



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:15 AM UTC

PDB ID : 2HWF / pdb_00002hwf
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

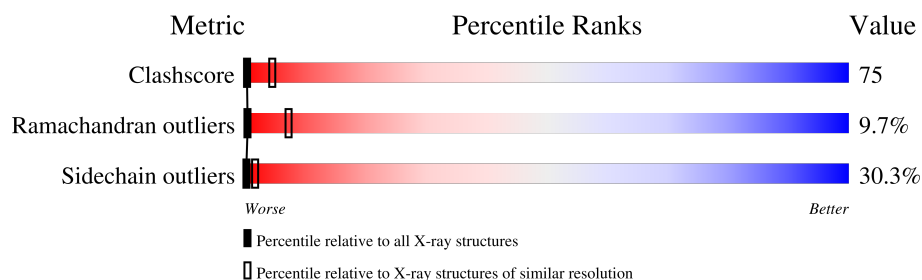
1 Overall quality at a glance

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	JEN	1	700	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6244 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			

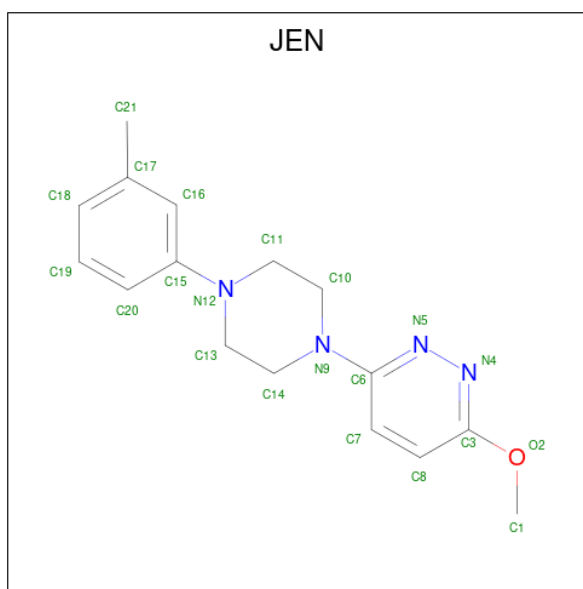
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

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 3-METHOXY-6-[4-(3-METHYLPHENYL)-1-PIPERAZINYL]PYRIDAZINE (CCD ID: JEN) (formula: C₁₆H₂₀N₄O).



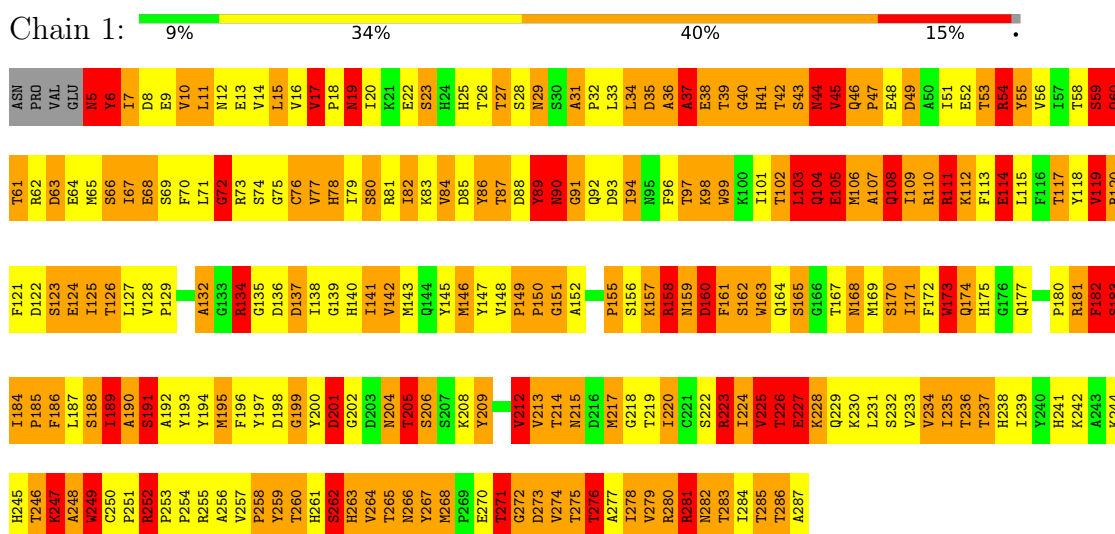
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			21	16	4	1		

3 Residue-property plots

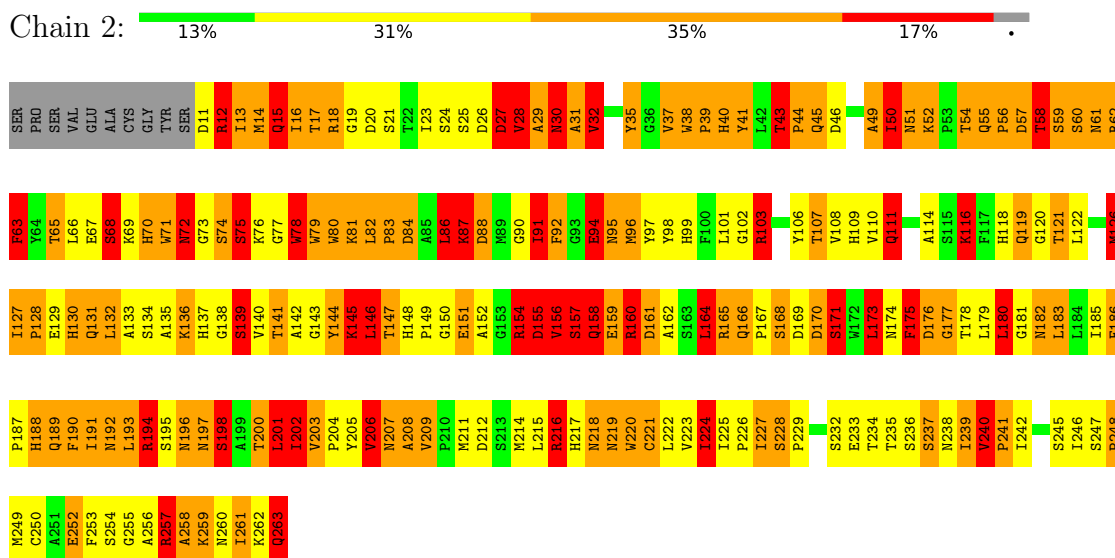
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

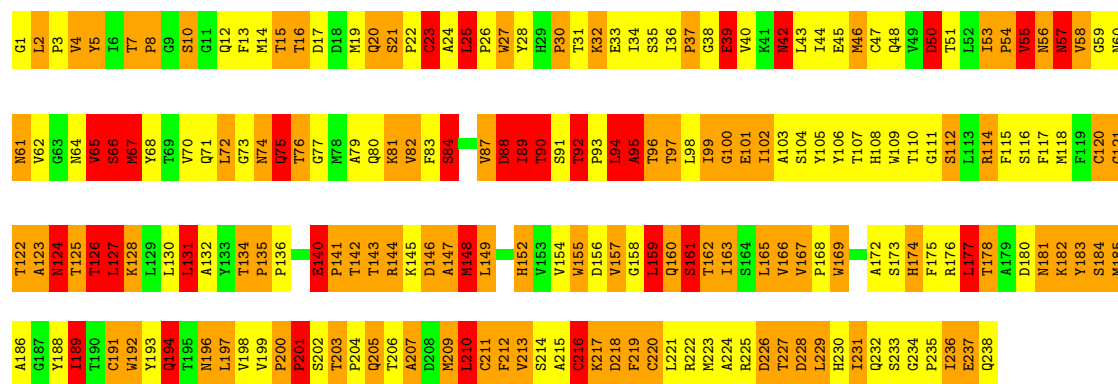


• Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)



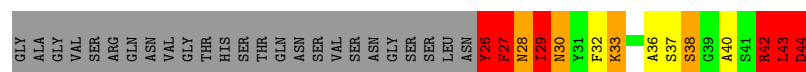
• Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)

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	6244	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: JEN

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	1.37	17/2322 (0.7%)	2.83	215/3162 (6.8%)
2	2	1.23	1/2033 (0.0%)	3.12	290/2770 (10.5%)
3	3	1.27	4/1878 (0.2%)	3.01	223/2570 (8.7%)
4	4	1.46	0/154	3.75	34/206 (16.5%)
All	All	1.30	22/6387 (0.3%)	3.00	762/8708 (8.8%)

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	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	118	TYR	C-N	-12.40	1.16	1.33
1	1	186	PHE	N-CA	-11.24	1.32	1.46
1	1	184	ILE	CA-C	-10.87	1.41	1.52
1	1	185	PRO	CA-C	-10.78	1.37	1.52
1	1	258	PRO	C-N	9.04	1.45	1.33
1	1	185	PRO	N-CA	-8.66	1.36	1.47
3	3	20	GLN	C-N	-8.25	1.22	1.33
1	1	184	ILE	CA-CB	-8.18	1.43	1.54
3	3	24	ALA	C-N	-7.24	1.27	1.33
1	1	183	SER	C-N	-7.17	1.25	1.33
1	1	252	ARG	N-CA	-6.20	1.40	1.46
1	1	165	SER	C-N	-5.98	1.24	1.33
1	1	184	ILE	N-CA	-5.93	1.39	1.46
1	1	185	PRO	C-O	5.91	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	183	SER	CA-C	-5.53	1.45	1.53
1	1	90	ASN	N-CA	5.47	1.53	1.46
3	3	27	TRP	NE1-CE2	-5.44	1.31	1.37
2	2	58	THR	CA-CB	5.43	1.62	1.53
3	3	25	LEU	N-CA	-5.34	1.41	1.46
1	1	99	TRP	NE1-CE2	-5.29	1.31	1.37
1	1	271	THR	N-CA	5.23	1.52	1.46
1	1	163	TRP	NE1-CE2	-5.20	1.31	1.37

All (762) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	249	TRP	O-C-N	-54.21	50.49	122.59
1	1	247	LYS	CA-C-O	-38.39	78.09	120.32
2	2	62	ARG	CD-NE-CZ	24.28	158.39	124.40
1	1	247	LYS	N-CA-C	24.14	147.88	108.52
1	1	249	TRP	CA-C-N	-16.22	84.35	122.31
1	1	249	TRP	C-N-CA	-16.22	84.35	122.31
1	1	247	LYS	CB-CA-C	-15.82	84.24	110.19
3	3	222	ARG	CD-NE-CZ	15.35	145.89	124.40
2	2	72	ASN	OD1-CG-ND2	14.94	137.54	122.60
3	3	235	PRO	CA-C-N	14.35	141.01	122.93
3	3	235	PRO	C-N-CA	14.35	141.01	122.93
1	1	68	GLU	CB-CG-CD	14.22	136.77	112.60
3	3	218	ASP	CA-CB-CG	-13.79	98.81	112.60
2	2	196	ASN	OD1-CG-ND2	13.74	136.34	122.60
3	3	212	PHE	CA-CB-CG	13.55	127.35	113.80
2	2	218	ASN	CA-CB-CG	13.43	126.03	112.60
3	3	203	THR	O-C-N	13.22	131.27	121.88
2	2	187	PRO	CB-CA-C	13.10	128.14	111.64
1	1	281	ARG	CA-CB-CG	13.07	140.23	114.10
2	2	154	ARG	CA-C-N	12.60	145.60	121.54
2	2	154	ARG	C-N-CA	12.60	145.60	121.54
3	3	64	ASN	OD1-CG-ND2	12.00	134.60	122.60
2	2	169	ASP	CA-CB-CG	11.79	124.39	112.60
3	3	144	ARG	CD-NE-CZ	11.75	140.85	124.40
3	3	232	GLN	N-CA-CB	11.59	126.22	110.57
4	4	27	PHE	CA-CB-CG	11.34	125.14	113.80
2	2	106	TYR	CA-C-N	11.26	138.65	122.77
2	2	106	TYR	C-N-CA	11.26	138.65	122.77
1	1	60	GLN	O-C-N	11.24	136.68	123.30
1	1	182	PHE	O-C-N	-11.20	107.83	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	216	ARG	NE-CZ-NH2	-11.05	109.25	119.20
1	1	10	VAL	CB-CA-C	10.98	120.73	111.06
2	2	241	PRO	CA-C-N	10.89	141.57	121.97
2	2	241	PRO	C-N-CA	10.89	141.57	121.97
1	1	134	ARG	NE-CZ-NH1	10.80	132.30	121.50
3	3	92	THR	CB-CA-C	10.79	131.44	110.17
1	1	61	THR	CA-CB-OG1	-10.77	93.44	109.60
1	1	185	PRO	O-C-N	10.76	137.16	122.64
1	1	172	PHE	CA-C-O	-10.63	108.88	120.36
3	3	207	ALA	O-C-N	10.55	134.71	123.42
1	1	77	VAL	O-C-N	10.55	132.64	121.78
3	3	73	GLY	CA-C-O	10.45	132.56	121.90
3	3	76	THR	O-C-N	10.42	132.81	122.07
3	3	57	ASN	CB-CG-ND2	-10.35	100.88	116.40
1	1	13	GLU	O-C-N	10.30	132.91	122.30
2	2	130	HIS	CA-CB-CG	-10.27	103.53	113.80
3	3	25	LEU	O-C-N	10.27	128.42	121.23
3	3	64	ASN	CA-CB-CG	-10.27	102.33	112.60
1	1	11	LEU	O-C-N	10.26	136.52	122.46
1	1	54	ARG	CG-CD-NE	10.22	134.50	112.00
3	3	56	ASN	CA-C-N	10.22	141.06	121.54
3	3	56	ASN	C-N-CA	10.22	141.06	121.54
3	3	67	MET	N-CA-CB	-10.18	93.29	110.49
2	2	240	VAL	CB-CA-C	10.16	120.73	111.08
1	1	280	ARG	NE-CZ-NH2	-10.10	110.11	119.20
2	2	17	THR	CB-CA-C	10.10	127.98	109.70
2	2	16	ILE	CA-C-O	-10.01	109.75	120.76
2	2	158	GLN	OE1-CD-NE2	9.98	132.58	122.60
2	2	237	SER	CA-C-O	9.91	130.87	119.27
4	4	30	ASN	CA-CB-CG	-9.87	102.73	112.60
3	3	53	ILE	N-CA-C	9.81	118.92	107.73
2	2	237	SER	N-CA-C	-9.79	101.09	113.23
2	2	169	ASP	CA-C-O	9.78	131.62	119.11
3	3	58	VAL	N-CA-C	9.76	121.83	108.17
2	2	161	ASP	N-CA-CB	9.75	124.61	109.69
3	3	232	GLN	O-C-N	9.74	134.05	122.46
4	4	28	ASN	OD1-CG-ND2	9.68	132.28	122.60
2	2	248	PRO	N-CA-C	-9.66	95.85	111.21
2	2	12	ARG	CD-NE-CZ	9.63	137.88	124.40
4	4	40	ALA	N-CA-C	-9.58	96.34	110.23
1	1	45	VAL	CB-CA-C	9.55	124.65	110.90
2	2	26	ASP	CA-CB-CG	9.48	122.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	10	VAL	CA-C-O	9.42	127.20	119.29
3	3	37	PRO	N-CA-CB	9.39	110.81	103.30
3	3	134	THR	CA-C-O	9.38	127.30	119.71
2	2	57	ASP	N-CA-CB	-9.34	95.66	110.69
2	2	20	ASP	N-CA-C	-9.30	101.45	113.17
2	2	164	LEU	O-C-N	9.27	133.95	123.01
3	3	74	ASN	OD1-CG-ND2	9.22	131.82	122.60
2	2	162	ALA	CB-CA-C	9.19	125.44	110.09
4	4	40	ALA	O-C-N	9.15	134.13	122.87
4	4	44	ASP	CA-CB-CG	9.13	121.73	112.60
3	3	227	THR	CA-C-O	9.11	131.89	121.87
1	1	19	ASN	OD1-CG-ND2	9.08	131.68	122.60
1	1	88	ASP	CA-C-O	9.06	130.00	120.30
2	2	71	TRP	CB-CA-C	9.05	125.55	110.79
1	1	206	SER	O-C-N	9.03	132.44	122.05
3	3	96	THR	CA-C-N	9.00	133.59	120.90
3	3	96	THR	C-N-CA	9.00	133.59	120.90
3	3	155	TRP	CA-C-O	-8.97	110.70	120.30
2	2	234	THR	CA-C-O	8.93	132.33	121.89
3	3	114	ARG	N-CA-C	8.92	122.95	108.41
2	2	49	ALA	CA-C-O	-8.91	107.77	120.51
4	4	37	SER	O-C-N	8.90	134.35	123.13
2	2	16	ILE	O-C-N	8.90	132.93	123.05
2	2	19	GLY	CA-C-N	8.89	137.21	122.54
2	2	19	GLY	C-N-CA	8.89	137.21	122.54
2	2	61	ASN	CB-CA-C	8.88	125.89	112.03
3	3	32	LYS	CA-C-O	-8.88	111.99	122.03
2	2	182	ASN	N-CA-C	-8.88	100.29	113.61
4	4	42	ARG	CD-NE-CZ	8.87	136.81	124.40
2	2	20	ASP	CA-C-O	8.86	129.71	119.35
2	2	107	THR	CA-CB-OG1	-8.85	96.32	109.60
1	1	12	ASN	CA-CB-CG	8.83	121.43	112.60
2	2	40	HIS	CA-CB-CG	-8.82	104.98	113.80
3	3	193	TYR	O-C-N	8.81	133.38	123.16
2	2	61	ASN	OD1-CG-ND2	8.81	131.41	122.60
2	2	81	LYS	O-C-N	8.80	133.66	123.27
2	2	57	ASP	CA-C-O	-8.79	111.40	120.71
3	3	54	PRO	CA-C-O	-8.76	110.67	120.92
3	3	108	HIS	CA-CB-CG	8.76	122.56	113.80
4	4	37	SER	CA-C-O	-8.72	111.12	120.46
3	3	203	THR	CA-C-O	-8.71	111.31	120.28
3	3	45	GLU	CB-CG-CD	8.66	127.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	101	LEU	CA-C-O	8.65	130.31	120.54
3	3	53	ILE	O-C-N	8.63	129.15	121.12
3	3	210	LEU	CA-C-N	-8.61	109.19	122.62
3	3	210	LEU	C-N-CA	-8.61	109.19	122.62
2	2	147	THR	N-CA-CB	8.57	124.01	110.73
2	2	63	PHE	N-CA-C	8.56	123.41	108.52
1	1	80	SER	CA-C-O	8.53	130.64	120.92
3	3	191	CYS	CA-C-O	-8.52	110.38	120.60
2	2	192	ASN	OD1-CG-ND2	8.52	131.12	122.60
1	1	70	PHE	N-CA-C	-8.45	100.70	112.45
3	3	226	ASP	CA-CB-CG	8.44	121.03	112.60
2	2	196	ASN	N-CA-CB	-8.41	98.86	110.38
3	3	205	GLN	OE1-CD-NE2	8.37	130.97	122.60
2	2	62	ARG	NH1-CZ-NH2	-8.35	108.45	119.30
2	2	92	PHE	CA-CB-CG	8.35	122.15	113.80
1	1	25	HIS	CA-C-O	-8.34	111.97	121.81
1	1	204	ASN	CA-C-O	8.34	130.29	120.70
3	3	218	ASP	N-CA-CB	-8.34	97.98	110.07
2	2	196	ASN	CA-CB-CG	-8.33	104.27	112.60
4	4	38	SER	O-C-N	8.31	133.65	122.59
2	2	135	ALA	CA-C-O	8.28	129.51	119.49
2	2	181	GLY	N-CA-C	-8.25	103.71	114.85
2	2	189	GLN	CA-CB-CG	8.25	130.60	114.10
1	1	46	GLN	O-C-N	8.23	130.78	121.32
2	2	220	TRP	CA-C-O	8.23	129.93	120.80
1	1	49	ASP	CA-CB-CG	-8.21	104.39	112.60
1	1	35	ASP	CA-C-O	-8.19	112.34	121.51
2	2	28	VAL	CA-CB-CG1	8.18	124.31	110.40
3	3	32	LYS	O-C-N	8.18	132.33	122.68
1	1	86	TYR	CB-CA-C	8.16	122.74	109.02
2	2	83	PRO	CB-CA-C	8.16	125.89	112.26
2	2	147	THR	O-C-N	8.16	131.96	122.25
1	1	59	SER	N-CA-CB	-8.16	96.70	110.49
3	3	206	THR	N-CA-C	-8.14	96.64	109.50
3	3	95	ALA	CA-C-O	-8.11	108.91	120.51
2	2	31	ALA	N-CA-CB	8.08	123.85	111.56
2	2	218	ASN	CB-CG-ND2	8.02	128.44	116.40
1	1	12	ASN	OD1-CG-ND2	-8.01	114.59	122.60
2	2	203	VAL	N-CA-CB	-8.00	100.01	111.21
2	2	257	ARG	NE-CZ-NH2	-7.96	112.04	119.20
1	1	25	HIS	O-C-N	7.95	131.91	122.85
3	3	227	THR	N-CA-C	7.93	120.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	91	ILE	N-CA-CB	7.93	124.31	111.23
1	1	5	ASN	CA-CB-CG	7.92	120.52	112.60
2	2	160	ARG	N-CA-CB	-7.90	98.30	111.57
2	2	183	LEU	O-C-N	7.88	132.99	122.43
3	3	90	THR	N-CA-CB	7.86	122.94	111.54
2	2	50	ILE	CA-CB-CG2	7.86	123.86	110.50
2	2	161	ASP	O-C-N	7.86	132.69	122.95
2	2	188	HIS	N-CA-C	7.86	118.61	108.24
3	3	50	ASP	CA-C-O	7.86	129.60	120.49
1	1	260	THR	O-C-N	7.83	133.01	122.59
3	3	36	ILE	N-CA-CB	7.83	122.16	111.21
1	1	28	SER	N-CA-C	7.80	122.11	109.40
2	2	156	VAL	CA-C-N	7.80	136.43	121.54
2	2	156	VAL	C-N-CA	7.80	136.43	121.54
3	3	199	VAL	O-C-N	7.80	129.99	121.10
2	2	156	VAL	CA-C-O	7.79	130.51	120.78
1	1	13	GLU	CA-C-O	-7.78	112.66	119.97
4	4	38	SER	CA-C-O	-7.78	109.39	120.51
1	1	168	ASN	CA-C-N	-7.76	112.29	123.00
1	1	168	ASN	C-N-CA	-7.76	112.29	123.00
3	3	233	SER	CA-C-O	7.76	131.29	122.37
2	2	29	ALA	N-CA-CB	7.75	123.48	110.69
3	3	42	ASN	OD1-CG-ND2	7.74	130.34	122.60
4	4	43	LEU	N-CA-C	7.69	122.57	112.72
2	2	119	GLN	OE1-CD-NE2	7.69	130.29	122.60
1	1	285	THR	CA-C-O	-7.62	111.48	120.10
2	2	72	ASN	CA-CB-CG	-7.62	104.98	112.60
3	3	55	VAL	CB-CA-C	7.61	123.78	111.29
3	3	168	PRO	CA-C-N	-7.59	112.97	122.84
3	3	168	PRO	C-N-CA	-7.59	112.97	122.84
2	2	161	ASP	CA-CB-CG	-7.59	105.01	112.60
3	3	35	SER	CA-C-O	-7.59	112.08	120.81
2	2	160	ARG	N-CA-C	7.59	119.67	108.14
1	1	44	ASN	CA-CB-CG	-7.57	105.03	112.60
1	1	134	ARG	NH1-CZ-NH2	-7.57	109.46	119.30
2	2	32	VAL	O-C-N	7.57	131.45	123.05
4	4	42	ARG	CA-C-N	-7.55	108.88	122.46
4	4	42	ARG	C-N-CA	-7.55	108.88	122.46
2	2	12	ARG	CG-CD-NE	7.54	128.58	112.00
1	1	38	GLU	CB-CG-CD	7.53	125.40	112.60
2	2	111	GLN	CB-CG-CD	7.53	125.40	112.60
2	2	182	ASN	O-C-N	7.51	131.06	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	200	PRO	N-CA-C	-7.48	101.57	110.70
1	1	202	GLY	CA-C-N	7.48	135.99	121.18
1	1	202	GLY	C-N-CA	7.48	135.99	121.18
4	4	32	PHE	CA-C-N	7.47	131.17	120.79
4	4	32	PHE	C-N-CA	7.47	131.17	120.79
2	2	169	ASP	N-CA-C	-7.46	104.15	113.18
2	2	224	ILE	CB-CA-C	7.45	120.48	110.42
1	1	34	LEU	CA-C-O	-7.45	112.80	120.54
2	2	233	GLU	CA-C-O	7.42	127.23	119.51
1	1	70	PHE	O-C-N	7.41	133.17	122.28
3	3	30	PRO	O-C-N	7.41	132.19	123.01
3	3	57	ASN	CA-CB-CG	-7.40	105.20	112.60
1	1	49	ASP	N-CA-C	7.39	119.12	111.14
3	3	160	GLN	OE1-CD-NE2	-7.37	115.23	122.60
3	3	185	MET	N-CA-CB	7.34	121.02	109.71
3	3	89	ILE	CB-CA-C	-7.33	99.28	111.29
2	2	70	HIS	CA-C-N	-7.31	112.73	123.11
2	2	70	HIS	C-N-CA	-7.31	112.73	123.11
2	2	233	GLU	CG-CD-OE2	7.30	135.19	118.40
2	2	126	MET	CA-CB-CG	-7.29	99.52	114.10
3	3	163	ILE	N-CA-C	-7.29	97.98	108.48
1	1	31	ALA	O-C-N	7.28	128.20	120.85
2	2	86	LEU	CA-C-O	7.28	129.35	120.55
3	3	50	ASP	CA-CB-CG	7.26	119.86	112.60
1	1	5	ASN	N-CA-CB	7.26	122.84	110.50
1	1	8	ASP	CA-CB-CG	-7.25	105.35	112.60
2	2	155	ASP	CA-CB-CG	7.24	119.84	112.60
1	1	173	TRP	CA-CB-CG	7.22	127.32	113.60
3	3	201	PRO	N-CA-C	7.21	127.31	112.47
1	1	16	VAL	CB-CA-C	7.20	122.19	111.31
2	2	52	LYS	CG-CD-CE	7.19	127.84	111.30
3	3	123	ALA	CA-C-O	-7.19	111.86	120.56
3	3	67	MET	CA-C-N	7.18	133.52	122.24
3	3	67	MET	C-N-CA	7.18	133.52	122.24
3	3	161	SER	CA-C-N	-7.18	111.68	122.74
3	3	161	SER	C-N-CA	-7.18	111.68	122.74
2	2	78	TRP	CA-CB-CG	7.17	127.23	113.60
3	3	218	ASP	CA-C-N	7.17	135.22	121.54
3	3	218	ASP	C-N-CA	7.17	135.22	121.54
1	1	23	SER	CA-C-O	7.16	129.88	121.58
1	1	55	TYR	O-C-N	7.14	132.09	122.59
3	3	161	SER	CB-CA-C	-7.14	96.21	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	130	HIS	O-C-N	7.13	132.17	122.83
2	2	220	TRP	CA-C-N	7.12	133.71	122.74
2	2	220	TRP	C-N-CA	7.12	133.71	122.74
3	3	114	ARG	NE-CZ-NH1	-7.11	114.39	121.50
3	3	70	VAL	CA-C-N	-7.10	112.18	122.19
3	3	70	VAL	C-N-CA	-7.10	112.18	122.19
1	1	186	PHE	N-CA-C	-7.10	99.16	109.59
3	3	216	CYS	CA-C-O	-7.08	113.16	121.44
2	2	147	THR	N-CA-C	-7.07	103.76	112.88
2	2	176	ASP	N-CA-C	-7.07	104.30	114.12
2	2	114	ALA	CA-C-O	-7.05	110.42	120.51
2	2	256	ALA	CA-C-O	-7.04	113.88	121.56
3	3	237	GLU	CA-C-O	7.04	130.58	120.51
1	1	82	ILE	CB-CA-C	-7.04	99.75	111.29
3	3	218	ASP	CA-C-O	7.01	127.92	120.70
2	2	127	ILE	O-C-N	7.01	129.09	121.10
1	1	199	GLY	O-C-N	7.00	129.69	123.60
2	2	205	TYR	CA-C-O	-6.99	113.10	120.58
2	2	52	LYS	CA-CB-CG	6.98	128.07	114.10
3	3	101	GLU	CA-C-O	6.98	128.02	120.20
1	1	134	ARG	CD-NE-CZ	6.98	134.17	124.40
2	2	134	SER	CA-C-O	6.96	128.93	120.92
2	2	168	SER	CA-C-O	6.96	128.23	120.43
1	1	61	THR	CB-CA-C	6.95	121.25	109.50
1	1	252	ARG	N-CA-CB	-6.95	104.13	111.29
4	4	28	ASN	CA-C-N	-6.94	109.48	121.97
4	4	28	ASN	C-N-CA	-6.94	109.48	121.97
3	3	210	LEU	CA-C-O	-6.94	113.09	121.28
2	2	190	PHE	CA-CB-CG	6.93	120.73	113.80
1	1	246	THR	N-CA-C	6.93	120.74	110.48
3	3	201	PRO	CA-C-N	-6.93	112.17	122.36
3	3	201	PRO	C-N-CA	-6.93	112.17	122.36
2	2	67	GLU	CA-C-O	-6.92	113.16	121.05
2	2	82	LEU	N-CA-C	6.92	125.09	109.81
2	2	237	SER	CB-CA-C	6.89	123.54	109.55
4	4	43	LEU	O-C-N	6.89	130.56	122.09
1	1	41	HIS	CA-C-N	-6.88	111.78	122.87
1	1	41	HIS	C-N-CA	-6.88	111.78	122.87
1	1	283	THR	O-C-N	6.88	131.25	123.27
3	3	160	GLN	O-C-N	6.88	131.74	122.59
3	3	70	VAL	O-C-N	6.88	129.16	122.97
2	2	126	MET	CA-C-O	-6.87	113.25	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	29	ILE	O-C-N	6.86	131.15	122.57
1	1	8	ASP	CA-C-N	6.84	133.75	121.92
1	1	8	ASP	C-N-CA	6.84	133.75	121.92
1	1	71	LEU	CA-C-O	-6.83	112.29	120.56
1	1	287	ALA	CA-C-O	-6.83	109.19	120.80
3	3	225	ARG	NE-CZ-NH1	-6.83	114.67	121.50
2	2	70	HIS	CA-CB-CG	-6.82	106.98	113.80
3	3	160	GLN	N-CA-CB	6.81	121.99	110.49
2	2	87	LYS	CB-CG-CD	6.80	126.94	111.30
3	3	146	ASP	CB-CG-OD2	-6.80	102.77	118.40
3	3	15	THR	CB-CA-C	6.79	123.44	110.27
1	1	78	HIS	CA-CB-CG	-6.77	107.03	113.80
3	3	89	ILE	CA-C-O	-6.77	112.32	120.78
3	3	234	GLY	O-C-N	6.75	128.52	121.77
2	2	119	GLN	CB-CA-C	6.75	121.47	109.65
3	3	65	VAL	N-CA-CB	6.74	120.18	110.68
2	2	80	TRP	N-CA-CB	6.74	123.19	111.00
3	3	58	VAL	CA-C-O	6.73	127.62	120.48
2	2	171	SER	CA-C-N	6.71	131.44	120.63
2	2	171	SER	C-N-CA	6.71	131.44	120.63
1	1	64	GLU	CA-CB-CG	6.71	127.52	114.10
2	2	31	ALA	O-C-N	6.71	130.10	123.46
1	1	91	GLY	CA-C-N	-6.70	113.86	122.77
1	1	91	GLY	C-N-CA	-6.70	113.86	122.77
1	1	256	ALA	CA-C-N	-6.70	109.74	122.13
1	1	256	ALA	C-N-CA	-6.70	109.74	122.13
2	2	198	SER	CB-CA-C	-6.69	97.33	113.19
1	1	45	VAL	O-C-N	6.69	130.13	122.97
1	1	55	TYR	CA-C-N	-6.69	113.48	122.98
1	1	55	TYR	C-N-CA	-6.69	113.48	122.98
3	3	90	THR	N-CA-C	-6.68	102.34	111.56
1	1	63	ASP	CA-C-O	-6.67	114.03	120.90
2	2	158	GLN	CB-CG-CD	-6.67	101.26	112.60
2	2	83	PRO	CA-C-N	6.67	135.84	121.64
2	2	83	PRO	C-N-CA	6.67	135.84	121.64
3	3	203	THR	N-CA-C	-6.67	97.55	108.82
1	1	53	THR	N-CA-CB	-6.66	101.25	110.38
3	3	206	THR	CA-CB-OG1	-6.64	99.64	109.60
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	6.62	129.22	122.60
3	3	147	ALA	CA-C-N	6.62	131.19	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	147	ALA	C-N-CA	6.62	131.19	120.60
2	2	155	ASP	N-CA-CB	6.61	121.66	110.49
3	3	128	LYS	CB-CA-C	-6.58	102.80	111.42
2	2	150	GLY	O-C-N	6.57	131.24	122.70
3	3	94	LEU	CA-C-O	-6.55	111.14	120.51
2	2	168	SER	CA-C-N	6.55	134.35	121.58
2	2	168	SER	C-N-CA	6.55	134.35	121.58
3	3	87	VAL	N-CA-C	6.54	121.20	112.04
1	1	62	ARG	N-CA-C	-6.54	103.63	112.26
3	3	169	TRP	CB-CA-C	6.54	121.24	110.78
2	2	130	HIS	CA-C-O	-6.53	113.76	122.51
1	1	52	GLU	O-C-N	6.53	130.68	122.84
2	2	232	SER	N-CA-CB	6.53	121.62	110.65
3	3	88	ASP	CA-CB-CG	6.53	119.13	112.60
3	3	10	SER	CB-CA-C	6.53	120.08	109.90
2	2	202	ILE	CA-C-O	-6.52	113.37	120.67
2	2	161	ASP	CB-CA-C	-6.51	99.75	109.90
2	2	68	SER	CA-CB-OG	6.50	124.11	111.10
1	1	281	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	1	280	ARG	NH1-CZ-NH2	6.50	127.75	119.30
3	3	15	THR	N-CA-CB	-6.50	98.98	110.42
3	3	165	LEU	O-C-N	6.50	130.96	123.29
3	3	70	VAL	CA-C-O	-6.49	114.44	120.22
2	2	180	LEU	CA-C-O	-6.48	113.90	120.96
1	1	52	GLU	CA-C-N	6.48	133.24	121.06
1	1	52	GLU	C-N-CA	6.48	133.24	121.06
3	3	56	ASN	CA-CB-CG	-6.47	106.13	112.60
3	3	16	THR	CA-CB-CG2	6.43	121.44	110.50
3	3	64	ASN	CB-CG-ND2	-6.43	106.76	116.40
3	3	206	THR	OG1-CB-CG2	6.43	122.16	109.30
1	1	201	ASP	CA-C-N	6.43	129.69	120.56
1	1	201	ASP	C-N-CA	6.43	129.69	120.56
3	3	106	TYR	CA-C-O	-6.42	113.93	121.44
1	1	132	ALA	CA-C-O	6.42	127.61	120.43
3	3	72	LEU	N-CA-C	-6.41	98.76	108.96
1	1	204	ASN	N-CA-CB	6.41	119.64	109.51
1	1	275	THR	O-C-N	6.41	130.79	123.48
2	2	54	THR	N-CA-CB	6.41	120.73	110.16
2	2	206	VAL	CB-CA-C	6.40	120.36	110.83
2	2	50	ILE	CB-CA-C	6.39	121.77	111.29
2	2	103	ARG	CD-NE-CZ	6.39	133.34	124.40
2	2	91	ILE	CA-C-O	-6.38	112.80	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	117	THR	CB-CA-C	-6.38	101.06	110.95
1	1	66	SER	O-C-N	6.37	130.88	123.30
2	2	152	ALA	N-CA-CB	-6.37	100.08	110.14
1	1	201	ASP	O-C-N	6.36	129.40	122.15
2	2	176	ASP	CB-CA-C	6.35	120.06	109.38
3	3	226	ASP	OD1-CG-OD2	-6.35	107.65	122.90
2	2	157	SER	CA-C-N	-6.35	112.14	122.81
2	2	157	SER	C-N-CA	-6.35	112.14	122.81
4	4	42	ARG	NE-CZ-NH1	6.35	127.85	121.50
2	2	228	SER	CA-C-N	6.35	126.37	119.90
2	2	228	SER	C-N-CA	6.35	126.37	119.90
1	1	285	THR	CA-CB-OG1	-6.33	100.10	109.60
2	2	228	SER	O-C-N	6.33	128.38	121.36
1	1	49	ASP	CA-C-N	6.32	131.43	120.68
1	1	49	ASP	C-N-CA	6.32	131.43	120.68
1	1	5	ASN	O-C-N	6.32	133.11	123.00
2	2	183	LEU	CA-C-O	-6.32	111.61	119.38
2	2	238	ASN	O-C-N	6.32	130.51	122.93
2	2	68	SER	N-CA-CB	6.32	120.02	110.42
4	4	40	ALA	N-CA-CB	6.32	119.37	109.83
2	2	183	LEU	N-CA-C	-6.31	104.84	112.54
1	1	47	PRO	CB-CA-C	6.31	121.97	111.56
1	1	174	GLN	CB-CG-CD	6.31	123.33	112.60
1	1	20	ILE	O-C-N	6.30	132.03	122.76
1	1	201	ASP	CA-C-O	-6.30	113.74	120.42
1	1	39	THR	O-C-N	6.30	131.16	122.46
3	3	235	PRO	CA-C-O	6.30	135.32	120.20
3	3	100	GLY	O-C-N	6.29	128.36	122.13
1	1	190	ALA	O-C-N	6.29	130.06	122.96
3	3	77	GLY	CA-C-O	6.29	130.74	122.75
2	2	56	PRO	CA-C-O	6.28	128.19	121.03
1	1	19	ASN	CA-CB-CG	-6.28	106.32	112.60
2	2	81	LYS	CA-CB-CG	6.28	126.66	114.10
2	2	233	GLU	CG-CD-OE1	-6.27	103.98	118.40
3	3	148	MET	CG-SD-CE	6.25	114.66	100.90
1	1	66	SER	CA-CB-OG	-6.24	98.61	111.10
1	1	175	HIS	N-CA-CB	-6.24	99.58	109.19
3	3	234	GLY	N-CA-C	-6.24	99.62	112.34
3	3	8	PRO	CA-C-N	6.22	133.60	121.41
3	3	8	PRO	C-N-CA	6.22	133.60	121.41
1	1	114	GLU	CB-CG-CD	6.22	123.17	112.60
4	4	30	ASN	CB-CA-C	6.22	122.79	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	205	THR	OG1-CB-CG2	6.20	121.70	109.30
2	2	95	ASN	N-CA-C	-6.20	105.58	113.01
2	2	212	ASP	CA-C-N	6.19	130.70	121.72
2	2	212	ASP	C-N-CA	6.19	130.70	121.72
2	2	262	LYS	CB-CA-C	6.19	122.36	109.68
3	3	181	ASN	O-C-N	6.18	130.92	123.26
2	2	95	ASN	OD1-CG-ND2	6.18	128.78	122.60
4	4	44	ASP	CA-C-O	6.18	131.30	120.80
1	1	19	ASN	CB-CG-OD1	-6.18	108.45	120.80
2	2	56	PRO	N-CA-C	-6.16	101.50	110.80
1	1	69	SER	N-CA-C	-6.15	105.42	113.17
2	2	196	ASN	N-CA-C	6.15	117.97	110.41
1	1	117	THR	N-CA-CB	6.15	118.89	109.98
3	3	123	ALA	O-C-N	6.14	129.39	122.32
2	2	128	PRO	CB-CA-C	6.12	119.00	110.98
2	2	39	PRO	CB-CA-C	-6.12	103.57	111.46
2	2	221	CYS	CA-C-O	6.11	127.11	120.32
3	3	134	THR	CB-CA-C	6.11	115.94	110.44
2	2	228	SER	N-CA-CB	6.09	118.91	110.01
1	1	45	VAL	CA-C-O	-6.08	114.58	121.75
1	1	248	ALA	CA-C-N	6.07	133.13	121.54
1	1	248	ALA	C-N-CA	6.07	133.13	121.54
2	2	27	ASP	CA-C-O	-6.06	113.28	120.43
1	1	60	GLN	N-CA-C	-6.04	99.06	108.90
2	2	70	HIS	CB-CA-C	-6.04	99.57	109.53
2	2	236	SER	CA-C-N	6.02	132.26	121.66
2	2	236	SER	C-N-CA	6.02	132.26	121.66
1	1	87	THR	CA-C-O	6.01	127.31	121.00
3	3	4	VAL	O-C-N	6.00	129.39	122.97
3	3	71	GLN	O-C-N	6.00	130.06	123.22
3	3	228	ASP	CB-CA-C	-6.00	99.58	110.56
1	1	286	THR	CA-C-O	-5.99	113.67	120.32
2	2	116	LYS	CB-CA-C	-5.98	99.30	110.36
2	2	161	ASP	CA-C-N	-5.97	112.68	122.54
2	2	161	ASP	C-N-CA	-5.97	112.68	122.54
2	2	173	LEU	CB-CA-C	5.97	120.06	110.09
3	3	89	ILE	CA-CB-CG2	5.97	120.65	110.50
1	1	183	SER	CA-C-N	-5.96	111.10	122.13
1	1	183	SER	C-N-CA	-5.96	111.10	122.13
4	4	32	PHE	CA-CB-CG	-5.95	107.85	113.80
3	3	194	GLN	N-CA-C	-5.94	103.49	112.04
1	1	62	ARG	O-C-N	5.93	129.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	155	ASP	O-C-N	5.93	130.48	122.59
3	3	56	ASN	OD1-CG-ND2	5.92	128.53	122.60
2	2	61	ASN	CA-C-N	5.92	131.84	122.36
2	2	61	ASN	C-N-CA	5.92	131.84	122.36
2	2	225	ILE	CA-C-O	5.91	123.01	119.94
2	2	71	TRP	CA-C-O	5.89	126.77	120.46
2	2	114	ALA	N-CA-C	-5.89	98.24	110.80
3	3	178	THR	N-CA-CB	5.88	119.36	110.30
2	2	209	VAL	CA-C-N	5.88	126.29	119.47
2	2	209	VAL	C-N-CA	5.88	126.29	119.47
2	2	215	LEU	CA-C-O	-5.88	111.90	120.13
3	3	73	GLY	N-CA-C	5.88	121.00	112.60
3	3	181	ASN	OD1-CG-ND2	5.88	128.47	122.60
2	2	238	ASN	N-CA-CB	5.87	119.55	110.21
3	3	75	GLN	CA-C-N	5.87	128.07	120.44
3	3	75	GLN	C-N-CA	5.87	128.07	120.44
2	2	12	ARG	CB-CA-C	-5.86	99.97	110.70
2	2	94	GLU	CA-C-O	5.85	127.31	119.47
4	4	40	ALA	CA-C-O	-5.85	114.75	121.19
2	2	59	SER	CA-C-O	5.85	126.57	119.38
3	3	198	VAL	O-C-N	5.83	129.09	123.14
1	1	81	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	2	38	TRP	CA-C-N	5.82	125.76	119.76
2	2	38	TRP	C-N-CA	5.82	125.76	119.76
3	3	92	THR	N-CA-C	-5.82	96.94	109.81
1	1	90	ASN	OD1-CG-ND2	-5.82	116.78	122.60
3	3	161	SER	O-C-N	5.82	130.33	122.59
2	2	239	ILE	CB-CA-C	5.82	119.50	110.83
1	1	205	THR	CA-CB-OG1	-5.81	100.89	109.60
1	1	63	ASP	O-C-N	5.81	128.30	122.03
2	2	197	ASN	CA-C-N	5.81	131.91	122.39
2	2	197	ASN	C-N-CA	5.81	131.91	122.39
4	4	42	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
3	3	191	CYS	O-C-N	5.80	130.35	123.33
1	1	10	VAL	N-CA-CB	-5.80	101.15	112.75
3	3	180	ASP	CA-C-O	5.80	126.33	120.88
2	2	155	ASP	CB-CG-OD2	-5.80	105.07	118.40
2	2	14	MET	CA-C-O	5.79	127.78	121.06
1	1	204	ASN	CB-CG-ND2	5.79	125.09	116.40
2	2	28	VAL	CB-CA-C	-5.79	101.80	111.29
1	1	283	THR	CA-CB-OG1	-5.78	100.92	109.60
1	1	36	ALA	CA-C-N	5.77	132.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	36	ALA	C-N-CA	5.77	132.56	121.54
2	2	175	PHE	CA-CB-CG	5.76	119.56	113.80
3	3	222	ARG	NH1-CZ-NH2	-5.76	111.81	119.30
3	3	57	ASN	OD1-CG-ND2	5.76	128.36	122.60
3	3	165	LEU	CA-C-O	-5.76	114.10	120.38
1	1	282	ASN	CA-C-O	5.75	126.63	120.70
2	2	154	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	1	68	GLU	CA-C-O	5.74	125.46	119.14
1	1	68	GLU	CA-CB-CG	5.74	125.57	114.10
1	1	171	ILE	CB-CA-C	5.71	119.04	110.98
1	1	235	ILE	O-C-N	5.71	129.02	123.03
2	2	154	ARG	CG-CD-NE	5.71	124.56	112.00
2	2	241	PRO	O-C-N	-5.71	114.94	122.64
1	1	175	HIS	CB-CA-C	5.70	116.81	109.80
2	2	157	SER	O-C-N	5.70	130.16	122.59
2	2	62	ARG	NE-CZ-NH1	5.69	127.19	121.50
3	3	71	GLN	N-CA-CB	5.69	119.54	110.16
3	3	120	CYS	CA-CB-SG	-5.69	101.32	114.40
3	3	96	THR	N-CA-C	5.68	122.90	110.80
2	2	227	ILE	N-CA-CB	5.67	120.59	111.23
1	1	37	ALA	N-CA-CB	-5.67	100.91	110.49
1	1	90	ASN	CB-CA-C	5.67	121.70	110.42
2	2	74	SER	O-C-N	5.67	128.89	122.20
3	3	180	ASP	CB-CA-C	5.67	116.77	109.80
2	2	90	GLY	CA-C-O	5.67	130.43	120.57
1	1	173	TRP	O-C-N	5.66	130.27	123.36
2	2	67	GLU	OE1-CD-OE2	5.66	136.49	122.90
2	2	176	ASP	CA-CB-CG	-5.66	106.94	112.60
3	3	185	MET	O-C-N	5.65	130.08	122.96
1	1	43	SER	CA-C-O	5.65	128.08	121.87
3	3	126	THR	O-C-N	5.65	129.71	123.33
3	3	162	THR	CB-CA-C	5.65	119.92	109.70
2	2	96	MET	CA-C-O	5.64	126.50	120.24
1	1	252	ARG	N-CA-C	5.64	113.09	108.07
1	1	246	THR	N-CA-CB	-5.63	101.73	110.29
2	2	12	ARG	CA-C-O	-5.63	113.99	120.24
3	3	155	TRP	O-C-N	5.63	129.80	123.27
3	3	156	ASP	CA-CB-CG	5.63	118.23	112.60
3	3	135	PRO	CA-C-O	5.62	128.72	120.56
1	1	276	THR	CA-CB-OG1	-5.61	101.18	109.60
3	3	81	LYS	N-CA-C	5.61	119.25	110.32
1	1	276	THR	O-C-N	5.61	130.44	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	84	ASP	CA-C-O	-5.61	113.16	120.00
1	1	281	ARG	N-CA-CB	-5.61	101.88	110.85
3	3	112	SER	CA-C-N	5.61	131.77	121.85
3	3	112	SER	C-N-CA	5.61	131.77	121.85
3	3	204	PRO	CA-C-O	-5.60	114.95	121.95
3	3	172	ALA	N-CA-C	-5.60	103.00	111.56
1	1	72	GLY	CA-C-N	5.59	130.69	121.86
1	1	72	GLY	C-N-CA	5.59	130.69	121.86
2	2	160	ARG	CG-CD-NE	5.59	124.29	112.00
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
2	2	41	TYR	O-C-N	5.58	129.26	122.96
1	1	164	GLN	OE1-CD-NE2	-5.57	117.03	122.60
3	3	146	ASP	N-CA-CB	5.56	119.89	110.49
1	1	71	LEU	CB-CA-C	5.56	121.43	111.03
2	2	263	GLN	OE1-CD-NE2	5.56	128.16	122.60
2	2	135	ALA	N-CA-CB	-5.55	100.88	110.32
1	1	282	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	1	84	VAL	O-C-N	5.55	127.53	122.65
3	3	46	MET	CA-C-O	5.54	126.36	120.10
1	1	259	TYR	O-C-N	5.54	129.22	122.68
1	1	286	THR	O-C-N	5.53	129.78	123.31
2	2	158	GLN	CA-C-N	5.53	130.89	122.65
2	2	158	GLN	C-N-CA	5.53	130.89	122.65
3	3	66	SER	CA-C-O	5.53	128.41	120.51
2	2	75	SER	O-C-N	5.52	129.38	122.86
1	1	161	PHE	O-C-N	5.52	129.93	122.59
3	3	89	ILE	N-CA-C	5.51	120.81	109.34
3	3	55	VAL	O-C-N	5.51	129.46	122.57
3	3	67	MET	O-C-N	-5.51	115.26	122.59
3	3	224	ALA	CA-C-O	5.51	127.33	121.16
1	1	258	PRO	O-C-N	5.50	129.34	123.01
2	2	43	THR	CA-C-N	5.50	126.71	119.84
2	2	43	THR	C-N-CA	5.50	126.71	119.84
1	1	10	VAL	N-CA-C	-5.49	107.47	112.96
2	2	73	GLY	N-CA-C	-5.49	106.22	115.62
3	3	89	ILE	CB-CG1-CD1	-5.49	102.27	113.80
1	1	117	THR	O-C-N	5.49	127.96	122.03
1	1	76	CYS	CA-C-O	-5.49	114.66	120.92
2	2	131	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	1	70	PHE	N-CA-CB	5.48	118.42	110.26
1	1	17	VAL	CA-C-N	5.48	126.24	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	17	VAL	C-N-CA	5.48	126.24	120.11
1	1	94	ILE	N-CA-C	5.47	116.55	108.45
2	2	261	ILE	O-C-N	5.47	129.23	123.00
1	1	42	THR	O-C-N	5.47	130.05	123.16
3	3	227	THR	OG1-CB-CG2	5.47	120.23	109.30
2	2	31	ALA	N-CA-C	-5.46	100.01	108.42
1	1	158	ARG	NE-CZ-NH2	5.46	124.12	119.20
2	2	142	ALA	CA-C-N	5.46	127.52	120.64
2	2	142	ALA	C-N-CA	5.46	127.52	120.64
2	2	106	TYR	N-CA-C	5.46	117.70	109.41
3	3	167	VAL	N-CA-CB	5.46	118.85	111.21
1	1	134	ARG	CA-C-O	5.45	125.81	119.32
2	2	150	GLY	CA-C-O	-5.45	111.09	120.57
1	1	82	ILE	N-CA-CB	5.44	120.21	111.23
1	1	89	TYR	CA-C-N	-5.44	111.16	121.54
1	1	89	TYR	C-N-CA	-5.44	111.16	121.54
2	2	94	GLU	CG-CD-OE1	-5.44	105.89	118.40
3	3	33	GLU	CG-CD-OE2	-5.44	105.90	118.40
2	2	30	ASN	N-CA-CB	-5.43	101.31	110.49
1	1	27	THR	CA-CB-OG1	-5.43	101.45	109.60
3	3	124	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	1	86	TYR	N-CA-C	-5.43	107.31	114.31
1	1	90	ASN	CB-CG-ND2	5.42	124.54	116.40
1	1	258	PRO	CA-C-N	-5.42	111.31	120.95
1	1	258	PRO	C-N-CA	-5.42	111.31	120.95
2	2	139	SER	N-CA-CB	-5.42	102.04	110.98
2	2	227	ILE	CA-C-N	-5.42	113.38	121.83
2	2	227	ILE	C-N-CA	-5.42	113.38	121.83
2	2	256	ALA	O-C-N	5.42	129.25	122.86
1	1	51	ILE	CA-CB-CG2	5.41	119.70	110.50
2	2	72	ASN	N-CA-C	5.41	118.53	110.52
2	2	237	SER	CA-CB-OG	5.41	121.92	111.10
3	3	152	HIS	O-C-N	5.41	128.77	122.99
1	1	172	PHE	O-C-N	5.40	129.73	123.30
1	1	252	ARG	NE-CZ-NH2	5.40	124.06	119.20
4	4	27	PHE	CA-C-O	5.39	128.22	120.51
1	1	279	VAL	CB-CA-C	5.39	118.93	111.38
1	1	120	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	3	131	LEU	O-C-N	5.39	129.95	123.16
3	3	235	PRO	N-CD-CG	-5.38	97.34	103.80
3	3	235	PRO	CB-CA-C	-5.38	98.56	112.00
2	2	86	LEU	O-C-N	-5.37	115.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	168	ASN	O-C-N	5.37	130.29	122.94
1	1	76	CYS	CB-CA-C	5.37	118.27	109.90
2	2	141	THR	O-C-N	5.37	128.95	122.94
3	3	226	ASP	CB-CA-C	5.36	118.59	109.53
3	3	182	LYS	O-C-N	5.36	127.80	122.12
3	3	226	ASP	CB-CG-OD1	5.36	130.72	118.40
3	3	5	TYR	CA-C-N	5.36	129.07	122.37
3	3	5	TYR	C-N-CA	5.36	129.07	122.37
2	2	24	SER	CA-C-N	5.35	128.82	121.33
2	2	24	SER	C-N-CA	5.35	128.82	121.33
1	1	181	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	1	111	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	1	40	GLY	N-CA-C	-5.35	108.34	115.40
3	3	114	ARG	N-CA-CB	-5.34	102.31	110.65
2	2	201	LEU	CA-C-N	5.33	130.35	122.94
2	2	201	LEU	C-N-CA	5.33	130.35	122.94
2	2	87	LYS	CB-CA-C	5.32	121.00	110.42
2	2	134	SER	N-CA-CB	5.32	118.85	110.23
2	2	223	VAL	N-CA-CB	-5.32	102.72	111.44
2	2	219	ASN	CB-CA-C	5.31	119.72	110.79
2	2	127	ILE	CA-C-O	-5.31	112.83	119.95
1	1	110	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	2	190	PHE	O-C-N	5.31	130.35	122.81
1	1	88	ASP	CA-CB-CG	5.31	117.91	112.60
1	1	89	TYR	N-CA-C	-5.30	101.05	109.59
2	2	108	VAL	CB-CA-C	5.30	118.56	111.19
3	3	201	PRO	N-CA-CB	-5.30	97.68	103.25
2	2	144	TYR	CA-C-N	5.29	131.64	121.54
2	2	144	TYR	C-N-CA	5.29	131.64	121.54
2	2	35	TYR	N-CA-CB	-5.29	104.22	112.41
1	1	201	ASP	CA-CB-CG	-5.28	107.32	112.60
3	3	57	ASN	N-CA-CB	-5.28	101.57	110.49
3	3	77	GLY	N-CA-C	-5.27	103.44	112.30
2	2	81	LYS	CA-C-O	-5.27	114.53	120.32
3	3	165	LEU	CA-C-N	-5.26	114.16	122.64
3	3	165	LEU	C-N-CA	-5.26	114.16	122.64
2	2	63	PHE	CA-CB-CG	-5.26	108.54	113.80
1	1	69	SER	CB-CA-C	5.26	118.87	110.09
3	3	228	ASP	CB-CG-OD2	-5.26	106.31	118.40
2	2	141	THR	CA-C-O	-5.26	115.52	121.72
1	1	155	PRO	O-C-N	5.25	128.71	122.98
1	1	45	VAL	N-CA-C	-5.25	100.80	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	247	LYS	N-CA-CB	5.25	118.80	110.55
1	1	82	ILE	O-C-N	5.24	129.12	122.57
1	1	204	ASN	N-CA-C	-5.24	102.15	109.96
2	2	45	GLN	N-CA-CB	5.24	119.65	110.27
2	2	37	VAL	O-C-N	5.24	128.84	123.18
3	3	157	VAL	CA-C-N	-5.23	113.30	120.57
3	3	157	VAL	C-N-CA	-5.23	113.30	120.57
2	2	157	SER	N-CA-CB	5.23	119.33	110.49
2	2	202	ILE	O-C-N	5.23	128.69	123.10
2	2	224	ILE	CA-CB-CG2	5.23	119.39	110.50
3	3	154	VAL	N-CA-C	-5.22	102.11	109.21
2	2	45	GLN	O-C-N	5.22	128.35	122.19
3	3	127	LEU	N-CA-CB	-5.22	102.80	111.57
4	4	42	ARG	CA-C-O	-5.22	113.90	120.84
2	2	20	ASP	CA-CB-CG	5.22	117.82	112.60
4	4	42	ARG	N-CA-C	5.21	116.71	109.31
2	2	96	MET	N-CA-CB	-5.21	102.43	110.20
3	3	141	PRO	CA-C-N	5.21	129.54	120.68
3	3	141	PRO	C-N-CA	5.21	129.54	120.68
2	2	165	ARG	N-CA-C	-5.21	99.71	110.80
3	3	142	THR	N-CA-CB	-5.20	102.29	110.30
3	3	15	THR	N-CA-C	-5.20	107.01	113.19
2	2	76	LYS	CA-CB-CG	-5.18	103.73	114.10
2	2	166	GLN	N-CA-CB	-5.18	102.65	110.32
1	1	267	TYR	O-C-N	-5.18	117.25	123.31
3	3	66	SER	CA-C-N	5.18	131.44	121.54
3	3	66	SER	C-N-CA	5.18	131.44	121.54
2	2	62	ARG	NE-CZ-NH2	5.17	123.86	119.20
2	2	79	TRP	CA-C-N	5.17	131.11	122.73
2	2	79	TRP	C-N-CA	5.17	131.11	122.73
2	2	97	TYR	N-CA-CB	-5.17	102.38	110.44
1	1	86	TYR	CA-C-O	5.17	124.51	118.77
2	2	194	ARG	NH1-CZ-NH2	5.17	126.02	119.30
2	2	186	PHE	N-CA-C	-5.17	102.64	110.39
3	3	39	GLU	CB-CG-CD	5.16	121.38	112.60
3	3	79	ALA	O-C-N	5.16	131.54	122.09
3	3	160	GLN	CG-CD-NE2	5.16	124.14	116.40
2	2	182	ASN	CA-CB-CG	5.16	117.76	112.60
4	4	29	ILE	CB-CA-C	5.15	119.74	111.29
2	2	146	LEU	N-CA-CB	5.15	118.22	110.65
1	1	270	GLU	O-C-N	5.15	129.30	122.56
2	2	171	SER	N-CA-C	5.15	119.44	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	163	ILE	N-CA-CB	5.14	120.34	111.39
1	1	43	SER	N-CA-CB	5.14	117.61	110.26
1	1	18	PRO	O-C-N	5.14	128.88	122.71
2	2	111	GLN	CB-CA-C	5.14	118.11	109.48
4	4	30	ASN	O-C-N	5.14	129.42	122.59
2	2	252	GLU	CG-CD-OE1	-5.13	106.61	118.40
2	2	257	ARG	O-C-N	5.13	129.41	122.59
1	1	223	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	2	68	SER	O-C-N	5.12	128.67	122.68
2	2	12	ARG	CA-CB-CG	-5.12	103.87	114.10
1	1	267	TYR	CA-C-N	-5.11	109.32	121.80
1	1	267	TYR	C-N-CA	-5.11	109.32	121.80
2	2	160	ARG	NE-CZ-NH1	-5.11	116.39	121.50
3	3	97	THR	N-CA-CB	5.10	117.80	109.69
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
3	3	184	SER	CA-C-N	5.10	128.58	121.24
3	3	184	SER	C-N-CA	5.10	128.58	121.24
2	2	20	ASP	CA-C-N	5.09	130.31	122.93
2	2	20	ASP	C-N-CA	5.09	130.31	122.93
2	2	160	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	2	152	ALA	N-CA-C	5.09	118.26	111.75
2	2	215	LEU	O-C-N	5.09	128.85	122.19
3	3	122	THR	N-CA-CB	5.09	118.55	110.87
3	3	167	VAL	O-C-N	5.08	126.90	121.10
2	2	79	TRP	CA-CB-CG	5.08	123.25	113.60
3	3	12	GLN	CA-C-N	5.07	130.72	121.89
3	3	12	GLN	C-N-CA	5.07	130.72	121.89
3	3	76	THR	N-CA-CB	5.07	117.36	110.01
1	1	186	PHE	CA-CB-CG	-5.07	108.73	113.80
3	3	200	PRO	O-C-N	5.06	127.43	121.46
3	3	140	GLU	CB-CA-C	5.06	117.56	109.62
1	1	83	LYS	N-CA-C	-5.06	99.09	107.99
1	1	70	PHE	CA-C-N	-5.06	112.56	121.81
1	1	70	PHE	C-N-CA	-5.06	112.56	121.81
1	1	283	THR	N-CA-CB	-5.05	102.13	111.53
1	1	62	ARG	CD-NE-CZ	-5.05	117.33	124.40
4	4	26	TYR	N-CA-CB	5.05	119.08	110.50
3	3	177	LEU	N-CA-CB	-5.04	102.19	110.41
1	1	18	PRO	CA-C-N	-5.04	114.02	123.05
1	1	18	PRO	C-N-CA	-5.04	114.02	123.05
2	2	11	ASP	O-C-N	5.04	131.07	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	148	MET	CA-C-O	5.04	125.59	119.49
3	3	111	GLY	CA-C-O	5.04	128.99	122.59
4	4	33	LYS	N-CA-C	5.03	117.16	111.02
2	2	94	GLU	N-CA-C	-5.03	106.49	113.18
2	2	31	ALA	CA-C-N	-5.03	115.47	122.71
2	2	31	ALA	C-N-CA	-5.03	115.47	122.71
3	3	189	ILE	CA-C-O	-5.03	115.23	120.76
3	3	84	SER	CA-C-N	5.02	129.09	122.51
3	3	84	SER	C-N-CA	5.02	129.09	122.51
3	3	114	ARG	O-C-N	5.02	129.09	123.27
1	1	189	ILE	O-C-N	-5.02	116.30	122.57
1	1	170	SER	CB-CA-C	5.01	117.86	110.14
2	2	15	GLN	CA-C-N	-5.01	115.49	122.71
2	2	15	GLN	C-N-CA	-5.01	115.49	122.71
2	2	121	THR	N-CA-CB	-5.01	102.32	110.59
2	2	14	MET	O-C-N	-5.01	117.46	123.27
3	3	222	ARG	N-CA-C	5.00	115.75	108.14
3	3	125	THR	CB-CA-C	-5.00	99.42	109.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	247	LYS	Mainchain
1	1	249	TRP	Mainchain

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	533	1
2	2	1979	0	1922	250	1
3	3	1831	0	1810	266	0
4	4	151	0	136	19	0
5	1	21	0	20	9	0
All	All	6244	0	6080	929	1

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 75.

All (929) 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)
1:1:125:ILE:HG21	1:1:182:PHE:CE1	1.52	1.41
1:1:261:HIS:CD2	2:2:138:GLY:C	2.06	1.31
1:1:267:TYR:O	1:1:268:MET:CG	1.78	1.29
1:1:183:SER:O	1:1:184:ILE:CG1	1.79	1.29
1:1:261:HIS:CD2	2:2:138:GLY:O	1.85	1.27
1:1:267:TYR:O	1:1:268:MET:HG2	1.11	1.26
1:1:261:HIS:NE2	2:2:138:GLY:C	1.94	1.25
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.21
1:1:101:ILE:HD11	1:1:217:MET:O	1.36	1.20
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
1:1:255:ARG:HD2	1:1:259:TYR:CE2	1.78	1.17
1:1:125:ILE:CG2	1:1:182:PHE:CE1	2.26	1.17
1:1:163:TRP:CH2	1:1:222:SER:O	1.99	1.14
1:1:98:LYS:O	1:1:98:LYS:HG2	1.43	1.14
1:1:183:SER:O	1:1:184:ILE:HG12	1.44	1.14
1:1:271:THR:O	1:1:273:ASP:N	1.78	1.14
1:1:104:GLN:O	3:3:236:ILE:HD13	1.48	1.13
2:2:18:ARG:HH12	2:2:249:MET:HE2	1.06	1.13
1:1:125:ILE:CG2	1:1:182:PHE:HE1	1.61	1.13
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.13
1:1:260:THR:CG2	1:1:261:HIS:H	1.44	1.11
1:1:260:THR:CG2	1:1:261:HIS:N	2.00	1.10
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.12	1.09
1:1:215:ASN:HD22	1:1:215:ASN:N	1.47	1.09
1:1:252:ARG:CG	1:1:253:PRO:HD2	1.82	1.09
1:1:260:THR:HG22	1:1:261:HIS:N	1.31	1.08
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.07
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.31	1.07
1:1:191:SER:OG	2:2:208:ALA:O	1.72	1.07
1:1:125:ILE:O	1:1:181:ARG:HG2	1.55	1.06
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.06
1:1:103:LEU:HD11	5:1:700:JEN:H8	1.33	1.06
1:1:103:LEU:C	1:1:104:GLN:HG2	1.79	1.05
1:1:113:PHE:HB3	1:1:195:MET:HE3	1.36	1.05
1:1:189:ILE:O	3:3:31:THR:HG21	1.55	1.05
1:1:230:LYS:HG2	1:1:231:LEU:HD22	1.37	1.05
1:1:183:SER:O	1:1:184:ILE:HG13	1.55	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:VAL:O	1:1:192:ALA:HB1	1.56	1.04
1:1:189:ILE:O	3:3:31:THR:CG2	2.06	1.04
1:1:146:MET:HE1	1:1:162:SER:O	1.58	1.03
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
1:1:255:ARG:CD	1:1:259:TYR:CE2	2.42	1.02
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.02
1:1:261:HIS:NE2	2:2:138:GLY:CA	2.23	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
1:1:273:ASP:O	1:1:274:VAL:HG12	1.59	1.01
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	1.01
1:1:129:PRO:HG2	1:1:173:TRP:CE2	1.95	1.00
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	1.00
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.00
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.00
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
1:1:193:TYR:CE1	1:1:217:MET:HE1	1.97	0.99
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.44	0.99
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	0.99
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.93	0.98
1:1:163:TRP:HH2	1:1:222:SER:O	1.41	0.98
1:1:252:ARG:HG3	1:1:253:PRO:HD2	1.46	0.98
1:1:108:GLN:CD	3:3:226:ASP:OD2	2.06	0.98
1:1:261:HIS:NE2	2:2:138:GLY:HA2	1.79	0.97
3:3:117:PHE:CD1	3:3:211:CYS:HB3	2.00	0.97
1:1:103:LEU:O	1:1:104:GLN:HG2	1.62	0.97
1:1:173:TRP:CD1	1:1:180:PRO:HD3	1.99	0.96
1:1:146:MET:CE	1:1:162:SER:O	2.13	0.96
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
3:3:28:TYR:O	3:3:30:PRO:HD3	1.64	0.96
1:1:113:PHE:O	1:1:115:LEU:N	1.99	0.95
1:1:103:LEU:O	1:1:104:GLN:CG	2.14	0.95
1:1:214:THR:C	1:1:215:ASN:HD22	1.73	0.95
1:1:249:TRP:HA	3:3:39:GLU:HA	1.44	0.95
1:1:158:ARG:O	1:1:163:TRP:NE1	1.99	0.94
1:1:267:TYR:O	1:1:268:MET:CB	2.13	0.94
1:1:189:ILE:O	3:3:31:THR:CB	2.15	0.94
1:1:212:VAL:CG1	1:1:263:HIS:CD2	2.51	0.93
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:VAL:HG12	1:1:225:VAL:CB	1.98	0.93
1:1:104:GLN:O	3:3:236:ILE:CD1	2.17	0.93
1:1:248:ALA:O	3:3:40:VAL:N	2.02	0.92
1:1:101:ILE:CD1	1:1:217:MET:HB2	1.98	0.92
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
1:1:183:SER:C	1:1:184:ILE:HG13	1.94	0.92
1:1:212:VAL:HG12	1:1:263:HIS:CG	2.04	0.92
1:1:260:THR:HG22	1:1:261:HIS:CA	1.99	0.91
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.50	0.91
1:1:212:VAL:CG1	1:1:263:HIS:CG	2.52	0.91
1:1:117:THR:O	1:1:195:MET:HB2	1.70	0.91
1:1:142:VAL:CG1	1:1:225:VAL:HB	2.01	0.90
1:1:138:ILE:HG13	1:1:139:GLY:N	1.86	0.90
1:1:158:ARG:O	1:1:163:TRP:CD1	2.24	0.90
1:1:173:TRP:HD1	1:1:180:PRO:CD	1.85	0.89
1:1:197:TYR:CD2	1:1:214:THR:HG22	2.07	0.89
1:1:189:ILE:O	3:3:31:THR:HB	1.71	0.89
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.88
1:1:147:TYR:CD1	5:1:700:JEN:H213	2.08	0.88
1:1:261:HIS:HD2	2:2:138:GLY:O	1.43	0.88
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.88
1:1:183:SER:C	1:1:184:ILE:CG1	2.43	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
1:1:125:ILE:O	1:1:181:ARG:CG	2.22	0.88
2:2:159:GLU:C	2:2:160:ARG:HG2	1.97	0.88
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.87
1:1:101:ILE:HD11	1:1:217:MET:HB2	1.56	0.87
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:96:PHE:CE2	1:1:157:LYS:HA	2.11	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
1:1:248:ALA:O	3:3:39:GLU:CA	2.25	0.85
1:1:125:ILE:HG21	1:1:182:PHE:HE1	0.85	0.85
1:1:122:ASP:OD2	4:4:36:ALA:HA	1.77	0.85
1:1:91:GLY:O	1:1:157:LYS:HB3	1.77	0.84
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.38	0.84
1:1:126:THR:HG23	1:1:181:ARG:HG3	1.57	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
1:1:108:GLN:NE2	3:3:226:ASP:OD2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:215:ASN:N	1:1:215:ASN:ND2	2.20	0.84
1:1:101:ILE:CD1	1:1:217:MET:O	2.23	0.83
1:1:260:THR:HG22	1:1:261:HIS:H	0.95	0.83
1:1:260:THR:CG2	1:1:261:HIS:CD2	2.61	0.83
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.83
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.14	0.83
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.83
1:1:101:ILE:HD11	1:1:217:MET:C	2.04	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
1:1:112:LYS:O	1:1:115:LEU:HB2	1.79	0.82
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
1:1:89:TYR:HE2	1:1:227:GLU:C	1.87	0.82
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.95	0.82
1:1:186:PHE:CE1	3:3:31:THR:HG22	2.13	0.82
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.82
1:1:97:THR:HG23	1:1:222:SER:HB3	1.60	0.82
1:1:186:PHE:HE1	3:3:31:THR:HG22	1.42	0.82
1:1:92:GLN:C	1:1:94:ILE:HD12	2.05	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.82
1:1:113:PHE:CB	1:1:195:MET:HE3	2.10	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:158:ARG:NH2	1:1:225:VAL:O	2.13	0.81
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.14	0.80
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.98	0.80
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.12	0.80
1:1:260:THR:HG22	1:1:261:HIS:CB	2.12	0.80
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.80
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:212:VAL:CG1	1:1:263:HIS:HB3	2.12	0.80
1:1:76:CYS:HA	1:1:239:ILE:O	1.81	0.80
1:1:141:ILE:CG2	1:1:141:ILE:O	2.30	0.80
1:1:212:VAL:HB	1:1:263:HIS:CD2	2.17	0.80
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.45	0.79
1:1:248:ALA:O	3:3:39:GLU:HA	1.82	0.79
1:1:214:THR:C	1:1:215:ASN:ND2	2.41	0.79
1:1:252:ARG:HG2	1:1:253:PRO:HD2	1.63	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
1:1:147:TYR:CD1	5:1:700:JEN:C21	2.66	0.79
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
1:1:142:VAL:CG1	1:1:225:VAL:CG2	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.78
1:1:252:ARG:CG	1:1:253:PRO:CD	2.61	0.78
1:1:110:ARG:O	1:1:114:GLU:HG3	1.82	0.78
1:1:126:THR:HG21	3:3:13:PHE:CE1	2.19	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.64	0.77
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.64	0.77
1:1:197:TYR:H	2:2:131:GLN:HE21	1.31	0.77
1:1:261:HIS:NE2	2:2:139:SER:N	2.33	0.77
3:3:55:VAL:C	3:3:57:ASN:H	1.93	0.77
1:1:212:VAL:HG11	1:1:263:HIS:CB	2.15	0.77
1:1:252:ARG:HG2	1:1:253:PRO:CD	2.15	0.76
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.62	0.76
1:1:92:GLN:O	1:1:93:ASP:HB2	1.85	0.76
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:261:HIS:ND1	2:2:139:SER:HB3	2.01	0.76
1:1:101:ILE:HG12	1:1:218:GLY:O	1.86	0.76
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
1:1:225:VAL:O	1:1:227:GLU:N	2.15	0.75
1:1:91:GLY:C	1:1:94:ILE:HD13	2.12	0.75
1:1:103:LEU:HD21	5:1:700:JEN:H7	1.67	0.75
1:1:184:ILE:HG23	1:1:185:PRO:HD2	1.69	0.75
1:1:149:PRO:HB2	1:1:150:PRO:HD2	1.69	0.75
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.75
1:1:193:TYR:CD1	1:1:217:MET:HE1	2.22	0.74
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
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
1:1:125:ILE:CG2	1:1:182:PHE:CD1	2.70	0.74
1:1:260:THR:HG21	1:1:261:HIS:HD2	1.53	0.74
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.52	0.74
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.70	0.74
1:1:252:ARG:HG3	2:2:186:PHE:HZ	1.53	0.74
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:212:VAL:HG11	1:1:263:HIS:CG	2.24	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
1:1:92:GLN:C	1:1:94:ILE:CD1	2.62	0.73
1:1:124:GLU:CD	1:1:181:ARG:HH11	1.97	0.73
1:1:99:TRP:NE1	1:1:105:GLU:OE2	2.22	0.73
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.71	0.73
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.73
1:1:138:ILE:CG1	1:1:139:GLY:N	2.51	0.73
1:1:212:VAL:CG1	1:1:263:HIS:CB	2.67	0.73
1:1:271:THR:C	1:1:273:ASP:N	2.47	0.73
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72
2:2:183:LEU:HD12	2:2:186:PHE:HD2	1.52	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:CD	2.52	0.72
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.24	0.72
1:1:117:THR:O	1:1:195:MET:CB	2.38	0.72
1:1:212:VAL:CB	1:1:263:HIS:CD2	2.72	0.72
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.72
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.72
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.06	0.71
1:1:140:HIS:HE1	1:1:174:GLN:OE1	1.73	0.71
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71
1:1:212:VAL:HG11	1:1:263:HIS:CD2	2.24	0.71
1:1:80:SER:HB3	1:1:237:THR:HG23	1.73	0.71
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.71
1:1:252:ARG:HG2	1:1:253:PRO:N	2.06	0.70
3:3:25:LEU:N	3:3:25:LEU:HD12	2.06	0.70
1:1:124:GLU:OE1	1:1:181:ARG:NH1	2.23	0.70
1:1:138:ILE:HG13	1:1:139:GLY:H	1.57	0.70
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.91	0.70
1:1:104:GLN:C	1:1:106:MET:H	1.97	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.70
1:1:252:ARG:HG3	2:2:186:PHE:CZ	2.26	0.70
1:1:101:ILE:HD12	1:1:217:MET:HB2	1.73	0.70
1:1:142:VAL:HG12	1:1:225:VAL:CG2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
1:1:138:ILE:CG1	1:1:139:GLY:H	2.03	0.69
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
1:1:249:TRP:CA	3:3:39:GLU:HA	2.22	0.69
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.71	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.93	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.69
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.69
1:1:124:GLU:CG	1:1:242:LYS:HB3	2.22	0.69
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.69
1:1:254:PRO:CG	3:3:101:GLU:HG2	2.23	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
1:1:197:TYR:CD2	1:1:214:THR:CG2	2.76	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.69
1:1:156:SER:C	1:1:157:LYS:HG3	2.16	0.68
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.68
1:1:260:THR:HG21	1:1:261:HIS:CD2	2.28	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
1:1:197:TYR:HD2	1:1:214:THR:HG22	1.53	0.68
1:1:222:SER:O	1:1:223:ARG:CB	2.42	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.94	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.68
2:2:174:ASN:C	2:2:175:PHE:HD1	2.02	0.67
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.30	0.67
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67
1:1:230:LYS:CG	1:1:231:LEU:HD22	2.19	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
1:1:125:ILE:CB	1:1:182:PHE:CE1	2.77	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.66
1:1:262:SER:HB2	3:3:238:GLN:HA	1.77	0.66
1:1:146:MET:HE2	1:1:162:SER:O	1.95	0.66
1:1:197:TYR:HD1	1:1:198:ASP:H	1.43	0.66
2:2:91:ILE:O	2:2:92:PHE:C	2.38	0.66
1:1:141:ILE:O	1:1:141:ILE:HG22	1.95	0.66
3:3:91:SER:O	3:3:92:THR:C	2.39	0.66
1:1:163:TRP:CG	1:1:223:ARG:HE	2.14	0.65
1:1:190:ALA:C	3:3:31:THR:HG21	2.21	0.65
1:1:268:MET:O	2:2:137:HIS:ND1	2.30	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.31	0.65
1:1:267:TYR:OH	2:2:170:ASP:CB	2.45	0.65
1:1:142:VAL:H	1:1:226:THR:HG23	1.60	0.65
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.65
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.62	0.65
1:1:145:TYR:HB2	1:1:171:ILE:HG23	1.77	0.65
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.65
1:1:125:ILE:CB	1:1:182:PHE:HE1	2.10	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.27	0.64
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.64
1:1:173:TRP:CD1	1:1:180:PRO:CD	2.70	0.64
1:1:222:SER:O	1:1:223:ARG:HB3	1.96	0.64
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
1:1:101:ILE:HB	5:1:700:JEN:H131	1.79	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:201:ASP:OD1	1:1:208:LYS:HB2	1.98	0.64
1:1:171:ILE:HD11	1:1:180:PRO:CB	2.27	0.64
1:1:136:ASP:O	1:1:137:ASP:HB2	1.97	0.63
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.63
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.63
1:1:129:PRO:HG2	1:1:173:TRP:CZ2	2.31	0.63
1:1:271:THR:C	1:1:273:ASP:H	2.04	0.63
1:1:142:VAL:CG1	1:1:225:VAL:HG21	2.29	0.63
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.63
1:1:199:GLY:HA2	2:2:216:ARG:O	1.99	0.63
1:1:212:VAL:HG11	1:1:263:HIS:HB3	1.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.34	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
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
2:2:235:THR:C	2:2:237:SER:H	2.06	0.62
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.62
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.62
3:3:145:LYS:O	3:3:148:MET:HE3	1.98	0.62
1:1:163:TRP:CZ3	1:1:223:ARG:HB3	2.35	0.62
1:1:255:ARG:HD2	1:1:259:TYR:CD2	2.34	0.62
1:1:255:ARG:HD3	1:1:259:TYR:CZ	2.35	0.62
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.15	0.61
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.61
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:124:GLU:O	1:1:124:GLU:HG3	1.98	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
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.16	0.61
1:1:209:TYR:OH	2:2:131:GLN:HA	2.00	0.61
2:2:183:LEU:HD12	2:2:186:PHE:CD2	2.34	0.61
1:1:92:GLN:N	1:1:94:ILE:CD1	2.63	0.61
1:1:158:ARG:HG2	1:1:159:ASN:N	2.14	0.61
1:1:261:HIS:CE1	2:2:139:SER:CB	2.84	0.61
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:78:HIS:O	1:1:239:ILE:HB	2.02	0.60
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.84	0.60
1:1:255:ARG:NE	1:1:257:VAL:O	2.34	0.60
1:1:91:GLY:O	1:1:157:LYS:CB	2.47	0.60
1:1:101:ILE:HG23	1:1:220:ILE:CG2	2.30	0.60
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.60
1:1:165:SER:OG	1:1:170:SER:OG	2.16	0.60
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.60
1:1:225:VAL:C	1:1:227:GLU:H	2.05	0.60
1:1:248:ALA:O	3:3:39:GLU:C	2.44	0.60
1:1:255:ARG:CD	1:1:259:TYR:CD2	2.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.29	0.60
2:2:84:ASP:OD1	2:2:87:LYS:HE2	2.02	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
2:2:159:GLU:C	2:2:160:ARG:CG	2.71	0.60
1:1:89:TYR:CE2	1:1:227:GLU:C	2.75	0.60
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.67	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.59
1:1:150:PRO:O	1:1:151:GLY:C	2.45	0.59
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.59
3:3:25:LEU:HD12	3:3:25:LEU:H	1.68	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
1:1:260:THR:HG22	1:1:261:HIS:CG	2.36	0.59
1:1:67:ILE:HD13	1:1:248:ALA:HB3	1.84	0.59
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.59
1:1:226:THR:O	1:1:227:GLU:CB	2.50	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
1:1:103:LEU:CD2	5:1:700:JEN:H7	2.33	0.59
1:1:104:GLN:C	1:1:106:MET:N	2.61	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.59
2:2:14:MET:HE1	2:2:31:ALA:HB2	1.83	0.58
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.58
1:1:89:TYR:HE2	1:1:228:LYS:N	2.01	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
1:1:261:HIS:C	1:1:262:SER:O	2.45	0.58
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.58
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.58
1:1:244:LYS:HE3	4:4:38:SER:O	2.03	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.86	0.58
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
1:1:184:ILE:CG2	1:1:187:LEU:HD21	2.33	0.58
1:1:209:TYR:CD1	1:1:209:TYR:C	2.80	0.58
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.58
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.58
1:1:149:PRO:CB	1:1:150:PRO:CD	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:261:HIS:CE1	2:2:139:SER:OG	2.58	0.57
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
1:1:125:ILE:HB	1:1:182:PHE:CD1	2.40	0.57
1:1:224:ILE:O	1:1:224:ILE:HG23	2.05	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
1:1:273:ASP:O	1:1:274:VAL:CG1	2.43	0.57
1:1:189:ILE:HG23	1:1:190:ALA:H	1.70	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.56
1:1:103:LEU:CD1	5:1:700:JEN:H8	2.23	0.56
1:1:101:ILE:CG1	1:1:218:GLY:O	2.53	0.56
3:3:25:LEU:N	3:3:25:LEU:CD1	2.68	0.56
1:1:113:PHE:CD2	1:1:195:MET:CE	2.88	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:74:SER:HA	1:1:241:HIS:O	2.06	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
1:1:267:TYR:CE1	1:1:268:MET:HE2	2.41	0.56
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.56
1:1:91:GLY:C	1:1:94:ILE:CD1	2.78	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
1:1:267:TYR:OH	2:2:168:SER:OG	2.21	0.56
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.87	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:101:ILE:CG2	1:1:220:ILE:CG2	2.85	0.55
1:1:271:THR:O	1:1:273:ASP:CA	2.52	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
1:1:141:ILE:O	1:1:141:ILE:HG23	2.07	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.55
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
1:1:146:MET:O	1:1:146:MET:HG3	1.99	0.55
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.88	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
1:1:260:THR:CG2	1:1:261:HIS:HD2	2.08	0.54
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.54
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.23	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:224:ILE:O	1:1:225:VAL:O	2.26	0.54
1:1:250:CYS:HB3	2:2:35:TYR:CZ	2.42	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.26	0.54
1:1:200:TYR:HA	1:1:208:LYS:O	2.07	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
3:3:107:THR:HG21	3:3:223:MET:HE2	1.89	0.54
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
1:1:257:VAL:HG13	1:1:258:PRO:HD2	1.90	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
2:2:168:SER:HG	2:2:170:ASP:HB2	1.73	0.54
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.54
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
1:1:107:ALA:O	1:1:109:ILE:N	2.41	0.54
1:1:195:MET:O	1:1:196:PHE:CG	2.61	0.54
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.54
1:1:125:ILE:CG2	1:1:126:THR:N	2.71	0.54
1:1:126:THR:HG23	1:1:181:ARG:CG	2.32	0.54
1:1:171:ILE:HD11	1:1:180:PRO:HB3	1.90	0.54
1:1:248:ALA:O	3:3:39:GLU:CB	2.56	0.54
1:1:147:TYR:CE1	5:1:700:JEN:H213	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:14:MET:C	3:3:16:THR:H	2.16	0.53
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	0.53
1:1:80:SER:O	1:1:236:THR:HA	2.07	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.53
1:1:124:GLU:HB3	1:1:244:LYS:HD3	1.89	0.53
1:1:197:TYR:HD1	1:1:198:ASP:N	2.06	0.53
1:1:197:TYR:CD1	1:1:198:ASP:N	2.77	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:94:ILE:HD12	1:1:94:ILE:N	2.23	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.53
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.53
1:1:244:LYS:NZ	4:4:38:SER:H	2.07	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:255:ARG:HD2	1:1:259:TYR:HE2	1.60	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.53
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.53
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.53
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.52
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.52
1:1:128:VAL:HG12	1:1:128:VAL:O	2.07	0.52
1:1:184:ILE:CG2	1:1:185:PRO:HD2	2.37	0.52
1:1:194:TYR:HB2	1:1:214:THR:OG1	2.08	0.52
3:3:43:LEU:CD2	3:3:46:MET:HE2	2.39	0.52
4:4:26:TYR:CD1	4:4:29:ILE:CD1	2.91	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.91	0.52
1:1:181:ARG:O	3:3:21:SER:HB3	2.09	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
3:3:26:PRO:HB2	3:3:27:TRP:CE3	2.44	0.52
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.44	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
1:1:92:GLN:O	1:1:94:ILE:HD11	2.10	0.52
1:1:93:ASP:N	1:1:94:ILE:HD12	2.24	0.52
1:1:101:ILE:HG23	1:1:220:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.52
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.52
1:1:148:VAL:CG1	1:1:152:ALA:HB3	2.40	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:103:LEU:O	1:1:104:GLN:CB	2.58	0.51
1:1:200:TYR:CE2	1:1:209:TYR:HB2	2.46	0.51
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
1:1:97:THR:HG23	1:1:222:SER:CB	2.38	0.51
1:1:103:LEU:C	1:1:104:GLN:CG	2.57	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:22:PRO:C	3:3:23:CYS:O	2.52	0.51
1:1:96:PHE:CZ	1:1:155:PRO:O	2.64	0.51
1:1:261:HIS:CE1	2:2:139:SER:N	2.79	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.51
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.10	0.51
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.72	0.51
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.43	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
1:1:185:PRO:HB2	1:1:186:PHE:O	2.11	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
1:1:149:PRO:HB2	1:1:150:PRO:CD	2.38	0.51
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.46	0.51
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.26	0.51
1:1:126:THR:HG21	3:3:13:PHE:CD1	2.46	0.50
1:1:101:ILE:HD11	1:1:217:MET:CB	2.36	0.50
1:1:188:SER:OG	1:1:193:TYR:CD1	2.56	0.50
1:1:255:ARG:NE	1:1:259:TYR:CD2	2.79	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.50
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.50
1:1:261:HIS:CD2	2:2:138:GLY:CA	2.86	0.50
1:1:271:THR:O	1:1:272:GLY:C	2.52	0.50
2:2:175:PHE:CD1	2:2:175:PHE:N	2.79	0.50
1:1:111:ARG:HA	1:1:259:TYR:OH	2.11	0.50
3:3:72:LEU:HD12	3:3:72:LEU:N	2.26	0.50
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.50
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.50
1:1:117:THR:C	1:1:195:MET:HB2	2.37	0.50
1:1:186:PHE:CZ	1:1:188:SER:HB2	2.47	0.50
1:1:191:SER:HB3	3:3:34:ILE:HG12	1.92	0.50
1:1:254:PRO:O	2:2:178:THR:HG22	2.11	0.50
1:1:145:TYR:N	1:1:145:TYR:CD1	2.80	0.50
1:1:260:THR:CG2	1:1:261:HIS:CG	2.95	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.50
1:1:111:ARG:NH2	3:3:101:GLU:OE2	2.39	0.49
1:1:197:TYR:H	2:2:131:GLN:NE2	2.07	0.49
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.49
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD2	2.48	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.49
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:99:TRP:CZ3	1:1:101:ILE:HA	2.48	0.49
1:1:191:SER:N	3:3:31:THR:HG21	2.28	0.49
1:1:125:ILE:HG23	1:1:126:THR:N	2.28	0.49
1:1:140:HIS:HE1	1:1:174:GLN:CD	2.19	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
3:3:25:LEU:O	3:3:25:LEU:HD13	2.12	0.49
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.47	0.49
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.49
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.49
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.49
2:2:126:MET:HE3	2:2:126:MET:HA	1.94	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.49
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.49
1:1:142:VAL:H	1:1:226:THR:CG2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.49
1:1:125:ILE:HG22	1:1:182:PHE:CD1	2.47	0.49
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.49
1:1:120:ARG:HD2	1:1:191:SER:O	2.13	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.48
1:1:163:TRP:CZ3	1:1:222:SER:O	2.62	0.48
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.48
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.48
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.78	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.48
1:1:200:TYR:CG	1:1:209:TYR:HB2	2.47	0.48
1:1:253:PRO:HB2	2:2:178:THR:HB	1.96	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
1:1:261:HIS:CE1	2:2:139:SER:HB3	2.48	0.48
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.48
1:1:132:ALA:HB3	1:1:234:VAL:HG13	1.96	0.48
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.48
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.48
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
1:1:261:HIS:O	1:1:262:SER:O	2.32	0.48
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.48
1:1:143:MET:HG2	1:1:145:TYR:CZ	2.49	0.48
1:1:120:ARG:O	1:1:121:PHE:HB3	2.13	0.48
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.48
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.48
3:3:82:VAL:HG12	3:3:83:PHE:H	1.77	0.48
1:1:117:THR:HA	1:1:252:ARG:HH21	1.78	0.47
1:1:125:ILE:CB	1:1:182:PHE:CD1	2.97	0.47
1:1:195:MET:O	1:1:196:PHE:CD2	2.67	0.47
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.47
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:186:PHE:CD1	1:1:186:PHE:C	2.91	0.47
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.47
1:1:266:ASN:HA	2:2:133:ALA:HB1	1.95	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD1	2.49	0.47
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:101:ILE:CG2	1:1:220:ILE:HG22	2.43	0.47
1:1:182:PHE:HD1	1:1:182:PHE:H	1.60	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.47
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.47
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.47
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
3:3:216:CYS:C	3:3:218:ASP:H	2.23	0.47
1:1:244:LYS:NZ	4:4:38:SER:O	2.47	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
1:1:141:ILE:HA	1:1:226:THR:HG21	1.96	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.47
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
1:1:137:ASP:O	1:1:231:LEU:HB2	2.14	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.47
3:3:43:LEU:HD23	3:3:46:MET:HE2	1.97	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
1:1:113:PHE:CD2	1:1:195:MET:HE3	2.49	0.47
1:1:248:ALA:O	3:3:39:GLU:HB2	2.15	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
1:1:38:GLU:C	1:1:40:GLY:N	2.73	0.47
1:1:163:TRP:CH2	1:1:223:ARG:HB3	2.50	0.47
1:1:261:HIS:ND1	2:2:139:SER:CB	2.77	0.47
1:1:267:TYR:OH	2:2:170:ASP:HB2	2.14	0.47
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
1:1:89:TYR:HD1	1:1:89:TYR:HA	1.49	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.46
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.46
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:142:VAL:HB	1:1:226:THR:HG23	1.97	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
1:1:134:ARG:HD3	1:1:234:VAL:HG12	1.97	0.46
1:1:253:PRO:CD	2:2:185:ILE:HG21	2.41	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.14	0.46
1:1:67:ILE:CD1	1:1:248:ALA:HB3	2.46	0.46
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.46
1:1:212:VAL:HG12	1:1:263:HIS:CD2	2.33	0.46
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.46
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.03	0.46
1:1:244:LYS:CE	4:4:38:SER:O	2.64	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
3:3:91:SER:C	3:3:92:THR:O	2.58	0.46
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.46
1:1:92:GLN:C	1:1:94:ILE:HD11	2.39	0.46
1:1:261:HIS:HB2	1:1:264:VAL:HG21	1.98	0.46
3:3:14:MET:C	3:3:16:THR:N	2.74	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	0.46
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.46
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.46
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.97	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
1:1:249:TRP:HA	3:3:39:GLU:CA	2.31	0.45
1:1:264:VAL:HG12	2:2:141:THR:HG22	1.98	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:197:TYR:N	2:2:131:GLN:HE21	2.08	0.45
1:1:89:TYR:CE2	1:1:228:LYS:N	2.83	0.45
1:1:113:PHE:HD2	1:1:195:MET:CE	2.29	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:240:VAL:HA	2:2:241:PRO:HD2	1.88	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
2:2:228:SER:HA	2:2:229:PRO:HD2	1.69	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:157:LYS:HE2	1:1:157:LYS:HB2	1.40	0.45
1:1:197:TYR:HE2	1:1:213:VAL:CG1	2.29	0.45
1:1:249:TRP:HA	3:3:38:GLY:O	2.17	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:39:THR:C	1:1:41:HIS:H	2.24	0.45
1:1:257:VAL:HG11	1:1:267:TYR:HB2	1.98	0.45
1:1:261:HIS:CD2	2:2:139:SER:N	2.74	0.45
1:1:104:GLN:O	1:1:106:MET:N	2.50	0.45
1:1:126:THR:HG23	1:1:181:ARG:HB2	1.98	0.45
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.45
3:3:42:ASN:CG	3:3:44:ILE:HG22	2.38	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
1:1:111:ARG:NH2	3:3:101:GLU:CD	2.75	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
2:2:144:TYR:C	2:2:146:LEU:H	2.25	0.45
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.45
1:1:197:TYR:CE2	1:1:213:VAL:CG1	2.99	0.44
1:1:214:THR:CA	1:1:215:ASN:HD22	2.30	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.17	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:230:LYS:HG2	1:1:231:LEU:N	2.32	0.44
2:2:18:ARG:HD3	2:2:18:ARG:HA	1.57	0.44
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.44
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.44
1:1:90:ASN:N	1:1:90:ASN:HD22	2.16	0.44
1:1:214:THR:OG1	1:1:215:ASN:ND2	2.51	0.44
1:1:244:LYS:HZ1	4:4:38:SER:H	1.66	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
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.44
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.44
2:2:83:PRO:CG	2:2:218:ASN:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.44
3:3:65:VAL:C	3:3:67:MET:N	2.74	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.44
1:1:61:THR:CG2	1:1:63:ASP:CG	2.91	0.43
1:1:111:ARG:HH21	3:3:101:GLU:HG3	1.83	0.43
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.43
1:1:92:GLN:O	1:1:94:ILE:CD1	2.66	0.43
3:3:25:LEU:HA	3:3:26:PRO:HD2	1.77	0.43
3:3:88:ASP:OD1	3:3:186:ALA:N	2.39	0.43
3:3:159:LEU:HA	3:3:159:LEU:HD23	1.72	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:155:PRO:CG	1:1:163:TRP:CZ2	3.01	0.43
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.43
2:2:247:SER:O	2:2:248:PRO:C	2.60	0.43
3:3:102:ILE:C	3:3:104:SER:N	2.76	0.43
1:1:247:LYS:HB3	1:1:249:TRP:CZ3	2.54	0.43
2:2:126:MET:HB3	2:2:126:MET:HE2	1.61	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:85:ASP:OD1	1:1:85:ASP:C	2.61	0.43
1:1:188:SER:HB3	1:1:189:ILE:H	1.17	0.43
1:1:267:TYR:OH	2:2:170:ASP:HB3	2.18	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.51	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.43
1:1:148:VAL:HG13	1:1:152:ALA:CB	2.48	0.43
1:1:248:ALA:C	3:3:39:GLU:HA	2.42	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
4:4:26:TYR:HD1	4:4:29:ILE:HD11	1.78	0.43
1:1:111:ARG:HH22	3:3:101:GLU:CD	2.25	0.43
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.43
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43
1:1:182:PHE:CD1	1:1:182:PHE:N	2.83	0.43
3:3:22:PRO:O	3:3:23:CYS:O	2.36	0.43
1:1:36:ALA:C	1:1:38:GLU:H	2.27	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.43
1:1:251:PRO:HG3	3:3:40:VAL:CG2	2.49	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
1:1:184:ILE:HA	1:1:185:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:249:TRP:CD1	3:3:39:GLU:HB3	2.53	0.42
2:2:154:ARG:HH11	2:2:154:ARG:HG2	1.83	0.42
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.42
1:1:98:LYS:O	1:1:98:LYS:CG	2.33	0.42
1:1:125:ILE:O	1:1:181:ARG:HG3	2.15	0.42
1:1:129:PRO:HA	1:1:237:THR:HA	2.02	0.42
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.42
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.42
1:1:165:SER:C	1:1:167:THR:N	2.77	0.42
1:1:249:TRP:CA	3:3:38:GLY:O	2.68	0.42
1:1:160:ASP:H	1:1:163:TRP:HD1	1.66	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:127:ILE:N	2:2:221:CYS:O	2.53	0.42
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
1:1:197:TYR:CE2	1:1:213:VAL:HG11	2.55	0.42
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.42
2:2:178:THR:O	2:2:179:LEU:C	2.62	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
1:1:103:LEU:HD11	5:1:700:JEN:C8	2.23	0.42
1:1:113:PHE:CG	1:1:195:MET:HE3	2.55	0.42
1:1:196:PHE:CD2	1:1:252:ARG:NH2	2.88	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.42
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.42
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:94:LEU:HA	3:3:94:LEU:HD23	1.83	0.42
3:3:158:GLY:C	3:3:160:GLN:N	2.77	0.42
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:46:MET:HE3	3:3:102:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
1:1:77:VAL:HG22	1:1:239:ILE:CG2	2.44	0.41
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.56	0.41
1:1:212:VAL:HG12	1:1:263:HIS:CB	2.41	0.41
3:3:143:THR:C	3:3:192:TRP:CH2	2.97	0.41
1:1:119:VAL:HG13	1:1:120:ARG:N	2.35	0.41
1:1:145:TYR:O	1:1:171:ILE:HG22	2.20	0.41
1:1:225:VAL:C	1:1:227:GLU:N	2.71	0.41
1:1:66:SER:O	1:1:67:ILE:C	2.60	0.41
1:1:150:PRO:O	1:1:152:ALA:N	2.52	0.41
1:1:197:TYR:HE2	1:1:213:VAL:HG12	1.86	0.41
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	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	2.56	0.41
3:3:2:LEU:HA	3:3:2:LEU:HD23	1.80	0.41
1:1:149:PRO:O	1:1:150:PRO:O	2.39	0.41
1:1:267:TYR:OH	2:2:170:ASP:OD2	2.38	0.41
2:2:61:ASN:HB2	2:2:248:PRO:C	2.45	0.41
2:2:63:PHE:CD1	2:2:247:SER:HB2	2.55	0.41
2:2:94:GLU:C	2:2:96:MET:N	2.76	0.41
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.41
1:1:82:ILE:HD13	1:1:82:ILE:HG21	1.81	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.41
1:1:184:ILE:CG2	1:1:185:PRO:CD	2.99	0.41
1:1:235:ILE:HG22	1:1:236:THR:N	2.34	0.41
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.41
1:1:146:MET:HA	1:1:169:MET:O	2.20	0.41
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.41
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.41
2:2:155:ASP:C	2:2:157:SER:H	2.29	0.41
3:3:43:LEU:HD23	3:3:43:LEU:HA	1.78	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
1:1:145:TYR:HE2	1:1:237:THR:OG1	2.04	0.41
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.55	0.41
2:2:192:ASN:C	2:2:194:ARG:N	2.79	0.41
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.41
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.41
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.41
1:1:92:GLN:N	1:1:94:ILE:HD11	2.36	0.41
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:TRP:HB3	1:1:223:ARG:HH21	1.86	0.41
1:1:220:ILE:O	1:1:220:ILE:HG13	2.11	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
3:3:43:LEU:HD22	3:3:46:MET:HE2	2.02	0.41
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.41
1:1:86:TYR:CE2	1:1:229:GLN:HB2	2.54	0.41
1:1:199:GLY:C	1:1:200:TYR:CD1	2.99	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
2:2:51:ASN:H	2:2:51:ASN:ND2	2.15	0.40
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.40
1:1:9:GLU:OE2	4:4:42:ARG:HG3	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:46:GLN:CD	3:3:217:LYS:HG3	2.47	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.02	0.40
3:3:145:LYS:O	3:3:146:ASP:C	2.65	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
1:1:119:VAL:CG1	1:1:121:PHE:HE1	2.35	0.40
1:1:123:SER:N	1:1:184:ILE:O	2.49	0.40
1:1:157:LYS:O	1:1:158:ARG:C	2.64	0.40
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.40
2:2:164:LEU:C	2:2:166:GLN:N	2.80	0.40
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
2:2:202:ILE:HD13	2:2:249:MET:HE3	2.02	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:114:ARG:NH2	3:3:215:ALA:O	2.55	0.40
3:3:115:PHE:CE1	3:3:167:VAL:HG21	2.57	0.40

All (1) 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)
1:1:27:THR:OG1	2:2:18:ARG:NH2[2_655]	2.09	0.11

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	1	281/287 (98%)	196 (70%)	46 (16%)	39 (14%)	0	3
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1	14
3	3	236/238 (99%)	176 (75%)	39 (16%)	21 (9%)	0	9
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1	15
All	All	785/832 (94%)	582 (74%)	127 (16%)	76 (10%)	0	7

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	102	THR
1	1	114	GLU
1	1	151	GLY
1	1	158	ARG
1	1	189	ILE
1	1	191	SER
1	1	223	ARG
1	1	225	VAL
1	1	226	THR
1	1	262	SER
1	1	263	HIS
1	1	264	VAL
1	1	271	THR
1	1	272	GLY
1	1	273	ASP
1	1	274	VAL
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	23	CYS

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Mol	Chain	Res	Type
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE
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	104	GLN
1	1	108	GLN
1	1	119	VAL
1	1	137	ASP
1	1	150	PRO
1	1	266	ASN
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	159	LEU
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	103	LEU
1	1	105	GLU
1	1	227	GLU
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE
1	1	160	ASP
1	1	268	MET

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Mol	Chain	Res	Type
2	2	260	ASN
1	1	107	ALA
1	1	161	PHE
1	1	205	THR
1	1	212	VAL
2	2	87	LYS
2	2	259	LYS
1	1	149	PRO
3	3	220	CYS
3	3	121	GLY
2	2	44	PRO
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%)	175 (69%)	79 (31%)	0	1
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%)	486 (70%)	211 (30%)	0	2

All (211) 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

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Mol	Chain	Res	Type
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	98	LYS
1	1	102	THR
1	1	103	LEU
1	1	104	GLN
1	1	105	GLU
1	1	106	MET
1	1	108	GLN
1	1	109	ILE
1	1	111	ARG
1	1	112	LYS
1	1	119	VAL
1	1	123	SER
1	1	124	GLU
1	1	125	ILE
1	1	126	THR
1	1	127	LEU
1	1	134	ARG
1	1	141	ILE
1	1	142	VAL
1	1	146	MET
1	1	157	LYS
1	1	159	ASN
1	1	160	ASP
1	1	162	SER
1	1	168	ASN
1	1	173	TRP
1	1	177	GLN
1	1	182	PHE
1	1	183	SER
1	1	188	SER
1	1	189	ILE
1	1	191	SER
1	1	195	MET
1	1	201	ASP
1	1	209	TYR

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Mol	Chain	Res	Type
1	1	212	VAL
1	1	213	VAL
1	1	214	THR
1	1	215	ASN
1	1	217	MET
1	1	219	THR
1	1	220	ILE
1	1	223	ARG
1	1	224	ILE
1	1	225	VAL
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	252	ARG
1	1	262	SER
1	1	265	THR
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
3	3	21	SER
3	3	23	CYS
3	3	25	LEU
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

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Mol	Chain	Res	Type
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
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
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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	95	ASN
1	1	108	GLN
1	1	140	HIS

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Mol	Chain	Res	Type
1	1	159	ASN
1	1	204	ASN
1	1	215	ASN
1	1	261	HIS
1	1	263	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
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
3	3	205	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	JEN	1	700	-	23,23,23	0.85	1 (4%)	30,31,31	0.89	1 (3%)

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	JEN	1	700	-	-	4/10/20/20	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	700	JEN	C8-C7	-2.68	1.34	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	700	JEN	C7-C6-N5	-2.00	120.91	123.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	700	JEN	N4-C3-O2-C1

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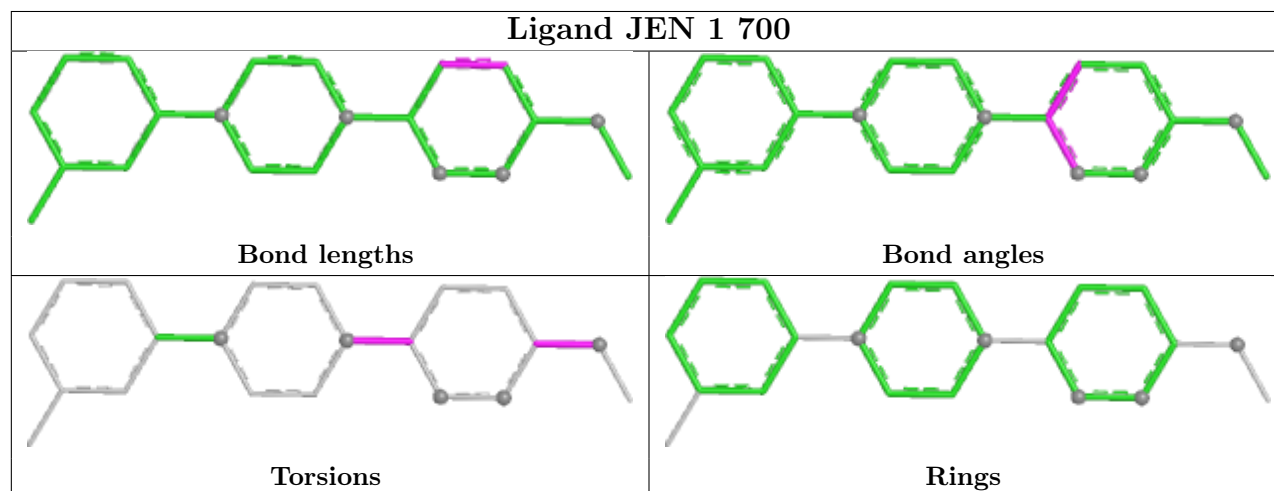
Mol	Chain	Res	Type	Atoms
5	1	700	JEN	C8-C3-O2-C1
5	1	700	JEN	N5-C6-N9-C10
5	1	700	JEN	C7-C6-N9-C10

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	700	JEN	9	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	118:TYR	C	119:VAL	N	1.16

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.