-CA	12.92	140.20	120.82
2	2	154	ARG	CA-C-N	12.56	145.53	121.54
2	2	154	ARG	C-N-CA	12.56	145.53	121.54
1	1	211	SER	CA-C-O	-12.43	107.12	121.66
3	3	64	ASN	OD1-CG-ND2	11.97	134.57	122.60
2	2	169	ASP	CA-CB-CG	11.74	124.34	112.60
3	3	144	ARG	CD-NE-CZ	11.74	140.84	124.40
3	3	232	GLN	N-CA-CB	11.61	126.24	110.57
3	3	24	ALA	CA-C-O	-11.42	109.31	121.87
4	4	27	PHE	CA-CB-CG	11.33	125.13	113.80
1	1	60	GLN	O-C-N	11.32	136.77	123.30
2	2	106	TYR	CA-C-N	11.27	138.66	122.77
2	2	106	TYR	C-N-CA	11.27	138.66	122.77
1	1	10	VAL	CB-CA-C	11.00	120.74	111.06
2	2	216	ARG	NE-CZ-NH2	-10.98	109.32	119.20
2	2	241	PRO	CA-C-N	10.87	141.53	121.97
2	2	241	PRO	C-N-CA	10.87	141.53	121.97
1	1	134	ARG	NE-CZ-NH1	10.85	132.35	121.50
3	3	92	THR	CB-CA-C	10.78	131.41	110.17
1	1	61	THR	CA-CB-OG1	-10.75	93.48	109.60
1	1	199	GLY	O-C-N	10.74	132.94	123.60
1	1	214	THR	N-CA-CB	10.72	126.90	111.25
1	1	77	VAL	O-C-N	10.58	132.68	121.78
1	1	213	VAL	O-C-N	10.58	134.12	122.06
1	1	172	PHE	CA-C-O	-10.58	108.94	120.36
3	3	73	GLY	CA-C-O	10.57	132.68	121.90
3	3	207	ALA	O-C-N	10.55	134.71	123.42
1	1	227	GLU	CB-CG-CD	10.51	130.47	112.60
3	3	76	THR	O-C-N	10.39	132.78	122.07
3	3	57	ASN	CB-CG-ND2	-10.34	100.89	116.40
1	1	255	ARG	CD-NE-CZ	10.33	138.86	124.40
1	1	13	GLU	O-C-N	10.30	132.91	122.30
3	3	64	ASN	CA-CB-CG	-10.30	102.30	112.60
2	2	130	HIS	CA-CB-CG	-10.29	103.51	113.80
3	3	56	ASN	CA-C-N	10.28	141.16	121.54
3	3	56	ASN	C-N-CA	10.28	141.16	121.54
1	1	11	LEU	O-C-N	10.27	136.52	122.46
1	1	54	ARG	CG-CD-NE	10.24	134.52	112.00
2	2	240	VAL	CB-CA-C	10.21	120.78	111.08
3	3	67	MET	N-CA-CB	-10.16	93.31	110.49
1	1	280	ARG	NE-CZ-NH2	-10.15	110.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	17	THR	CB-CA-C	10.09	127.96	109.70
2	2	16	ILE	CA-C-O	-10.01	109.75	120.76
2	2	158	GLN	OE1-CD-NE2	9.99	132.59	122.60
2	2	237	SER	CA-C-O	9.88	130.83	119.27
4	4	30	ASN	CA-CB-CG	-9.86	102.74	112.60
3	3	53	ILE	N-CA-C	9.82	118.93	107.73
2	2	237	SER	N-CA-C	-9.80	101.08	113.23
2	2	169	ASP	CA-C-O	9.78	131.63	119.11
3	3	58	VAL	N-CA-C	9.77	121.84	108.17
2	2	161	ASP	N-CA-CB	9.74	124.60	109.69
2	2	248	PRO	N-CA-C	-9.70	95.79	111.21
3	3	232	GLN	O-C-N	9.66	133.96	122.46
2	2	12	ARG	CD-NE-CZ	9.64	137.90	124.40
4	4	28	ASN	OD1-CG-ND2	9.63	132.23	122.60
4	4	40	ALA	N-CA-C	-9.57	96.35	110.23
1	1	257	VAL	CB-CA-C	9.54	120.57	110.37
1	1	45	VAL	CB-CA-C	9.49	124.56	110.90
3	3	134	THR	CA-C-O	9.44	127.36	119.71
1	1	10	VAL	CA-C-O	9.42	127.20	119.29
2	2	26	ASP	CA-CB-CG	9.40	122.00	112.60
3	3	37	PRO	N-CA-CB	9.39	110.81	103.30
2	2	57	ASP	N-CA-CB	-9.33	95.67	110.69
2	2	164	LEU	O-C-N	9.30	133.99	123.01
2	2	20	ASP	N-CA-C	-9.29	101.47	113.17
1	1	154	ILE	O-C-N	9.25	130.03	121.61
3	3	74	ASN	OD1-CG-ND2	9.24	131.84	122.60
1	1	188	SER	CA-C-O	-9.20	110.39	121.06
1	1	19	ASN	OD1-CG-ND2	9.17	131.77	122.60
3	3	227	THR	CA-C-O	9.16	131.94	121.87
4	4	44	ASP	CA-CB-CG	9.12	121.72	112.60
4	4	40	ALA	O-C-N	9.11	134.07	122.87
1	1	88	ASP	CA-C-O	9.09	130.03	120.30
1	1	206	SER	O-C-N	9.07	132.48	122.05
2	2	71	TRP	CB-CA-C	9.03	125.51	110.79
3	3	96	THR	CA-C-N	8.99	133.58	120.90
3	3	96	THR	C-N-CA	8.99	133.58	120.90
2	2	16	ILE	O-C-N	8.96	133.00	123.05
3	3	155	TRP	CA-C-O	-8.94	110.73	120.30
2	2	61	ASN	CB-CA-C	8.93	125.95	112.03
4	4	42	ARG	CD-NE-CZ	8.92	136.88	124.40
2	2	182	ASN	N-CA-C	-8.91	100.25	113.61
3	3	114	ARG	N-CA-C	8.90	122.92	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	19	GLY	CA-C-N	8.90	137.22	122.54
2	2	19	GLY	C-N-CA	8.90	137.22	122.54
3	3	32	LYS	CA-C-O	-8.89	111.98	122.03
2	2	49	ALA	CA-C-O	-8.87	107.83	120.51
2	2	20	ASP	CA-C-O	8.87	129.73	119.35
4	4	37	SER	O-C-N	8.87	134.31	123.13
2	2	234	THR	CA-C-O	8.85	132.25	121.89
2	2	40	HIS	CA-CB-CG	-8.84	104.96	113.80
2	2	107	THR	CA-CB-OG1	-8.82	96.37	109.60
2	2	81	LYS	O-C-N	8.81	133.66	123.27
1	1	12	ASN	CA-CB-CG	8.80	121.40	112.60
2	2	162	ALA	CB-CA-C	8.79	125.42	110.56
3	3	54	PRO	CA-C-O	-8.77	110.66	120.92
2	2	57	ASP	CA-C-O	-8.76	111.42	120.71
2	2	61	ASN	OD1-CG-ND2	8.76	131.36	122.60
3	3	193	TYR	O-C-N	8.76	133.32	123.16
4	4	37	SER	CA-C-O	-8.76	111.09	120.46
3	3	108	HIS	CA-CB-CG	8.75	122.55	113.80
1	1	159	ASN	CA-CB-CG	8.72	121.32	112.60
3	3	53	ILE	O-C-N	8.71	129.22	121.12
3	3	45	GLU	CB-CG-CD	8.69	127.37	112.60
3	3	203	THR	CA-C-O	-8.68	111.34	120.28
2	2	101	LEU	CA-C-O	8.66	130.33	120.54
3	3	210	LEU	CA-C-N	-8.58	109.23	122.62
3	3	210	LEU	C-N-CA	-8.58	109.23	122.62
2	2	147	THR	N-CA-CB	8.54	123.97	110.73
2	2	63	PHE	N-CA-C	8.54	123.37	108.52
1	1	213	VAL	N-CA-C	-8.52	99.62	111.89
3	3	191	CYS	CA-C-O	-8.51	110.39	120.60
1	1	80	SER	CA-C-O	8.50	130.61	120.92
2	2	92	PHE	CA-CB-CG	8.46	122.26	113.80
1	1	70	PHE	N-CA-C	-8.45	100.71	112.45
3	3	205	GLN	OE1-CD-NE2	8.44	131.03	122.60
3	3	226	ASP	CA-CB-CG	8.43	121.03	112.60
3	3	26	PRO	O-C-N	8.40	133.39	123.06
1	1	204	ASN	CA-C-O	8.39	130.32	120.58
2	2	192	ASN	OD1-CG-ND2	8.39	130.99	122.60
3	3	218	ASP	N-CA-CB	-8.38	97.91	110.07
1	1	25	HIS	CA-C-O	-8.38	111.92	121.81
2	2	196	ASN	N-CA-CB	-8.37	98.91	110.38
2	2	62	ARG	NH1-CZ-NH2	-8.34	108.45	119.30
4	4	38	SER	O-C-N	8.34	133.68	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	196	ASN	CA-CB-CG	-8.32	104.28	112.60
2	2	135	ALA	CA-C-O	8.27	129.49	119.49
2	2	189	GLN	CA-CB-CG	8.26	130.62	114.10
1	1	216	ASP	CB-CA-C	8.26	125.44	111.41
1	1	35	ASP	CA-C-O	-8.22	112.30	121.51
2	2	181	GLY	N-CA-C	-8.21	103.76	114.85
1	1	252	ARG	O-C-N	8.21	127.95	121.55
1	1	49	ASP	CA-CB-CG	-8.19	104.41	112.60
3	3	32	LYS	O-C-N	8.18	132.34	122.68
1	1	86	TYR	CB-CA-C	8.18	122.76	109.02
2	2	220	TRP	CA-C-O	8.18	129.88	120.80
3	3	95	ALA	CA-C-O	-8.16	108.84	120.51
2	2	147	THR	O-C-N	8.16	131.96	122.25
2	2	83	PRO	CB-CA-C	8.15	125.87	112.26
1	1	46	GLN	O-C-N	8.14	130.69	121.32
1	1	59	SER	N-CA-CB	-8.13	96.75	110.49
2	2	28	VAL	CA-CB-CG1	8.12	124.21	110.40
3	3	206	THR	N-CA-C	-8.11	96.69	109.50
2	2	31	ALA	N-CA-CB	8.08	123.84	111.56
1	1	270	GLU	N-CA-CB	8.07	122.64	109.88
2	2	218	ASN	CB-CG-ND2	8.05	128.48	116.40
2	2	203	VAL	N-CA-CB	-8.00	100.01	111.21
1	1	12	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	1	251	PRO	CA-C-O	7.93	130.76	121.56
2	2	91	ILE	N-CA-CB	7.93	124.32	111.23
2	2	257	ARG	NE-CZ-NH2	-7.92	112.07	119.20
1	1	5	ASN	CA-CB-CG	7.92	120.52	112.60
3	3	227	THR	N-CA-C	7.91	120.79	110.43
2	2	160	ARG	N-CA-CB	-7.91	98.28	111.57
1	1	25	HIS	O-C-N	7.91	131.86	122.85
2	2	183	LEU	O-C-N	7.90	133.02	122.43
2	2	188	HIS	N-CA-C	7.87	118.63	108.24
3	3	90	THR	N-CA-CB	7.87	122.95	111.54
1	1	234	VAL	CA-C-O	7.87	129.00	120.43
2	2	50	ILE	CA-CB-CG2	7.86	123.87	110.50
1	1	146	MET	CA-C-N	7.85	133.55	122.72
1	1	146	MET	C-N-CA	7.85	133.55	122.72
2	2	161	ASP	O-C-N	7.84	132.67	122.95
3	3	36	ILE	N-CA-CB	7.84	122.18	111.21
3	3	50	ASP	CA-C-O	7.84	129.58	120.49
1	1	28	SER	N-CA-C	7.80	122.12	109.40
3	3	199	VAL	O-C-N	7.78	129.97	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	38	SER	CA-C-O	-7.77	109.39	120.51
2	2	156	VAL	CA-C-N	7.77	136.39	121.54
2	2	156	VAL	C-N-CA	7.77	136.39	121.54
3	3	233	SER	CA-C-O	7.77	131.30	122.37
4	4	43	LEU	N-CA-C	7.77	122.66	112.72
2	2	156	VAL	CA-C-O	7.74	130.45	120.78
1	1	168	ASN	CA-C-N	-7.73	112.33	123.00
1	1	168	ASN	C-N-CA	-7.73	112.33	123.00
1	1	13	GLU	CA-C-O	-7.73	112.70	119.97
1	1	100	LYS	O-C-N	7.73	132.02	123.13
2	2	29	ALA	N-CA-CB	7.72	123.42	110.69
3	3	42	ASN	OD1-CG-ND2	7.71	130.31	122.60
2	2	119	GLN	OE1-CD-NE2	7.68	130.28	122.60
1	1	285	THR	CA-C-O	-7.67	111.44	120.10
3	3	168	PRO	CA-C-N	-7.64	112.91	122.84
3	3	168	PRO	C-N-CA	-7.64	112.91	122.84
1	1	255	ARG	CA-C-O	-7.63	111.92	120.54
1	1	44	ASN	CA-CB-CG	-7.62	104.98	112.60
1	1	227	GLU	CG-CD-OE1	7.62	135.93	118.40
2	2	182	ASN	O-C-N	7.62	131.19	122.20
2	2	160	ARG	N-CA-C	7.61	119.70	108.14
3	3	55	VAL	CB-CA-C	7.60	123.76	111.29
1	1	134	ARG	NH1-CZ-NH2	-7.60	109.42	119.30
2	2	72	ASN	CA-CB-CG	-7.59	105.01	112.60
3	3	35	SER	CA-C-O	-7.58	112.09	120.81
1	1	275	THR	OG1-CB-CG2	7.57	124.45	109.30
1	1	38	GLU	CB-CG-CD	7.56	125.45	112.60
2	2	12	ARG	CG-CD-NE	7.55	128.60	112.00
2	2	161	ASP	CA-CB-CG	-7.55	105.05	112.60
2	2	111	GLN	CB-CG-CD	7.54	125.42	112.60
2	2	169	ASP	N-CA-C	-7.52	104.08	113.18
2	2	224	ILE	CB-CA-C	7.50	120.55	110.42
3	3	160	GLN	OE1-CD-NE2	-7.50	115.10	122.60
4	4	42	ARG	CA-C-N	-7.50	108.97	122.46
4	4	42	ARG	C-N-CA	-7.50	108.97	122.46
1	1	70	PHE	O-C-N	7.48	133.28	122.28
1	1	34	LEU	CA-C-O	-7.46	112.78	120.54
1	1	202	GLY	CA-C-N	7.46	135.95	121.18
1	1	202	GLY	C-N-CA	7.46	135.95	121.18
2	2	32	VAL	O-C-N	7.46	131.33	123.05
3	3	200	PRO	N-CA-C	-7.45	101.61	110.70
4	4	32	PHE	CA-C-N	7.45	131.14	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	32	PHE	C-N-CA	7.45	131.14	120.79
2	2	233	GLU	CA-C-O	7.41	127.22	119.51
1	1	159	ASN	CA-C-O	-7.39	112.41	121.58
3	3	57	ASN	CA-CB-CG	-7.39	105.20	112.60
1	1	111	ARG	CD-NE-CZ	7.39	134.75	124.40
3	3	185	MET	N-CA-CB	7.38	121.08	109.71
1	1	271	THR	CA-CB-OG1	-7.36	98.55	109.60
1	1	226	THR	N-CA-C	7.33	126.42	110.80
1	1	49	ASP	N-CA-C	7.33	119.05	111.14
2	2	86	LEU	CA-C-O	7.33	129.41	120.55
3	3	89	ILE	CB-CA-C	-7.31	99.30	111.29
1	1	5	ASN	N-CA-CB	7.30	122.92	110.50
2	2	70	HIS	CA-C-N	-7.30	112.74	123.11
2	2	70	HIS	C-N-CA	-7.30	112.74	123.11
3	3	163	ILE	N-CA-C	-7.30	97.97	108.48
2	2	233	GLU	CG-CD-OE2	7.29	135.18	118.40
2	2	126	MET	CA-CB-CG	-7.29	99.51	114.10
1	1	8	ASP	CA-CB-CG	-7.29	105.31	112.60
3	3	50	ASP	CA-CB-CG	7.28	119.88	112.60
2	2	155	ASP	CA-CB-CG	7.27	119.87	112.60
1	1	16	VAL	CB-CA-C	7.26	122.27	111.31
1	1	31	ALA	O-C-N	7.25	128.17	120.85
1	1	158	ARG	CD-NE-CZ	7.24	134.53	124.40
3	3	161	SER	CA-C-N	-7.22	111.62	122.74
3	3	161	SER	C-N-CA	-7.22	111.62	122.74
3	3	123	ALA	CA-C-O	-7.22	111.83	120.56
1	1	173	TRP	CA-CB-CG	7.20	127.28	113.60
3	3	201	PRO	N-CA-C	7.19	127.28	112.47
3	3	218	ASP	CA-C-N	7.18	135.25	121.54
3	3	218	ASP	C-N-CA	7.18	135.25	121.54
2	2	52	LYS	CG-CD-CE	7.16	127.77	111.30
2	2	78	TRP	CA-CB-CG	7.16	127.20	113.60
3	3	161	SER	CB-CA-C	-7.14	96.20	110.42
1	1	231	LEU	CA-CB-CG	7.14	141.29	116.30
1	1	23	SER	CA-C-O	7.13	129.86	121.58
1	1	233	VAL	CB-CA-C	-7.13	99.60	111.29
2	2	220	TRP	CA-C-N	7.13	133.72	122.74
2	2	220	TRP	C-N-CA	7.13	133.72	122.74
3	3	67	MET	CA-C-N	7.12	133.42	122.24
3	3	67	MET	C-N-CA	7.12	133.42	122.24
3	3	216	CYS	CA-C-O	-7.12	113.11	121.44
1	1	164	GLN	CG-CD-OE1	7.12	135.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	176	ASP	N-CA-C	-7.09	104.26	114.12
1	1	231	LEU	CB-CA-C	7.09	121.40	109.84
3	3	114	ARG	NE-CZ-NH1	-7.09	114.41	121.50
2	2	127	ILE	O-C-N	7.09	129.18	121.10
1	1	55	TYR	O-C-N	7.08	132.01	122.59
1	1	82	ILE	CB-CA-C	-7.08	99.67	111.29
2	2	114	ALA	CA-C-O	-7.08	110.39	120.51
2	2	147	THR	N-CA-C	-7.07	103.75	112.88
1	1	163	TRP	N-CA-C	-7.07	104.66	112.72
3	3	70	VAL	CA-C-N	-7.06	112.23	122.19
3	3	70	VAL	C-N-CA	-7.06	112.23	122.19
2	2	256	ALA	CA-C-O	-7.05	113.87	121.56
2	2	168	SER	CA-C-O	7.04	128.31	120.43
2	2	52	LYS	CA-CB-CG	7.02	128.15	114.10
2	2	205	TYR	CA-C-O	-7.01	113.08	120.58
1	1	190	ALA	CA-C-O	-6.99	113.47	121.72
2	2	134	SER	CA-C-O	6.99	128.96	120.92
1	1	134	ARG	CD-NE-CZ	6.98	134.18	124.40
3	3	101	GLU	CA-C-O	6.98	128.02	120.20
3	3	218	ASP	CA-C-O	6.97	127.88	120.70
2	2	190	PHE	CA-CB-CG	6.96	120.76	113.80
1	1	61	THR	CB-CA-C	6.96	121.25	109.50
1	1	246	THR	N-CA-C	6.94	120.75	110.48
2	2	67	GLU	CA-C-O	-6.93	113.15	121.05
4	4	43	LEU	O-C-N	6.93	130.62	122.09
2	2	237	SER	CB-CA-C	6.93	123.62	109.55
4	4	28	ASN	CA-C-N	-6.93	109.50	121.97
4	4	28	ASN	C-N-CA	-6.93	109.50	121.97
1	1	224	ILE	CB-CG1-CD1	-6.92	99.27	113.80
3	3	210	LEU	CA-C-O	-6.92	113.11	121.28
3	3	201	PRO	CA-C-N	-6.92	112.19	122.36
3	3	201	PRO	C-N-CA	-6.92	112.19	122.36
2	2	82	LEU	N-CA-C	6.91	125.08	109.81
2	2	126	MET	CA-C-O	-6.90	113.22	121.56
1	1	243	ALA	CA-C-O	6.88	127.70	120.54
4	4	29	ILE	O-C-N	6.88	131.17	122.57
1	1	216	ASP	O-C-N	6.88	131.10	122.84
1	1	283	THR	O-C-N	6.88	131.25	123.27
1	1	287	ALA	CA-C-O	-6.88	109.11	120.80
3	3	160	GLN	O-C-N	6.87	131.73	122.59
1	1	41	HIS	CA-C-N	-6.87	111.81	122.87
1	1	41	HIS	C-N-CA	-6.87	111.81	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	160	GLN	N-CA-CB	6.86	122.08	110.49
1	1	8	ASP	CA-C-N	6.86	133.78	121.92
1	1	8	ASP	C-N-CA	6.86	133.78	121.92
3	3	225	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	1	152	ALA	N-CA-CB	-6.83	103.93	111.10
3	3	70	VAL	O-C-N	6.83	129.12	122.97
1	1	138	ILE	N-CA-C	6.82	122.35	113.07
1	1	248	ALA	CA-C-N	6.81	133.15	122.94
1	1	248	ALA	C-N-CA	6.81	133.15	122.94
2	2	70	HIS	CA-CB-CG	-6.80	107.00	113.80
3	3	15	THR	CB-CA-C	6.80	123.46	110.27
2	2	87	LYS	CB-CG-CD	6.79	126.92	111.30
3	3	146	ASP	CB-CG-OD2	-6.78	102.81	118.40
1	1	179	PHE	O-C-N	6.77	126.93	121.38
2	2	119	GLN	CB-CA-C	6.76	121.48	109.65
3	3	89	ILE	CA-C-O	-6.75	112.34	120.78
3	3	58	VAL	CA-C-O	6.74	127.62	120.48
1	1	71	LEU	CA-C-O	-6.74	112.41	120.56
1	1	78	HIS	CA-CB-CG	-6.73	107.07	113.80
2	2	80	TRP	N-CA-CB	6.73	123.18	111.00
3	3	234	GLY	O-C-N	6.72	128.49	121.77
2	2	171	SER	CA-C-N	6.72	131.44	120.63
2	2	171	SER	C-N-CA	6.72	131.44	120.63
2	2	198	SER	CB-CA-C	-6.70	97.30	113.19
3	3	65	VAL	N-CA-CB	6.70	120.12	110.68
1	1	64	GLU	CA-CB-CG	6.69	127.49	114.10
1	1	275	THR	CA-CB-OG1	-6.69	99.56	109.60
2	2	31	ALA	O-C-N	6.68	130.08	123.46
2	2	158	GLN	CB-CG-CD	-6.68	101.24	112.60
3	3	90	THR	N-CA-C	-6.68	102.34	111.56
1	1	55	TYR	CA-C-N	-6.68	113.50	122.98
1	1	55	TYR	C-N-CA	-6.68	113.50	122.98
3	3	206	THR	CA-CB-OG1	-6.67	99.59	109.60
1	1	268	MET	O-C-N	6.65	128.97	121.32
3	3	203	THR	N-CA-C	-6.65	97.58	108.82
1	1	45	VAL	O-C-N	6.64	130.08	122.97
2	2	83	PRO	CA-C-N	6.64	135.78	121.64
2	2	83	PRO	C-N-CA	6.64	135.78	121.64
1	1	63	ASP	CA-C-O	-6.63	114.07	120.90
2	2	177	GLY	CA-C-N	6.63	131.77	121.76
2	2	177	GLY	C-N-CA	6.63	131.77	121.76
3	3	71	GLN	OE1-CD-NE2	6.63	129.23	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	155	ASP	N-CA-CB	6.63	121.69	110.49
2	2	150	GLY	O-C-N	6.62	131.31	122.70
3	3	128	LYS	CB-CA-C	-6.62	102.74	111.42
1	1	53	THR	N-CA-CB	-6.62	101.31	110.38
1	1	164	GLN	N-CA-C	-6.61	104.24	112.90
3	3	147	ALA	CA-C-N	6.61	131.18	120.60
3	3	147	ALA	C-N-CA	6.61	131.18	120.60
3	3	94	LEU	CA-C-O	-6.61	111.06	120.51
1	1	281	ARG	NE-CZ-NH2	-6.59	113.27	119.20
3	3	88	ASP	CA-CB-CG	6.57	119.17	112.60
3	3	169	TRP	CB-CA-C	6.55	121.26	110.78
2	2	168	SER	CA-C-N	6.55	134.34	121.58
2	2	168	SER	C-N-CA	6.55	134.34	121.58
3	3	165	LEU	O-C-N	6.54	131.01	123.29
3	3	87	VAL	N-CA-C	6.54	121.19	112.04
2	2	202	ILE	CA-C-O	-6.53	113.35	120.67
2	2	232	SER	N-CA-CB	6.53	121.62	110.65
3	3	10	SER	CB-CA-C	6.53	120.08	109.90
1	1	52	GLU	O-C-N	6.53	130.67	122.84
1	1	62	ARG	N-CA-C	-6.51	103.66	112.26
1	1	270	GLU	O-C-N	6.51	131.33	122.48
2	2	68	SER	CA-CB-OG	6.50	124.09	111.10
2	2	161	ASP	CB-CA-C	-6.50	99.76	109.90
1	1	52	GLU	CA-C-N	6.49	133.26	121.06
1	1	52	GLU	C-N-CA	6.49	133.26	121.06
3	3	15	THR	N-CA-CB	-6.49	99.00	110.42
3	3	70	VAL	CA-C-O	-6.47	114.46	120.22
1	1	132	ALA	CA-C-O	6.47	127.68	120.43
1	1	280	ARG	NH1-CZ-NH2	6.47	127.71	119.30
1	1	201	ASP	CA-C-N	6.46	129.74	120.56
1	1	201	ASP	C-N-CA	6.46	129.74	120.56
1	1	175	HIS	N-CA-CB	-6.46	99.58	110.49
3	3	56	ASN	CA-CB-CG	-6.45	106.15	112.60
1	1	234	VAL	CB-CA-C	6.43	120.45	110.28
3	3	206	THR	OG1-CB-CG2	6.43	122.17	109.30
3	3	72	LEU	N-CA-C	-6.43	98.74	108.96
2	2	180	LEU	CA-C-O	-6.43	113.96	120.96
2	2	54	THR	N-CA-CB	6.42	120.75	110.16
1	1	180	PRO	CB-CA-C	6.41	119.88	110.85
2	2	91	ILE	CA-C-O	-6.41	112.77	120.78
3	3	16	THR	CA-CB-CG2	6.40	121.38	110.50
1	1	204	ASN	N-CA-CB	6.40	119.57	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	64	ASN	CB-CG-ND2	-6.40	106.80	116.40
2	2	50	ILE	CB-CA-C	6.40	121.78	111.29
3	3	106	TYR	CA-C-O	-6.40	113.96	121.44
2	2	206	VAL	CB-CA-C	6.39	120.35	110.83
2	2	94	GLU	CA-C-O	6.39	127.24	119.64
2	2	228	SER	CA-C-N	6.38	126.40	119.90
2	2	228	SER	C-N-CA	6.38	126.40	119.90
2	2	103	ARG	CD-NE-CZ	6.37	133.32	124.40
2	2	176	ASP	CB-CA-C	6.37	120.08	109.38
1	1	216	ASP	CA-CB-CG	6.36	118.96	112.60
1	1	201	ASP	O-C-N	6.36	129.40	122.15
2	2	157	SER	CA-C-N	-6.36	112.13	122.81
2	2	157	SER	C-N-CA	-6.36	112.13	122.81
2	2	238	ASN	O-C-N	6.35	130.55	122.93
1	1	201	ASP	CA-C-O	-6.34	113.70	120.42
2	2	152	ALA	N-CA-CB	-6.34	100.13	110.14
3	3	226	ASP	OD1-CG-OD2	-6.33	107.71	122.90
3	3	77	GLY	CA-C-O	6.32	130.78	122.75
1	1	47	PRO	CB-CA-C	6.32	121.98	111.56
1	1	39	THR	O-C-N	6.31	131.17	122.46
1	1	94	ILE	O-C-N	6.31	130.19	123.00
2	2	183	LEU	CA-C-O	-6.31	111.62	119.38
1	1	5	ASN	O-C-N	6.31	133.09	123.00
1	1	49	ASP	CA-C-N	6.31	131.40	120.68
1	1	49	ASP	C-N-CA	6.31	131.40	120.68
2	2	183	LEU	N-CA-C	-6.30	104.85	112.54
1	1	121	PHE	CB-CA-C	-6.30	99.19	110.03
1	1	66	SER	O-C-N	6.30	130.79	123.30
1	1	211	SER	O-C-N	6.29	131.10	122.41
1	1	285	THR	CA-CB-OG1	-6.29	100.16	109.60
2	2	68	SER	N-CA-CB	6.29	119.98	110.42
4	4	40	ALA	N-CA-CB	6.29	119.33	109.83
3	3	235	PRO	CA-C-O	6.29	135.29	120.20
4	4	42	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	1	20	ILE	O-C-N	6.28	131.99	122.76
3	3	27	TRP	CA-C-N	-6.28	114.34	123.00
3	3	27	TRP	C-N-CA	-6.28	114.34	123.00
2	2	81	LYS	CA-CB-CG	6.27	126.65	114.10
2	2	56	PRO	CA-C-O	6.27	128.18	121.03
2	2	233	GLU	CG-CD-OE1	-6.27	103.98	118.40
2	2	161	ASP	CA-C-N	-6.26	112.63	122.65
2	2	161	ASP	C-N-CA	-6.26	112.63	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	228	SER	O-C-N	6.26	128.31	121.36
1	1	174	GLN	CB-CG-CD	6.26	123.24	112.60
1	1	268	MET	CA-CB-CG	-6.26	101.58	114.10
1	1	19	ASN	CA-CB-CG	-6.25	106.35	112.60
2	2	95	ASN	N-CA-C	-6.24	105.53	113.01
3	3	148	MET	CG-SD-CE	6.24	114.62	100.90
3	3	234	GLY	N-CA-C	-6.23	99.63	112.34
2	2	212	ASP	CA-C-N	6.23	130.75	121.72
2	2	212	ASP	C-N-CA	6.23	130.75	121.72
1	1	117	THR	CB-CA-C	-6.22	101.06	110.90
1	1	214	THR	N-CA-C	6.22	121.39	111.81
3	3	100	GLY	O-C-N	6.22	128.29	122.13
3	3	8	PRO	CA-C-N	6.22	133.59	121.41
3	3	8	PRO	C-N-CA	6.22	133.59	121.41
1	1	66	SER	CA-CB-OG	-6.21	98.68	111.10
2	2	130	HIS	O-C-N	6.21	132.10	122.67
1	1	154	ILE	N-CA-C	-6.20	100.73	108.05
1	1	155	PRO	CA-C-N	6.20	128.59	120.28
1	1	155	PRO	C-N-CA	6.20	128.59	120.28
1	1	19	ASN	CB-CG-OD1	-6.20	108.40	120.80
4	4	30	ASN	CB-CA-C	6.20	122.75	110.42
3	3	123	ALA	O-C-N	6.17	129.42	122.32
4	4	44	ASP	CA-C-O	6.17	131.30	120.80
1	1	205	THR	OG1-CB-CG2	6.17	121.64	109.30
1	1	69	SER	N-CA-C	-6.16	105.41	113.17
2	2	262	LYS	CB-CA-C	6.16	122.30	109.68
3	3	181	ASN	O-C-N	6.15	130.88	123.26
2	2	196	ASN	N-CA-C	6.14	117.96	110.41
2	2	128	PRO	CB-CA-C	6.13	119.02	110.98
2	2	39	PRO	CB-CA-C	-6.13	103.56	111.46
1	1	235	ILE	CA-C-O	6.13	127.70	120.72
1	1	161	PHE	N-CA-C	-6.11	97.79	110.80
2	2	56	PRO	N-CA-C	-6.10	101.58	110.80
2	2	95	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	1	189	ILE	CA-C-N	6.09	134.32	122.07
1	1	189	ILE	C-N-CA	6.09	134.32	122.07
1	1	121	PHE	CA-CB-CG	6.09	119.89	113.80
3	3	4	VAL	O-C-N	6.09	129.49	122.97
2	2	221	CYS	CA-C-O	6.08	127.07	120.32
3	3	26	PRO	N-CA-CB	6.08	108.98	103.33
3	3	134	THR	CB-CA-C	6.05	115.89	110.44
3	3	71	GLN	O-C-N	6.05	130.12	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	131	ILE	N-CA-C	6.05	116.41	107.15
2	2	225	ILE	CA-C-O	6.05	123.08	119.94
2	2	228	SER	N-CA-CB	6.04	118.83	110.01
1	1	117	THR	N-CA-CB	6.04	118.82	110.07
2	2	27	ASP	CA-C-O	-6.04	113.31	120.43
2	2	236	SER	CA-C-N	6.04	132.28	121.66
2	2	236	SER	C-N-CA	6.04	132.28	121.66
1	1	276	THR	O-C-N	6.03	130.47	123.17
1	1	45	VAL	CA-C-O	-6.02	114.65	121.75
1	1	60	GLN	N-CA-C	-6.01	99.10	108.90
1	1	94	ILE	N-CA-C	6.01	118.55	108.81
1	1	237	THR	CA-CB-OG1	-6.00	100.60	109.60
2	2	70	HIS	CB-CA-C	-6.00	99.63	109.53
3	3	228	ASP	CB-CA-C	-5.99	99.60	110.56
2	2	116	LYS	CB-CA-C	-5.98	99.29	110.36
1	1	189	ILE	CA-C-O	5.98	127.26	119.85
3	3	56	ASN	OD1-CG-ND2	5.97	128.57	122.60
3	3	181	ASN	OD1-CG-ND2	5.97	128.57	122.60
1	1	286	THR	CA-C-O	-5.96	113.71	120.32
3	3	194	GLN	N-CA-C	-5.95	103.47	112.04
3	3	89	ILE	CA-CB-CG2	5.95	120.62	110.50
1	1	227	GLU	OE1-CD-OE2	-5.95	108.63	122.90
2	2	173	LEU	CB-CA-C	5.95	120.02	110.09
1	1	233	VAL	CA-C-O	5.94	128.21	120.78
2	2	155	ASP	O-C-N	5.94	130.49	122.59
2	2	238	ASN	N-CA-CB	5.93	119.64	110.21
1	1	129	PRO	CA-C-N	5.92	131.12	122.77
1	1	129	PRO	C-N-CA	5.92	131.12	122.77
2	2	71	TRP	CA-C-O	5.92	126.79	120.46
2	2	61	ASN	CA-C-N	5.91	131.82	122.36
2	2	61	ASN	C-N-CA	5.91	131.82	122.36
1	1	236	THR	CB-CA-C	5.91	120.27	111.17
1	1	62	ARG	O-C-N	5.91	129.76	122.20
2	2	215	LEU	CA-C-O	-5.90	111.86	120.13
4	4	32	PHE	CA-CB-CG	-5.90	107.90	113.80
1	1	87	THR	CA-C-O	5.89	127.18	121.00
3	3	75	GLN	CA-C-N	5.89	128.10	120.44
3	3	75	GLN	C-N-CA	5.89	128.10	120.44
3	3	198	VAL	O-C-N	5.89	129.15	123.14
2	2	114	ALA	N-CA-C	-5.89	98.26	110.80
3	3	178	THR	N-CA-CB	5.89	119.36	110.30
1	1	273	ASP	CA-C-O	-5.88	115.32	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	81	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	1	274	VAL	O-C-N	5.87	129.41	122.66
3	3	161	SER	O-C-N	5.86	130.38	122.59
1	1	210	GLY	CA-C-O	5.85	126.32	121.05
1	1	163	TRP	CB-CA-C	5.85	120.59	110.94
2	2	209	VAL	CA-C-N	5.84	126.25	119.47
2	2	209	VAL	C-N-CA	5.84	126.25	119.47
1	1	283	THR	CA-CB-OG1	-5.83	100.85	109.60
3	3	180	ASP	CA-C-O	5.83	126.36	120.88
2	2	12	ARG	CB-CA-C	-5.83	100.04	110.70
3	3	73	GLY	N-CA-C	5.82	120.93	112.60
1	1	90	ASN	OD1-CG-ND2	-5.82	116.78	122.60
4	4	40	ALA	CA-C-O	-5.82	114.79	121.19
2	2	28	VAL	CB-CA-C	-5.82	101.75	111.29
3	3	92	THR	N-CA-C	-5.81	96.97	109.81
2	2	38	TRP	CA-C-N	5.81	125.74	119.76
2	2	38	TRP	C-N-CA	5.81	125.74	119.76
2	2	59	SER	CA-C-O	5.81	126.52	119.38
2	2	239	ILE	CB-CA-C	5.80	119.48	110.83
1	1	205	THR	CA-CB-OG1	-5.80	100.91	109.60
1	1	10	VAL	N-CA-CB	-5.78	101.18	112.75
2	2	155	ASP	CB-CG-OD2	-5.78	105.11	118.40
2	2	14	MET	CA-C-O	5.78	127.76	121.06
3	3	191	CYS	O-C-N	5.78	130.32	123.33
1	1	121	PHE	N-CA-C	5.77	117.25	108.07
4	4	42	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
2	2	62	ARG	NE-CZ-NH1	5.77	127.27	121.50
3	3	165	LEU	CA-C-O	-5.76	114.10	120.38
1	1	36	ALA	CA-C-N	5.76	132.54	121.54
1	1	36	ALA	C-N-CA	5.76	132.54	121.54
1	1	204	ASN	CB-CG-ND2	5.76	125.04	116.40
3	3	24	ALA	N-CA-CB	-5.76	102.03	110.26
1	1	63	ASP	O-C-N	5.76	128.25	122.03
1	1	282	ASN	CA-C-O	5.76	126.63	120.70
2	2	197	ASN	CA-C-N	5.74	131.81	122.39
2	2	197	ASN	C-N-CA	5.74	131.81	122.39
1	1	143	MET	CA-C-O	-5.74	114.40	121.06
1	1	273	ASP	CA-CB-CG	-5.74	106.86	112.60
3	3	222	ARG	NH1-CZ-NH2	-5.74	111.84	119.30
3	3	71	GLN	N-CA-CB	5.73	119.62	110.16
3	3	180	ASP	CB-CA-C	5.73	116.85	109.80
1	1	106	MET	N-CA-C	5.73	116.94	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	68	GLU	CA-C-O	5.72	125.44	119.14
1	1	220	ILE	CB-CA-C	-5.72	103.92	110.73
1	1	68	GLU	CA-CB-CG	5.72	125.55	114.10
1	1	259	TYR	CB-CA-C	-5.72	100.41	113.33
3	3	126	THR	O-C-N	5.71	129.78	123.33
3	3	57	ASN	OD1-CG-ND2	5.71	128.31	122.60
2	2	175	PHE	CA-CB-CG	5.70	119.50	113.80
2	2	241	PRO	O-C-N	-5.70	114.94	122.64
3	3	96	THR	N-CA-C	5.70	122.94	110.80
1	1	171	ILE	CB-CA-C	5.70	119.01	110.98
2	2	157	SER	O-C-N	5.69	130.16	122.59
1	1	126	THR	O-C-N	5.69	130.21	123.27
2	2	154	ARG	CG-CD-NE	5.69	124.52	112.00
3	3	120	CYS	CA-CB-SG	-5.69	101.31	114.40
3	3	155	TRP	O-C-N	5.69	129.87	123.27
3	3	162	THR	CB-CA-C	5.68	119.98	109.70
1	1	90	ASN	CB-CA-C	5.68	121.72	110.42
2	2	154	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	1	173	TRP	O-C-N	5.67	130.28	123.36
3	3	156	ASP	CA-CB-CG	5.67	118.27	112.60
2	2	227	ILE	N-CA-CB	5.67	120.58	111.23
1	1	37	ALA	N-CA-CB	-5.67	100.92	110.49
1	1	158	ARG	NE-CZ-NH1	5.66	127.16	121.50
2	2	12	ARG	CA-C-O	-5.66	113.96	120.24
1	1	266	ASN	O-C-N	5.65	130.10	122.59
1	1	246	THR	N-CA-CB	-5.65	101.71	110.29
2	2	84	ASP	CA-C-O	-5.64	113.11	120.00
2	2	74	SER	O-C-N	5.64	128.86	122.20
2	2	90	GLY	CA-C-O	5.64	130.38	120.57
2	2	96	MET	CA-C-O	5.64	126.50	120.24
3	3	135	PRO	CA-C-O	5.63	128.73	120.56
1	1	43	SER	CA-C-O	5.63	128.06	121.87
1	1	120	ARG	NE-CZ-NH2	5.62	124.26	119.20
3	3	81	LYS	N-CA-C	5.62	119.26	110.32
2	2	67	GLU	OE1-CD-OE2	5.62	136.39	122.90
3	3	172	ALA	N-CA-C	-5.62	102.96	111.56
2	2	176	ASP	CA-CB-CG	-5.62	106.98	112.60
3	3	185	MET	O-C-N	5.62	130.03	122.96
1	1	72	GLY	CA-C-N	5.61	130.73	121.86
1	1	72	GLY	C-N-CA	5.61	130.73	121.86
1	1	162	SER	CA-C-N	-5.61	113.69	122.73
1	1	162	SER	C-N-CA	-5.61	113.69	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	112	SER	CA-C-N	5.61	131.78	121.85
3	3	112	SER	C-N-CA	5.61	131.78	121.85
1	1	276	THR	CA-CB-OG1	-5.61	101.19	109.60
2	2	131	GLN	OE1-CD-NE2	-5.60	117.00	122.60
3	3	204	PRO	CA-C-O	-5.60	114.95	121.95
1	1	145	TYR	O-C-N	5.59	129.73	123.19
2	2	160	ARG	CG-CD-NE	5.59	124.29	112.00
2	2	75	SER	O-C-N	5.58	129.45	122.86
3	3	66	SER	CA-C-O	5.58	128.50	120.51
2	2	56	PRO	CA-C-N	-5.58	114.84	122.93
2	2	56	PRO	C-N-CA	-5.58	114.84	122.93
3	3	27	TRP	CA-C-O	-5.58	114.06	120.98
3	3	46	MET	CA-C-O	5.58	126.40	120.10
1	1	281	ARG	N-CA-CB	-5.58	101.93	110.85
1	1	71	LEU	CB-CA-C	5.57	121.45	111.03
2	2	135	ALA	N-CA-CB	-5.57	100.86	110.32
1	1	10	VAL	N-CA-C	-5.56	107.40	112.96
1	1	217	MET	O-C-N	5.56	129.50	122.28
1	1	70	PHE	N-CA-CB	5.55	118.53	110.26
3	3	146	ASP	N-CA-CB	5.55	119.87	110.49
2	2	263	GLN	OE1-CD-NE2	5.55	128.15	122.60
1	1	42	THR	O-C-N	5.54	130.15	123.16
2	2	158	GLN	CA-C-N	5.54	130.91	122.65
2	2	158	GLN	C-N-CA	5.54	130.91	122.65
1	1	153	PRO	N-CD-CG	-5.54	94.88	103.20
2	2	41	TYR	O-C-N	5.54	129.22	122.96
1	1	250	CYS	CA-C-N	5.54	125.49	119.78
1	1	250	CYS	C-N-CA	5.54	125.49	119.78
2	2	43	THR	CA-C-N	5.53	126.76	119.84
2	2	43	THR	C-N-CA	5.53	126.76	119.84
3	3	167	VAL	N-CA-CB	5.53	118.95	111.21
1	1	286	THR	O-C-N	5.52	129.76	123.31
1	1	282	ASN	OD1-CG-ND2	5.51	128.12	122.60
3	3	89	ILE	N-CA-C	5.51	120.81	109.34
2	2	142	ALA	CA-C-N	5.51	127.58	120.64
2	2	142	ALA	C-N-CA	5.51	127.58	120.64
2	2	261	ILE	O-C-N	5.50	129.28	123.00
1	1	76	CYS	CA-C-O	-5.50	114.64	120.92
3	3	55	VAL	O-C-N	5.50	129.45	122.57
2	2	94	GLU	N-CA-C	-5.50	106.50	113.43
3	3	124	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	1	124	GLU	N-CA-C	-5.49	102.77	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	157	LYS	CA-C-O	5.49	126.51	120.31
3	3	224	ALA	CA-C-O	5.49	127.31	121.16
1	1	86	TYR	N-CA-C	-5.48	107.24	114.31
2	2	31	ALA	N-CA-C	-5.47	99.99	108.42
1	1	251	PRO	N-CA-CB	5.47	108.11	103.35
2	2	150	GLY	CA-C-O	-5.47	111.05	120.57
2	2	73	GLY	N-CA-C	-5.47	106.27	115.62
3	3	89	ILE	CB-CG1-CD1	-5.47	102.32	113.80
3	3	33	GLU	CG-CD-OE2	-5.46	105.83	118.40
1	1	134	ARG	CA-C-O	5.46	125.81	119.32
2	2	106	TYR	N-CA-C	5.46	117.71	109.41
2	2	256	ALA	O-C-N	5.45	129.29	122.86
1	1	270	GLU	CB-CA-C	-5.45	102.16	110.88
3	3	235	PRO	N-CD-CG	-5.45	97.26	103.80
1	1	89	TYR	CA-C-N	-5.45	111.14	121.54
1	1	89	TYR	C-N-CA	-5.45	111.14	121.54
1	1	111	ARG	CA-C-O	5.45	127.06	121.07
1	1	275	THR	CA-C-O	5.45	126.48	120.71
1	1	17	VAL	CA-C-N	5.44	126.21	120.11
1	1	17	VAL	C-N-CA	5.44	126.21	120.11
1	1	82	ILE	N-CA-CB	5.44	120.21	111.23
3	3	28	TYR	CB-CG-CD2	5.44	128.96	120.80
4	4	27	PHE	CA-C-O	5.44	128.29	120.51
2	2	30	ASN	N-CA-CB	-5.43	101.32	110.49
2	2	94	GLU	CG-CD-OE1	-5.42	105.93	118.40
3	3	131	LEU	O-C-N	5.42	129.99	123.16
1	1	90	ASN	CB-CG-ND2	5.42	124.53	116.40
1	1	27	THR	CA-CB-OG1	-5.41	101.48	109.60
2	2	139	SER	N-CA-CB	-5.41	102.06	110.98
1	1	175	HIS	CA-C-O	5.41	128.24	120.51
1	1	223	ARG	O-C-N	-5.40	117.58	123.52
2	2	237	SER	CA-CB-OG	5.40	121.91	111.10
3	3	235	PRO	CB-CA-C	-5.40	98.50	112.00
2	2	201	LEU	CA-C-N	5.40	130.45	122.94
2	2	201	LEU	C-N-CA	5.40	130.45	122.94
3	3	227	THR	OG1-CB-CG2	5.40	120.10	109.30
2	2	72	ASN	N-CA-C	5.40	118.51	110.52
1	1	279	VAL	CB-CA-C	5.40	118.93	111.38
2	2	86	LEU	O-C-N	-5.39	115.30	122.20
1	1	51	ILE	CA-CB-CG2	5.39	119.66	110.50
2	2	141	THR	O-C-N	5.39	128.98	122.94
3	3	67	MET	O-C-N	-5.38	115.43	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	152	HIS	O-C-N	5.38	128.74	122.99
1	1	40	GLY	N-CA-C	-5.38	108.30	115.40
2	2	130	HIS	CA-C-O	-5.38	113.76	122.20
1	1	76	CYS	CB-CA-C	5.37	118.28	109.90
1	1	181	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	1	208	LYS	O-C-N	5.36	129.02	122.96
2	2	219	ASN	CB-CA-C	5.36	119.80	110.79
3	3	226	ASP	CB-CA-C	5.36	118.58	109.53
3	3	5	TYR	CA-C-N	5.35	129.06	122.37
3	3	5	TYR	C-N-CA	5.35	129.06	122.37
1	1	172	PHE	O-C-N	5.35	129.66	123.30
1	1	255	ARG	CA-C-N	-5.34	113.95	122.29
1	1	255	ARG	C-N-CA	-5.34	113.95	122.29
2	2	227	ILE	CA-C-N	-5.34	113.49	121.83
2	2	227	ILE	C-N-CA	-5.34	113.49	121.83
3	3	226	ASP	CB-CG-OD1	5.34	130.69	118.40
2	2	190	PHE	O-C-N	5.34	130.40	122.81
2	2	127	ILE	CA-C-O	-5.34	112.80	119.95
3	3	114	ARG	N-CA-CB	-5.33	102.33	110.65
2	2	134	SER	N-CA-CB	5.33	118.86	110.23
1	1	274	VAL	CA-CB-CG1	5.32	119.45	110.40
2	2	24	SER	CA-C-N	5.31	128.77	121.33
2	2	24	SER	C-N-CA	5.31	128.77	121.33
2	2	87	LYS	CB-CA-C	5.31	120.99	110.42
2	2	223	VAL	N-CA-CB	-5.31	102.73	111.44
2	2	35	TYR	N-CA-CB	-5.31	104.18	112.41
3	3	77	GLY	N-CA-C	-5.31	103.38	112.30
3	3	182	LYS	O-C-N	5.30	127.74	122.12
1	1	89	TYR	N-CA-C	-5.30	101.06	109.59
2	2	20	ASP	CA-CB-CG	5.30	117.90	112.60
1	1	168	ASN	O-C-N	5.30	130.20	122.94
2	2	108	VAL	CB-CA-C	5.30	118.55	111.19
1	1	201	ASP	CA-CB-CG	-5.29	107.31	112.60
1	1	247	LYS	CB-CA-C	-5.29	98.32	109.38
3	3	201	PRO	N-CA-CB	-5.29	97.70	103.25
1	1	88	ASP	CA-CB-CG	5.29	117.89	112.60
2	2	96	MET	N-CA-CB	-5.29	102.32	110.20
2	2	141	THR	CA-C-O	-5.29	115.48	121.72
3	3	165	LEU	CA-C-N	-5.28	114.14	122.64
3	3	165	LEU	C-N-CA	-5.28	114.14	122.64
2	2	63	PHE	CA-CB-CG	-5.27	108.53	113.80
1	1	223	ARG	NE-CZ-NH2	5.27	123.94	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	69	SER	CB-CA-C	5.27	118.89	110.09
3	3	157	VAL	CA-C-N	-5.27	113.25	120.57
3	3	157	VAL	C-N-CA	-5.27	113.25	120.57
2	2	144	TYR	CA-C-N	5.26	131.58	121.54
2	2	144	TYR	C-N-CA	5.26	131.58	121.54
2	2	202	ILE	O-C-N	5.25	128.72	123.10
2	2	81	LYS	CA-C-O	-5.25	114.55	120.32
4	4	42	ARG	N-CA-C	5.24	116.76	109.31
1	1	242	LYS	CA-C-O	5.24	126.69	120.66
2	2	165	ARG	N-CA-C	-5.24	99.64	110.80
3	3	141	PRO	CA-C-N	5.24	129.59	120.68
3	3	141	PRO	C-N-CA	5.24	129.59	120.68
3	3	154	VAL	N-CA-C	-5.24	102.09	109.21
3	3	160	GLN	CG-CD-NE2	5.24	124.25	116.40
3	3	57	ASN	N-CA-CB	-5.23	101.64	110.49
1	1	45	VAL	N-CA-C	-5.23	100.83	108.99
3	3	228	ASP	CB-CG-OD2	-5.23	106.36	118.40
2	2	157	SER	N-CA-CB	5.23	119.33	110.49
4	4	42	ARG	CA-C-O	-5.23	113.88	120.84
2	2	45	GLN	N-CA-CB	5.23	119.63	110.27
2	2	166	GLN	N-CA-CB	-5.23	102.58	110.32
3	3	127	LEU	N-CA-CB	-5.23	102.79	111.57
3	3	15	THR	N-CA-C	-5.22	106.98	113.19
1	1	236	THR	CA-CB-CG2	5.21	119.36	110.50
1	1	154	ILE	N-CA-CB	5.21	117.83	111.21
2	2	37	VAL	O-C-N	5.21	128.80	123.18
3	3	66	SER	CA-C-N	5.21	131.48	121.54
3	3	66	SER	C-N-CA	5.21	131.48	121.54
1	1	226	THR	CA-CB-OG1	-5.20	101.80	109.60
2	2	224	ILE	CA-CB-CG2	5.20	119.34	110.50
1	1	232	SER	N-CA-CB	5.20	117.36	110.29
3	3	79	ALA	O-C-N	5.20	131.60	122.09
3	3	142	THR	N-CA-CB	-5.19	102.31	110.30
1	1	82	ILE	O-C-N	5.18	129.05	122.57
2	2	182	ASN	CA-CB-CG	5.18	117.78	112.60
2	2	68	SER	O-C-N	5.18	128.74	122.68
3	3	163	ILE	N-CA-CB	5.18	120.40	111.39
2	2	45	GLN	O-C-N	5.17	128.30	122.19
2	2	186	PHE	N-CA-C	-5.17	102.63	110.39
4	4	29	ILE	CB-CA-C	5.17	119.78	111.29
1	1	18	PRO	O-C-N	5.17	128.92	122.71
2	2	76	LYS	CA-CB-CG	-5.17	103.77	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	146	LEU	N-CA-CB	5.16	118.23	110.65
1	1	86	TYR	CA-C-O	5.16	124.49	118.77
2	2	252	GLU	CG-CD-OE1	-5.16	106.54	118.40
1	1	43	SER	N-CA-CB	5.15	117.63	110.26
1	1	125	ILE	O-C-N	5.15	129.00	122.57
2	2	111	GLN	CB-CA-C	5.15	118.13	109.48
2	2	97	TYR	N-CA-CB	-5.14	102.42	110.44
1	1	125	ILE	CB-CA-C	-5.13	102.87	111.29
2	2	20	ASP	CA-C-N	5.13	130.37	122.93
2	2	20	ASP	C-N-CA	5.13	130.37	122.93
2	2	12	ARG	CA-CB-CG	-5.13	103.83	114.10
2	2	215	LEU	O-C-N	5.13	128.91	122.19
3	3	167	VAL	O-C-N	5.13	126.95	121.10
1	1	237	THR	OG1-CB-CG2	5.12	119.54	109.30
3	3	39	GLU	CB-CG-CD	5.12	121.31	112.60
3	3	184	SER	CA-C-N	5.12	128.61	121.24
3	3	184	SER	C-N-CA	5.12	128.61	121.24
2	2	171	SER	N-CA-C	5.12	119.39	111.56
2	2	257	ARG	O-C-N	5.12	129.39	122.59
2	2	194	ARG	NH1-CZ-NH2	5.11	125.94	119.30
2	2	160	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	2	152	ALA	N-CA-C	5.10	118.28	111.75
4	4	30	ASN	O-C-N	5.10	129.38	122.59
1	1	204	ASN	N-CA-C	-5.10	102.09	109.59
3	3	149	LEU	N-CA-CB	-5.10	102.37	110.22
3	3	183	TYR	CB-CG-CD1	5.10	128.45	120.80
2	2	160	ARG	NE-CZ-NH1	-5.10	116.40	121.50
2	2	79	TRP	CA-C-N	5.09	130.98	122.73
2	2	79	TRP	C-N-CA	5.09	130.98	122.73
3	3	200	PRO	O-C-N	5.09	127.47	121.46
2	2	62	ARG	NE-CZ-NH2	5.09	123.78	119.20
3	3	97	THR	N-CA-CB	5.09	117.78	109.69
3	3	76	THR	N-CA-CB	5.09	117.39	110.01
2	2	14	MET	O-C-N	-5.08	117.38	123.27
4	4	26	TYR	N-CA-CB	5.08	119.13	110.50
1	1	145	TYR	CA-C-N	-5.07	111.61	121.91
1	1	145	TYR	C-N-CA	-5.07	111.61	121.91
3	3	122	THR	N-CA-CB	5.07	118.53	110.87
1	1	18	PRO	CA-C-N	-5.07	113.98	123.05
1	1	18	PRO	C-N-CA	-5.07	113.98	123.05
1	1	228	LYS	CD-CE-NZ	5.06	128.08	111.90
1	1	83	LYS	N-CA-C	-5.05	99.09	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	62	ARG	CD-NE-CZ	-5.05	117.33	124.40
2	2	11	ASP	O-C-N	5.04	131.07	123.00
2	2	79	TRP	CA-CB-CG	5.04	123.19	113.60
3	3	84	SER	CA-C-N	5.04	129.11	122.51
3	3	84	SER	C-N-CA	5.04	129.11	122.51
4	4	33	LYS	N-CA-C	5.04	117.17	111.02
1	1	121	PHE	O-C-N	5.04	127.94	123.41
3	3	140	GLU	CB-CA-C	5.04	117.53	109.62
3	3	177	LEU	N-CA-CB	-5.04	102.20	110.41
3	3	105	TYR	N-CA-C	-5.03	107.12	114.12
1	1	175	HIS	CB-CA-C	5.03	120.43	110.42
1	1	283	THR	N-CA-CB	-5.03	102.17	111.53
3	3	170	VAL	CB-CA-C	5.03	117.91	110.77
3	3	189	ILE	CA-C-O	-5.03	115.23	120.76
1	1	70	PHE	CA-C-N	-5.02	112.62	121.81
1	1	70	PHE	C-N-CA	-5.02	112.62	121.81
2	2	15	GLN	CA-C-N	-5.02	115.47	122.71
2	2	15	GLN	C-N-CA	-5.02	115.47	122.71
2	2	243	THR	CA-CB-CG2	5.02	119.04	110.50
2	2	31	ALA	CA-C-N	-5.02	115.48	122.71
2	2	31	ALA	C-N-CA	-5.02	115.48	122.71
3	3	12	GLN	CA-C-N	5.02	130.62	121.89
3	3	12	GLN	C-N-CA	5.02	130.62	121.89
3	3	111	GLY	CA-C-O	5.02	128.97	122.59
1	1	170	SER	CB-CA-C	5.02	117.86	110.14
3	3	222	ARG	N-CA-C	5.01	115.76	108.14
1	1	27	THR	CA-CB-CG2	5.01	119.01	110.50
1	1	42	THR	CA-CB-OG1	-5.01	102.09	109.60
2	2	228	SER	CB-CA-C	5.00	115.56	109.85
4	4	26	TYR	O-C-N	5.00	131.00	123.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	110	ARG	Mainchain
1	1	150	PRO	Peptide
1	1	186	PHE	Mainchain
1	1	211	SER	Mainchain
1	1	223	ARG	Mainchain
1	1	98	LYS	Mainchain,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	1	2262	0	2192	403	1
2	2	1979	0	1922	223	2
3	3	1831	0	1810	247	1
4	4	151	0	136	18	0
5	1	25	0	20	3	0
All	All	6248	0	6080	795	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (795) 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)
1:1:101:ILE:H	1:1:101:ILE:CD1	1.07	1.45
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.55	1.45
1:1:101:ILE:N	1:1:101:ILE:HD13	1.26	1.25
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.69	1.25
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.59	1.20
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.20
1:1:108:GLN:CD	3:3:226:ASP:OD2	1.85	1.20
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
1:1:104:GLN:O	3:3:236:ILE:HD11	1.42	1.17
1:1:218:GLY:O	1:1:219:THR:HG22	0.98	1.16
1:1:211:SER:C	1:1:212:VAL:HG12	1.68	1.16
1:1:218:GLY:C	1:1:219:THR:HG22	1.63	1.16
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.15
1:1:104:GLN:O	3:3:236:ILE:CD1	1.95	1.14
1:1:101:ILE:HG21	1:1:217:MET:O	1.46	1.14
2:2:18:ARG:HH12	2:2:249:MET:HE2	1.06	1.14
1:1:218:GLY:C	1:1:219:THR:CG2	2.21	1.14
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.12
1:1:98:LYS:HA	1:1:220:ILE:O	1.50	1.11
1:1:154:ILE:CG2	1:1:221:CYS:SG	2.41	1.08
1:1:254:PRO:CG	3:3:101:GLU:HG2	1.81	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.07
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.06
1:1:146:MET:HE1	1:1:162:SER:O	1.54	1.06
1:1:119:VAL:CG1	1:1:121:PHE:HE1	1.70	1.05
1:1:108:GLN:OE1	3:3:226:ASP:CG	2.00	1.04
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
1:1:100:LYS:C	1:1:101:ILE:HD13	1.84	1.02
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:100:LYS:CA	1:1:101:ILE:HD13	1.89	1.02
1:1:150:PRO:O	1:1:151:GLY:C	1.99	1.02
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.02
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.01
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.01
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.91	1.00
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	0.99
1:1:101:ILE:H	1:1:101:ILE:HD12	1.23	0.99
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.94	0.98
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.98
1:1:223:ARG:HG2	1:1:223:ARG:HH11	1.29	0.97
3:3:117:PHE:CD1	3:3:211:CYS:HB3	2.00	0.97
1:1:211:SER:N	1:1:212:VAL:HG12	1.80	0.97
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
1:1:100:LYS:HA	1:1:101:ILE:CD1	1.96	0.95
1:1:211:SER:C	1:1:212:VAL:CG1	2.27	0.94
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93
1:1:163:TRP:CH2	1:1:222:SER:O	2.21	0.93
1:1:100:LYS:HA	1:1:101:ILE:HD13	1.49	0.93
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
1:1:217:MET:O	1:1:217:MET:HG2	1.70	0.92
1:1:101:ILE:HD12	1:1:219:THR:HA	1.53	0.91
3:3:24:ALA:O	3:3:25:LEU:HB2	1.71	0.91
1:1:113:PHE:O	1:1:115:LEU:N	2.04	0.90
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.90
1:1:96:PHE:CE2	1:1:157:LYS:HA	2.06	0.90
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.89
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:97:THR:HG23	1:1:222:SER:HB3	1.53	0.88
1:1:119:VAL:CG1	1:1:121:PHE:CE1	2.56	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.08	0.88
2:2:159:GLU:C	2:2:160:ARG:HG2	1.96	0.88
3:3:237:GLU:HG2	3:3:238:GLN:H	1.38	0.88
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.55	0.88
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.87
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.87
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	0.86
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.10	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:119:VAL:HG11	1:1:121:PHE:HE1	1.38	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.56	0.86
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.85
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.85
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.39	0.84
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.84
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.84
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.84
1:1:217:MET:O	1:1:217:MET:CG	2.22	0.84
1:1:97:THR:O	1:1:222:SER:N	2.12	0.83
1:1:101:ILE:CD1	1:1:101:ILE:N	1.88	0.83
1:1:101:ILE:HG13	1:1:218:GLY:CA	2.09	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.83
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.83
1:1:212:VAL:C	1:1:214:THR:N	2.37	0.82
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
1:1:102:THR:HG23	1:1:103:LEU:N	1.93	0.82
1:1:150:PRO:O	1:1:152:ALA:N	2.13	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.96	0.80
1:1:223:ARG:HG2	1:1:223:ARG:NH1	1.90	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:68:SER:C	2:2:69:LYS:HG2	2.06	0.80
1:1:148:VAL:HG11	1:1:154:ILE:HG13	1.63	0.80
1:1:104:GLN:O	3:3:236:ILE:HD13	1.80	0.79
1:1:124:GLU:O	1:1:125:ILE:HG12	1.82	0.79
1:1:119:VAL:HG13	1:1:121:PHE:HE1	1.47	0.79
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.79
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.18	0.79
3:3:237:GLU:CG	3:3:238:GLN:H	1.95	0.79
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
2:2:173:LEU:O	2:2:174:ASN:HB2	1.84	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
1:1:107:ALA:O	1:1:109:ILE:N	2.18	0.77
1:1:215:ASN:CG	1:1:215:ASN:O	2.27	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
3:3:55:VAL:C	3:3:57:ASN:H	1.93	0.76
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.76
1:1:211:SER:CA	1:1:212:VAL:HG12	2.16	0.76
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
1:1:99:TRP:CE3	1:1:220:ILE:HD12	2.22	0.75
1:1:261:HIS:HA	3:3:237:GLU:O	1.87	0.75
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.75
1:1:96:PHE:HB2	1:1:222:SER:O	1.86	0.75
4:4:26:TYR:CD1	4:4:29:ILE:HD11	2.22	0.74
2:2:65:THR:OG1	2:2:245:SER:OG	2.05	0.74
1:1:101:ILE:HG13	1:1:218:GLY:N	2.02	0.74
1:1:125:ILE:HD13	5:1:500:W54:C2B	2.17	0.74
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.74
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.74
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.73
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.53	0.73
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:TYR:H	2:2:131:GLN:HE21	1.36	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.22	0.73
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.73
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	0.73
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.72
1:1:211:SER:N	1:1:212:VAL:CG1	2.51	0.72
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
2:2:183:LEU:HD12	2:2:186:PHE:HD2	1.52	0.72
1:1:97:THR:O	1:1:221:CYS:HA	1.89	0.72
1:1:145:TYR:N	1:1:145:TYR:CD1	2.54	0.72
3:3:173:SER:O	3:3:175:PHE:N	2.23	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
1:1:212:VAL:H	1:1:214:THR:H	1.37	0.72
1:1:101:ILE:HG13	1:1:217:MET:C	2.15	0.72
1:1:124:GLU:O	1:1:125:ILE:CG1	2.37	0.72
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.72
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
2:2:148:HIS:N	2:2:149:PRO:HD3	2.05	0.71
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.71
1:1:101:ILE:HD12	1:1:219:THR:CA	2.19	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.71
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.23	0.71
1:1:104:GLN:HB2	1:1:262:SER:HB2	1.73	0.71
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.71
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:97:THR:HG23	1:1:222:SER:CB	2.20	0.70
1:1:99:TRP:HE3	1:1:220:ILE:HD12	1.54	0.70
1:1:107:ALA:O	1:1:110:ARG:N	2.22	0.70
1:1:146:MET:HB2	1:1:169:MET:O	1.91	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
1:1:101:ILE:CG2	1:1:217:MET:O	2.35	0.70
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.02	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.71	0.70
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.69
1:1:269:PRO:HG2	1:1:272:GLY:O	1.93	0.69
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.92	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:110:ARG:O	1:1:114:GLU:HG3	1.93	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.27	0.69
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.68
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68
1:1:160:ASP:H	1:1:163:TRP:CD1	2.11	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.93	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.67
2:2:78:TRP:HE3	2:2:78:TRP:N	1.92	0.67
2:2:174:ASN:C	2:2:175:PHE:HD1	2.03	0.67
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.67
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.67
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.67
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.77	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67
2:2:107:THR:OG1	2:2:249:MET:HE3	1.95	0.66
1:1:163:TRP:HH2	1:1:222:SER:O	1.73	0.66
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.66
2:2:91:ILE:O	2:2:92:PHE:C	2.39	0.66
3:3:91:SER:O	3:3:92:THR:C	2.39	0.66
1:1:260:THR:C	1:1:261:HIS:CD2	2.74	0.66
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
1:1:102:THR:C	1:1:103:LEU:HD23	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.65
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.65
2:2:155:ASP:O	2:2:156:VAL:HB	1.97	0.65
1:1:215:ASN:O	1:1:215:ASN:ND2	2.30	0.64
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:210:GLY:C	1:1:212:VAL:HG13	2.22	0.64
1:1:127:LEU:O	1:1:180:PRO:HD2	1.98	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.64
1:1:163:TRP:CZ3	1:1:223:ARG:HB2	2.33	0.64
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.64
1:1:212:VAL:N	1:1:214:THR:H	1.96	0.63
1:1:186:PHE:HE1	3:3:31:THR:HG22	1.63	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.99	0.63
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.63
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.63
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
1:1:197:TYR:HD1	1:1:198:ASP:H	1.46	0.62
3:3:145:LYS:O	3:3:148:MET:HE3	1.98	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.62
1:1:182:PHE:HA	3:3:21:SER:HB2	1.82	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.62
2:2:235:THR:C	2:2:237:SER:H	2.06	0.62
1:1:145:TYR:N	1:1:145:TYR:HD1	1.97	0.62
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.62
1:1:141:ILE:HA	1:1:226:THR:HG21	1.81	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.61
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:145:TYR:O	1:1:170:SER:HA	2.01	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.61
1:1:104:GLN:HA	1:1:110:ARG:HG3	1.82	0.61
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:LEU:HD12	2:2:186:PHE:CD2	2.34	0.61
1:1:94:ILE:HD12	1:1:94:ILE:N	2.16	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.60
1:1:125:ILE:HD12	1:1:182:PHE:HE1	1.66	0.60
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.36	0.60
1:1:146:MET:O	1:1:146:MET:HG2	1.96	0.60
1:1:260:THR:C	1:1:261:HIS:HD2	2.09	0.60
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.60
2:2:84:ASP:OD1	2:2:87:LYS:HE2	2.02	0.60
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.60
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.37	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.60
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.60
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
1:1:210:GLY:C	1:1:212:VAL:CG1	2.75	0.59
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.29	0.59
1:1:149:PRO:O	1:1:150:PRO:O	2.20	0.59
1:1:155:PRO:HD2	1:1:221:CYS:SG	2.41	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:150:PRO:O	1:1:152:ALA:CB	2.51	0.59
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.59
1:1:260:THR:O	1:1:261:HIS:HB2	2.03	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.66	0.59
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.59
2:2:14:MET:HE1	2:2:31:ALA:HB2	1.83	0.59
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.76	0.58
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.58
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.58
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.58
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.57
1:1:89:TYR:HE2	1:1:227:GLU:C	2.12	0.57
1:1:97:THR:H	1:1:222:SER:HB3	1.69	0.57
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.57
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:101:ILE:HG13	1:1:218:GLY:C	2.29	0.57
1:1:201:ASP:OD1	1:1:213:VAL:HG22	2.05	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.57
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
1:1:119:VAL:HG13	1:1:121:PHE:CD1	2.40	0.56
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.56
1:1:150:PRO:O	1:1:152:ALA:HB2	2.05	0.56
1:1:244:LYS:HZ1	4:4:38:SER:H	1.53	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.88	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.56
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.21	0.56
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.41	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.56
1:1:260:THR:O	1:1:261:HIS:CB	2.53	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.55
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.55
2:2:154:ARG:HD3	2:2:155:ASP:H	1.71	0.55
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:92:GLN:N	1:1:94:ILE:CD1	2.69	0.55
1:1:184:ILE:HG22	1:1:185:PRO:O	2.06	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.55
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.55
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
1:1:98:LYS:CA	1:1:220:ILE:O	2.40	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.55
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	0.55
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
1:1:260:THR:HB	1:1:261:HIS:HD2	1.71	0.55
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.55
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.55
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.22	0.54
3:3:107:THR:HG21	3:3:223:MET:HE2	1.89	0.54
3:3:237:GLU:CG	3:3:238:GLN:N	2.68	0.54
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.54
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.06	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
1:1:19:ASN:HA	1:1:58:THR:HG23	1.89	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
1:1:163:TRP:CH2	1:1:222:SER:C	2.86	0.54
1:1:183:SER:O	1:1:184:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.54
1:1:183:SER:C	1:1:184:ILE:CG1	2.80	0.54
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.54
1:1:261:HIS:CD2	1:1:261:HIS:N	2.76	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.54
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.70	0.53
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.53
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.53
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.53
1:1:186:PHE:CD1	1:1:186:PHE:C	2.86	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53
3:3:14:MET:C	3:3:16:THR:H	2.16	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.23	0.53
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.53
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.53
4:4:26:TYR:CD1	4:4:29:ILE:CD1	2.91	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:145:TYR:HD1	1:1:145:TYR:H	1.56	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.24	0.52
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:200:TYR:CE2	1:1:209:TYR:HB2	2.44	0.52
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.52
3:3:43:LEU:CD2	3:3:46:MET:HE2	2.39	0.52
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
1:1:101:ILE:CD1	1:1:219:THR:CA	2.87	0.52
1:1:197:TYR:HD1	1:1:198:ASP:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.28	0.52
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
1:1:197:TYR:CD1	1:1:198:ASP:N	2.78	0.52
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.52
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.51
1:1:260:THR:HB	1:1:261:HIS:CD2	2.44	0.51
1:1:265:THR:HG1	2:2:133:ALA:HB2	1.75	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.51
1:1:141:ILE:O	1:1:141:ILE:CG1	2.51	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.51
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
1:1:101:ILE:CD1	1:1:219:THR:N	2.73	0.51
1:1:101:ILE:CD1	1:1:219:THR:HA	2.35	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.51
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.51
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51
1:1:101:ILE:CG1	1:1:217:MET:C	2.84	0.51
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
1:1:102:THR:O	1:1:103:LEU:HD23	2.11	0.50
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.11	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
1:1:119:VAL:HG11	1:1:121:PHE:CE1	2.30	0.50
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.50
3:3:72:LEU:HD12	3:3:72:LEU:N	2.26	0.50
1:1:244:LYS:CE	4:4:38:SER:O	2.60	0.50
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.50
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD2	2.47	0.49
1:1:104:GLN:HB2	1:1:262:SER:CB	2.41	0.49
2:2:126:MET:HE3	2:2:126:MET:HA	1.94	0.49
2:2:175:PHE:CD1	2:2:175:PHE:N	2.79	0.49
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.49
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.49
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.49
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.49
1:1:191:SER:CB	3:3:34:ILE:HG12	2.43	0.49
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.49
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.49
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.48	0.49
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.49
2:2:18:ARG:HA	2:2:18:ARG:HD3	1.57	0.49
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.48
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.48
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.48
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.48
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.48
1:1:218:GLY:C	1:1:219:THR:HG23	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.78	0.48
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.48
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.48
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.48
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.48
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.48
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.48
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.48
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.48
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:212:VAL:C	1:1:214:THR:H	2.19	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD1	2.49	0.47
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.47
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
1:1:271:THR:O	1:1:272:GLY:C	2.58	0.47
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.47
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.27	0.47
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.47
3:3:216:CYS:C	3:3:218:ASP:H	2.22	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.47
1:1:186:PHE:CE1	3:3:31:THR:HG22	2.46	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.47
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.47
3:3:43:LEU:HD23	3:3:46:MET:HE2	1.97	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
3:3:237:GLU:HG2	3:3:238:GLN:N	2.18	0.47
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:TYR:HD1	1:1:89:TYR:HA	1.49	0.47
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.45	0.47
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.77	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.47
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.47
3:3:82:VAL:HG12	3:3:83:PHE:H	1.78	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.47
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.47
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:190:ALA:C	3:3:31:THR:HG21	2.38	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.46
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.46
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.46
1:1:125:ILE:HD12	1:1:182:PHE:CE1	2.47	0.46
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.97	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.15	0.46
1:1:101:ILE:HD12	1:1:219:THR:N	2.30	0.46
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.46
1:1:262:SER:O	1:1:263:HIS:HB2	2.14	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.49	0.46
1:1:224:ILE:HG21	1:1:224:ILE:HD13	1.46	0.46
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.46
3:3:91:SER:C	3:3:92:THR:O	2.58	0.46
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.46
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.46
1:1:122:ASP:OD1	1:1:245:HIS:HB2	2.16	0.46
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.98	0.46
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.46
2:2:160:ARG:HH11	2:2:160:ARG:HD2	1.57	0.45
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.45
3:3:14:MET:C	3:3:16:THR:N	2.74	0.45
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.56	0.45
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.04	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:103:LEU:HG	5:1:500:W54:C4	2.47	0.45
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.45
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.45
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.45
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.45
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.45
1:1:75:GLY:N	1:1:240:TYR:HD1	2.15	0.45
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.98	0.45
1:1:124:GLU:C	1:1:125:ILE:CG1	2.89	0.45
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.82	0.45
1:1:39:THR:C	1:1:41:HIS:H	2.24	0.45
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
1:1:101:ILE:CD1	1:1:218:GLY:C	2.90	0.45
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.54	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.45
3:3:42:ASN:CG	3:3:44:ILE:HG22	2.38	0.45
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.47	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:144:TYR:C	2:2:146:LEU:H	2.26	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:165:SER:C	1:1:167:THR:N	2.73	0.44
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.44
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
3:3:65:VAL:C	3:3:67:MET:N	2.74	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.17	0.44
1:1:101:ILE:HG13	1:1:218:GLY:HA3	1.97	0.44
1:1:127:LEU:HD12	1:1:239:ILE:HG12	2.00	0.44
1:1:148:VAL:C	1:1:149:PRO:O	2.57	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
1:1:90:ASN:HD22	1:1:90:ASN:N	2.16	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.33	0.44
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.44
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.44
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.44
2:2:155:ASP:HB3	2:2:156:VAL:H	1.61	0.44
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
1:1:61:THR:CG2	1:1:63:ASP:CG	2.91	0.43
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.43
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.43
1:1:85:ASP:OD1	1:1:85:ASP:C	2.61	0.43
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.43
1:1:197:TYR:H	2:2:131:GLN:NE2	2.12	0.43
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.43
3:3:102:ILE:C	3:3:104:SER:N	2.76	0.43
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.43
1:1:244:LYS:NZ	4:4:38:SER:O	2.52	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.43
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.43
1:1:149:PRO:C	1:1:150:PRO:O	2.62	0.43
2:2:126:MET:HB3	2:2:126:MET:HE2	1.61	0.43
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.43
2:2:247:SER:O	2:2:248:PRO:C	2.60	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.43
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.43
1:1:129:PRO:HA	1:1:237:THR:HA	2.01	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.52	0.43
1:1:36:ALA:C	1:1:38:GLU:H	2.26	0.43
1:1:99:TRP:CE3	1:1:220:ILE:CD1	2.98	0.43
2:2:57:ASP:O	2:2:58:THR:CG2	2.66	0.43
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.43
2:2:83:PRO:CG	2:2:218:ASN:HA	2.32	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
2:2:154:ARG:HH11	2:2:154:ARG:HG2	1.83	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.42
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.42
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.42
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.42
1:1:197:TYR:N	2:2:131:GLN:HE21	2.11	0.42
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
3:3:88:ASP:OD1	3:3:186:ALA:N	2.39	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.42
1:1:98:LYS:HA	1:1:220:ILE:C	2.37	0.42
1:1:182:PHE:CA	3:3:21:SER:HB2	2.47	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
3:3:46:MET:HE3	3:3:102:ILE:HD11	2.01	0.42
4:4:26:TYR:HD1	4:4:29:ILE:HD11	1.78	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:94:GLU:C	2:2:96:MET:N	2.76	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.42
2:2:178:THR:O	2:2:179:LEU:C	2.62	0.42
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.02	0.42
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.42
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:TRP:O	1:1:219:THR:HA	2.20	0.42
2:2:21:SER:OG	2:2:63:PHE:HB2	2.19	0.42
3:3:143:THR:C	3:3:192:TRP:CH2	2.97	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:159:LEU:HD23	3:3:159:LEU:HA	1.72	0.42
1:1:98:LYS:HB3	1:1:221:CYS:SG	2.60	0.41
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.41
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.41
1:1:66:SER:O	1:1:67:ILE:C	2.60	0.41
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.41
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.41
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.41
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.55	0.41
3:3:88:ASP:O	3:3:91:SER:OG	2.35	0.41
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.41
1:1:7:ILE:N	1:1:7:ILE:CD1	2.76	0.41
1:1:124:GLU:N	1:1:242:LYS:O	2.41	0.41
1:1:125:ILE:HD11	1:1:184:ILE:HD12	2.02	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
1:1:183:SER:C	1:1:184:ILE:HG12	2.45	0.41
1:1:261:HIS:H	3:3:237:GLU:H	1.68	0.41
2:2:61:ASN:HB2	2:2:248:PRO:C	2.45	0.41
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.41
1:1:136:ASP:O	1:1:137:ASP:CB	2.67	0.41
2:2:63:PHE:CD1	2:2:247:SER:HB2	2.55	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:71:LEU:HD13	1:1:113:PHE:CE1	2.56	0.41
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.41
2:2:155:ASP:O	2:2:156:VAL:CB	2.68	0.41
3:3:30:PRO:O	3:3:31:THR:C	2.62	0.41
3:3:158:GLY:C	3:3:160:GLN:N	2.77	0.41
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	0.41
1:1:184:ILE:HG23	1:1:185:PRO:HD2	2.01	0.41
1:1:199:GLY:C	1:1:200:TYR:CD1	2.98	0.41
1:1:124:GLU:HB3	1:1:242:LYS:HB3	2.02	0.41
1:1:148:VAL:HA	1:1:149:PRO:HD2	1.79	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
2:2:155:ASP:C	2:2:157:SER:H	2.29	0.41
1:1:38:GLU:C	1:1:40:GLY:N	2.73	0.41
1:1:101:ILE:O	1:1:102:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:ILE:HD13	1:1:125:ILE:HG21	1.79	0.41
1:1:125:ILE:HD13	5:1:500:W54:C1B	2.50	0.41
3:3:43:LEU:HD23	3:3:43:LEU:HA	1.78	0.41
3:3:43:LEU:HD22	3:3:46:MET:HE2	2.02	0.41
3:3:72:LEU:CD1	3:3:209:MET:HB3	2.48	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
1:1:169:MET:CE	1:1:171:ILE:CB	2.96	0.41
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.41
2:2:192:ASN:C	2:2:194:ARG:N	2.79	0.41
1:1:9:GLU:OE2	4:4:42:ARG:HG3	2.21	0.40
1:1:45:VAL:N	3:3:114:ARG:HH12	2.12	0.40
1:1:255:ARG:NH1	1:1:265:THR:O	2.36	0.40
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.03	0.40
2:2:55:GLN:HA	2:2:56:PRO:HD2	1.98	0.40
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.40
1:1:110:ARG:HD3	1:1:259:TYR:CZ	2.56	0.40
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.40
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.40
3:3:145:LYS:O	3:3:146:ASP:C	2.65	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.40
2:2:228:SER:HA	2:2:229:PRO:HD2	1.68	0.40
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.40
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:252:ARG:HB3	1:1:253:PRO:HD2	2.04	0.40
2:2:144:TYR:C	2:2:146:LEU:N	2.78	0.40
2:2:164:LEU:C	2:2:166:GLN:N	2.80	0.40
3:3:53:ILE:HG13	3:3:212:PHE:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:113:ASN:OD1	3:3:195:THR:OG1[3_665]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:25:HIS:CB	2:2:17:THR:O[2_655]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	281/287 (98%)	207 (74%)	50 (18%)	24 (8%)	0	9
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1	14
3	3	236/238 (99%)	178 (75%)	38 (16%)	20 (8%)	0	9
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1	15
All	All	785/832 (94%)	595 (76%)	130 (17%)	60 (8%)	1	11

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU
1	1	150	PRO
1	1	158	ARG
1	1	212	VAL
1	1	219	THR
1	1	226	THR
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE

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Mol	Chain	Res	Type
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA
1	1	67	ILE
1	1	90	ASN
1	1	99	TRP
1	1	227	GLU
2	2	91	ILE
2	2	129	GLU
2	2	155	ASP
2	2	193	LEU
2	2	208	ALA
2	2	257	ARG
3	3	59	GLY
3	3	66	SER
3	3	67	MET
3	3	95	ALA
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	137	ASP
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	159	LEU
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	125	ILE
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
2	2	44	PRO
3	3	121	GLY

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Mol	Chain	Res	Type
1	1	101	ILE
3	3	82	VAL

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	1	254/258 (98%)	184 (72%)	70 (28%)	0	3
2	2	219/227 (96%)	149 (68%)	70 (32%)	0	1
3	3	209/209 (100%)	153 (73%)	56 (27%)	0	3
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	495 (71%)	202 (29%)	0	2

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	ASN
1	1	6	TYR
1	1	7	ILE
1	1	15	LEU
1	1	17	VAL
1	1	19	ASN
1	1	26	THR
1	1	29	ASN
1	1	44	ASN
1	1	45	VAL
1	1	54	ARG
1	1	60	GLN
1	1	87	THR
1	1	89	TYR
1	1	90	ASN
1	1	97	THR
1	1	100	LYS
1	1	101	ILE
1	1	102	THR

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Mol	Chain	Res	Type
1	1	103	LEU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
1	1	121	PHE
1	1	123	SER
1	1	126	THR
1	1	127	LEU
1	1	134	ARG
1	1	141	ILE
1	1	142	VAL
1	1	143	MET
1	1	145	TYR
1	1	146	MET
1	1	157	LYS
1	1	158	ARG
1	1	160	ASP
1	1	162	SER
1	1	168	ASN
1	1	173	TRP
1	1	186	PHE
1	1	187	LEU
1	1	201	ASP
1	1	212	VAL
1	1	213	VAL
1	1	215	ASN
1	1	216	ASP
1	1	217	MET
1	1	219	THR
1	1	223	ARG
1	1	224	ILE
1	1	226	THR
1	1	227	GLU
1	1	228	LYS
1	1	232	SER
1	1	234	VAL
1	1	236	THR
1	1	237	THR
1	1	246	THR
1	1	247	LYS
1	1	250	CYS

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Mol	Chain	Res	Type
1	1	259	TYR
1	1	265	THR
1	1	274	VAL
1	1	275	THR
1	1	276	THR
1	1	278	ILE
1	1	279	VAL
1	1	281	ARG
1	1	286	THR
2	2	12	ARG
2	2	13	ILE
2	2	15	GLN
2	2	17	THR
2	2	18	ARG
2	2	25	SER
2	2	27	ASP
2	2	28	VAL
2	2	30	ASN
2	2	32	VAL
2	2	43	THR
2	2	50	ILE
2	2	51	ASN
2	2	52	LYS
2	2	55	GLN
2	2	58	THR
2	2	60	SER
2	2	62	ARG
2	2	63	PHE
2	2	65	THR
2	2	68	SER
2	2	72	ASN
2	2	75	SER
2	2	78	TRP
2	2	86	LEU
2	2	87	LYS
2	2	88	ASP
2	2	91	ILE
2	2	94	GLU
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	119	GLN

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Mol	Chain	Res	Type
2	2	126	MET
2	2	132	LEU
2	2	136	LYS
2	2	139	SER
2	2	140	VAL
2	2	145	LYS
2	2	146	LEU
2	2	151	GLU
2	2	154	ARG
2	2	158	GLN
2	2	159	GLU
2	2	160	ARG
2	2	164	LEU
2	2	170	ASP
2	2	171	SER
2	2	173	LEU
2	2	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	194	ARG
2	2	195	SER
2	2	197	ASN
2	2	198	SER
2	2	200	THR
2	2	201	LEU
2	2	202	ILE
2	2	206	VAL
2	2	207	ASN
2	2	216	ARG
2	2	219	ASN
2	2	222	LEU
2	2	224	ILE
2	2	239	ILE
2	2	240	VAL
2	2	257	ARG
2	2	261	ILE
2	2	263	GLN
3	3	2	LEU
3	3	4	VAL
3	3	5	TYR
3	3	7	THR
3	3	19	MET

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Mol	Chain	Res	Type
3	3	21	SER
3	3	23	CYS
3	3	32	LYS
3	3	39	GLU
3	3	42	ASN
3	3	50	ASP
3	3	55	VAL
3	3	60	ASN
3	3	61	ASN
3	3	65	VAL
3	3	66	SER
3	3	75	GLN
3	3	84	SER
3	3	89	ILE
3	3	90	THR
3	3	92	THR
3	3	99	ILE
3	3	102	ILE
3	3	116	SER
3	3	124	ASN
3	3	126	THR
3	3	127	LEU
3	3	131	LEU
3	3	134	THR
3	3	140	GLU
3	3	142	THR
3	3	143	THR
3	3	148	MET
3	3	157	VAL
3	3	159	LEU
3	3	161	SER
3	3	166	VAL
3	3	177	LEU
3	3	182	LYS
3	3	189	ILE
3	3	192	TRP
3	3	194	GLN
3	3	196	ASN
3	3	197	LEU
3	3	201	PRO
3	3	205	GLN
3	3	209	MET

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Mol	Chain	Res	Type
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE
3	3	213	VAL
3	3	216	CYS
3	3	217	LYS
3	3	231	ILE
3	3	236	ILE
3	3	238	GLN
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	159	ASN
1	1	174	GLN
1	1	175	HIS
1	1	204	ASN
1	1	215	ASN
1	1	261	HIS
1	1	282	ASN
2	2	15	GLN
2	2	30	ASN
2	2	51	ASN
2	2	72	ASN
2	2	109	HIS
2	2	111	GLN
2	2	131	GLN
2	2	192	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
3	3	12	GLN
3	3	20	GLN

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Mol	Chain	Res	Type
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN
3	3	75	GLN
3	3	80	GLN
3	3	124	ASN
3	3	194	GLN
4	4	28	ASN
4	4	30	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	W54	1	500	-	27,27,27	3.05	4 (14%)	35,36,36	2.71	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W54	1	500	-	-	5/13/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	13.12	1.43	1.27
5	1	500	W54	C4A-N3A	-6.89	1.36	1.47
5	1	500	W54	O1A-C2A	-4.22	1.29	1.36
5	1	500	W54	O1A-C5A	-3.12	1.38	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-9.58	109.97	118.25
5	1	500	W54	C4A-N3A-C2A	6.81	112.80	106.75
5	1	500	W54	O1A-C2A-C4B	6.48	124.03	115.85
5	1	500	W54	O1B-C1B-C6B	-4.87	115.21	121.14
5	1	500	W54	O1A-C5A-C4A	4.02	111.71	104.24
5	1	500	W54	O1B-C1B-C2B	3.33	125.20	121.14
5	1	500	W54	C5A-C4A-N3A	-2.68	98.58	104.42
5	1	500	W54	C5C-O1B-C1B	2.06	120.39	114.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

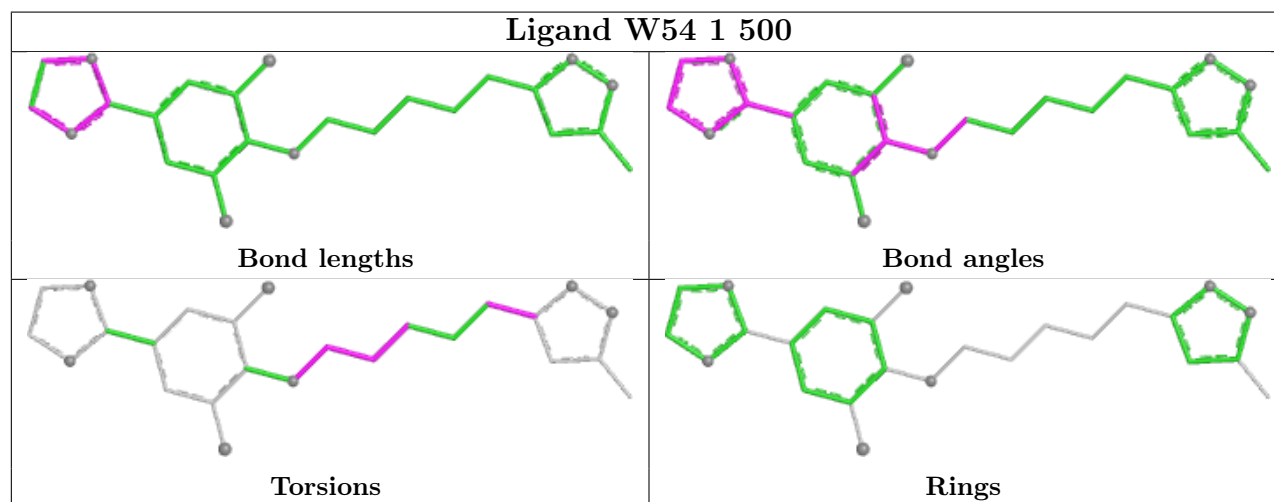
Mol	Chain	Res	Type	Atoms
5	1	500	W54	C3C-C4C-C5C-O1B
5	1	500	W54	C2C-C3C-C4C-C5C
5	1	500	W54	C2C-C1C-C5-O1
5	1	500	W54	C2C-C1C-C5-C4
5	1	500	W54	C4C-C5C-O1B-C1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	500	W54	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	213:VAL	C	214:THR	N	1.61
1	1	118:TYR	C	119:VAL	N	1.19
1	1	98:LYS	C	99:TRP	N	1.15
1	1	146:MET	C	147:TYR	N	0.98

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.