



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:45 AM UTC

PDB ID : 2HWD / pdb_00002hwd
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

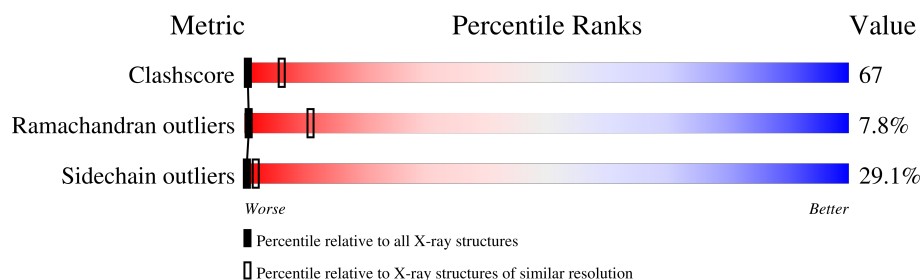
1 Overall quality at a glance

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	W91	1	700	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6246 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			

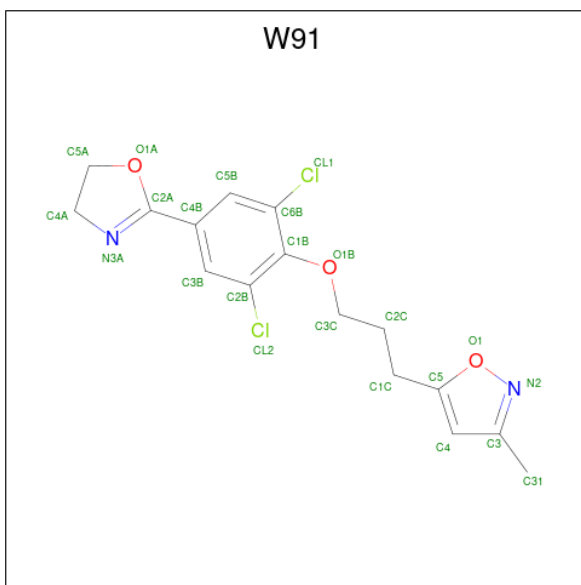
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

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-(3-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)PROPYL)-3-METHYL ISOXAZOLE (CCD ID: W91) (formula: C₁₆H₁₆Cl₂N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1	1	Total 23	C 16	Cl 2	N 2	O 3	0	0

A186	T122	M61	G1
G187	A123	V62	L2
I188	M124	G63	P3
T190	T125	M64	V4
C191	T126	V65	Y5
M192	L127	S66	I6
I193	K128	M67	T7
Q194	L129	V68	P8
T195	L130	T69	G9
M196	L131	V70	S10
L197	A132	Q71	G11
V198	T133	L72	Q12
V199	T134	G73	F13
P200	P135	M74	M14
P201	P136	Q75	T15
S202		T76	T16
T203	F140	G77	D17
T204	P141	M78	D18
Q205	T142	A79	M19
T206	T143	Q80	Q20
A207	R144	K81	S21
D208	K145	V82	P22
M209	D146	F83	C23
L210	M148	S84	A24
C211	L149		L25
F212		V87	P26
V213	H152	D88	W27
S214	V153	I89	Y28
K215	V154	T90	H29
C216	M155	S91	P30
K217	D156	T92	T31
D218	V157	P93	K32
F219	G158	A95	E33
C220	L159	T96	I34
L221	Q160	T97	S35
R222	S161	L98	I36
M223	T162	T99	P37
A224	I163	G100	G38
R225	L164	E101	C39
D226	S165	I102	V40
T227	V166	A103	K41
D228	V167	S104	M42
L229	P168	V105	L43
T230	W169	V106	I44
I231		T107	E45
Q232	A172	H108	M46
S233	H173	W109	C47
G234	S174	T110	Q48
P235	F175	G111	V49
T236	R176	S112	D50
E237	L177	L113	L52
Q238	T178	R114	I53
	A179	F115	P54
	D180	S116	V55
	M181	F117	M56
	K182	M118	S57
	Y183	F119	V58
	S184	C120	G59
	M185	C121	M60

GLY	ALA	GLY	VAL	SER	ARG	GLN	VAL	GLY	THR	HTS	SER	THR	GLN	ASN	SER	VAL	SER	SER	GLN	ASN	SER	LEU	ASN	Y26	F77	F28	T29	N30	Y31	F32	K33	S37	S38	G39	A40	S41	R42	L43	D44
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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	6246	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: W91

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	31/2322 (1.3%)	3.26	308/3162 (9.7%)
2	2	1.23	2/2033 (0.1%)	3.12	290/2770 (10.5%)
3	3	1.22	0/1878	3.04	224/2570 (8.7%)
4	4	1.46	0/154	3.75	34/206 (16.5%)
All	All	1.39	33/6387 (0.5%)	3.16	856/8708 (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	6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	213	VAL	C-N	19.66	1.61	1.33
1	1	98	LYS	C-N	-13.05	1.15	1.33
1	1	145	TYR	C-N	12.48	1.48	1.33
1	1	118	TYR	C-N	-12.01	1.19	1.33
1	1	223	ARG	C-N	11.82	1.49	1.33
1	1	146	MET	C-N	-9.47	1.20	1.33
1	1	150	PRO	C-N	-9.40	1.25	1.33
1	1	218	GLY	CA-C	-7.88	1.40	1.51
1	1	144	GLN	C-N	7.75	1.44	1.33
1	1	149	PRO	CA-C	-7.69	1.45	1.52
1	1	184	ILE	N-CA	-7.64	1.37	1.46
1	1	101	ILE	N-CA	-7.26	1.37	1.46
1	1	219	THR	N-CA	-7.08	1.37	1.46
1	1	124	GLU	N-CA	6.91	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	123	SER	CA-C	6.86	1.60	1.52
1	1	196	PHE	N-CA	6.75	1.53	1.46
1	1	148	VAL	CA-C	-6.72	1.45	1.52
1	1	100	LYS	C-N	-6.65	1.24	1.33
1	1	214	THR	CA-C	-6.02	1.45	1.53
1	1	123	SER	N-CA	5.83	1.53	1.45
1	1	217	MET	CA-C	-5.83	1.47	1.53
1	1	211	SER	C-N	-5.82	1.25	1.33
1	1	101	ILE	C-N	-5.69	1.25	1.33
1	1	90	ASN	N-CA	5.51	1.53	1.46
2	2	58	THR	CA-CB	5.42	1.62	1.53
1	1	218	GLY	N-CA	-5.37	1.37	1.45
1	1	102	THR	CA-C	-5.35	1.45	1.52
1	1	99	TRP	NE1-CE2	-5.34	1.31	1.37
1	1	102	THR	N-CA	-5.33	1.39	1.46
1	1	182	PHE	C-N	-5.20	1.26	1.33
1	1	181	ARG	C-N	-5.07	1.26	1.33
1	1	101	ILE	CA-CB	-5.04	1.47	1.54
2	2	127	ILE	CA-CB	5.01	1.60	1.54

All (856) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-39.27	77.72	123.27
1	1	150	PRO	CA-C-N	-31.02	87.55	120.43
1	1	150	PRO	C-N-CA	-31.02	87.55	120.43
2	2	62	ARG	CD-NE-CZ	24.22	158.31	124.40
1	1	146	MET	O-C-N	20.67	143.93	123.46
1	1	98	LYS	CA-C-N	18.47	156.83	121.54
1	1	98	LYS	C-N-CA	18.47	156.83	121.54
1	1	218	GLY	O-C-N	16.52	144.18	122.70
1	1	164	GLN	OE1-CD-NE2	-16.45	106.16	122.60
1	1	187	LEU	CA-C-O	-15.46	102.68	122.63
3	3	222	ARG	CD-NE-CZ	15.29	145.81	124.40
2	2	72	ASN	OD1-CG-ND2	14.95	137.55	122.60
1	1	211	SER	CA-C-N	-14.87	95.20	121.97
1	1	211	SER	C-N-CA	-14.87	95.20	121.97
1	1	151	GLY	N-CA-C	-14.53	90.69	111.03
3	3	235	PRO	CA-C-N	14.36	141.03	122.93
3	3	235	PRO	C-N-CA	14.36	141.03	122.93
1	1	68	GLU	CB-CG-CD	14.25	136.83	112.60
3	3	218	ASP	CA-CB-CG	-13.85	98.75	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	213	VAL	CA-C-N	-13.82	102.58	123.17
1	1	213	VAL	C-N-CA	-13.82	102.58	123.17
2	2	196	ASN	OD1-CG-ND2	13.76	136.36	122.60
3	3	212	PHE	CA-CB-CG	13.58	127.38	113.80
2	2	218	ASN	CA-CB-CG	13.35	125.94	112.60
1	1	214	THR	CB-CA-C	-13.33	88.58	111.23
3	3	203	THR	O-C-N	13.14	131.21	121.88
1	1	274	VAL	N-CA-CB	13.12	125.38	110.82
2	2	187	PRO	CB-CA-C	13.10	128.15	111.64
1	1	281	ARG	CA-CB-CG	13.06	140.22	114.10
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	12.58	145.57	121.54
2	2	154	ARG	C-N-CA	12.58	145.57	121.54
1	1	211	SER	CA-C-O	-12.44	107.11	121.66
3	3	64	ASN	OD1-CG-ND2	11.98	134.58	122.60
2	2	169	ASP	CA-CB-CG	11.78	124.38	112.60
3	3	144	ARG	CD-NE-CZ	11.74	140.84	124.40
3	3	232	GLN	N-CA-CB	11.60	126.23	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	11.31	136.76	123.30
2	2	106	TYR	CA-C-N	11.25	138.64	122.77
2	2	106	TYR	C-N-CA	11.25	138.64	122.77
2	2	216	ARG	NE-CZ-NH2	-11.07	109.23	119.20
1	1	10	VAL	CB-CA-C	10.96	120.71	111.06
2	2	241	PRO	CA-C-N	10.86	141.52	121.97
2	2	241	PRO	C-N-CA	10.86	141.52	121.97
1	1	134	ARG	NE-CZ-NH1	10.79	132.29	121.50
3	3	92	THR	CB-CA-C	10.79	131.43	110.17
1	1	100	LYS	O-C-N	10.74	135.46	123.22
1	1	61	THR	CA-CB-OG1	-10.72	93.53	109.60
1	1	214	THR	N-CA-CB	10.67	126.83	111.25
1	1	172	PHE	CA-C-O	-10.61	108.90	120.36
1	1	199	GLY	O-C-N	10.61	132.83	123.60
1	1	213	VAL	O-C-N	10.59	134.13	122.06
3	3	73	GLY	CA-C-O	10.59	132.70	121.90
1	1	77	VAL	O-C-N	10.55	132.64	121.78
1	1	227	GLU	CB-CG-CD	10.52	130.48	112.60
3	3	207	ALA	O-C-N	10.51	134.67	123.42
3	3	76	THR	O-C-N	10.40	132.78	122.07
1	1	255	ARG	CD-NE-CZ	10.39	138.94	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	57	ASN	CB-CG-ND2	-10.33	100.90	116.40
3	3	64	ASN	CA-CB-CG	-10.32	102.28	112.60
2	2	130	HIS	CA-CB-CG	-10.31	103.49	113.80
1	1	13	GLU	O-C-N	10.30	132.91	122.30
1	1	11	LEU	O-C-N	10.27	136.52	122.46
1	1	54	ARG	CG-CD-NE	10.21	134.47	112.00
3	3	56	ASN	CA-C-N	10.18	140.99	121.54
3	3	56	ASN	C-N-CA	10.18	140.99	121.54
2	2	240	VAL	CB-CA-C	10.14	120.72	111.08
3	3	67	MET	N-CA-CB	-10.13	93.37	110.49
1	1	280	ARG	NE-CZ-NH2	-10.12	110.09	119.20
2	2	17	THR	CB-CA-C	10.06	127.91	109.70
2	2	16	ILE	CA-C-O	-10.02	109.74	120.76
2	2	158	GLN	OE1-CD-NE2	9.93	132.53	122.60
2	2	237	SER	CA-C-O	9.91	130.86	119.27
4	4	30	ASN	CA-CB-CG	-9.89	102.71	112.60
3	3	53	ILE	N-CA-C	9.87	118.98	107.73
2	2	237	SER	N-CA-C	-9.82	101.05	113.23
3	3	58	VAL	N-CA-C	9.80	121.90	108.17
2	2	161	ASP	N-CA-CB	9.78	124.65	109.69
2	2	169	ASP	CA-C-O	9.73	131.56	119.11
3	3	232	GLN	O-C-N	9.70	134.00	122.46
2	2	248	PRO	N-CA-C	-9.69	95.80	111.21
2	2	12	ARG	CD-NE-CZ	9.64	137.90	124.40
4	4	28	ASN	OD1-CG-ND2	9.64	132.24	122.60
1	1	257	VAL	CB-CA-C	9.59	120.63	110.37
4	4	40	ALA	N-CA-C	-9.57	96.35	110.23
1	1	45	VAL	CB-CA-C	9.51	124.59	110.90
2	2	26	ASP	CA-CB-CG	9.45	122.05	112.60
1	1	10	VAL	CA-C-O	9.43	127.21	119.29
3	3	134	THR	CA-C-O	9.42	127.34	119.71
3	3	37	PRO	N-CA-CB	9.39	110.81	103.30
1	1	260	THR	CA-C-O	-9.35	108.57	119.98
2	2	57	ASP	N-CA-CB	-9.33	95.67	110.69
1	1	154	ILE	O-C-N	9.32	130.09	121.61
2	2	164	LEU	O-C-N	9.31	134.00	123.01
2	2	20	ASP	N-CA-C	-9.25	101.52	113.17
3	3	74	ASN	OD1-CG-ND2	9.24	131.84	122.60
1	1	188	SER	CA-C-O	-9.23	110.35	121.06
1	1	19	ASN	OD1-CG-ND2	9.17	131.77	122.60
3	3	227	THR	CA-C-O	9.14	131.93	121.87
4	4	44	ASP	CA-CB-CG	9.14	121.74	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	40	ALA	O-C-N	9.12	134.09	122.87
2	2	71	TRP	CB-CA-C	9.08	125.59	110.79
1	1	88	ASP	CA-C-O	9.06	129.99	120.30
1	1	206	SER	O-C-N	9.04	132.45	122.05
3	3	96	THR	CA-C-N	9.02	133.62	120.90
3	3	96	THR	C-N-CA	9.02	133.62	120.90
2	2	16	ILE	O-C-N	9.00	133.04	123.05
3	3	155	TRP	CA-C-O	-8.97	110.71	120.30
2	2	20	ASP	CA-C-O	8.96	129.83	119.35
2	2	61	ASN	CB-CA-C	8.94	125.98	112.03
2	2	234	THR	CA-C-O	8.93	132.34	121.89
3	3	114	ARG	N-CA-C	8.92	122.95	108.41
2	2	182	ASN	N-CA-C	-8.92	100.23	113.61
4	4	42	ARG	CD-NE-CZ	8.92	136.88	124.40
2	2	49	ALA	CA-C-O	-8.90	107.78	120.51
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
4	4	37	SER	O-C-N	8.86	134.29	123.13
2	2	107	THR	CA-CB-OG1	-8.84	96.34	109.60
2	2	40	HIS	CA-CB-CG	-8.81	104.99	113.80
2	2	81	LYS	O-C-N	8.80	133.65	123.27
2	2	57	ASP	CA-C-O	-8.79	111.39	120.71
2	2	162	ALA	CB-CA-C	8.78	125.40	110.56
1	1	12	ASN	CA-CB-CG	8.77	121.37	112.60
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	54	PRO	CA-C-O	-8.76	110.68	120.92
3	3	108	HIS	CA-CB-CG	8.75	122.55	113.80
3	3	45	GLU	CB-CG-CD	8.69	127.37	112.60
3	3	203	THR	CA-C-O	-8.69	111.33	120.28
1	1	159	ASN	CA-CB-CG	8.66	121.26	112.60
2	2	101	LEU	CA-C-O	8.64	130.31	120.54
3	3	53	ILE	O-C-N	8.63	129.15	121.12
1	1	213	VAL	N-CA-C	-8.57	99.54	111.89
2	2	147	THR	N-CA-CB	8.57	124.01	110.73
3	3	210	LEU	CA-C-N	-8.56	109.27	122.62
3	3	210	LEU	C-N-CA	-8.56	109.27	122.62
2	2	63	PHE	N-CA-C	8.56	123.41	108.52
2	2	192	ASN	OD1-CG-ND2	8.51	131.11	122.60
3	3	191	CYS	CA-C-O	-8.51	110.39	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	80	SER	CA-C-O	8.48	130.58	120.92
1	1	70	PHE	N-CA-C	-8.44	100.71	112.45
2	2	92	PHE	CA-CB-CG	8.43	122.23	113.80
1	1	25	HIS	CA-C-O	-8.43	111.86	121.81
3	3	26	PRO	O-C-N	8.41	133.41	123.06
3	3	226	ASP	CA-CB-CG	8.40	121.00	112.60
3	3	218	ASP	N-CA-CB	-8.37	97.93	110.07
2	2	196	ASN	N-CA-CB	-8.36	98.93	110.38
2	2	62	ARG	NH1-CZ-NH2	-8.36	108.44	119.30
4	4	38	SER	O-C-N	8.34	133.69	122.59
3	3	205	GLN	OE1-CD-NE2	8.33	130.93	122.60
1	1	204	ASN	CA-C-O	8.33	130.28	120.70
2	2	196	ASN	CA-CB-CG	-8.30	104.30	112.60
2	2	135	ALA	CA-C-O	8.29	129.52	119.49
2	2	189	GLN	CA-CB-CG	8.26	130.63	114.10
2	2	220	TRP	CA-C-O	8.23	129.93	120.80
1	1	35	ASP	CA-C-O	-8.20	112.33	121.51
1	1	49	ASP	CA-CB-CG	-8.19	104.41	112.60
2	2	181	GLY	N-CA-C	-8.19	103.79	114.85
1	1	86	TYR	CB-CA-C	8.17	122.75	109.02
3	3	32	LYS	O-C-N	8.17	132.32	122.68
3	3	95	ALA	CA-C-O	-8.16	108.84	120.51
3	3	206	THR	N-CA-C	-8.16	96.61	109.50
2	2	83	PRO	CB-CA-C	8.14	125.86	112.26
2	2	147	THR	O-C-N	8.13	131.92	122.25
2	2	28	VAL	CA-CB-CG1	8.12	124.21	110.40
1	1	252	ARG	O-C-N	8.12	127.88	121.55
1	1	59	SER	N-CA-CB	-8.11	96.78	110.49
2	2	31	ALA	N-CA-CB	8.07	123.83	111.56
1	1	46	GLN	O-C-N	8.06	130.59	121.32
1	1	270	GLU	N-CA-CB	8.06	122.62	109.88
2	2	218	ASN	CB-CG-ND2	8.02	128.43	116.40
1	1	102	THR	O-C-N	8.00	133.23	122.59
2	2	203	VAL	N-CA-CB	-8.00	100.01	111.21
1	1	12	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	1	5	ASN	CA-CB-CG	7.95	120.55	112.60
2	2	91	ILE	N-CA-CB	7.95	124.35	111.23
1	1	25	HIS	O-C-N	7.95	131.91	122.85
1	1	251	PRO	CA-C-O	7.94	130.77	121.56
2	2	257	ARG	NE-CZ-NH2	-7.92	112.07	119.20
2	2	188	HIS	N-CA-C	7.91	118.69	108.24
2	2	183	LEU	O-C-N	7.90	133.02	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	227	THR	N-CA-C	7.90	120.78	110.43
2	2	160	ARG	N-CA-CB	-7.88	98.33	111.57
1	1	101	ILE	N-CA-CB	-7.88	98.22	111.23
2	2	161	ASP	O-C-N	7.87	132.71	122.95
3	3	90	THR	N-CA-CB	7.87	122.95	111.54
2	2	50	ILE	CA-CB-CG2	7.86	123.87	110.50
1	1	234	VAL	CA-C-O	7.85	128.99	120.43
3	3	36	ILE	N-CA-CB	7.84	122.18	111.21
3	3	50	ASP	CA-C-O	7.83	129.57	120.49
4	4	38	SER	CA-C-O	-7.83	109.31	120.51
1	1	28	SER	N-CA-C	7.81	122.14	109.40
2	2	156	VAL	CA-C-N	7.80	136.44	121.54
2	2	156	VAL	C-N-CA	7.80	136.44	121.54
2	2	156	VAL	CA-C-O	7.79	130.52	120.78
3	3	199	VAL	O-C-N	7.78	129.97	121.10
4	4	43	LEU	N-CA-C	7.77	122.66	112.72
1	1	13	GLU	CA-C-O	-7.76	112.67	119.97
1	1	168	ASN	CA-C-N	-7.76	112.30	123.00
1	1	168	ASN	C-N-CA	-7.76	112.30	123.00
3	3	42	ASN	OD1-CG-ND2	7.74	130.34	122.60
2	2	29	ALA	N-CA-CB	7.73	123.45	110.69
3	3	233	SER	CA-C-O	7.71	131.23	122.37
3	3	168	PRO	CA-C-N	-7.69	112.85	122.84
3	3	168	PRO	C-N-CA	-7.69	112.85	122.84
1	1	255	ARG	CA-C-O	-7.68	111.86	120.54
1	1	196	PHE	CA-C-O	-7.68	113.24	121.38
1	1	285	THR	CA-C-O	-7.66	111.44	120.10
2	2	72	ASN	CA-CB-CG	-7.66	104.94	112.60
2	2	119	GLN	OE1-CD-NE2	7.64	130.24	122.60
3	3	55	VAL	CB-CA-C	7.63	123.81	111.29
2	2	160	ARG	N-CA-C	7.62	119.72	108.14
1	1	227	GLU	CG-CD-OE1	7.62	135.91	118.40
3	3	35	SER	CA-C-O	-7.61	112.06	120.81
1	1	275	THR	OG1-CB-CG2	7.59	124.49	109.30
2	2	182	ASN	O-C-N	7.58	131.15	122.20
1	1	44	ASN	CA-CB-CG	-7.58	105.02	112.60
2	2	161	ASP	CA-CB-CG	-7.56	105.04	112.60
1	1	134	ARG	NH1-CZ-NH2	-7.55	109.48	119.30
2	2	111	GLN	CB-CG-CD	7.55	125.43	112.60
2	2	12	ARG	CG-CD-NE	7.53	128.57	112.00
2	2	32	VAL	O-C-N	7.53	131.41	123.05
1	1	38	GLU	CB-CG-CD	7.52	125.38	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	224	ILE	CB-CA-C	7.50	120.55	110.42
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
2	2	169	ASP	N-CA-C	-7.49	104.11	113.18
1	1	202	GLY	CA-C-N	7.49	136.00	121.18
1	1	202	GLY	C-N-CA	7.49	136.00	121.18
1	1	34	LEU	CA-C-O	-7.47	112.77	120.54
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
4	4	32	PHE	C-N-CA	7.45	131.14	120.79
3	3	57	ASN	CA-CB-CG	-7.42	105.18	112.60
1	1	70	PHE	O-C-N	7.42	133.18	122.28
2	2	233	GLU	CA-C-O	7.42	127.22	119.51
3	3	160	GLN	OE1-CD-NE2	-7.39	115.21	122.60
3	3	185	MET	N-CA-CB	7.39	121.09	109.71
1	1	49	ASP	N-CA-C	7.37	119.10	111.14
1	1	159	ASN	CA-C-O	-7.37	112.44	121.58
1	1	271	THR	CA-CB-OG1	-7.36	98.55	109.60
2	2	70	HIS	CA-C-N	-7.35	112.68	123.11
2	2	70	HIS	C-N-CA	-7.35	112.68	123.11
1	1	226	THR	N-CA-C	7.34	126.44	110.80
2	2	233	GLU	CG-CD-OE2	7.33	135.25	118.40
2	2	126	MET	CA-CB-CG	-7.32	99.47	114.10
1	1	8	ASP	CA-CB-CG	-7.31	105.29	112.60
3	3	89	ILE	CB-CA-C	-7.31	99.31	111.29
3	3	163	ILE	N-CA-C	-7.31	97.96	108.48
3	3	50	ASP	CA-CB-CG	7.28	119.88	112.60
1	1	16	VAL	CB-CA-C	7.27	122.29	111.31
1	1	5	ASN	N-CA-CB	7.26	122.84	110.50
2	2	86	LEU	CA-C-O	7.26	129.33	120.55
1	1	158	ARG	CD-NE-CZ	7.25	134.56	124.40
3	3	123	ALA	CA-C-O	-7.22	111.83	120.56
3	3	161	SER	CA-C-N	-7.21	111.63	122.74
3	3	161	SER	C-N-CA	-7.21	111.63	122.74
1	1	31	ALA	O-C-N	7.21	128.13	120.85
1	1	173	TRP	CA-CB-CG	7.20	127.28	113.60
2	2	155	ASP	CA-CB-CG	7.19	119.79	112.60
3	3	201	PRO	N-CA-C	7.19	127.28	112.47
3	3	218	ASP	CA-C-N	7.17	135.23	121.54
3	3	218	ASP	C-N-CA	7.17	135.23	121.54
3	3	161	SER	CB-CA-C	-7.16	96.17	110.42
2	2	78	TRP	CA-CB-CG	7.15	127.18	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	52	LYS	CG-CD-CE	7.14	127.73	111.30
3	3	67	MET	CA-C-N	7.14	133.46	122.24
3	3	67	MET	C-N-CA	7.14	133.46	122.24
1	1	23	SER	CA-C-O	7.14	129.86	121.58
1	1	164	GLN	CG-CD-OE1	7.13	135.06	120.80
1	1	233	VAL	CB-CA-C	-7.13	99.60	111.29
1	1	231	LEU	CA-CB-CG	7.12	141.24	116.30
3	3	70	VAL	CA-C-N	-7.12	112.14	122.19
3	3	70	VAL	C-N-CA	-7.12	112.14	122.19
3	3	216	CYS	CA-C-O	-7.12	113.11	121.44
2	2	147	THR	N-CA-C	-7.12	103.70	112.88
3	3	237	GLU	CA-C-O	7.09	130.65	120.51
2	2	220	TRP	CA-C-N	7.08	133.65	122.74
2	2	220	TRP	C-N-CA	7.08	133.65	122.74
2	2	256	ALA	CA-C-O	-7.08	113.84	121.56
2	2	114	ALA	CA-C-O	-7.08	110.39	120.51
3	3	114	ARG	NE-CZ-NH1	-7.08	114.42	121.50
1	1	231	LEU	CB-CA-C	7.07	121.37	109.84
1	1	163	TRP	N-CA-C	-7.07	104.66	112.72
1	1	55	TYR	O-C-N	7.07	131.99	122.59
1	1	82	ILE	CB-CA-C	-7.05	99.72	111.29
2	2	176	ASP	N-CA-C	-7.03	104.34	114.12
1	1	134	ARG	CD-NE-CZ	7.02	134.22	124.40
2	2	127	ILE	O-C-N	7.02	129.10	121.10
2	2	168	SER	CA-C-O	7.02	128.29	120.43
3	3	101	GLU	CA-C-O	7.01	128.06	120.20
1	1	190	ALA	CA-C-O	-6.99	113.47	121.72
2	2	52	LYS	CA-CB-CG	6.99	128.08	114.10
2	2	205	TYR	CA-C-O	-6.98	113.12	120.58
1	1	121	PHE	CB-CA-C	-6.97	98.03	110.03
2	2	134	SER	CA-C-O	6.97	128.94	120.92
3	3	201	PRO	CA-C-N	-6.96	112.12	122.36
3	3	201	PRO	C-N-CA	-6.96	112.12	122.36
1	1	61	THR	CB-CA-C	6.95	121.24	109.50
3	3	210	LEU	CA-C-O	-6.94	113.09	121.28
2	2	67	GLU	CA-C-O	-6.94	113.14	121.05
3	3	218	ASP	CA-C-O	6.94	127.85	120.70
2	2	82	LEU	N-CA-C	6.93	125.13	109.81
2	2	237	SER	CB-CA-C	6.92	123.59	109.55
4	4	28	ASN	CA-C-N	-6.92	109.52	121.97
4	4	28	ASN	C-N-CA	-6.92	109.52	121.97
1	1	224	ILE	CB-CG1-CD1	-6.91	99.29	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	43	LEU	O-C-N	6.90	130.58	122.09
2	2	70	HIS	CA-CB-CG	-6.90	106.90	113.80
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	287	ALA	CA-C-O	-6.88	109.11	120.80
2	2	190	PHE	CA-CB-CG	6.88	120.67	113.80
3	3	70	VAL	O-C-N	6.87	129.16	122.97
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
1	1	138	ILE	N-CA-C	6.87	122.41	113.07
3	3	225	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	1	152	ALA	N-CA-CB	-6.86	103.90	111.10
2	2	126	MET	CA-C-O	-6.86	113.26	121.56
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
1	1	184	ILE	N-CA-CB	-6.85	101.61	111.21
3	3	160	GLN	O-C-N	6.85	131.70	122.59
1	1	283	THR	O-C-N	6.82	131.18	123.27
3	3	160	GLN	N-CA-CB	6.81	122.00	110.49
2	2	87	LYS	CB-CG-CD	6.80	126.95	111.30
3	3	146	ASP	CB-CG-OD2	-6.80	102.77	118.40
3	3	15	THR	CB-CA-C	6.79	123.45	110.27
1	1	248	ALA	CA-C-N	6.78	133.11	122.94
1	1	248	ALA	C-N-CA	6.78	133.11	122.94
1	1	78	HIS	CA-CB-CG	-6.76	107.03	113.80
3	3	234	GLY	O-C-N	6.76	128.53	121.77
2	2	119	GLN	CB-CA-C	6.74	121.45	109.65
1	1	71	LEU	CA-C-O	-6.74	112.41	120.56
1	1	275	THR	CA-CB-OG1	-6.74	99.50	109.60
1	1	179	PHE	O-C-N	6.73	126.90	121.38
2	2	80	TRP	N-CA-CB	6.73	123.17	111.00
3	3	71	GLN	OE1-CD-NE2	6.72	129.32	122.60
2	2	198	SER	CB-CA-C	-6.72	97.27	113.19
3	3	89	ILE	CA-C-O	-6.72	112.38	120.78
2	2	171	SER	CA-C-N	6.69	131.41	120.63
2	2	171	SER	C-N-CA	6.69	131.41	120.63
3	3	90	THR	N-CA-C	-6.69	102.32	111.56
1	1	45	VAL	O-C-N	6.68	130.12	122.97
3	3	58	VAL	CA-C-O	6.68	127.56	120.48
3	3	203	THR	N-CA-C	-6.67	97.54	108.82
1	1	63	ASP	CA-C-O	-6.67	114.03	120.90
3	3	65	VAL	N-CA-CB	6.67	120.08	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	64	GLU	CA-CB-CG	6.66	127.42	114.10
2	2	31	ALA	O-C-N	6.66	130.05	123.46
2	2	150	GLY	O-C-N	6.66	131.35	122.70
2	2	177	GLY	CA-C-N	6.65	131.80	121.76
2	2	177	GLY	C-N-CA	6.65	131.80	121.76
3	3	147	ALA	CA-C-N	6.65	131.23	120.60
3	3	147	ALA	C-N-CA	6.65	131.23	120.60
2	2	83	PRO	CA-C-N	6.64	135.79	121.64
2	2	83	PRO	C-N-CA	6.64	135.79	121.64
1	1	55	TYR	CA-C-N	-6.64	113.55	122.98
1	1	55	TYR	C-N-CA	-6.64	113.55	122.98
1	1	164	GLN	N-CA-C	-6.64	104.21	112.90
2	2	158	GLN	CB-CG-CD	-6.63	101.34	112.60
3	3	128	LYS	CB-CA-C	-6.62	102.74	111.42
3	3	206	THR	CA-CB-OG1	-6.62	99.67	109.60
1	1	53	THR	N-CA-CB	-6.62	101.31	110.38
2	2	155	ASP	N-CA-CB	6.62	121.67	110.49
1	1	268	MET	O-C-N	6.60	128.91	121.32
1	1	121	PHE	CA-CB-CG	6.60	120.40	113.80
1	1	281	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	1	121	PHE	N-CA-C	6.58	118.53	108.07
3	3	94	LEU	CA-C-O	-6.58	111.10	120.51
3	3	87	VAL	N-CA-C	6.55	121.21	112.04
3	3	165	LEU	O-C-N	6.55	131.01	123.29
2	2	232	SER	N-CA-CB	6.54	121.64	110.65
1	1	246	THR	N-CA-C	6.54	120.72	110.32
2	2	168	SER	CA-C-N	6.54	134.33	121.58
2	2	168	SER	C-N-CA	6.54	134.33	121.58
1	1	102	THR	CB-CA-C	-6.53	97.42	110.42
1	1	52	GLU	O-C-N	6.52	130.66	122.84
1	1	132	ALA	CA-C-O	6.51	127.72	120.43
3	3	169	TRP	CB-CA-C	6.51	121.20	110.78
1	1	62	ARG	N-CA-C	-6.51	103.67	112.26
3	3	88	ASP	CA-CB-CG	6.51	119.11	112.60
2	2	68	SER	CA-CB-OG	6.51	124.12	111.10
1	1	52	GLU	CA-C-N	6.50	133.28	121.06
1	1	52	GLU	C-N-CA	6.50	133.28	121.06
1	1	270	GLU	O-C-N	6.50	131.32	122.48
2	2	202	ILE	CA-C-O	-6.50	113.39	120.67
3	3	10	SER	CB-CA-C	6.49	120.03	109.90
2	2	161	ASP	CB-CA-C	-6.49	99.78	109.90
3	3	15	THR	N-CA-CB	-6.49	99.00	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	56	ASN	CA-CB-CG	-6.48	106.12	112.60
3	3	70	VAL	CA-C-O	-6.47	114.46	120.22
1	1	280	ARG	NH1-CZ-NH2	6.47	127.71	119.30
3	3	206	THR	OG1-CB-CG2	6.46	122.23	109.30
1	1	175	HIS	N-CA-CB	-6.46	99.58	110.49
2	2	180	LEU	CA-C-O	-6.46	113.92	120.96
3	3	72	LEU	N-CA-C	-6.43	98.74	108.96
3	3	16	THR	CA-CB-CG2	6.42	121.41	110.50
2	2	103	ARG	CD-NE-CZ	6.42	133.38	124.40
1	1	204	ASN	N-CA-CB	6.42	119.65	109.51
1	1	234	VAL	CB-CA-C	6.41	120.41	110.28
1	1	201	ASP	CA-C-N	6.40	129.65	120.56
1	1	201	ASP	C-N-CA	6.40	129.65	120.56
2	2	94	GLU	CA-C-O	6.40	127.25	119.64
2	2	54	THR	N-CA-CB	6.40	120.72	110.16
3	3	64	ASN	CB-CG-ND2	-6.40	106.80	116.40
3	3	106	TYR	CA-C-O	-6.40	113.96	121.44
1	1	180	PRO	CB-CA-C	6.39	119.86	110.85
2	2	206	VAL	CB-CA-C	6.39	120.35	110.83
2	2	50	ILE	CB-CA-C	6.38	121.75	111.29
2	2	157	SER	CA-C-N	-6.37	112.11	122.81
2	2	157	SER	C-N-CA	-6.37	112.11	122.81
1	1	20	ILE	O-C-N	6.37	132.12	122.76
2	2	228	SER	CA-C-N	6.37	126.40	119.90
2	2	228	SER	C-N-CA	6.37	126.40	119.90
1	1	201	ASP	O-C-N	6.37	129.41	122.15
2	2	176	ASP	CB-CA-C	6.36	120.07	109.38
3	3	226	ASP	OD1-CG-OD2	-6.36	107.63	122.90
1	1	263	HIS	O-C-N	6.36	129.95	122.00
2	2	91	ILE	CA-C-O	-6.36	112.84	120.78
2	2	152	ALA	N-CA-CB	-6.35	100.11	110.14
1	1	66	SER	O-C-N	6.33	130.84	123.30
2	2	238	ASN	O-C-N	6.33	130.52	122.93
1	1	49	ASP	CA-C-N	6.32	131.42	120.68
1	1	49	ASP	C-N-CA	6.32	131.42	120.68
1	1	39	THR	O-C-N	6.32	131.18	122.46
2	2	228	SER	O-C-N	6.32	128.37	121.36
1	1	5	ASN	O-C-N	6.31	133.10	123.00
2	2	68	SER	N-CA-CB	6.31	120.02	110.42
1	1	94	ILE	O-C-N	6.31	130.20	123.00
4	4	40	ALA	N-CA-CB	6.31	119.36	109.83
2	2	183	LEU	CA-C-O	-6.31	111.62	119.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	235	PRO	CA-C-O	6.31	135.34	120.20
1	1	201	ASP	CA-C-O	-6.30	113.74	120.42
3	3	77	GLY	CA-C-O	6.30	130.75	122.75
1	1	285	THR	CA-CB-OG1	-6.29	100.16	109.60
2	2	81	LYS	CA-CB-CG	6.29	126.68	114.10
2	2	183	LEU	N-CA-C	-6.28	104.88	112.54
4	4	42	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	1	174	GLN	CB-CG-CD	6.28	123.27	112.60
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	233	GLU	CG-CD-OE1	-6.28	103.97	118.40
1	1	19	ASN	CA-CB-CG	-6.27	106.33	112.60
1	1	211	SER	O-C-N	6.27	131.06	122.41
1	1	47	PRO	CB-CA-C	6.27	121.90	111.56
1	1	214	THR	N-CA-C	6.26	121.45	111.81
1	1	268	MET	CA-CB-CG	-6.26	101.58	114.10
3	3	148	MET	CG-SD-CE	6.26	114.67	100.90
2	2	161	ASP	CA-C-N	-6.25	112.64	122.65
2	2	161	ASP	C-N-CA	-6.25	112.64	122.65
1	1	155	PRO	CA-C-N	6.25	128.66	120.28
1	1	155	PRO	C-N-CA	6.25	128.66	120.28
1	1	66	SER	CA-CB-OG	-6.25	98.61	111.10
3	3	234	GLY	N-CA-C	-6.24	99.61	112.34
1	1	117	THR	CB-CA-C	-6.24	101.04	110.90
2	2	95	ASN	N-CA-C	-6.24	105.53	113.01
2	2	212	ASP	CA-C-N	6.23	130.76	121.72
2	2	212	ASP	C-N-CA	6.23	130.76	121.72
4	4	30	ASN	CB-CA-C	6.22	122.80	110.42
2	2	56	PRO	CA-C-O	6.22	128.12	121.03
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
3	3	100	GLY	O-C-N	6.21	128.28	122.13
3	3	134	THR	CB-CA-C	6.21	116.03	110.44
1	1	19	ASN	CB-CG-OD1	-6.21	108.38	120.80
1	1	114	GLU	CB-CG-CD	6.21	123.16	112.60
2	2	130	HIS	O-C-N	6.20	132.09	122.67
1	1	154	ILE	N-CA-C	-6.19	100.75	108.05
1	1	205	THR	OG1-CB-CG2	6.19	121.68	109.30
1	1	235	ILE	CA-C-O	6.19	127.78	120.72
4	4	44	ASP	CA-C-O	6.18	131.31	120.80
2	2	262	LYS	CB-CA-C	6.17	122.33	109.68
3	3	181	ASN	O-C-N	6.16	130.90	123.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	69	SER	N-CA-C	-6.12	105.45	113.17
1	1	189	ILE	CA-C-N	6.12	134.37	122.07
1	1	189	ILE	C-N-CA	6.12	134.37	122.07
1	1	161	PHE	N-CA-C	-6.11	97.79	110.80
2	2	225	ILE	CA-C-O	6.11	123.12	119.94
2	2	56	PRO	N-CA-C	-6.10	101.58	110.80
2	2	39	PRO	CB-CA-C	-6.10	103.59	111.46
3	3	71	GLN	O-C-N	6.10	130.17	123.22
2	2	95	ASN	OD1-CG-ND2	6.09	128.69	122.60
2	2	196	ASN	N-CA-C	6.09	117.90	110.41
3	3	4	VAL	O-C-N	6.09	129.49	122.97
2	2	128	PRO	CB-CA-C	6.08	118.95	110.98
3	3	123	ALA	O-C-N	6.08	129.31	122.32
2	2	236	SER	CA-C-N	6.08	132.35	121.66
2	2	236	SER	C-N-CA	6.08	132.35	121.66
3	3	26	PRO	N-CA-CB	6.08	108.98	103.33
1	1	131	ILE	N-CA-C	6.07	116.43	107.15
2	2	27	ASP	CA-C-O	-6.06	113.27	120.43
2	2	221	CYS	CA-C-O	6.06	127.05	120.32
1	1	117	THR	N-CA-CB	6.06	118.85	110.07
1	1	45	VAL	CA-C-O	-6.05	114.61	121.75
2	2	228	SER	N-CA-CB	6.05	118.84	110.01
1	1	94	ILE	N-CA-C	6.04	118.60	108.81
1	1	148	VAL	O-C-N	6.03	126.75	120.96
1	1	276	THR	O-C-N	6.03	130.47	123.17
1	1	122	ASP	N-CA-C	-6.02	101.62	110.52
2	2	70	HIS	CB-CA-C	-6.00	99.62	109.53
3	3	228	ASP	CB-CA-C	-5.99	99.61	110.56
1	1	237	THR	CA-CB-OG1	-5.98	100.63	109.60
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
1	1	60	GLN	N-CA-C	-5.98	99.16	108.90
3	3	56	ASN	OD1-CG-ND2	5.97	128.57	122.60
1	1	286	THR	CA-C-O	-5.96	113.71	120.32
1	1	129	PRO	CA-C-N	5.96	131.17	122.77
1	1	129	PRO	C-N-CA	5.96	131.17	122.77
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	233	VAL	CA-C-O	5.94	128.21	120.78
1	1	87	THR	CA-C-O	5.94	127.24	121.00
1	1	81	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	1	227	GLU	OE1-CD-OE2	-5.93	108.66	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	71	TRP	CA-C-O	5.93	126.80	120.46
2	2	173	LEU	CB-CA-C	5.93	119.99	110.09
2	2	155	ASP	O-C-N	5.92	130.47	122.59
2	2	209	VAL	CA-C-N	5.92	126.34	119.47
2	2	209	VAL	C-N-CA	5.92	126.34	119.47
2	2	114	ALA	N-CA-C	-5.92	98.20	110.80
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
3	3	181	ASN	OD1-CG-ND2	5.91	128.51	122.60
1	1	273	ASP	CA-C-O	-5.90	115.29	121.55
4	4	32	PHE	CA-CB-CG	-5.90	107.90	113.80
2	2	215	LEU	CA-C-O	-5.90	111.87	120.13
3	3	178	THR	N-CA-CB	5.89	119.37	110.30
1	1	236	THR	CB-CA-C	5.87	120.22	111.17
2	2	238	ASN	N-CA-CB	5.87	119.54	110.21
1	1	274	VAL	O-C-N	5.87	129.41	122.66
1	1	62	ARG	O-C-N	5.86	129.70	122.20
3	3	161	SER	O-C-N	5.85	130.37	122.59
1	1	163	TRP	CB-CA-C	5.85	120.59	110.94
3	3	73	GLY	N-CA-C	5.84	120.96	112.60
3	3	75	GLN	CA-C-N	5.84	128.03	120.44
3	3	75	GLN	C-N-CA	5.84	128.03	120.44
4	4	40	ALA	CA-C-O	-5.83	114.78	121.19
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
2	2	38	TRP	CA-C-N	5.83	125.76	119.76
2	2	38	TRP	C-N-CA	5.83	125.76	119.76
2	2	28	VAL	CB-CA-C	-5.82	101.75	111.29
1	1	273	ASP	CA-CB-CG	-5.81	106.79	112.60
3	3	198	VAL	O-C-N	5.81	129.07	123.14
2	2	239	ILE	CB-CA-C	5.80	119.48	110.83
1	1	260	THR	O-C-N	5.80	130.45	123.26
2	2	59	SER	CA-C-O	5.80	126.51	119.38
3	3	92	THR	N-CA-C	-5.80	96.99	109.81
1	1	63	ASP	O-C-N	5.79	128.29	122.03
3	3	222	ARG	NH1-CZ-NH2	-5.79	111.77	119.30
1	1	282	ASN	CA-C-O	5.79	126.66	120.70
1	1	10	VAL	N-CA-CB	-5.79	101.18	112.75
1	1	204	ASN	CB-CG-ND2	5.78	125.07	116.40
2	2	14	MET	CA-C-O	5.78	127.76	121.06
2	2	155	ASP	CB-CG-OD2	-5.78	105.12	118.40
3	3	191	CYS	O-C-N	5.78	130.32	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	205	THR	CA-CB-OG1	-5.77	100.94	109.60
1	1	220	ILE	CB-CA-C	-5.77	103.86	110.73
2	2	154	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	1	90	ASN	OD1-CG-ND2	-5.77	116.83	122.60
4	4	42	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	1	283	THR	CA-CB-OG1	-5.76	100.95	109.60
3	3	165	LEU	CA-C-O	-5.76	114.10	120.38
3	3	24	ALA	N-CA-CB	-5.76	102.03	110.26
1	1	143	MET	CA-C-O	-5.76	114.38	121.06
1	1	210	GLY	CA-C-O	5.75	126.23	121.05
2	2	197	ASN	CA-C-N	5.75	131.82	122.39
2	2	197	ASN	C-N-CA	5.75	131.82	122.39
2	2	62	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	1	36	ALA	CA-C-N	5.74	132.50	121.54
1	1	36	ALA	C-N-CA	5.74	132.50	121.54
1	1	68	GLU	CA-CB-CG	5.73	125.57	114.10
2	2	175	PHE	CA-CB-CG	5.73	119.53	113.80
1	1	68	GLU	CA-C-O	5.72	125.44	119.14
3	3	57	ASN	OD1-CG-ND2	5.72	128.32	122.60
2	2	176	ASP	CA-CB-CG	-5.72	106.88	112.60
2	2	157	SER	O-C-N	5.72	130.19	122.59
3	3	180	ASP	CB-CA-C	5.71	116.83	109.80
2	2	154	ARG	CG-CD-NE	5.71	124.55	112.00
3	3	155	TRP	O-C-N	5.71	129.89	123.27
1	1	259	TYR	CB-CA-C	-5.70	100.45	113.33
3	3	96	THR	N-CA-C	5.70	122.94	110.80
1	1	90	ASN	CB-CA-C	5.70	121.75	110.42
1	1	171	ILE	CB-CA-C	5.70	119.01	110.98
3	3	120	CYS	CA-CB-SG	-5.69	101.31	114.40
3	3	126	THR	O-C-N	5.69	129.76	123.33
3	3	71	GLN	N-CA-CB	5.68	119.54	110.16
2	2	241	PRO	O-C-N	-5.68	114.98	122.64
2	2	96	MET	CA-C-O	5.67	126.53	120.24
2	2	227	ILE	N-CA-CB	5.67	120.58	111.23
2	2	74	SER	O-C-N	5.67	128.89	122.20
1	1	266	ASN	O-C-N	5.66	130.12	122.59
3	3	162	THR	CB-CA-C	5.66	119.94	109.70
1	1	37	ALA	N-CA-CB	-5.66	100.93	110.49
1	1	158	ARG	NE-CZ-NH1	5.65	127.15	121.50
2	2	12	ARG	CA-C-O	-5.65	113.97	120.24
2	2	41	TYR	O-C-N	5.64	129.34	122.96
2	2	90	GLY	CA-C-O	5.64	130.38	120.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	135	PRO	CA-C-O	5.64	128.73	120.56
3	3	156	ASP	CA-CB-CG	5.64	118.24	112.60
1	1	173	TRP	O-C-N	5.63	130.23	123.36
3	3	185	MET	O-C-N	5.63	130.05	122.96
1	1	120	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	1	43	SER	CA-C-O	5.62	128.05	121.87
2	2	67	GLU	OE1-CD-OE2	5.62	136.38	122.90
3	3	112	SER	CA-C-N	5.62	131.79	121.85
3	3	112	SER	C-N-CA	5.62	131.79	121.85
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
1	1	281	ARG	N-CA-CB	-5.61	101.88	110.85
2	2	84	ASP	CA-C-O	-5.61	113.16	120.00
3	3	27	TRP	CA-C-O	-5.60	114.03	120.98
1	1	276	THR	CA-CB-OG1	-5.60	101.20	109.60
3	3	172	ALA	N-CA-C	-5.60	102.99	111.56
1	1	72	GLY	CA-C-N	5.60	130.70	121.86
1	1	72	GLY	C-N-CA	5.60	130.70	121.86
2	2	160	ARG	CG-CD-NE	5.60	124.31	112.00
3	3	204	PRO	CA-C-O	-5.59	114.96	121.95
1	1	71	LEU	CB-CA-C	5.59	121.48	111.03
1	1	70	PHE	N-CA-CB	5.58	118.58	110.26
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	146	ASP	N-CA-CB	5.57	119.90	110.49
1	1	250	CYS	CA-C-N	5.57	125.51	119.78
1	1	250	CYS	C-N-CA	5.57	125.51	119.78
2	2	135	ALA	N-CA-CB	-5.57	100.86	110.32
3	3	66	SER	CA-C-O	5.57	128.47	120.51
3	3	46	MET	CA-C-O	5.56	126.38	120.10
1	1	184	ILE	N-CA-C	5.56	120.88	108.88
2	2	131	GLN	OE1-CD-NE2	-5.54	117.06	122.60
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	145	TYR	O-C-N	5.53	129.66	123.19
1	1	157	LYS	CA-C-O	5.53	126.56	120.31
2	2	263	GLN	OE1-CD-NE2	5.53	128.12	122.60
3	3	55	VAL	O-C-N	5.53	129.48	122.57
1	1	282	ASN	OD1-CG-ND2	5.52	128.12	122.60
3	3	89	ILE	N-CA-C	5.52	120.83	109.34
1	1	153	PRO	N-CD-CG	-5.52	94.92	103.20
1	1	275	THR	CA-C-O	5.52	126.56	120.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	42	THR	O-C-N	5.52	130.11	123.16
3	3	81	LYS	N-CA-C	5.52	119.23	109.96
1	1	286	THR	O-C-N	5.52	129.76	123.31
2	2	75	SER	O-C-N	5.51	129.36	122.86
3	3	224	ALA	CA-C-O	5.50	127.32	121.16
3	3	167	VAL	N-CA-CB	5.50	118.91	111.21
1	1	10	VAL	N-CA-C	-5.50	107.46	112.96
3	3	124	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	1	76	CYS	CA-C-O	-5.49	114.66	120.92
1	1	111	ARG	CA-C-O	5.49	127.11	121.07
2	2	94	GLU	N-CA-C	-5.49	106.51	113.43
2	2	150	GLY	CA-C-O	-5.49	111.02	120.57
2	2	43	THR	CA-C-N	5.48	126.69	119.84
2	2	43	THR	C-N-CA	5.48	126.69	119.84
2	2	142	ALA	CA-C-N	5.48	127.55	120.64
2	2	142	ALA	C-N-CA	5.48	127.55	120.64
3	3	89	ILE	CB-CG1-CD1	-5.48	102.29	113.80
1	1	134	ARG	CA-C-O	5.47	125.83	119.32
2	2	256	ALA	O-C-N	5.47	129.32	122.86
1	1	251	PRO	N-CA-CB	5.47	108.11	103.35
2	2	73	GLY	N-CA-C	-5.45	106.30	115.62
1	1	86	TYR	N-CA-C	-5.45	107.28	114.31
1	1	270	GLU	CB-CA-C	-5.45	102.16	110.88
3	3	33	GLU	CG-CD-OE2	-5.45	105.87	118.40
2	2	30	ASN	N-CA-CB	-5.44	101.29	110.49
1	1	89	TYR	CA-C-N	-5.44	111.15	121.54
1	1	89	TYR	C-N-CA	-5.44	111.15	121.54
2	2	31	ALA	N-CA-C	-5.44	100.04	108.42
2	2	94	GLU	CG-CD-OE1	-5.44	105.89	118.40
2	2	261	ILE	O-C-N	5.44	129.20	123.00
3	3	28	TYR	CB-CG-CD2	5.44	128.96	120.80
2	2	237	SER	CA-CB-OG	5.44	121.97	111.10
3	3	131	LEU	O-C-N	5.43	130.00	123.16
4	4	27	PHE	CA-C-O	5.43	128.28	120.51
2	2	139	SER	N-CA-CB	-5.43	102.02	110.98
1	1	27	THR	CA-CB-OG1	-5.42	101.46	109.60
2	2	106	TYR	N-CA-C	5.42	117.66	109.41
2	2	141	THR	O-C-N	5.42	129.01	122.94
3	3	67	MET	O-C-N	-5.42	115.38	122.59
3	3	235	PRO	N-CD-CG	-5.42	97.30	103.80
3	3	227	THR	OG1-CB-CG2	5.42	120.13	109.30
1	1	82	ILE	N-CA-CB	5.41	120.16	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	223	ARG	O-C-N	-5.40	117.58	123.52
3	3	152	HIS	O-C-N	5.40	128.77	122.99
1	1	51	ILE	CA-CB-CG2	5.40	119.68	110.50
1	1	90	ASN	CB-CG-ND2	5.40	124.50	116.40
1	1	17	VAL	CA-C-N	5.40	126.16	120.11
1	1	17	VAL	C-N-CA	5.40	126.16	120.11
2	2	72	ASN	N-CA-C	5.38	118.47	110.52
3	3	235	PRO	CB-CA-C	-5.38	98.56	112.00
3	3	226	ASP	CB-CG-OD1	5.37	130.76	118.40
1	1	40	GLY	N-CA-C	-5.37	108.31	115.40
2	2	227	ILE	CA-C-N	-5.37	113.45	121.83
2	2	227	ILE	C-N-CA	-5.37	113.45	121.83
3	3	226	ASP	CB-CA-C	5.36	118.59	109.53
2	2	86	LEU	O-C-N	-5.36	115.34	122.20
1	1	175	HIS	CA-C-O	5.36	128.17	120.51
3	3	114	ARG	N-CA-CB	-5.35	102.30	110.65
2	2	87	LYS	CB-CA-C	5.35	121.07	110.42
1	1	110	ARG	O-C-N	5.35	127.79	122.12
1	1	172	PHE	O-C-N	5.35	129.66	123.30
1	1	181	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	1	279	VAL	CB-CA-C	5.35	118.86	111.38
2	2	201	LEU	CA-C-N	5.34	130.37	122.94
2	2	201	LEU	C-N-CA	5.34	130.37	122.94
2	2	219	ASN	CB-CA-C	5.34	119.77	110.79
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
3	3	201	PRO	N-CA-CB	-5.34	97.64	103.25
1	1	274	VAL	CA-CB-CG1	5.34	119.47	110.40
2	2	141	THR	CA-C-O	-5.33	115.42	121.72
2	2	24	SER	CA-C-N	5.33	128.80	121.33
2	2	24	SER	C-N-CA	5.33	128.80	121.33
3	3	5	TYR	CA-C-N	5.33	129.04	122.37
3	3	5	TYR	C-N-CA	5.33	129.04	122.37
1	1	76	CYS	CB-CA-C	5.33	118.22	109.90
1	1	208	LYS	O-C-N	5.33	128.99	122.96
2	2	130	HIS	CA-C-O	-5.33	113.83	122.20
2	2	134	SER	N-CA-CB	5.33	118.86	110.23
1	1	246	THR	N-CA-CB	-5.33	101.73	110.41
2	2	127	ILE	CA-C-O	-5.33	112.81	119.95
2	2	35	TYR	N-CA-CB	-5.32	104.16	112.41
2	2	108	VAL	CB-CA-C	5.32	118.58	111.19
2	2	190	PHE	O-C-N	5.32	130.36	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	223	VAL	N-CA-CB	-5.32	102.72	111.44
3	3	182	LYS	O-C-N	5.32	127.75	122.12
1	1	168	ASN	O-C-N	5.31	130.22	122.94
3	3	57	ASN	N-CA-CB	-5.31	101.52	110.49
3	3	165	LEU	CA-C-N	-5.30	114.11	122.64
3	3	165	LEU	C-N-CA	-5.30	114.11	122.64
1	1	201	ASP	CA-CB-CG	-5.30	107.30	112.60
2	2	20	ASP	CA-CB-CG	5.29	117.89	112.60
2	2	81	LYS	CA-C-O	-5.29	114.50	120.32
2	2	96	MET	N-CA-CB	-5.29	102.32	110.20
1	1	88	ASP	CA-CB-CG	5.29	117.89	112.60
3	3	77	GLY	N-CA-C	-5.29	103.42	112.30
1	1	69	SER	CB-CA-C	5.29	118.92	110.09
3	3	157	VAL	CA-C-N	-5.28	113.23	120.57
3	3	157	VAL	C-N-CA	-5.28	113.23	120.57
1	1	223	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	1	261	HIS	CA-CB-CG	-5.28	108.52	113.80
1	1	89	TYR	N-CA-C	-5.28	101.09	109.59
1	1	247	LYS	CB-CA-C	-5.26	98.38	109.38
2	2	63	PHE	CA-CB-CG	-5.26	108.54	113.80
2	2	202	ILE	O-C-N	5.25	128.72	123.10
1	1	232	SER	N-CA-CB	5.25	117.43	110.29
2	2	45	GLN	N-CA-CB	5.25	119.67	110.27
1	1	204	ASN	N-CA-C	-5.25	102.14	109.96
3	3	228	ASP	CB-CG-OD2	-5.25	106.33	118.40
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
3	3	15	THR	N-CA-C	-5.24	106.95	113.19
3	3	66	SER	CA-C-N	5.24	131.55	121.54
3	3	66	SER	C-N-CA	5.24	131.55	121.54
2	2	144	TYR	CA-C-N	5.24	131.55	121.54
2	2	144	TYR	C-N-CA	5.24	131.55	121.54
3	3	154	VAL	N-CA-C	-5.24	102.09	109.21
1	1	45	VAL	N-CA-C	-5.23	100.83	108.99
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
3	3	127	LEU	N-CA-CB	-5.23	102.79	111.57
2	2	165	ARG	N-CA-C	-5.23	99.67	110.80
2	2	224	ILE	CA-CB-CG2	5.22	119.38	110.50
3	3	141	PRO	CA-C-N	5.22	129.55	120.68
3	3	141	PRO	C-N-CA	5.22	129.55	120.68
1	1	86	TYR	CA-C-O	5.21	124.56	118.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	226	THR	CA-CB-OG1	-5.21	101.79	109.60
3	3	160	GLN	CG-CD-NE2	5.21	124.21	116.40
2	2	166	GLN	N-CA-CB	-5.20	102.63	110.32
1	1	236	THR	CA-CB-CG2	5.20	119.34	110.50
3	3	79	ALA	O-C-N	5.20	131.60	122.09
1	1	43	SER	N-CA-CB	5.18	117.67	110.26
1	1	154	ILE	N-CA-CB	5.18	117.79	111.21
3	3	142	THR	N-CA-CB	-5.18	102.33	110.30
1	1	82	ILE	O-C-N	5.17	129.04	122.57
2	2	37	VAL	O-C-N	5.17	128.77	123.18
2	2	45	GLN	O-C-N	5.17	128.30	122.19
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	257	ARG	O-C-N	5.17	129.47	122.59
2	2	186	PHE	N-CA-C	-5.17	102.64	110.39
2	2	68	SER	O-C-N	5.17	128.72	122.68
2	2	76	LYS	CA-CB-CG	-5.17	103.77	114.10
2	2	111	GLN	CB-CA-C	5.16	118.16	109.48
2	2	146	LEU	N-CA-CB	5.16	118.24	110.65
1	1	262	SER	O-C-N	5.16	130.02	123.11
2	2	182	ASN	CA-CB-CG	5.16	117.76	112.60
2	2	79	TRP	CA-C-N	5.15	131.08	122.73
2	2	79	TRP	C-N-CA	5.15	131.08	122.73
2	2	160	ARG	NE-CZ-NH1	-5.15	116.35	121.50
3	3	163	ILE	N-CA-CB	5.15	120.35	111.39
2	2	252	GLU	CG-CD-OE1	-5.14	106.57	118.40
4	4	30	ASN	O-C-N	5.14	129.43	122.59
2	2	97	TYR	N-CA-CB	-5.14	102.42	110.44
1	1	183	SER	N-CA-C	5.14	115.83	108.74
2	2	194	ARG	NH1-CZ-NH2	5.14	125.98	119.30
2	2	62	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	2	12	ARG	CA-CB-CG	-5.13	103.83	114.10
2	2	171	SER	N-CA-C	5.13	119.41	111.56
3	3	167	VAL	O-C-N	5.13	126.95	121.10
2	2	20	ASP	CA-C-N	5.12	130.36	122.93
2	2	20	ASP	C-N-CA	5.12	130.36	122.93
3	3	39	GLU	CB-CG-CD	5.12	121.31	112.60
1	1	237	THR	OG1-CB-CG2	5.12	119.54	109.30
2	2	215	LEU	O-C-N	5.12	128.90	122.19
2	2	160	ARG	NE-CZ-NH2	5.11	123.80	119.20
3	3	184	SER	CA-C-N	5.11	128.59	121.24
3	3	184	SER	C-N-CA	5.11	128.59	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	152	ALA	N-CA-C	5.10	118.28	111.75
3	3	183	TYR	CB-CG-CD1	5.10	128.45	120.80
3	3	97	THR	N-CA-CB	5.09	117.78	109.69
3	3	149	LEU	N-CA-CB	-5.08	102.39	110.22
3	3	200	PRO	O-C-N	5.08	127.45	121.46
1	1	18	PRO	CA-C-N	-5.07	113.97	123.05
1	1	18	PRO	C-N-CA	-5.07	113.97	123.05
3	3	122	THR	N-CA-CB	5.07	118.53	110.87
4	4	26	TYR	N-CA-CB	5.07	119.11	110.50
1	1	228	LYS	CD-CE-NZ	5.06	128.10	111.90
2	2	14	MET	O-C-N	-5.06	117.40	123.27
1	1	145	TYR	CA-C-N	-5.06	111.64	121.91
1	1	145	TYR	C-N-CA	-5.06	111.64	121.91
2	2	79	TRP	CA-CB-CG	5.05	123.20	113.60
1	1	83	LYS	N-CA-C	-5.05	99.10	107.99
3	3	76	THR	N-CA-CB	5.04	117.31	110.01
4	4	33	LYS	N-CA-C	5.04	117.17	111.02
1	1	62	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	1	175	HIS	CB-CA-C	5.04	120.44	110.42
2	2	66	LEU	CA-C-N	5.04	128.62	121.42
2	2	66	LEU	C-N-CA	5.04	128.62	121.42
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
3	3	140	GLU	CB-CA-C	5.04	117.53	109.62
1	1	283	THR	N-CA-CB	-5.03	102.17	111.53
2	2	11	ASP	O-C-N	5.03	131.05	123.00
2	2	15	GLN	CA-C-N	-5.03	115.47	122.71
2	2	15	GLN	C-N-CA	-5.03	115.47	122.71
3	3	222	ARG	N-CA-C	5.03	115.78	108.14
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	128.96	122.59
1	1	262	SER	CA-C-O	-5.01	115.59	121.46
1	1	27	THR	CA-CB-CG2	5.01	119.02	110.50
1	1	70	PHE	CA-C-N	-5.01	112.64	121.81
1	1	70	PHE	C-N-CA	-5.01	112.64	121.81
1	1	42	THR	CA-CB-OG1	-5.01	102.09	109.60
2	2	121	THR	N-CA-CB	-5.01	102.33	110.59
1	1	170	SER	CB-CA-C	5.00	117.85	110.14

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2191	433	1
2	2	1979	0	1922	221	2
3	3	1831	0	1810	248	1
4	4	151	0	136	18	0
5	1	23	0	16	8	0
All	All	6246	0	6075	822	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 67.

All (822) 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)
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.54	1.45
1:1:101:ILE:H	1:1:101:ILE:CD1	1.12	1.39
1:1:100:LYS:HA	1:1:101:ILE:CD1	1.64	1.25
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.70	1.23
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.20
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
1:1:100:LYS:CA	1:1:101:ILE:HD13	1.73	1.19
1:1:108:GLN:CD	3:3:226:ASP:OD2	1.87	1.18
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.61	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	1.15
1:1:218:GLY:C	1:1:219:THR:HG22	1.63	1.15
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:ARG:HH12	2:2:249:MET:HE2	1.06	1.14
1:1:101:ILE:HD13	1:1:101:ILE:N	1.33	1.14
1:1:101:ILE:CD1	1:1:219:THR:HA	1.76	1.14
1:1:104:GLN:O	3:3:236:ILE:HD11	1.44	1.13
1:1:98:LYS:HA	1:1:220:ILE:O	1.50	1.12
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.12
1:1:104:GLN:O	3:3:236:ILE:CD1	1.99	1.11
1:1:147:TYR:CE1	5:1:700:W91:CL2	2.41	1.10
1:1:101:ILE:HG21	1:1:217:MET:O	1.51	1.09
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
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.07
1:1:124:GLU:O	1:1:124:GLU:HG3	1.52	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
1:1:218:GLY:C	1:1:219:THR:CG2	2.21	1.05
1:1:119:VAL:CG1	1:1:121:PHE:HE1	1.70	1.05
1:1:101:ILE:HD12	1:1:219:THR:HA	1.36	1.05
1:1:100:LYS:HA	1:1:101:ILE:HD13	1.17	1.04
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
1:1:104:GLN:HB2	1:1:262:SER:HB2	1.41	1.02
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	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
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	1.01
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.01
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.00
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
1:1:108:GLN:OE1	3:3:226:ASP:CG	2.04	1.00
1:1:100:LYS:C	1:1:101:ILE:HD13	1.87	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	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	1.93	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
1:1:101:ILE:O	1:1:102:THR:OG1	1.83	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	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.95
1:1:113:PHE:O	1:1:115:LEU:N	1.99	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
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
1:1:101:ILE:CD1	1:1:219:THR:CA	2.47	0.92
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.49	0.91
3:3:24:ALA:O	3:3:25:LEU:HB2	1.71	0.91
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
1:1:100:LYS:HA	1:1:101:ILE:HD11	1.52	0.89
1:1:101:ILE:HD12	1:1:219:THR:CA	2.01	0.89
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.89
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.89
1:1:119:VAL:HG11	1:1:121:PHE:HE1	1.36	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.08	0.88
1:1:119:VAL:CG1	1:1:121:PHE:CE1	2.56	0.88
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	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
3:3:54:PRO:O	3:3:93:PRO:HB2	1.73	0.87
1:1:97:THR:HG23	1:1:222:SER:HB3	1.54	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
1:1:215:ASN:CG	1:1:215:ASN:O	2.18	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	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
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.85
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.85
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.12	0.85
1:1:97:THR:O	1:1:222:SER:N	2.10	0.84
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.39	0.84
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.84
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.84
1:1:182:PHE:HE1	1:1:184:ILE:HD11	1.43	0.84
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:HD11	1:1:219:THR:HA	1.59	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
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
1:1:212:VAL:C	1:1:214:THR:N	2.37	0.82
1:1:107:ALA:O	1:1:109:ILE:N	2.12	0.82
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	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
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.16	0.81
1:1:197:TYR:H	2:2:131:GLN:HE21	1.28	0.81
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.95	0.81
1:1:182:PHE:HA	3:3:21:SER:HB2	1.62	0.81
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:223:ARG:HG2	1:1:223:ARG:NH1	1.90	0.80
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.80
1:1:102:THR:CG2	1:1:263:HIS:CE1	2.65	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
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.79
1:1:110:ARG:O	1:1:114:GLU:HG3	1.82	0.79
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
1:1:101:ILE:HD11	1:1:219:THR:CA	2.12	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	1.83	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
1:1:104:GLN:HB2	1:1:262:SER:CB	2.13	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
1:1:113:PHE:C	1:1:115:LEU:H	1.93	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
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.19	0.76
1:1:119:VAL:HG13	1:1:121:PHE:HE1	1.50	0.76
1:1:99:TRP:CE3	1:1:220:ILE:HD12	2.21	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	0.75
1:1:102:THR:HG22	1:1:103:LEU:H	1.50	0.75
1:1:211:SER:CA	1:1:212:VAL:HG12	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	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
1:1:147:TYR:HE1	5:1:700:W91:CL2	2.02	0.74
1:1:100:LYS:CA	1:1:101:ILE:CD1	2.44	0.74
4:4:26:TYR:CD1	4:4:29:ILE:HD11	2.22	0.74
1:1:182:PHE:HD1	1:1:183:SER:N	1.84	0.74
1:1:104:GLN:O	3:3:236:ILE:HD13	1.87	0.74
2:2:65:THR:OG1	2:2:245:SER:OG	2.05	0.74
1:1:182:PHE:CE1	1:1:184:ILE:HD11	2.23	0.74
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.74
1:1:215:ASN:O	1:1:215:ASN:ND2	2.21	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.74
1:1:148:VAL:HG11	1:1:154:ILE:HG13	1.68	0.73
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
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
1:1:124:GLU:O	1:1:124:GLU:CG	2.35	0.73
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.73
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.72
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	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
1:1:211:SER:N	1:1:212:VAL:CG1	2.51	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	2.22	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
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.72
2:2:148:HIS:N	2:2:149:PRO:HD3	2.05	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	0.71
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.71
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.71
1:1:97:THR:O	1:1:221:CYS:HA	1.91	0.70
1:1:101:ILE:H	1:1:101:ILE:HD13	0.71	0.70
1:1:146:MET:HB2	1:1:169:MET:O	1.91	0.70
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
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.02	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	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
1:1:97:THR:HG23	1:1:222:SER:CB	2.21	0.70
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.70
1:1:182:PHE:CD1	1:1:183:SER:N	2.60	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
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
1:1:99:TRP:HE3	1:1:220:ILE:HD12	1.54	0.69
1:1:127:LEU:O	1:1:180:PRO:HD2	1.92	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.69
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.68
1:1:160:ASP:H	1:1:163:TRP:CD1	2.11	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.93	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:260:THR:C	1:1:261:HIS:HD2	2.02	0.68
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.20	0.68
1:1:265:THR:HG1	2:2:133:ALA:HB2	1.58	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.67
1:1:260:THR:C	1:1:261:HIS:CD2	2.71	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
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:23:SER:OG	1:1:53:THR:CG2	2.30	0.67
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.29	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
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
2:2:107:THR:OG1	2:2:249:MET:HE3	1.95	0.67
1:1:182:PHE:HE1	1:1:184:ILE:CD1	2.08	0.66
1:1:107:ALA:O	1:1:110:ARG:N	2.26	0.66
1:1:101:ILE:C	1:1:102:THR:HG1	2.01	0.66
1:1:163:TRP:HH2	1:1:222:SER:O	1.73	0.66
1:1:183:SER:C	1:1:184:ILE:CG1	2.67	0.66
2:2:91:ILE:O	2:2:92:PHE:C	2.39	0.66
1:1:183:SER:C	1:1:184:ILE:HG13	2.20	0.66
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.66
3:3:91:SER:O	3:3:92:THR:C	2.39	0.66
1:1:104:GLN:HG3	1:1:263:HIS:HD1	1.59	0.65
1:1:182:PHE:CD1	1:1:182:PHE:C	2.74	0.65
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
1:1:98:LYS:CA	1:1:220:ILE:O	2.39	0.65
1:1:104:GLN:HG3	1:1:263:HIS:ND1	2.11	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
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	1.98	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
1:1:101:ILE:CD1	1:1:219:THR:N	2.59	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:101:ILE:C	1:1:102:THR:OG1	2.37	0.64
1:1:104:GLN:HA	1:1:110:ARG:HG3	1.79	0.64
1:1:210:GLY:C	1:1:212:VAL:HG13	2.23	0.64
1:1:181:ARG:HG2	1:1:182:PHE:N	2.12	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	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
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.64
1:1:102:THR:HG21	1:1:263:HIS:CE1	2.32	0.63
1:1:212:VAL:N	1:1:214:THR:H	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:113:PHE:HE2	1:1:121:PHE:CZ	2.16	0.63
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.63
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	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
3:3:145:LYS:O	3:3:148:MET:HE3	1.98	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.14	0.62
1:1:195:MET:O	1:1:196:PHE:CD1	2.53	0.62
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.62
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.15	0.62
1:1:145:TYR:N	1:1:145:TYR:HD1	1.97	0.62
2:2:235:THR:C	2:2:237:SER:H	2.06	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
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
1:1:124:GLU:OE1	1:1:181:ARG:HD3	2.00	0.61
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
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.61
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
1:1:102:THR:CG2	1:1:103:LEU:H	2.05	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61
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
1:1:113:PHE:C	1:1:115:LEU:N	2.52	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
1:1:79: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
1:1:249: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
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.37	0.60
1:1:101:ILE:CD1	1:1:101:ILE:N	1.97	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.29	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:149:PRO:O	1:1:150:PRO:O	2.20	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:210:GLY:C	1:1:212:VAL:CG1	2.75	0.59
1:1:150:PRO:O	1:1:152:ALA:CB	2.51	0.59
1:1:155:PRO:HD2	1:1:221:CYS:SG	2.41	0.59
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	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	1.66	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	1.67	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
1:1:123:SER:HA	1:1:242:LYS:O	2.02	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
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.58
1:1:101:ILE:HD12	1:1:219:THR:N	2.18	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
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
1:1:278:ILE:HA	3:3:92:THR:HG21	1.86	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:102:THR:CG2	1:1:263:HIS:HE1	2.16	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
1:1:119:VAL:HG13	1:1:121:PHE:CD1	2.39	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
1:1:197:TYR:HD1	1:1:198:ASP:H	1.52	0.58
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.57
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.57
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.86	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	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
1:1:72: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
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:99:TRP:NE1	1:1:105:GLU:OE2	2.38	0.57
1:1:201:ASP:OD1	1:1:213:VAL:HG22	2.05	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
1:1:261:HIS:H	3:3:237:GLU:H	1.52	0.56
1:1:127:LEU:CB	1:1:180:PRO:HG2	2.30	0.56
1:1:181:ARG:O	1:1:182:PHE:HB3	2.05	0.56
1:1:217:MET:O	1:1:217:MET:CG	2.53	0.56
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.56
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.56
1:1:150:PRO:O	1:1:152:ALA:HB2	2.05	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	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
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.56
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.41	0.56
1:1:147:TYR:CZ	5:1:700:W91:CL2	2.94	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	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
2:2:86:LEU:C	2:2:88:ASP:H	2.14	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	2.68	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:154:ARG:HD3	2:2:155:ASP:H	1.71	0.55
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.55
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
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
1:1:184:ILE:HG22	1:1:185:PRO:O	2.06	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	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
1:1:182:PHE:HE1	1:1:184:ILE:CG1	2.19	0.55
3:3:125:THR:CG2	3:3:126:THR:N	2.70	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
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	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	0.54
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
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	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
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
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	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
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.54
1:1:19:ASN:HA	1:1:58:THR:HG23	1.89	0.54
1:1:102:THR:HG23	1:1:263:HIS:CE1	2.42	0.54
1:1:183:SER:HG	3:3:21:SER:HG	1.54	0.54
1:1:119:VAL:HG11	1:1:121:PHE:CE1	2.28	0.54
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.70	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.53
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
1:1:186:PHE:CD1	1:1:186:PHE:C	2.86	0.53
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.53
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.53
3:3:14:MET:C	3:3:16:THR:H	2.16	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	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
1:1:113:PHE:CE2	1:1:121:PHE:CZ	2.96	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
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.24	0.53
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	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
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.53
1:1:145:TYR:HD1	1:1:145:TYR:H	1.56	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:181:ARG:HG2	1:1:182:PHE:H	1.72	0.53
1:1:261:HIS:CD2	1:1:261:HIS:N	2.74	0.53
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
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.52
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.52
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.52
3:3:43:LEU:CD2	3:3:46:MET:HE2	2.39	0.52
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.52
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	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
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	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
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.52
1:1:197:TYR:H	2:2:131:GLN:NE2	2.04	0.52
1:1:217:MET:SD	5:1:700:W91:O1	2.68	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:110:VAL:O	2:2:198:SER:HA	2.10	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.46	0.51
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	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
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:141:ILE:O	1:1:141:ILE:CG1	2.51	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:104:GLN:HA	1:1:110:ARG:CD	2.41	0.51
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.51
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.51
1:1:127:LEU:HD21	5:1:700:W91:H5A1	1.92	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
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.51
1:1:99:TRP:HE1	1:1:105:GLU:CD	2.19	0.51
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.50
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.50
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.50
1:1:124:GLU:HG2	1:1:242:LYS:CB	2.41	0.50
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.51	0.50
1:1:217:MET:O	1:1:217:MET:HG3	2.12	0.50
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.11	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
1:1:244:LYS:HZ1	4:4:38:SER:H	1.60	0.50
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
1:1:281: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
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.49
2:2:126:MET:HE3	2:2:126:MET:HA	1.94	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
3:3:231:ILE:CD1	3:3:231:ILE:N	2.69	0.49
2:2:175:PHE:CD1	2:2:175:PHE:N	2.79	0.49
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	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
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.47	0.49
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	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
2:2:18:ARG:HA	2:2:18:ARG:HD3	1.57	0.49
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.49
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.61	0.49
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.49
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.49
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.49
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
1:1:197:TYR:N	2:2:131:GLN:HE21	2.05	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.48
1:1:261:HIS:H	3:3:237:GLU:N	2.11	0.48
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.48
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.48
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.48
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.48
1:1:218:GLY:C	1:1:219:THR:HG23	2.26	0.48
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.48
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.48
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
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:197:TYR:HD1	1:1:198:ASP:N	2.10	0.48
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.48
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.48
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.48
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.48
1:1:197:TYR:CD1	1:1:198:ASP:N	2.81	0.48
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.48
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.44	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
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
1:1:271:THR:O	1:1:272:GLY:C	2.58	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
2:2:128:PRO:HD2	2:2:186:PHE:CD1	2.49	0.47
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.47
3:3:216:CYS:C	3:3:218:ASP:H	2.22	0.47
1:1:212:VAL:C	1:1:214:THR:H	2.20	0.47
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.47
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.47
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
2:2:192:ASN:C	2:2:194:ARG:H	2.21	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
3:3:43:LEU:HD23	3:3:46:MET:HE2	1.97	0.47
1:1:101:ILE:HG22	5:1:700:W91:H3C1	1.95	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.47
1:1:89:TYR:HD1	1:1:89:TYR:HA	1.49	0.47
1:1:104:GLN:HA	1:1:110:ARG:CG	2.44	0.47
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.45	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.49	0.47
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.77	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	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
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.47
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.47
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:113:PHE:HE2	1:1:121:PHE:CE1	2.33	0.46
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.46
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.46
1:1:124:GLU:OE1	1:1:181:ARG:CD	2.63	0.46
1:1:190:ALA:C	3:3:31:THR:HG21	2.38	0.46
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.46
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.46
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.15	0.46
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	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
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.98	0.46
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.46
1:1:224:ILE:HG21	1:1:224:ILE:HD13	1.46	0.46
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.46
3:3:91:SER:C	3:3:92:THR:O	2.58	0.46
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.46
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.46
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.34	0.46
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.46
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:147:THR:C	2:2:149:PRO:HD3	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:100:LYS:HG3	1:1:101:ILE:HG12	1.98	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
3:3:14:MET:C	3:3:16:THR:N	2.74	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	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
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.45
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.45
1:1:39:THR:C	1:1:41:HIS:H	2.24	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
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.82	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	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
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.50	0.45
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.45
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.45
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.55	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
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
2:2:144:TYR:C	2:2:146:LEU:H	2.26	0.44
3:3:42:ASN:CG	3:3:44:ILE:HG22	2.39	0.44
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:147:TYR:CD1	5:1:700:W91:H3B	2.53	0.44
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.44
1:1:165:SER:C	1:1:167:THR:N	2.74	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.44
1:1:148:VAL:C	1:1:149:PRO:O	2.57	0.44
1:1:90:ASN:HD22	1:1:90:ASN:N	2.16	0.44
1:1:182:PHE:CA	3:3:21:SER:HB2	2.40	0.44
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	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	1.62	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
1:1:54: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
1:1:85:ASP:OD1	1:1:85:ASP:C	2.61	0.43
1:1:129:PRO:HA	1:1:237:THR:HA	2.00	0.43
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.43
1:1:262:SER:O	1:1:263:HIS:HB2	2.18	0.43
1:1:101:ILE:HD11	1:1:219:THR:CB	2.49	0.43
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.43
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	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
2:2:247: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
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.43
1:1:99:TRP:CE3	1:1:220:ILE:CD1	2.98	0.43
1:1:125:ILE:HD13	5:1:700:W91:C6B	2.48	0.43
1:1:148:VAL:CG1	1:1:152:ALA:HB3	2.48	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
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43
1:1:260:THR:HB	1:1:261:HIS:CD2	2.53	0.43
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.43
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.43
1:1:36:ALA:C	1:1:38:GLU:H	2.26	0.43
1:1:260:THR:HB	1:1:261:HIS:HD2	1.84	0.43
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.43
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:106:MET:O	1:1:107:ALA:O	2.36	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.66	0.42
2:2:83:PRO:CG	2:2:218:ASN:HA	2.32	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
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.42
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	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
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.42
1:1:104:GLN:HG3	1:1:263:HIS:CE1	2.54	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
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
1:1:99:TRP:O	1:1:219:THR:HA	2.20	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:178:THR:O	2:2:179:LEU:C	2.62	0.42
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.42
2:2:94:GLU:C	2:2:96:MET:N	2.76	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
3:3:143:THR:C	3:3:192:TRP:CH2	2.97	0.42
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.42
2:2:21:SER:OG	2:2:63:PHE:HB2	2.19	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.41
1:1:261:HIS:HA	3:3:237:GLU:C	2.45	0.41
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.55	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
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.41
1:1:184:ILE:HG23	1:1:185:PRO:HD2	2.02	0.41
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.41
3:3:88:ASP:O	3:3:91:SER:OG	2.35	0.41
1:1:66:SER:O	1:1:67:ILE:C	2.60	0.41
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.41
2:2:61:ASN:HB2	2:2:248:PRO:C	2.45	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
1:1:122:ASP:OD1	1:1:245:HIS:HB2	2.20	0.41
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	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
3:3:158:GLY:C	3:3:160:GLN:N	2.77	0.41
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.02	0.41
3:3:30:PRO:O	3:3:31:THR:C	2.62	0.41
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
2:2:155:ASP:O	2:2:156:VAL:CB	2.68	0.41
1:1:111:ARG:HA	1:1:259:TYR:OH	2.21	0.41
1:1:148:VAL:HA	1:1:149:PRO:HD2	1.79	0.41
1:1:199:GLY:C	1:1:200:TYR:CD1	2.98	0.41
1:1:38:GLU:C	1:1:40:GLY:N	2.73	0.41
2:2:155:ASP:C	2:2:157:SER:H	2.29	0.41
1:1:98:LYS:HB3	1:1:221:CYS:SG	2.61	0.41
1:1:99:TRP:CZ3	1:1:220:ILE:HD12	2.55	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
2:2:192:ASN:C	2:2:194:ARG:N	2.79	0.41
3:3:43:LEU:HD23	3:3:43:LEU:HA	1.77	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
2:2:55:GLN:HA	2:2:56:PRO:HD2	1.98	0.41
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:43:LEU:HD22	3:3:46:MET:HE2	2.02	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
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	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
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.50	0.40
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.40
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.09	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.40
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.40
1:1:70:PHE:O	1:1:112:LYS:HE2	2.21	0.40
1:1:101:ILE:HG13	1:1:218:GLY:C	2.47	0.40
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
2:2:228:SER:HA	2:2:229:PRO:HD2	1.68	0.40
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	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
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.20	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
3:3:53:ILE:HG13	3:3:212:PHE:HA	2.03	0.40
3:3:94:LEU:HA	3:3:94:LEU:HD23	1.83	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]	2.11	0.09
1:1:25:HIS:CB	2:2:17:THR:O[2_655]	2.16	0.04

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%)	207 (74%)	49 (17%)	25 (9%)	0	9
2	2	251/263 (95%)	200 (80%)	36 (14%)	15 (6%)	1	14
3	3	236/238 (99%)	179 (76%)	37 (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%)	129 (16%)	61 (8%)	1	11

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	102	THR
1	1	104	GLN
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
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	101	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
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%)	182 (72%)	72 (28%)	0	2
2	2	219/227 (96%)	149 (68%)	70 (32%)	0	1
3	3	209/209 (100%)	154 (74%)	55 (26%)	0	3
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	494 (71%)	203 (29%)	0	2

All (203) 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
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
1	1	121	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	122	ASP
1	1	123	SER
1	1	124	GLU
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	195	MET
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
1	1	259	TYR
1	1	265	THR
1	1	274	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
2	2	126	MET
2	2	132	LEU
2	2	136	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
3	3	21	SER
3	3	23	CYS
3	3	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	W91	1	700	-	25,25,25	3.09	4 (16%)	33,34,34	2.46	6 (18%)

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	W91	1	700	-	-	1/11/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	700	W91	C2A-N3A	12.97	1.43	1.27
5	1	700	W91	C4A-N3A	-6.86	1.36	1.47
5	1	700	W91	O1A-C5A	-3.03	1.38	1.46
5	1	700	W91	O1A-C2A	-2.90	1.31	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	700	W91	O1A-C2A-N3A	-9.30	110.21	118.25
5	1	700	W91	C4A-N3A-C2A	6.16	112.22	106.75
5	1	700	W91	O1A-C2A-C4B	5.49	122.79	115.85
5	1	700	W91	O1A-C5A-C4A	4.09	111.85	104.24
5	1	700	W91	C5A-C4A-N3A	-2.26	99.50	104.42
5	1	700	W91	C3C-O1B-C1B	2.00	120.23	114.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	700	W91	C5-C1C-C2C-C3C

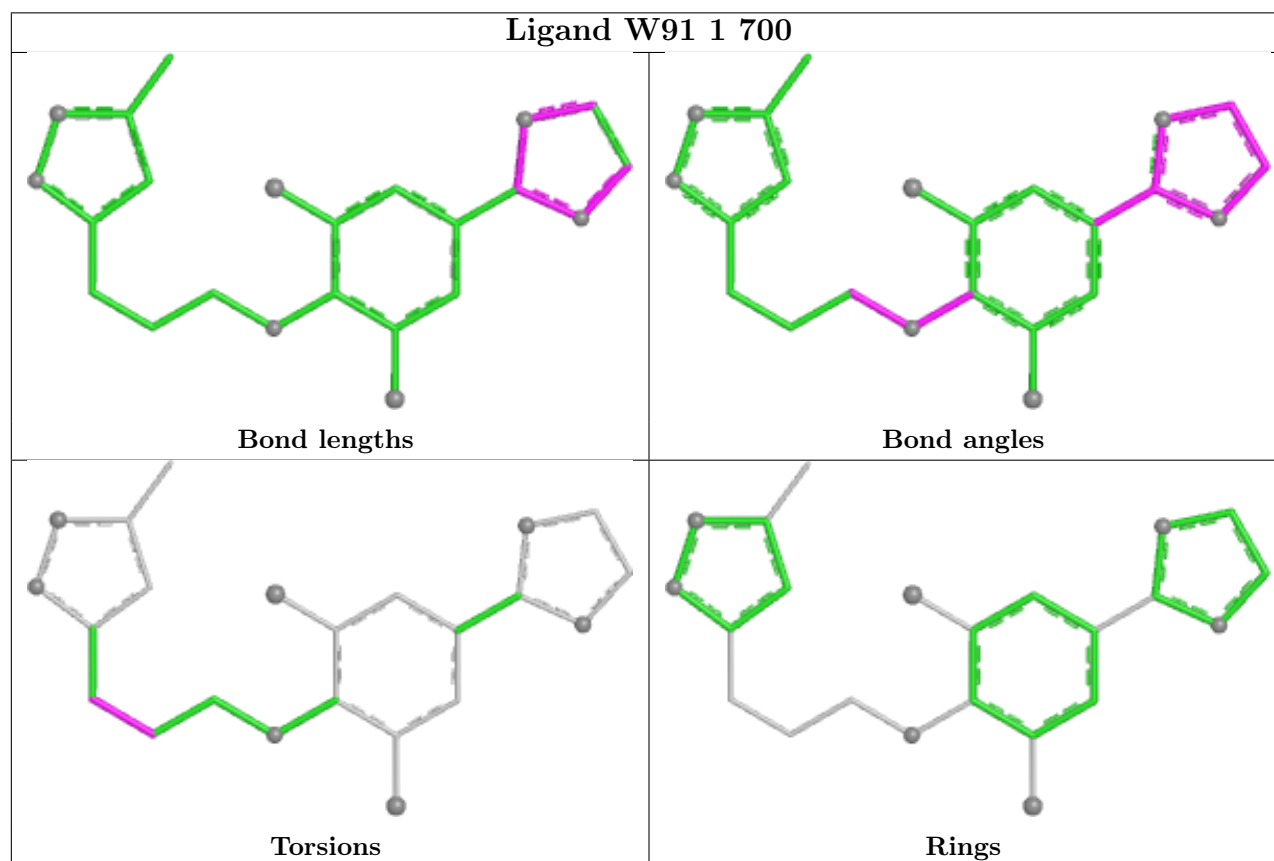
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	700	W91	8	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	146:MET	C	147:TYR	N	1.20
1	1	118:TYR	C	119:VAL	N	1.19
1	1	98:LYS	C	99:TRP	N	1.15

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.