



# Full wwPDB X-ray Structure Validation Report i

Mar 8, 2023 – 01:17 AM EST

PDB ID : 2HWE  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<span style="color: red;">NOT EXECUTED</span>
EDS	:	<span style="color: red;">NOT EXECUTED</span>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

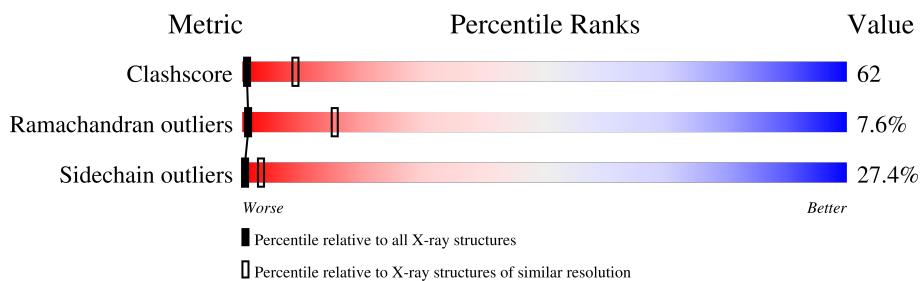
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

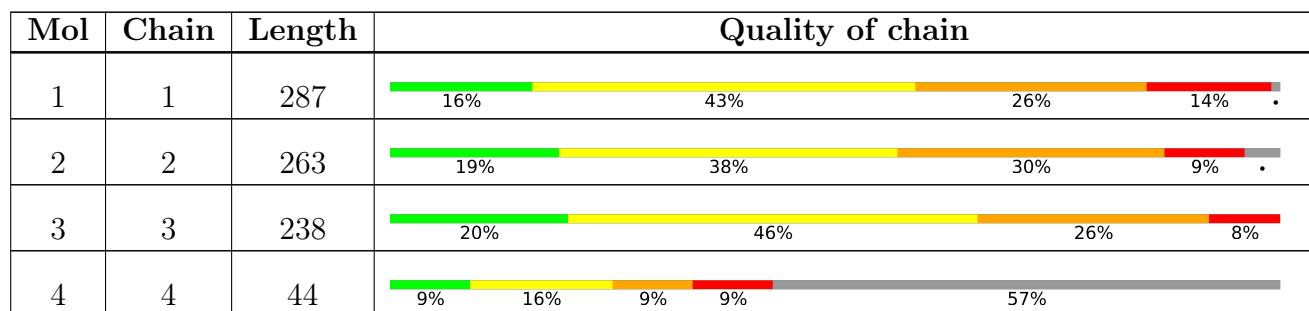
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 <=5%

Note EDS was not executed.



## 2 Entry composition [\(i\)](#)

There are 5 unique types of molecules in this entry. The entry contains 6248 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

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

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

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

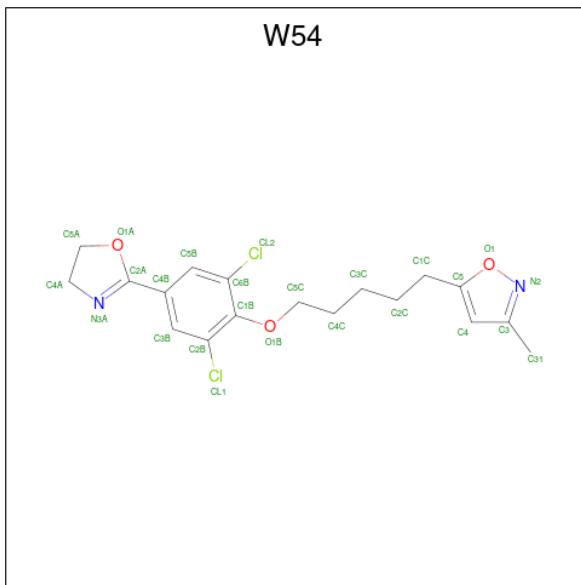
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

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

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

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

- Molecule 5 is 5-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYL ISOXAZOLE (three-letter code: W54) (formula: C<sub>18</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>).



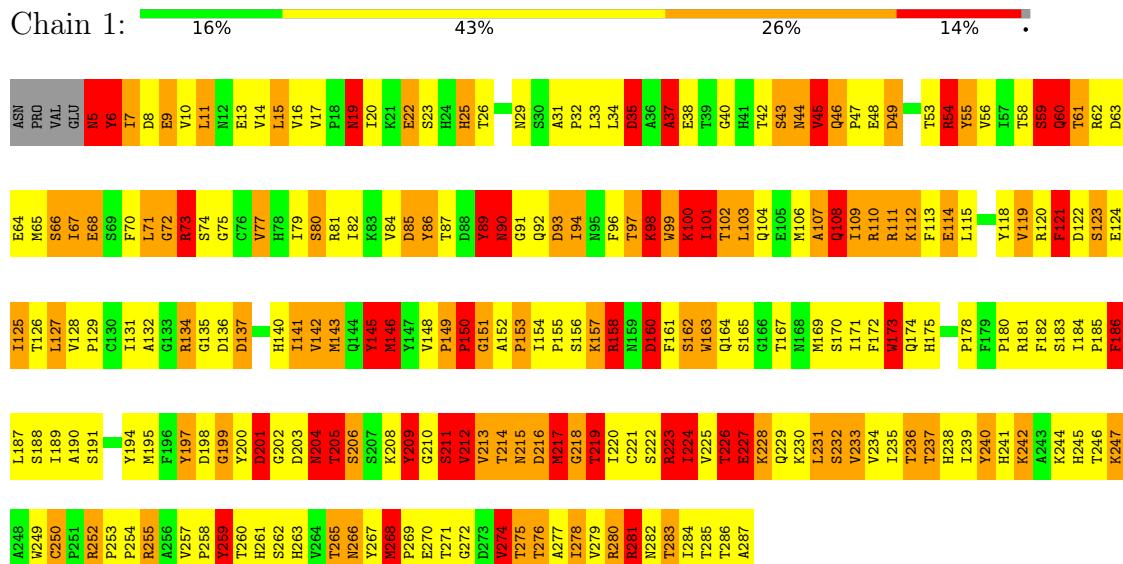
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5		1	Total	C	Cl	N	O	0	0
		1	25	18	2	2	3		

### 3 Residue-property plots

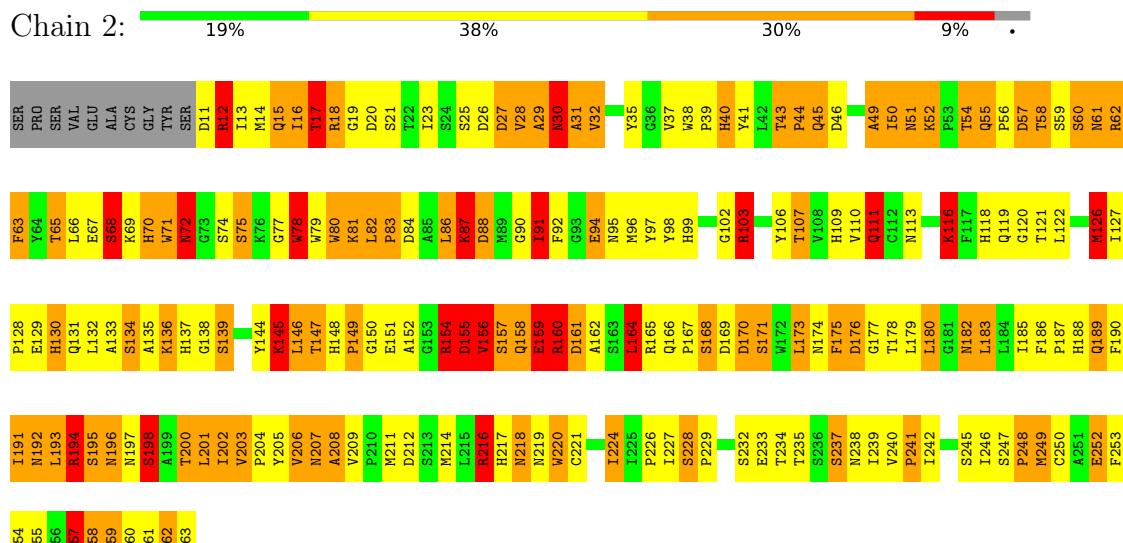
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

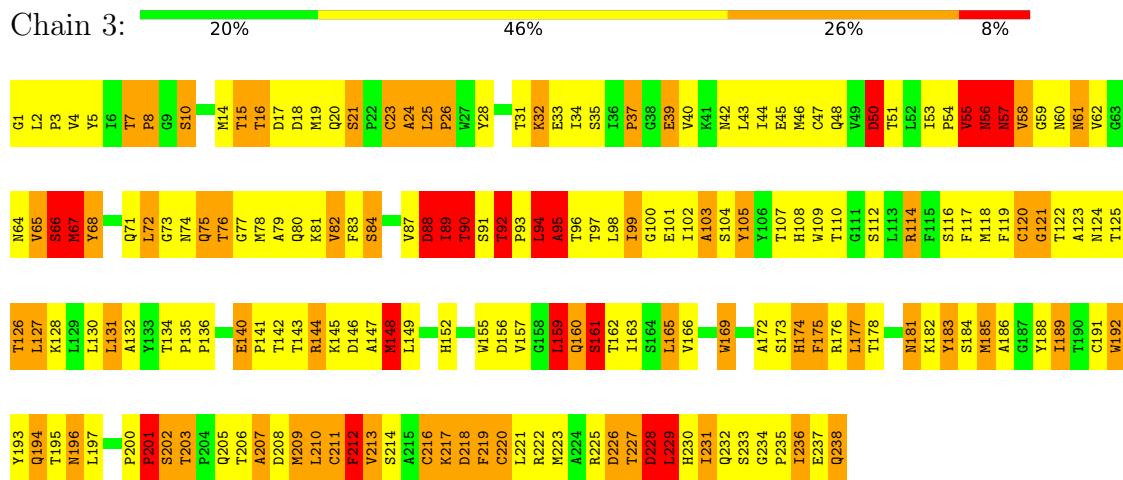
- Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)



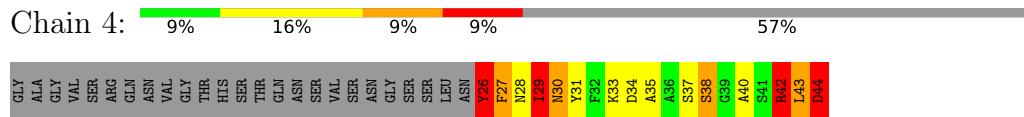
- Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)



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



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



## 4 Data and refinement statistics i

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, $\alpha$ , $\beta$ , $\gamma$	341.30 Å    341.30 Å    465.90 Å 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 <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R <sub>free</sub>	(Not available), (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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: W54

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1	1.19	8/2322 (0.3%)	2.59	143/3162 (4.5%)
2	2	0.95	0/2033	2.59	151/2770 (5.5%)
3	3	0.93	0/1878	2.46	110/2570 (4.3%)
4	4	1.25	0/154	3.15	21/206 (10.2%)
All	All	1.05	8/6387 (0.1%)	2.57	425/8708 (4.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	MET	C-N	-15.40	0.98	1.34
1	1	213	VAL	C-N	11.89	1.61	1.34
1	1	98	LYS	C-N	-8.12	1.15	1.34
1	1	218	GLY	CA-C	-6.92	1.40	1.51
1	1	223	ARG	C-N	6.78	1.49	1.34
1	1	118	TYR	C-N	-6.50	1.19	1.34
1	1	145	TYR	C-N	6.30	1.48	1.34
1	1	149	PRO	N-CA	-5.02	1.38	1.47

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-28.02	77.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	62	ARG	CD-NE-CZ	24.80	158.32	123.60
1	1	134	ARG	NE-CZ-NH1	24.10	132.35	120.30
2	2	216	ARG	NE-CZ-NH2	-21.96	109.32	120.30
1	1	280	ARG	NE-CZ-NH2	-20.47	110.06	120.30
3	3	146	ASP	CB-CG-OD2	-17.21	102.81	118.30
1	1	98	LYS	CA-C-N	16.79	154.13	117.20
1	1	150	PRO	C-N-CA	-16.53	87.58	122.30
2	2	257	ARG	NE-CZ-NH2	-16.45	112.07	120.30
3	3	222	ARG	CD-NE-CZ	15.87	145.82	123.60
4	4	42	ARG	NE-CZ-NH1	14.96	127.78	120.30
2	2	155	ASP	CB-CG-OD2	-14.66	105.11	118.30
1	1	81	ARG	NE-CZ-NH1	14.15	127.37	120.30
1	1	281	ARG	NE-CZ-NH2	-14.07	113.27	120.30
1	1	98	LYS	C-N-CA	14.02	156.75	121.70
2	2	62	ARG	NE-CZ-NH1	13.94	127.27	120.30
3	3	226	ASP	CB-CG-OD1	13.77	130.69	118.30
2	2	154	ARG	NE-CZ-NH1	13.75	127.18	120.30
1	1	158	ARG	NE-CZ-NH1	13.72	127.16	120.30
1	1	218	GLY	O-C-N	13.42	144.18	122.70
3	3	28	TYR	CB-CG-CD2	13.27	128.96	121.00
3	3	228	ASP	CB-CG-OD2	-13.26	106.36	118.30
3	3	183	TYR	CB-CG-CD1	12.41	128.45	121.00
3	3	144	ARG	CD-NE-CZ	12.31	140.84	123.60
1	1	227	GLU	OE1-CD-OE2	-12.23	108.63	123.30
1	1	281	ARG	CA-CB-CG	12.21	140.27	113.40
1	1	6	TYR	CB-CG-CD1	-12.09	113.75	121.00
1	1	93	ASP	CB-CG-OD1	-11.83	107.65	118.30
3	3	114	ARG	NE-CZ-NH1	-11.79	114.41	120.30
3	3	144	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	1	231	LEU	CA-CB-CG	11.30	141.29	115.30
3	3	225	ARG	NE-CZ-NH1	-11.28	114.66	120.30
3	3	50	ASP	CB-CG-OD2	-11.21	108.21	118.30
3	3	50	ASP	CB-CG-OD1	10.94	128.15	118.30
2	2	67	GLU	OE1-CD-OE2	10.91	136.39	123.30
1	1	255	ARG	CD-NE-CZ	10.90	138.86	123.60
2	2	35	TYR	CB-CG-CD2	10.85	127.51	121.00
1	1	54	ARG	CG-CD-NE	10.82	134.52	111.80
4	4	44	ASP	CB-CG-OD2	-10.74	108.63	118.30
1	1	211	SER	C-N-CA	-10.60	95.21	121.70
3	3	218	ASP	CB-CG-OD2	-10.36	108.97	118.30
2	2	12	ARG	NE-CZ-NH2	-10.27	115.16	120.30
2	2	12	ARG	CD-NE-CZ	10.21	137.90	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	162	ALA	CB-CA-C	10.21	125.42	110.10
2	2	205	TYR	CB-CG-CD2	10.17	127.10	121.00
2	2	62	ARG	NH1-CZ-NH2	-9.95	108.45	119.40
2	2	11	ASP	CB-CG-OD1	9.87	127.18	118.30
2	2	31	ALA	N-CA-CB	9.82	123.84	110.10
2	2	216	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	1	8	ASP	CB-CG-OD2	-9.63	109.63	118.30
3	3	67	MET	N-CA-CB	-9.61	93.31	110.60
2	2	154	ARG	C-N-CA	9.53	145.53	121.70
2	2	29	ALA	N-CA-CB	9.52	123.42	110.10
4	4	42	ARG	CD-NE-CZ	9.49	136.88	123.60
2	2	176	ASP	CB-CG-OD2	9.40	126.76	118.30
1	1	281	ARG	NE-CZ-NH1	9.32	124.96	120.30
2	2	165	ARG	NE-CZ-NH1	9.31	124.96	120.30
2	2	212	ASP	CB-CG-OD2	9.30	126.67	118.30
1	1	59	SER	N-CA-CB	-9.17	96.75	110.50
1	1	9	GLU	OE1-CD-OE2	9.15	134.28	123.30
1	1	134	ARG	NH1-CZ-NH2	-9.07	109.42	119.40
3	3	148	MET	CG-SD-CE	9.01	114.62	100.20
1	1	151	GLY	N-CA-C	-8.98	90.66	113.10
3	3	18	ASP	CB-CG-OD1	-8.98	110.22	118.30
1	1	218	GLY	CA-C-N	-8.93	97.55	117.20
2	2	165	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	2	28	VAL	CA-CB-CG1	8.87	124.21	110.90
1	1	146	MET	O-C-N	8.85	136.85	122.70
1	1	227	GLU	CG-CD-OE1	8.81	135.93	118.30
1	1	60	GLN	O-C-N	8.80	136.77	122.70
1	1	214	THR	N-CA-CB	8.74	126.90	110.30
2	2	35	TYR	CB-CG-CD1	-8.72	115.77	121.00
2	2	11	ASP	CB-CG-OD2	-8.72	110.45	118.30
2	2	154	ARG	NE-CZ-NH2	-8.69	115.96	120.30
3	3	232	GLN	N-CA-CB	8.69	126.24	110.60
1	1	55	TYR	CB-CG-CD2	-8.67	115.80	121.00
1	1	11	LEU	O-C-N	8.64	136.52	122.70
1	1	214	THR	CB-CA-C	-8.53	88.58	111.60
3	3	222	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	2	233	GLU	CG-CD-OE2	8.44	135.18	118.30
1	1	68	GLU	CB-CG-CD	8.37	136.79	114.20
3	3	28	TYR	CB-CG-CD1	-8.31	116.01	121.00
1	1	187	LEU	CA-C-O	-8.30	102.67	120.10
2	2	57	ASP	N-CA-CB	-8.30	95.67	110.60
2	2	12	ARG	NE-CZ-NH1	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	ASP	OD1-CG-OD2	-8.21	107.71	123.30
2	2	97	TYR	CB-CG-CD2	8.19	125.91	121.00
2	2	126	MET	CA-CB-CG	-8.11	99.51	113.30
2	2	12	ARG	CG-CD-NE	8.00	128.60	111.80
1	1	111	ARG	CD-NE-CZ	7.96	134.75	123.60
2	2	241	PRO	C-N-CA	7.93	141.53	121.70
1	1	120	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	1	49	ASP	CB-CG-OD1	-7.88	111.20	118.30
2	2	194	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	2	189	GLN	CA-CB-CG	7.83	130.62	113.40
1	1	158	ARG	CD-NE-CZ	7.81	134.53	123.60
1	1	55	TYR	CB-CG-CD1	7.80	125.68	121.00
2	2	160	ARG	NE-CZ-NH1	-7.79	116.40	120.30
2	2	26	ASP	CB-CG-OD2	7.79	125.31	118.30
3	3	56	ASN	C-N-CA	7.79	141.16	121.70
2	2	61	ASN	CB-CA-C	7.78	125.95	110.40
2	2	161	ASP	N-CA-CB	7.78	124.60	110.60
3	3	235	PRO	C-N-CA	7.73	141.02	121.70
1	1	93	ASP	CB-CG-OD2	7.68	125.21	118.30
2	2	94	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	1	6	TYR	CB-CG-CD2	7.64	125.58	121.00
1	1	213	VAL	C-N-CA	-7.63	102.61	121.70
2	2	159	GLU	OE1-CD-OE2	7.60	132.42	123.30
1	1	85	ASP	CB-CG-OD1	-7.59	111.46	118.30
2	2	161	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	1	134	ARG	CD-NE-CZ	7.56	134.18	123.60
1	1	280	ARG	NH1-CZ-NH2	7.55	127.71	119.40
2	2	71	TRP	CB-CA-C	7.55	125.51	110.40
1	1	73	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	1	216	ASP	CB-CA-C	7.52	125.44	110.40
3	3	207	ALA	O-C-N	7.50	134.71	122.70
1	1	111	ARG	NE-CZ-NH1	-7.48	116.56	120.30
3	3	68	TYR	CB-CG-CD2	7.47	125.48	121.00
2	2	252	GLU	OE1-CD-OE2	7.46	132.25	123.30
1	1	181	ARG	NE-CZ-NH2	7.45	124.03	120.30
2	2	232	SER	N-CA-CB	7.41	121.62	110.50
1	1	111	ARG	C-N-CA	7.40	140.20	121.70
1	1	61	THR	CA-CB-OG1	-7.39	93.48	109.00
4	4	34	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	1	89	TYR	CB-CG-CD1	-7.34	116.60	121.00
3	3	92	THR	CB-CA-C	7.34	131.41	111.60
3	3	161	SER	CB-CA-C	-7.32	96.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	223	ARG	NE-CZ-NH2	7.29	123.94	120.30
4	4	37	SER	O-C-N	7.25	134.31	122.70
3	3	95	ALA	CA-C-N	7.20	133.03	117.20
2	2	147	THR	N-CA-CB	7.19	123.97	110.30
2	2	233	GLU	CG-CD-OE1	-7.16	103.98	118.30
1	1	173	TRP	CA-CB-CG	7.15	127.28	113.70
1	1	213	VAL	O-C-N	7.14	134.12	122.70
1	1	228	LYS	CD-CE-NZ	7.12	128.08	111.70
2	2	152	ALA	N-CA-CB	-7.12	100.13	110.10
3	3	88	ASP	CB-CG-OD2	7.12	124.71	118.30
2	2	237	SER	CB-CA-C	7.12	123.62	110.10
4	4	40	ALA	O-C-N	7.11	134.07	122.70
2	2	78	TRP	CA-CB-CG	7.11	127.20	113.70
2	2	164	LEU	O-C-N	7.05	133.99	122.70
3	3	120	CYS	CA-CB-SG	-7.05	101.31	114.00
3	3	218	ASP	N-CA-CB	-7.05	97.91	110.60
3	3	232	GLN	O-C-N	7.04	133.96	122.70
2	2	160	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	2	80	TRP	N-CA-CB	6.99	123.18	110.60
2	2	62	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	2	103	ARG	CD-NE-CZ	6.94	133.32	123.60
1	1	45	VAL	CB-CA-C	6.93	124.56	111.40
4	4	42	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	1	259	TYR	CB-CG-CD2	-6.91	116.86	121.00
1	1	268	MET	CA-CB-CG	-6.89	101.58	113.30
4	4	31	TYR	CB-CG-CD1	6.88	125.13	121.00
3	3	222	ARG	NH1-CZ-NH2	-6.87	111.84	119.40
2	2	81	LYS	O-C-N	6.85	133.66	122.70
1	1	5	ASN	N-CA-CB	6.84	122.92	110.60
2	2	160	ARG	N-CA-CB	-6.84	98.28	110.60
1	1	164	GLN	OE1-CD-NE2	-6.83	106.18	121.90
2	2	72	ASN	OD1-CG-ND2	6.83	137.62	121.90
3	3	25	LEU	CA-CB-CG	6.80	130.94	115.30
2	2	106	TYR	C-N-CA	6.79	138.66	121.70
1	1	203	ASP	CB-CG-OD1	-6.78	112.20	118.30
2	2	198	SER	CB-CA-C	-6.74	97.30	110.10
1	1	164	GLN	CG-CD-OE1	6.72	135.04	121.60
3	3	73	GLY	CA-C-O	6.71	132.68	120.60
2	2	52	LYS	CA-CB-CG	6.70	128.15	113.40
1	1	270	GLU	N-CA-CB	6.69	122.64	110.60
3	3	26	PRO	O-C-N	6.68	133.39	122.70
3	3	218	ASP	CA-CB-CG	-6.68	98.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	90	THR	N-CA-CB	6.66	122.95	110.30
3	3	193	TYR	O-C-N	6.64	133.32	122.70
1	1	70	PHE	O-C-N	6.61	133.28	122.70
2	2	135	ALA	N-CA-CB	-6.60	100.86	110.10
1	1	19	ASN	CB-CG-OD1	-6.60	108.40	121.60
4	4	40	ALA	N-CA-CB	6.59	119.33	110.10
3	3	57	ASN	CB-CG-ND2	-6.59	100.89	116.70
1	1	37	ALA	N-CA-CB	-6.56	100.92	110.10
3	3	55	VAL	CB-CA-C	6.50	123.76	111.40
1	1	5	ASN	O-C-N	6.50	133.09	122.70
2	2	196	ASN	N-CA-CB	-6.50	98.91	110.60
2	2	50	ILE	CA-CB-CG2	6.48	123.87	110.90
1	1	213	VAL	CA-C-N	-6.46	102.99	117.20
2	2	187	PRO	CB-CA-C	6.45	128.13	112.00
2	2	183	LEU	O-C-N	6.45	133.02	122.70
2	2	16	ILE	O-C-N	6.43	133.00	122.70
3	3	16	THR	CA-CB-CG2	6.42	121.38	112.40
1	1	64	GLU	CA-CB-CG	6.40	127.49	113.40
1	1	199	GLY	O-C-N	6.40	132.94	122.70
1	1	13	GLU	O-C-N	6.38	132.91	122.70
2	2	28	VAL	CG1-CB-CG2	-6.38	100.69	110.90
3	3	160	GLN	N-CA-CB	6.38	122.08	110.60
3	3	222	ARG	NE-CZ-NH2	6.34	123.47	120.30
3	3	172	ALA	CB-CA-C	6.34	119.61	110.10
2	2	68	SER	N-CA-CB	6.32	119.98	110.50
3	3	235	PRO	CA-C-N	-6.30	103.34	117.20
2	2	26	ASP	OD1-CG-OD2	-6.30	111.33	123.30
1	1	201	ASP	CB-CG-OD2	6.30	123.97	118.30
2	2	196	ASN	OD1-CG-ND2	6.29	136.37	121.90
1	1	274	VAL	N-CA-CB	6.29	125.34	111.50
3	3	235	PRO	CA-C-O	6.29	135.29	120.20
1	1	275	THR	OG1-CB-CG2	6.28	124.45	110.00
1	1	146	MET	CA-C-N	-6.28	103.40	117.20
1	1	106	MET	CG-SD-CE	6.27	110.24	100.20
2	2	248	PRO	N-CA-C	-6.27	95.79	112.10
3	3	37	PRO	N-CA-CB	6.26	110.81	103.30
4	4	44	ASP	CB-CG-OD1	6.25	123.92	118.30
1	1	77	VAL	O-C-N	6.24	132.68	122.70
3	3	33	GLU	CG-CD-OE2	-6.23	105.83	118.30
2	2	161	ASP	O-C-N	6.23	132.67	122.70
1	1	233	VAL	CA-C-N	-6.22	103.52	117.20
1	1	233	VAL	CB-CA-C	-6.21	99.60	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	19	GLY	C-N-CA	6.21	137.22	121.70
3	3	94	LEU	CA-C-N	6.19	130.81	117.20
2	2	94	GLU	CG-CD-OE1	-6.19	105.93	118.30
1	1	211	SER	CA-C-O	-6.18	107.12	120.10
1	1	86	TYR	CB-CA-C	6.18	122.76	110.40
4	4	30	ASN	CB-CA-C	6.18	122.75	110.40
4	4	38	SER	O-C-N	6.16	133.68	123.20
2	2	155	ASP	N-CA-CB	6.16	121.69	110.60
2	2	205	TYR	CB-CG-CD1	-6.15	117.31	121.00
3	3	89	ILE	CB-CA-C	-6.15	99.30	111.60
1	1	16	VAL	CG1-CB-CG2	6.14	120.72	110.90
1	1	195	MET	CG-SD-CE	6.13	110.00	100.20
1	1	175	HIS	N-CA-CB	-6.12	99.58	110.60
1	1	206	SER	O-C-N	6.11	132.48	122.70
1	1	209	TYR	CB-CG-CD1	6.09	124.66	121.00
2	2	17	THR	CB-CA-C	6.06	127.96	111.60
2	2	154	ARG	CG-CD-NE	6.06	124.52	111.80
3	3	185	MET	CA-CB-CG	6.06	123.59	113.30
4	4	35	ALA	CB-CA-C	6.06	119.18	110.10
1	1	247	LYS	CB-CA-C	-6.04	98.32	110.40
1	1	35	ASP	CB-CG-OD2	6.03	123.73	118.30
2	2	57	ASP	CB-CG-OD1	-6.03	112.87	118.30
2	2	82	LEU	CA-CB-CG	-6.03	101.43	115.30
1	1	227	GLU	CB-CG-CD	6.03	130.47	114.20
2	2	81	LYS	CA-CB-CG	6.02	126.65	113.40
3	3	32	LYS	O-C-N	6.02	132.34	122.70
2	2	107	THR	CA-CB-OG1	-6.02	96.37	109.00
2	2	155	ASP	CB-CG-OD1	6.01	123.71	118.30
2	2	57	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	1	187	LEU	CA-C-N	5.99	130.37	117.20
3	3	105	TYR	CB-CG-CD2	5.96	124.58	121.00
1	1	82	ILE	CB-CA-C	-5.96	99.67	111.60
2	2	262	LYS	CB-CA-C	5.95	122.30	110.40
1	1	146	MET	CG-SD-CE	5.95	109.72	100.20
2	2	160	ARG	CG-CD-NE	5.95	124.29	111.80
2	2	194	ARG	NH1-CZ-NH2	5.95	125.94	119.40
3	3	15	THR	N-CA-CB	-5.95	99.00	110.30
2	2	130	HIS	CA-CB-CG	-5.93	103.51	113.60
1	1	71	LEU	CB-CA-C	5.92	121.45	110.20
4	4	26	TYR	CB-CG-CD1	5.91	124.55	121.00
1	1	68	GLU	OE1-CD-OE2	-5.90	116.22	123.30
3	3	233	SER	CA-C-N	-5.90	104.40	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	217	MET	CG-SD-CE	5.90	109.64	100.20
1	1	89	TYR	CB-CG-CD2	5.90	124.54	121.00
1	1	231	LEU	CB-CA-C	5.90	121.40	110.20
3	3	68	TYR	CB-CG-CD1	-5.89	117.46	121.00
2	2	87	LYS	CB-CG-CD	5.89	126.92	111.60
2	2	157	SER	N-CA-CB	5.89	119.33	110.50
2	2	208	ALA	N-CA-CB	5.88	118.33	110.10
2	2	252	GLU	CG-CD-OE1	-5.88	106.54	118.30
2	2	91	ILE	N-CA-CB	5.88	124.32	110.80
2	2	130	HIS	O-C-N	5.88	132.10	122.70
2	2	156	VAL	C-N-CA	5.88	136.39	121.70
3	3	183	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	2	49	ALA	CA-C-O	-5.84	107.83	120.10
3	3	201	PRO	N-CA-C	5.84	127.28	112.10
1	1	240	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	1	100	LYS	O-C-N	5.82	132.02	122.70
3	3	185	MET	N-CA-CB	5.82	121.08	110.60
1	1	55	TYR	O-C-N	5.82	132.01	122.70
1	1	85	ASP	CB-CG-OD2	5.81	123.53	118.30
1	1	20	ILE	O-C-N	5.81	131.99	122.70
1	1	49	ASP	OD1-CG-OD2	5.80	134.33	123.30
2	2	97	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	1	54	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	2	147	THR	O-C-N	5.79	131.96	122.70
2	2	234	THR	CA-C-O	5.78	132.25	120.10
2	2	249	MET	CA-CB-CG	5.78	123.13	113.30
3	3	24	ALA	N-CA-CB	-5.77	102.03	110.10
2	2	57	ASP	OD1-CG-OD2	5.75	134.23	123.30
1	1	25	HIS	O-C-N	5.73	131.86	122.70
1	1	250	CYS	CA-CB-SG	5.72	124.31	114.00
2	2	218	ASN	CA-CB-CG	5.72	125.99	113.40
1	1	16	VAL	CB-CA-C	5.72	122.27	111.40
2	2	257	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	1	226	THR	N-CA-C	5.71	126.42	111.00
2	2	134	SER	CA-C-N	-5.71	104.65	117.20
1	1	202	GLY	C-N-CA	5.70	135.95	121.70
1	1	81	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	1	274	VAL	CA-CB-CG1	5.70	119.45	110.90
1	1	204	ASN	CA-C-N	-5.68	104.71	117.20
1	1	90	ASN	CB-CA-C	5.66	121.72	110.40
3	3	77	GLY	CA-C-O	5.66	130.78	120.60
3	3	229	LEU	CA-CB-CG	5.65	128.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	232	SER	CB-CA-C	-5.65	99.37	110.10
3	3	160	GLN	O-C-N	5.64	131.73	122.70
3	3	227	THR	CA-C-O	5.64	131.94	120.10
2	2	249	MET	CG-SD-CE	5.64	109.22	100.20
2	2	83	PRO	C-N-CA	5.63	135.78	121.70
3	3	18	ASP	OD1-CG-OD2	5.63	134.00	123.30
3	3	103	ALA	CB-CA-C	5.63	118.55	110.10
3	3	45	GLU	OE1-CD-OE2	-5.63	116.54	123.30
3	3	76	THR	O-C-N	5.63	132.78	123.20
2	2	139	SER	N-CA-CB	-5.63	102.06	110.50
2	2	26	ASP	CB-CG-OD1	5.62	123.36	118.30
1	1	121	PHE	CB-CA-C	-5.61	99.19	110.40
3	3	212	PHE	CA-CB-CG	5.61	127.35	113.90
3	3	146	ASP	OD1-CG-OD2	5.60	133.94	123.30
2	2	49	ALA	CA-C-N	5.58	129.48	117.20
1	1	111	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	2	212	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	1	274	VAL	CA-C-N	-5.57	104.94	117.20
2	2	134	SER	N-CA-CB	5.57	118.86	110.50
3	3	79	ALA	O-C-N	5.57	131.60	122.70
2	2	116	LYS	CB-CA-C	-5.55	99.29	110.40
1	1	62	ARG	NE-CZ-NH1	-5.55	117.52	120.30
2	2	228	SER	N-CA-CB	5.55	118.83	110.50
2	2	83	PRO	CB-CA-C	5.55	125.87	112.00
2	2	220	TRP	CA-C-N	-5.54	105.00	117.20
1	1	153	PRO	N-CD-CG	-5.54	94.88	103.20
2	2	119	GLN	CB-CA-C	5.54	121.48	110.40
1	1	68	GLU	CA-CB-CG	5.52	125.55	113.40
2	2	149	PRO	CA-C-N	5.52	127.23	116.20
3	3	24	ALA	CA-C-N	5.51	129.33	117.20
3	3	64	ASN	OD1-CG-ND2	5.51	134.57	121.90
2	2	54	THR	N-CA-CB	5.50	120.75	110.30
2	2	169	ASP	CA-C-O	5.49	131.63	120.10
1	1	81	ARG	CD-NE-CZ	5.48	131.28	123.60
2	2	216	ARG	NH1-CZ-NH2	5.48	125.43	119.40
3	3	146	ASP	CB-CG-OD1	5.47	123.23	118.30
3	3	183	TYR	CG-CD2-CE2	5.46	125.67	121.30
2	2	90	GLY	CA-C-O	5.43	130.38	120.60
3	3	169	TRP	CB-CA-C	5.43	121.26	110.40
4	4	40	ALA	N-CA-C	-5.42	96.35	111.00
3	3	58	VAL	CA-CB-CG1	-5.42	102.77	110.90
3	3	218	ASP	C-N-CA	5.42	135.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	235	PRO	CB-CA-C	-5.40	98.50	112.00
3	3	228	ASP	CB-CA-C	-5.40	99.60	110.40
2	2	20	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	1	270	GLU	O-C-N	5.39	131.33	122.70
2	2	32	VAL	O-C-N	5.39	131.33	122.70
3	3	225	ARG	NE-CZ-NH2	5.39	123.00	120.30
3	3	234	GLY	N-CA-C	-5.39	99.63	113.10
2	2	70	HIS	CB-CA-C	-5.38	99.63	110.40
2	2	150	GLY	O-C-N	5.38	131.31	122.70
2	2	194	ARG	NE-CZ-NH1	-5.38	117.61	120.30
3	3	8	PRO	C-N-CA	5.38	133.59	122.30
3	3	95	ALA	CA-C-O	-5.36	108.84	120.10
1	1	283	THR	O-C-N	5.34	131.25	122.70
3	3	233	SER	CA-C-O	5.33	131.30	120.10
4	4	44	ASP	CA-C-O	5.33	131.30	120.10
3	3	88	ASP	OD1-CG-OD2	-5.33	113.18	123.30
2	2	96	MET	CA-C-N	-5.33	105.49	117.20
2	2	161	ASP	CB-CA-C	-5.32	99.76	110.40
2	2	111	GLN	CB-CG-CD	5.32	125.42	111.60
1	1	172	PHE	CA-C-O	-5.32	108.94	120.10
3	3	175	PHE	CB-CG-CD1	-5.32	117.08	120.80
2	2	182	ASN	O-C-N	5.31	131.19	122.70
2	2	150	GLY	CA-C-O	-5.30	111.05	120.60
1	1	201	ASP	CB-CG-OD1	-5.30	113.53	118.30
3	3	203	THR	O-C-N	5.30	131.17	121.10
3	3	206	THR	N-CA-C	-5.30	96.69	111.00
4	4	26	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	2	87	LYS	CB-CA-C	5.30	120.99	110.40
4	4	29	ILE	O-C-N	5.29	131.17	122.70
3	3	206	THR	OG1-CB-CG2	5.29	122.17	110.00
2	2	52	LYS	CG-CD-CE	5.29	127.77	111.90
2	2	165	ARG	C-N-CA	5.28	134.90	121.70
2	2	195	SER	CB-CA-C	5.28	120.13	110.10
3	3	114	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	3	108	HIS	CA-CB-CG	5.26	122.55	113.60
3	3	202	SER	CA-C-N	-5.26	105.63	117.20
3	3	35	SER	N-CA-CB	-5.25	102.62	110.50
3	3	10	SER	CB-CA-C	5.25	120.08	110.10
1	1	216	ASP	O-C-N	5.25	131.10	122.70
1	1	211	SER	O-C-N	5.25	131.10	122.70
1	1	287	ALA	CA-C-O	-5.23	109.11	120.10
2	2	11	ASP	O-C-N	5.23	131.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	224	ILE	CB-CG1-CD1	-5.23	99.27	113.90
2	2	203	VAL	N-CA-CB	-5.22	100.01	111.50
2	2	82	LEU	N-CA-C	5.21	125.08	111.00
1	1	242	LYS	CA-C-N	-5.20	105.75	117.20
3	3	92	THR	N-CA-C	-5.20	96.97	111.00
3	3	156	ASP	CB-CG-OD1	-5.20	113.62	118.30
3	3	165	LEU	O-C-N	5.19	131.01	122.70
4	4	26	TYR	O-C-N	5.19	131.00	122.70
2	2	12	ARG	CB-CA-C	-5.18	100.04	110.40
1	1	158	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
3	3	64	ASN	N-CA-CB	-5.17	101.29	110.60
1	1	22	GLU	CG-CD-OE2	5.17	128.64	118.30
2	2	173	LEU	CB-CA-C	5.17	120.02	110.20
3	3	76	THR	CA-C-N	-5.16	105.87	116.20
2	2	19	GLY	CA-C-N	-5.16	105.85	117.20
2	2	30	ASN	N-CA-CB	-5.16	101.32	110.60
3	3	146	ASP	N-CA-CB	5.15	119.87	110.60
3	3	24	ALA	CA-C-O	-5.14	109.31	120.10
1	1	43	SER	CA-C-N	-5.12	105.94	117.20
3	3	181	ASN	O-C-N	5.12	130.88	122.70
2	2	237	SER	CA-C-O	5.11	130.83	120.10
3	3	72	LEU	CB-CG-CD2	-5.10	102.33	111.00
4	4	38	SER	CA-C-O	-5.10	109.39	120.10
1	1	163	TRP	CB-CA-C	5.09	120.59	110.40
2	2	50	ILE	CB-CA-C	5.09	121.78	111.60
4	4	42	ARG	C-N-CA	-5.09	108.97	121.70
1	1	94	ILE	CA-C-N	-5.09	106.01	117.20
2	2	40	HIS	CA-CB-CG	-5.08	104.96	113.60
2	2	28	VAL	CB-CA-C	-5.08	101.75	111.40
1	1	178	PRO	CA-C-N	-5.08	106.03	117.20
1	1	205	THR	OG1-CB-CG2	5.06	121.64	110.00
1	1	66	SER	O-C-N	5.06	130.79	122.70
2	2	168	SER	C-N-CA	5.06	134.34	121.70
3	3	78	MET	CB-CA-C	5.06	120.52	110.40
1	1	189	ILE	C-N-CA	5.05	134.32	121.70
3	3	64	ASN	CA-CB-CG	-5.05	102.30	113.40
1	1	46	GLN	O-C-N	5.04	130.69	121.10
2	2	218	ASN	CB-CG-OD1	-5.04	111.53	121.60
2	2	238	ASN	N-CA-CB	5.02	119.64	110.60
1	1	175	HIS	CB-CA-C	5.02	120.43	110.40
2	2	45	GLN	N-CA-CB	5.02	119.63	110.60
3	3	131	LEU	CA-CB-CG	5.01	126.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	227	THR	CA-CB-CG2	-5.01	105.39	112.40
3	3	71	GLN	N-CA-CB	5.01	119.62	110.60
3	3	223	MET	CG-SD-CE	5.01	108.21	100.20
1	1	80	SER	CA-C-O	5.00	130.61	120.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	110	ARG	Mainchain
1	1	150	PRO	Peptide
1	1	186	PHE	Mainchain
1	1	211	SER	Mainchain
1	1	223	ARG	Mainchain
1	1	98	LYS	Peptide, Mainchain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2262	0	2191	391	1
2	2	1979	0	1920	214	2
3	3	1831	0	1809	235	1
4	4	151	0	136	18	0
5	1	25	0	20	3	0
All	All	6248	0	6076	762	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 62.

All (762) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:H	1:1:101:ILE:CD1	1.07	1.45
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.55	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:N	1:1:101:ILE:HD13	1.26	1.25
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.69	1.25
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.54	1.21
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.59	1.20
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
1:1:104:GLN:O	3:3:236:ILE:HD11	1.42	1.17
1:1:218:GLY:O	1:1:219:THR:HG22	0.98	1.16
1:1:108:GLN:CD	3:3:226:ASP:OD2	1.85	1.15
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.15
1:1:104:GLN:O	3:3:236:ILE:CD1	1.95	1.14
1:1:101:ILE:HG21	1:1:217:MET:O	1.46	1.14
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.12
1:1:98:LYS:HA	1:1:220:ILE:O	1.50	1.11
1:1:211:SER:C	1:1:212:VAL:HG12	1.68	1.11
1:1:218:GLY:C	1:1:219:THR:HG22	1.63	1.11
2:2:18:ARG:HH12	2:2:249:MET:HE2	0.99	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
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.06
1:1:119:VAL:CG1	1:1:121:PHE:HE1	1.70	1.05
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:100:LYS:CA	1:1:101:ILE:HD13	1.89	1.02
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.02
1:1:218:GLY:C	1:1:219:THR:CG2	2.21	1.01
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.01
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.01
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.91	1.00
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	1.00
1:1:108:GLN:OE1	3:3:226:ASP:CG	2.00	0.99
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	0.99
1:1:101:ILE:H	1:1:101:ILE:HD12	1.23	0.99
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.94	0.98
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.98
1:1:100:LYS:C	1:1:101:ILE:HD13	1.84	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:223:ARG:HG2	1:1:223:ARG:HH11	1.29	0.97
1:1:150:PRO:O	1:1:151:GLY:C	1.99	0.97
3:3:117:PHE:CD1	3:3:211:CYS:HB3	2.00	0.97
1:1:211:SER:N	1:1:212:VAL:HG12	1.80	0.97
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
1:1:100:LYS:HA	1:1:101:ILE:CD1	1.96	0.95
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93
1:1:163:TRP:CH2	1:1:222:SER:O	2.21	0.93
1:1:100:LYS:HA	1:1:101:ILE:HD13	1.49	0.93
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
1:1:217:MET:O	1:1:217:MET:HG2	1.70	0.92
1:1:101:ILE:HD12	1:1:219:THR:HA	1.53	0.91
1:1:211:SER:C	1:1:212:VAL:CG1	2.27	0.91
3:3:24:ALA:O	3:3:25:LEU:HB2	1.71	0.91
1:1:113:PHE:O	1:1:115:LEU:N	2.04	0.90
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.90
1:1:96:PHE:CE2	1:1:157:LYS:HA	2.06	0.90
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.89
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.89
1:1:97:THR:HG23	1:1:222:SER:HB3	1.53	0.88
1:1:119:VAL:CG1	1:1:121:PHE:CE1	2.56	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.08	0.88
3:3:237:GLU:HG2	3:3:238:GLN:H	1.38	0.88
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.55	0.88
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.87
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.87
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	0.86
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.10	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:119:VAL:HG11	1:1:121:PHE:HE1	1.38	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.56	0.86
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.85
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.85
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.39	0.84
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.84
1:1:217:MET:O	1:1:217:MET:CG	2.22	0.84
2:2:159:GLU:C	2:2:160:ARG:HG2	1.96	0.83
1:1:97:THR:O	1:1:222:SER:N	2.12	0.83
1:1:101:ILE:CD1	1:1:101:ILE:N	1.88	0.83
1:1:101:ILE:HG13	1:1:218:GLY:CA	2.09	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.83
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.61	0.83
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
1:1:102:THR:HG23	1:1:103:LEU:N	1.93	0.82
1:1:150:PRO:O	1:1:152:ALA:N	2.13	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.96	0.80
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.80
1:1:223:ARG:HG2	1:1:223:ARG:NH1	1.90	0.80
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.80
1:1:148:VAL:HG11	1:1:154:ILE:HG13	1.63	0.80
1:1:104:GLN:O	3:3:236:ILE:HD13	1.80	0.79
1:1:124:GLU:O	1:1:125:ILE:HG12	1.82	0.79
1:1:119:VAL:HG13	1:1:121:PHE:HE1	1.47	0.79
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.79
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.18	0.79
3:3:237:GLU:CG	3:3:238:GLN:H	1.95	0.79
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
2:2:173:LEU:O	2:2:174:ASN:HB2	1.84	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
1:1:107:ALA:O	1:1:109:ILE:N	2.18	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
1:1:212:VAL:C	1:1:214:THR:N	2.37	0.77
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:211:SER:CA	1:1:212:VAL:HG12	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
1:1:99:TRP:CE3	1:1:220:ILE:HD12	2.22	0.75
2:2:68:SER:C	2:2:69:LYS:HG2	2.06	0.75
1:1:261:HIS:HA	3:3:237:GLU:O	1.87	0.75
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.75
1:1:96:PHE:HB2	1:1:222:SER:O	1.86	0.75
4:4:26:TYR:CD1	4:4:29:ILE:HD11	2.22	0.74
1:1:101:ILE:HG13	1:1:218:GLY:N	2.02	0.74
1:1:125:ILE:HD13	5:1:500:W54:C2B	2.17	0.74
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.74
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.73
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.53	0.73
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.73
1:1:197:TYR:H	2:2:131:GLN:HE21	1.36	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.22	0.73
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	0.73
1:1:211:SER:N	1:1:212:VAL:CG1	2.51	0.72
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
2:2:183:LEU:HD12	2:2:186:PHE:HD2	1.52	0.72
1:1:97:THR:O	1:1:221:CYS:HA	1.89	0.72
1:1:145:TYR:N	1:1:145:TYR:CD1	2.54	0.72
3:3:173:SER:O	3:3:175:PHE:N	2.23	0.72
1:1:215:ASN:CG	1:1:215:ASN:O	2.27	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
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
1:1:124:GLU:O	1:1:125:ILE:CG1	2.37	0.72
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.72
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.72
2:2:148:HIS:N	2:2:149:PRO:HD3	2.05	0.71
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.71
1:1:101:ILE:HD12	1:1:219:THR:CA	2.19	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.23	0.71
1:1:104:GLN:HB2	1:1:262:SER:HB2	1.73	0.71
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.71

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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
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:97:THR:HG23	1:1:222:SER:CB	2.20	0.70
1:1:99:TRP:HE3	1:1:220:ILE:HD12	1.54	0.70
1:1:107:ALA:O	1:1:110:ARG:N	2.22	0.70
1:1:146:MET:HB2	1:1:169:MET:O	1.91	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
1:1:101:ILE:CG2	1:1:217:MET:O	2.35	0.70
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.02	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.70
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
1:1:269:PRO:HG2	1:1:272:GLY:O	1.93	0.69
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.92	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.69
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:110:ARG:O	1:1:114:GLU:HG3	1.93	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.27	0.69
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.68
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.93	0.68
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.68
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.67
2:2:78:TRP:HE3	2:2:78:TRP:N	1.92	0.67
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.67
1:1:101:ILE:HG13	1:1:217:MET:C	2.15	0.67
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.66
1:1:163:TRP:HH2	1:1:222:SER:O	1.73	0.66
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.66
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
2:2:126:MET:HE3	2:2:126:MET:HA	1.79	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.65
2:2:155:ASP:O	2:2:156:VAL:HB	1.97	0.65
1:1:215:ASN:O	1:1:215:ASN:ND2	2.30	0.64
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:127:LEU:O	1:1:180:PRO:HD2	1.98	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.64
1:1:163:TRP:CZ3	1:1:223:ARG:HB2	2.33	0.64
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.64
1:1:212:VAL:N	1:1:214:THR:H	1.96	0.63
1:1:186:PHE:HE1	3:3:31:THR:HG22	1.63	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.99	0.63
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.63
2:2:174:ASN:C	2:2:175:PHE:HD1	2.03	0.63
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.63
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.62
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
1:1:197:TYR:HD1	1:1:198:ASP:H	1.46	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:182:PHE:HA	3:3:21:SER:HB2	1.82	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.62
1:1:146:MET:CE	1:1:162:SER:O	2.48	0.62
1:1:145:TYR:N	1:1:145:TYR:HD1	1.97	0.62
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.62
1:1:141:ILE:HA	1:1:226:THR:HG21	1.81	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:145:TYR:O	1:1:170:SER:HA	2.01	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
1:1:104:GLN:HA	1:1:110:ARG:HG3	1.82	0.61
2:2:91:ILE:O	2:2:92:PHE:C	2.39	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61
3:3:91:SER:O	3:3:92:THR:C	2.39	0.61
1:1:260:THR:C	1:1:261:HIS:CD2	2.74	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
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.60
1:1:125:ILE:HD12	1:1:182:PHE:HE1	1.66	0.60
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.36	0.60
1:1:146:MET:O	1:1:146:MET:HG2	1.96	0.60
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.60
2:2:84:ASP:OD1	2:2:87:LYS:HE2	2.02	0.60
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.37	0.60
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.60
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
1:1:102:THR:C	1:1:103:LEU:HD23	2.22	0.60
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.60
2:2:65:THR:HG1	2:2:245:SER:HG	1.47	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
1:1:149:PRO:O	1:1:150:PRO:O	2.20	0.59
1:1:155:PRO:HD2	1:1:221:CYS:SG	2.41	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:210:GLY:C	1:1:212:VAL:HG13	2.22	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:150:PRO:O	1:1:152:ALA:CB	2.51	0.59
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.59
1:1:260:THR:O	1:1:261:HIS:HB2	2.03	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.66	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
3:3:145:LYS:HA	3:3:148:MET:HE2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.85	0.58
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.58
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.58
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.57
1:1:97: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
2:2:235:THR:C	2:2:237:SER:H	2.06	0.57
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:201:ASP:OD1	1:1:213:VAL:HG22	2.05	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.57
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.57
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.56
1:1:146:MET:HE1	1:1:162:SER:O	2.05	0.56
1:1:119:VAL:HG13	1:1:121:PHE:CD1	2.40	0.56
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.56
1:1:150:PRO:O	1:1:152:ALA:HB2	2.05	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.88	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.21	0.56
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.41	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.56
1:1:260:THR:C	1:1:261:HIS:HD2	2.09	0.56
1:1:260:THR:O	1:1:261:HIS:CB	2.53	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.55
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:92:GLN:N	1:1:94:ILE:CD1	2.69	0.55
1:1:184:ILE:HG22	1:1:185:PRO:O	2.06	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.55
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.55
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.55
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
1:1:98:LYS:CA	1:1:220:ILE:O	2.40	0.55
1:1:210:GLY:C	1:1:212:VAL:CG1	2.75	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.55
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
1:1:145:TYR:HE2	1:1:237:THR:HG1	1.53	0.55
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
1:1:260:THR:HB	1:1:261:HIS:HD2	1.71	0.55
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.55
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.55
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.54
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.22	0.54
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.54
3:3:237:GLU:CG	3:3:238:GLN:N	2.68	0.54
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.54
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.54
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.06	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
1:1:19:ASN:HA	1:1:58:THR:HG23	1.89	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
1:1:183:SER:O	1:1:184:ILE:HG12	2.08	0.54
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.54
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.54
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.54
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.54
1:1:261:HIS:CD2	1:1:261:HIS:N	2.76	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.54
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.70	0.53
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.53
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.23	0.53
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.53
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.53
4:4:26:TYR:CD1	4:4:29:ILE:CD1	2.91	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:89:TYR:HE2	1:1:227:GLU:C	2.12	0.53
1:1:145:TYR:HD1	1:1:145:TYR:H	1.56	0.53
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.24	0.52
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:200:TYR:CE2	1:1:209:TYR:HB2	2.44	0.52
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.38	0.52
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:CD1	1:1:219:THR:CA	2.87	0.52
1:1:101:ILE:HG13	1:1:218:GLY:C	2.29	0.52
1:1:197:TYR:HD1	1:1:198:ASP:N	2.07	0.52
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.28	0.52
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
1:1:197:TYR:CD1	1:1:198:ASP:N	2.78	0.52
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.51
1:1:260:THR:HB	1:1:261:HIS:CD2	2.44	0.51
1:1:265:THR:HG1	2:2:133:ALA:HB2	1.75	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.51
1:1:141:ILE:O	1:1:141:ILE:CG1	2.51	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.51
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.51
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.51
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
1:1:101:ILE:CD1	1:1:219:THR:N	2.73	0.51
1:1:101:ILE:CD1	1:1:219:THR:HA	2.35	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.51
2:2:202:ILE:HD13	2:2:249:MET:HE3	1.93	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
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
1:1:102:THR:O	1:1:103:LEU:HD23	2.11	0.50
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.50
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
1:1:119:VAL:HG11	1:1:121:PHE:CE1	2.30	0.50
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	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
1:1:146:MET:HE3	1:1:162:SER:O	2.12	0.49
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD2	2.47	0.49
1:1:104:GLN:HB2	1:1:262:SER:CB	2.41	0.49
1:1:183:SER:C	1:1:184:ILE:CG1	2.80	0.49
2:2:175:PHE:CD1	2:2:175:PHE:N	2.79	0.49
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.49
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.49
1:1:163:TRP:CH2	1:1:222:SER:C	2.86	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.49
1:1:191:SER:CB	3:3:34:ILE:HG12	2.43	0.49
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.49
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.49
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.49
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.48	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
3:3:14:MET:C	3:3:16:THR:H	2.16	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
1:1:186:PHE:CD1	1:1:186:PHE:C	2.86	0.49
2:2:18:ARG:HA	2:2:18:ARG:HD3	1.57	0.49
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.48
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.78	0.48
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.48
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.48
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.48
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.48
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.48
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.48
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.48
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.48
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	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
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.47
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.27	0.47
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.47
2:2:111:GLN:OE1	2:2:245:SER:OG	2.31	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.47
1:1:186:PHE:CE1	3:3:31:THR:HG22	2.46	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
3:3:237:GLU:HG2	3:3:238:GLN:N	2.18	0.47
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.47
1:1:89:TYR:HD1	1:1:89:TYR:HA	1.49	0.47
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.45	0.47
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.77	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.47
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.47
3:3:82:VAL:HG12	3:3:83:PHE:H	1.78	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.47
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.47
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.47
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.46
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.46
1:1:125:ILE:HD12	1:1:182:PHE:CE1	2.47	0.46
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.97	0.46
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.15	0.46
1:1:101:ILE:HD12	1:1:219:THR:N	2.30	0.46
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.46
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.46
1:1:262:SER:O	1:1:263:HIS:HB2	2.14	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.49	0.46
1:1:224:ILE:HG21	1:1:224:ILE:HD13	1.46	0.46
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.46
3:3:46:MET:HE3	3:3:102:ILE:HD11	1.98	0.46
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.46
1:1:122:ASP:OD1	1:1:245:HIS:HB2	2.16	0.46
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.46
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.98	0.46
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.46
2:2:160:ARG:HH11	2:2:160:ARG:HD2	1.57	0.45
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:101:ILE:CG1	1:1:217:MET:C	2.84	0.45
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.56	0.45
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.04	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:103:LEU:HG	5:1:500:W54:C4	2.47	0.45
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.45
3:3:161:SER:OG	3:3:162:THR:N	2.47	0.45
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.45
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.45
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.45
1:1:75:GLY:N	1:1:240:TYR:HD1	2.15	0.45
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.98	0.45
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.82	0.45
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.54	0.45
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.45
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.47	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.44
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.44
1:1:218:GLY:C	1:1:219:THR:HG23	2.27	0.44
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.17	0.44
1:1:101:ILE:HG13	1:1:218:GLY:HA3	1.97	0.44
1:1:127:LEU:HD12	1:1:239:ILE:HG12	2.00	0.44
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
1:1:90:ASN:HD22	1:1:90:ASN:N	2.16	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.33	0.44
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.44
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.44
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.44
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.44
2:2:155:ASP:HB3	2:2:156:VAL:H	1.61	0.44
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.43
2:2:126:MET:HE2	2:2:126:MET:HB3	1.80	0.43
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.43
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.43
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.43
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.43
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.43
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.43
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.43
1:1:197:TYR:H	2:2:131:GLN:NE2	2.12	0.43
2:2:43:THR:C	2:2:45:GLN:H	2.22	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
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.43
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.43
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.43
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.43
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.43
2:2:107:THR:OG1	2:2:249:MET:HE3	2.18	0.43
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.43
1:1:129:PRO:HA	1:1:237:THR:HA	2.01	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.52	0.43
1:1:99:TRP:CE3	1:1:220:ILE:CD1	2.98	0.43
1:1:271:THR:O	1:1:272:GLY:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:57:ASP:O	2:2:58:THR:CG2	2.66	0.43
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.43
2:2:83:PRO:CG	2:2:218:ASN:HA	2.32	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
2:2:154:ARG:HH11	2:2:154:ARG:HG2	1.83	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.42
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.42
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.42
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.42
1:1:197:TYR:N	2:2:131:GLN:HE21	2.11	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.42
3:3:88:ASP:OD1	3:3:186:ALA:N	2.39	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.42
1:1:182:PHE:CA	3:3:21:SER:HB2	2.47	0.42
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
4:4:26:TYR:HD1	4:4:29:ILE:HD11	1.78	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.42
3:3:216:CYS:C	3:3:218:ASP:H	2.22	0.42
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.02	0.42
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
1:1:99:TRP:O	1:1:219:THR:HA	2.20	0.42
1:1:190:ALA:C	3:3:31:THR:HG21	2.38	0.42
1:1:278:ILE:CD1	3:3:67:MET:HE3	2.40	0.42
2:2:21:SER:OG	2:2:63:PHE:HB2	2.19	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:159:LEU:HD23	3:3:159:LEU:HA	1.72	0.42
1:1:98:LYS:HB3	1:1:221:CYS:SG	2.60	0.41
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.41
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.41
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.41
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.41
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.41
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.55	0.41
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.41
1:1:7:ILE:N	1:1:7:ILE:CD1	2.76	0.41
1:1:124:GLU:N	1:1:242:LYS:O	2.41	0.41
1:1:125:ILE:HD11	1:1:184:ILE:HD12	2.02	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
1:1:261:HIS:H	3:3:237:GLU:H	1.68	0.41
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.41
1:1:136:ASP:O	1:1:137:ASP:CB	2.67	0.41
2:2:63:PHE:CD1	2:2:247:SER:HB2	2.55	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:71:LEU:HD13	1:1:113:PHE:CE1	2.56	0.41
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.41
1:1:165:SER:HG	1:1:170:SER:HG	1.55	0.41
2:2:155:ASP:O	2:2:156:VAL:CB	2.68	0.41
3:3:65:VAL:C	3:3:67:MET:N	2.74	0.41
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	0.41
1:1:184:ILE:HG23	1:1:185:PRO:HD2	2.01	0.41
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.41
3:3:91:SER:C	3:3:92:THR:O	2.58	0.41
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.41
1:1:124:GLU:HB3	1:1:242:LYS:HB3	2.02	0.41
1:1:148:VAL:HA	1:1:149:PRO:HD2	1.79	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
1:1:101:ILE:O	1:1:102:THR:HB	2.21	0.41
1:1:125:ILE:HD13	1:1:125:ILE:HG21	1.79	0.41
1:1:125:ILE:HD13	5:1:500:W54:C1B	2.50	0.41
1:1:165:SER:C	1:1:167:THR:N	2.73	0.41
2:2:175:PHE:HD1	2:2:175:PHE:N	2.18	0.41
3:3:43:LEU:HA	3:3:43:LEU:HD23	1.78	0.41
3:3:72:LEU:CD1	3:3:209:MET:HB3	2.48	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
1:1:169:MET:CE	1:1:171:ILE:CB	2.96	0.41
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.41
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:255:ARG:NH1	1:1:265:THR:O	2.36	0.40
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.03	0.40
2:2:55:GLN:HA	2:2:56:PRO:HD2	1.98	0.40
3:3:14:MET:C	3:3:16:THR:N	2.74	0.40
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.40
1:1:110:ARG:HD3	1:1:259:TYR:CZ	2.56	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.40
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.40
1:1:244:LYS:HZ1	4:4:38:SER:H	1.70	0.40
2:2:228:SER:HA	2:2:229:PRO:HD2	1.68	0.40
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.40
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:252:ARG:HB3	1:1:253:PRO:HD2	2.04	0.40
3:3:53:ILE:HG13	3:3:212:PHE:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:113:ASN:OD1	3:3:195:THR:OG1[3_665]	2.12	0.08
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%)	50 (18%)	24 (8%)	1 12
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1 20
3	3	236/238 (99%)	178 (75%)	38 (16%)	20 (8%)	1 12
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1 21
All	All	785/832 (94%)	595 (76%)	130 (17%)	60 (8%)	1 15

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU
1	1	150	PRO
1	1	158	ARG
1	1	212	VAL
1	1	219	THR
1	1	226	THR
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA
1	1	67	ILE
1	1	90	ASN
1	1	99	TRP
1	1	227	GLU
2	2	91	ILE
2	2	129	GLU
2	2	155	ASP
2	2	193	LEU
2	2	208	ALA
2	2	257	ARG
3	3	59	GLY
3	3	66	SER
3	3	67	MET

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Mol	Chain	Res	Type
3	3	95	ALA
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	137	ASP
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	159	LEU
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	125	ILE
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
2	2	44	PRO
3	3	121	GLY
1	1	101	ILE
3	3	82	VAL

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	254/258 (98%)	182 (72%)	72 (28%)	0   2
2	2	219/227 (96%)	159 (73%)	60 (27%)	0   3
3	3	209/209 (100%)	156 (75%)	53 (25%)	0   4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	4	15/35 (43%)	9 (60%)	6 (40%)	0   0
All	All	697/729 (96%)	506 (73%)	191 (27%)	0   3

All (191) 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	19	ASN
1	1	26	THR
1	1	35	ASP
1	1	44	ASN
1	1	45	VAL
1	1	54	ARG
1	1	60	GLN
1	1	73	ARG
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	103	LEU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
1	1	121	PHE
1	1	123	SER
1	1	126	THR
1	1	127	LEU
1	1	134	ARG
1	1	141	ILE
1	1	142	VAL
1	1	143	MET
1	1	145	TYR
1	1	146	MET
1	1	157	LYS
1	1	158	ARG

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Mol	Chain	Res	Type
1	1	160	ASP
1	1	161	PHE
1	1	162	SER
1	1	173	TRP
1	1	174	GLN
1	1	186	PHE
1	1	197	TYR
1	1	201	ASP
1	1	204	ASN
1	1	209	TYR
1	1	212	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	236	THR
1	1	237	THR
1	1	246	THR
1	1	247	LYS
1	1	250	CYS
1	1	252	ARG
1	1	259	TYR
1	1	265	THR
1	1	274	VAL
1	1	275	THR
1	1	276	THR
1	1	278	ILE
1	1	279	VAL
1	1	281	ARG
1	1	286	THR
2	2	12	ARG
2	2	15	GLN
2	2	17	THR
2	2	18	ARG
2	2	25	SER
2	2	27	ASP

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Mol	Chain	Res	Type
2	2	30	ASN
2	2	43	THR
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	94	GLU
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	126	MET
2	2	136	LYS
2	2	139	SER
2	2	145	LYS
2	2	146	LEU
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	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	192	ASN
2	2	194	ARG
2	2	195	SER
2	2	197	ASN
2	2	198	SER
2	2	200	THR

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Mol	Chain	Res	Type
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	224	ILE
2	2	239	ILE
2	2	240	VAL
2	2	257	ARG
2	2	261	ILE
2	2	262	LYS
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
3	3	39	GLU
3	3	50	ASP
3	3	55	VAL
3	3	56	ASN
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	90	THR
3	3	92	THR
3	3	99	ILE
3	3	116	SER
3	3	119	PHE
3	3	126	THR
3	3	127	LEU
3	3	134	THR
3	3	140	GLU
3	3	142	THR
3	3	143	THR
3	3	148	MET

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Mol	Chain	Res	Type
3	3	157	VAL
3	3	159	LEU
3	3	161	SER
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	201	PRO
3	3	205	GLN
3	3	208	ASP
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	228	ASP
3	3	231	ILE
3	3	236	ILE
3	3	238	GLN
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	204	ASN
1	1	215	ASN
1	1	261	HIS
1	1	282	ASN
2	2	15	GLN

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Mol	Chain	Res	Type
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	197	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
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	196	ASN
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 monosaccharides 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	W54	1	500	-	24,27,27	3.12	5 (20%)	31,36,36	2.83	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W54	1	500	-	-	4/12/20/20	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	12.18	1.43	1.27
5	1	500	W54	C4A-N3A	-6.36	1.36	1.47
5	1	500	W54	O1A-C2A	-4.08	1.29	1.36
5	1	500	W54	C4-C5	-3.64	1.34	1.39
5	1	500	W54	O1A-C5A	-3.13	1.38	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-9.61	109.97	118.23
5	1	500	W54	C4A-N3A-C2A	6.74	112.80	106.77
5	1	500	W54	O1A-C2A-C4B	6.18	124.03	115.85
5	1	500	W54	O1B-C1B-C6B	-4.60	115.21	121.17
5	1	500	W54	O1A-C5A-C4A	3.65	111.71	104.28
5	1	500	W54	O1B-C1B-C2B	3.11	125.20	121.17
5	1	500	W54	C5A-C4A-N3A	-2.42	98.58	104.35
5	1	500	W54	C1C-C5-C4	2.38	134.76	128.60
5	1	500	W54	C5C-O1B-C1B	2.04	120.39	114.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

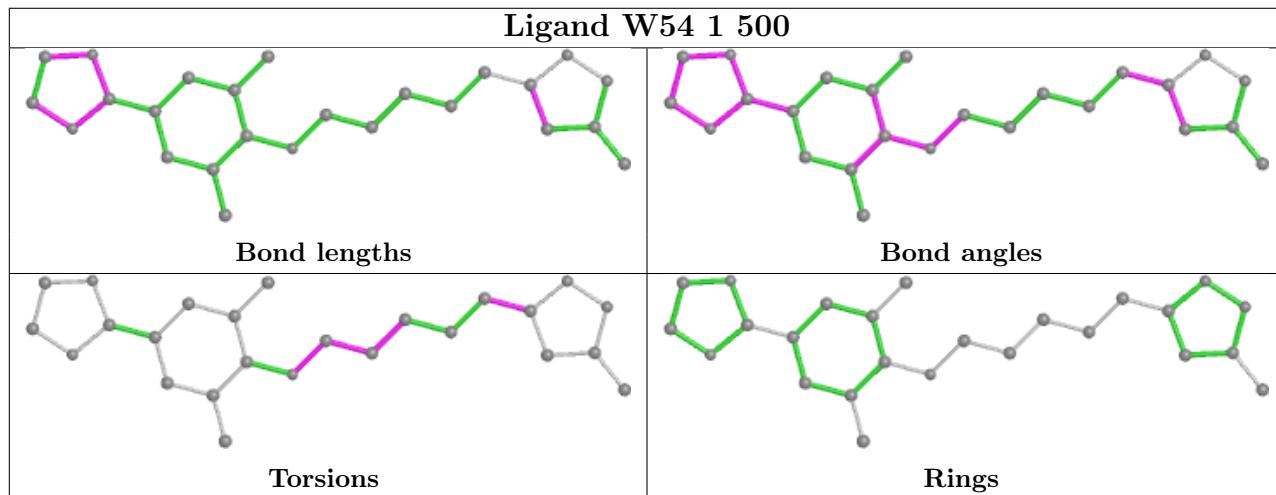
Mol	Chain	Res	Type	Atoms
5	1	500	W54	C2C-C1C-C5-C4
5	1	500	W54	C3C-C4C-C5C-O1B
5	1	500	W54	C2C-C3C-C4C-C5C
5	1	500	W54	C4C-C5C-O1B-C1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4

All chain breaks are listed below:

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

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [\(i\)](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [\(i\)](#)

EDS was not executed - this section is therefore empty.