



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:12 AM UTC

PDB ID : 1R1A / pdb_00001r1a
Title : CRYSTAL STRUCTURE OF HUMAN RHINOVIRUS SEROTYPE 1A (HRV1A)
Authors : Kim, S.; Rossmann, M.G.
Deposited on : 1989-03-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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
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

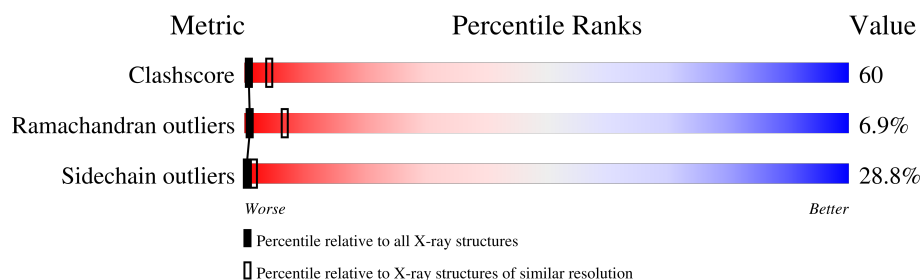
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
5	A	2	

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	GLC	A	1	X	-	X	-
5	FRU	A	2	-	-	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			

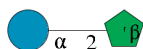
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

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 an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



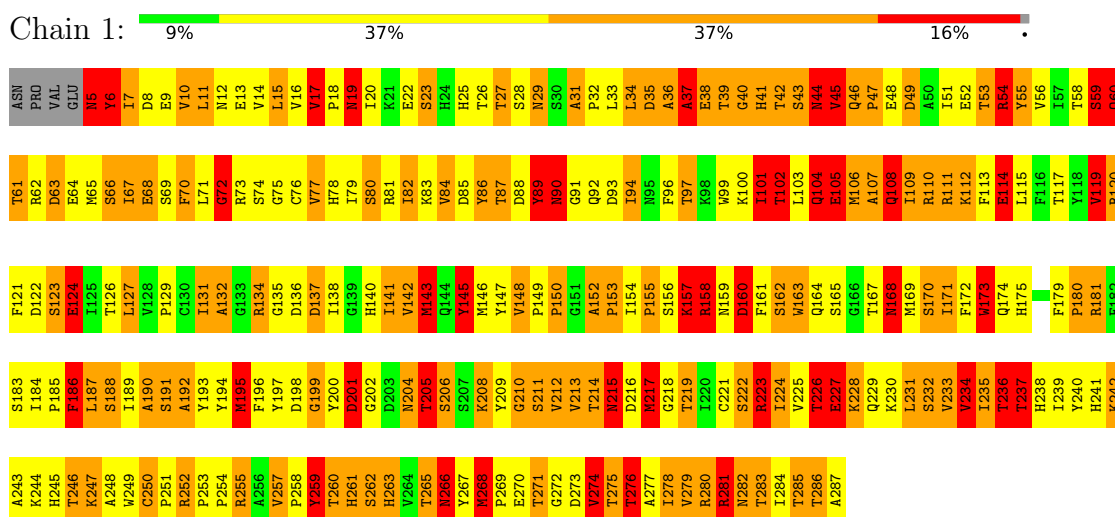
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	A	2	Total	C	O	0	0	0
			23	12	11			

3 Residue-property plots

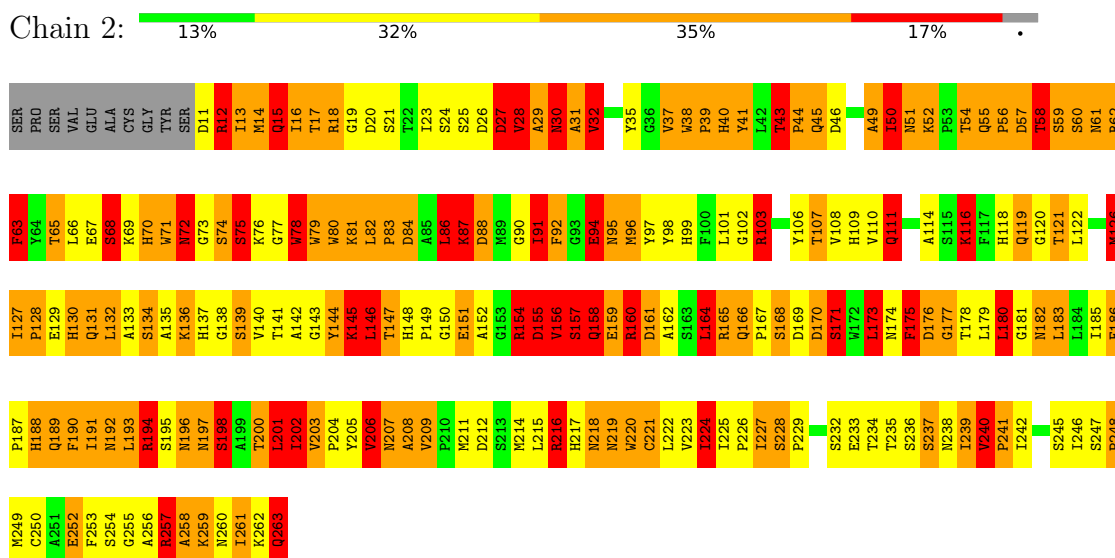
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

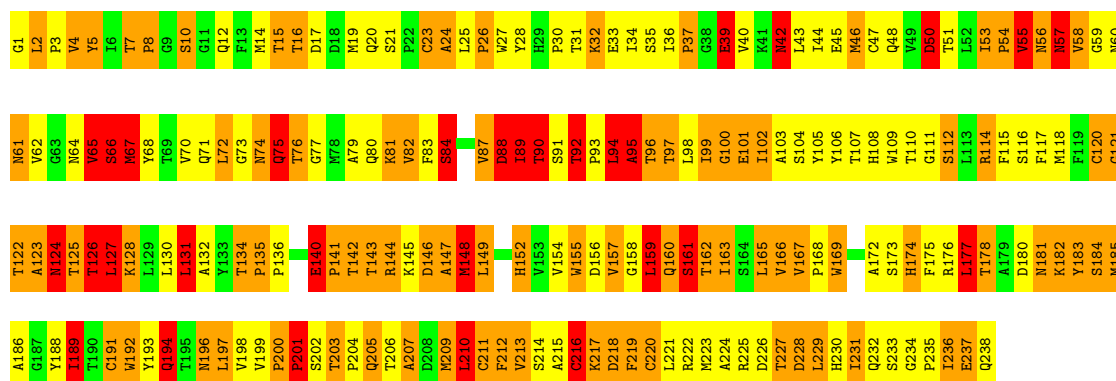
• Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)



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

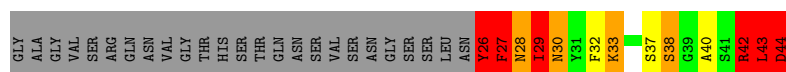


Chain 3:  14% 37% 37% 13%



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

Chain 4:  14% 7% 9% 14% 57%



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain A:  100%



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)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.293 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6246	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: GLC, FRU

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	1.25	1/2322 (0.0%)	3.10	330/3162 (10.4%)
2	2	1.23	1/2033 (0.0%)	3.12	291/2770 (10.5%)
3	3	1.22	0/1878	3.04	229/2570 (8.9%)
4	4	1.46	0/154	3.75	34/206 (16.5%)
All	All	1.24	2/6387 (0.0%)	3.10	884/8708 (10.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	90	ASN	N-CA	5.47	1.53	1.46
2	2	58	THR	CA-CB	5.43	1.62	1.53

All (884) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	62	ARG	CD-NE-CZ	24.28	158.39	124.40
1	1	164	GLN	OE1-CD-NE2	-16.43	106.17	122.60
3	3	222	ARG	CD-NE-CZ	15.35	145.89	124.40
2	2	72	ASN	OD1-CG-ND2	14.94	137.54	122.60
1	1	187	LEU	CA-C-O	-14.80	102.67	122.51
3	3	235	PRO	CA-C-N	14.35	141.01	122.93
3	3	235	PRO	C-N-CA	14.35	141.01	122.93
1	1	68	GLU	CB-CG-CD	14.22	136.77	112.60
3	3	218	ASP	CA-CB-CG	-13.79	98.81	112.60
2	2	196	ASN	OD1-CG-ND2	13.74	136.34	122.60
1	1	110	ARG	CD-NE-CZ	13.72	143.61	124.40
3	3	212	PHE	CA-CB-CG	13.55	127.35	113.80
2	2	218	ASN	CA-CB-CG	13.43	126.03	112.60
1	1	108	GLN	CA-C-N	13.28	142.85	121.34
1	1	108	GLN	C-N-CA	13.28	142.85	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	203	THR	O-C-N	13.22	131.27	121.88
2	2	187	PRO	CB-CA-C	13.10	128.14	111.64
1	1	274	VAL	N-CA-CB	13.07	125.33	110.82
1	1	281	ARG	CA-CB-CG	13.07	140.23	114.10
2	2	154	ARG	CA-C-N	12.60	145.60	121.54
2	2	154	ARG	C-N-CA	12.60	145.60	121.54
3	3	64	ASN	OD1-CG-ND2	12.00	134.60	122.60
2	2	169	ASP	CA-CB-CG	11.79	124.39	112.60
3	3	144	ARG	CD-NE-CZ	11.75	140.85	124.40
3	3	232	GLN	N-CA-CB	11.59	126.22	110.57
1	1	111	ARG	CA-C-N	11.56	136.15	120.54
1	1	111	ARG	C-N-CA	11.56	136.15	120.54
3	3	24	ALA	CA-C-O	-11.48	109.24	121.87
4	4	27	PHE	CA-CB-CG	11.34	125.14	113.80
2	2	106	TYR	CA-C-N	11.26	138.65	122.77
2	2	106	TYR	C-N-CA	11.26	138.65	122.77
1	1	60	GLN	O-C-N	11.24	136.68	123.30
2	2	216	ARG	NE-CZ-NH2	-11.05	109.25	119.20
1	1	10	VAL	CB-CA-C	10.98	120.73	111.06
2	2	241	PRO	CA-C-N	10.89	141.57	121.97
2	2	241	PRO	C-N-CA	10.89	141.57	121.97
1	1	134	ARG	NE-CZ-NH1	10.80	132.30	121.50
3	3	92	THR	CB-CA-C	10.79	131.44	110.17
1	1	61	THR	CA-CB-OG1	-10.77	93.44	109.60
1	1	199	GLY	O-C-N	10.73	132.93	123.60
1	1	172	PHE	CA-C-O	-10.63	108.88	120.36
3	3	207	ALA	O-C-N	10.55	134.71	123.42
1	1	77	VAL	O-C-N	10.55	132.64	121.78
1	1	227	GLU	CB-CG-CD	10.53	130.49	112.60
3	3	73	GLY	CA-C-O	10.45	132.56	121.90
3	3	76	THR	O-C-N	10.42	132.81	122.07
1	1	255	ARG	CD-NE-CZ	10.35	138.89	124.40
3	3	57	ASN	CB-CG-ND2	-10.35	100.88	116.40
1	1	13	GLU	O-C-N	10.30	132.91	122.30
2	2	130	HIS	CA-CB-CG	-10.27	103.53	113.80
3	3	64	ASN	CA-CB-CG	-10.27	102.33	112.60
1	1	11	LEU	O-C-N	10.26	136.52	122.46
3	3	56	ASN	CA-C-N	10.25	141.11	121.54
3	3	56	ASN	C-N-CA	10.25	141.11	121.54
1	1	54	ARG	CG-CD-NE	10.22	134.50	112.00
3	3	67	MET	N-CA-CB	-10.18	93.29	110.49
2	2	240	VAL	CB-CA-C	10.16	120.73	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	280	ARG	NE-CZ-NH2	-10.10	110.11	119.20
2	2	17	THR	CB-CA-C	10.10	127.98	109.70
2	2	16	ILE	CA-C-O	-10.01	109.75	120.76
2	2	158	GLN	OE1-CD-NE2	9.98	132.58	122.60
1	1	105	GLU	CA-CB-CG	9.95	134.00	114.10
2	2	237	SER	CA-C-O	9.91	130.87	119.27
4	4	30	ASN	CA-CB-CG	-9.87	102.73	112.60
3	3	53	ILE	N-CA-C	9.81	118.92	107.73
2	2	237	SER	N-CA-C	-9.79	101.09	113.23
2	2	169	ASP	CA-C-O	9.78	131.62	119.11
3	3	58	VAL	N-CA-C	9.76	121.83	108.17
2	2	161	ASP	N-CA-CB	9.75	124.61	109.69
3	3	232	GLN	O-C-N	9.74	134.05	122.46
4	4	28	ASN	OD1-CG-ND2	9.68	132.28	122.60
2	2	248	PRO	N-CA-C	-9.66	95.85	111.21
2	2	12	ARG	CD-NE-CZ	9.63	137.88	124.40
1	1	105	GLU	N-CA-C	-9.61	101.07	113.17
1	1	257	VAL	CB-CA-C	9.61	120.65	110.37
4	4	40	ALA	N-CA-C	-9.58	96.34	110.23
1	1	45	VAL	CB-CA-C	9.55	124.65	110.90
1	1	211	SER	O-C-N	9.49	135.22	122.59
2	2	26	ASP	CA-CB-CG	9.48	122.08	112.60
1	1	10	VAL	CA-C-O	9.42	127.20	119.29
3	3	37	PRO	N-CA-CB	9.39	110.81	103.30
3	3	134	THR	CA-C-O	9.38	127.30	119.71
1	1	110	ARG	NE-CZ-NH2	-9.37	110.77	119.20
1	1	260	THR	CA-C-O	-9.36	108.56	119.98
1	1	211	SER	CA-C-O	-9.35	107.13	120.51
1	1	154	ILE	O-C-N	9.34	130.11	121.61
2	2	57	ASP	N-CA-CB	-9.34	95.66	110.69
2	2	20	ASP	N-CA-C	-9.30	101.45	113.17
2	2	164	LEU	O-C-N	9.27	133.95	123.01
1	1	188	SER	CA-C-O	-9.24	110.34	121.06
3	3	74	ASN	OD1-CG-ND2	9.22	131.82	122.60
2	2	162	ALA	CB-CA-C	9.19	125.44	110.09
4	4	40	ALA	O-C-N	9.15	134.13	122.87
1	1	106	MET	CA-CB-CG	-9.14	95.82	114.10
4	4	44	ASP	CA-CB-CG	9.13	121.73	112.60
3	3	227	THR	CA-C-O	9.11	131.89	121.87
1	1	19	ASN	OD1-CG-ND2	9.08	131.68	122.60
1	1	88	ASP	CA-C-O	9.06	130.00	120.30
2	2	71	TRP	CB-CA-C	9.05	125.55	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	206	SER	O-C-N	9.03	132.44	122.05
3	3	96	THR	CA-C-N	9.00	133.59	120.90
3	3	96	THR	C-N-CA	9.00	133.59	120.90
3	3	155	TRP	CA-C-O	-8.97	110.70	120.30
2	2	234	THR	CA-C-O	8.93	132.33	121.89
3	3	114	ARG	N-CA-C	8.92	122.95	108.41
2	2	49	ALA	CA-C-O	-8.91	107.77	120.51
4	4	37	SER	O-C-N	8.90	134.35	123.13
2	2	16	ILE	O-C-N	8.90	132.93	123.05
2	2	19	GLY	CA-C-N	8.89	137.21	122.54
2	2	19	GLY	C-N-CA	8.89	137.21	122.54
2	2	61	ASN	CB-CA-C	8.88	125.89	112.03
3	3	32	LYS	CA-C-O	-8.88	111.99	122.03
2	2	182	ASN	N-CA-C	-8.88	100.29	113.61
4	4	42	ARG	CD-NE-CZ	8.87	136.81	124.40
1	1	101	ILE	N-CA-CB	-8.87	98.35	110.05
2	2	20	ASP	CA-C-O	8.86	129.71	119.35
2	2	107	THR	CA-CB-OG1	-8.85	96.32	109.60
1	1	12	ASN	CA-CB-CG	8.83	121.43	112.60
2	2	40	HIS	CA-CB-CG	-8.82	104.98	113.80
3	3	193	TYR	O-C-N	8.81	133.38	123.16
2	2	61	ASN	OD1-CG-ND2	8.81	131.41	122.60
2	2	81	LYS	O-C-N	8.80	133.66	123.27
2	2	57	ASP	CA-C-O	-8.79	111.40	120.71
3	3	54	PRO	CA-C-O	-8.76	110.67	120.92
3	3	108	HIS	CA-CB-CG	8.76	122.56	113.80
1	1	212	VAL	O-C-N	8.73	133.49	122.57
4	4	37	SER	CA-C-O	-8.72	111.12	120.46
3	3	203	THR	CA-C-O	-8.71	111.31	120.28
1	1	159	ASN	CA-CB-CG	8.70	121.30	112.60
3	3	45	GLU	CB-CG-CD	8.66	127.33	112.60
2	2	101	LEU	CA-C-O	8.65	130.31	120.54
3	3	53	ILE	O-C-N	8.63	129.15	121.12
3	3	210	LEU	CA-C-N	-8.61	109.19	122.62
3	3	210	LEU	C-N-CA	-8.61	109.19	122.62
2	2	147	THR	N-CA-CB	8.57	124.01	110.73
2	2	63	PHE	N-CA-C	8.56	123.41	108.52
1	1	80	SER	CA-C-O	8.53	130.64	120.92
3	3	191	CYS	CA-C-O	-8.52	110.38	120.60
2	2	192	ASN	OD1-CG-ND2	8.52	131.12	122.60
1	1	70	PHE	N-CA-C	-8.45	100.70	112.45
1	1	110	ARG	N-CA-C	-8.44	102.04	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	ASP	CA-CB-CG	8.44	121.03	112.60
2	2	196	ASN	N-CA-CB	-8.41	98.86	110.38
3	3	26	PRO	O-C-N	8.38	133.37	123.06
3	3	205	GLN	OE1-CD-NE2	8.37	130.97	122.60
2	2	62	ARG	NH1-CZ-NH2	-8.35	108.45	119.30
2	2	92	PHE	CA-CB-CG	8.35	122.15	113.80
1	1	25	HIS	CA-C-O	-8.34	111.97	121.81
1	1	204	ASN	CA-C-O	8.34	130.29	120.70
3	3	218	ASP	N-CA-CB	-8.34	97.98	110.07
2	2	196	ASN	CA-CB-CG	-8.33	104.27	112.60
4	4	38	SER	O-C-N	8.31	133.65	122.59
2	2	135	ALA	CA-C-O	8.28	129.51	119.49
2	2	181	GLY	N-CA-C	-8.25	103.71	114.85
2	2	189	GLN	CA-CB-CG	8.25	130.60	114.10
1	1	46	GLN	O-C-N	8.23	130.78	121.32
2	2	220	TRP	CA-C-O	8.23	129.93	120.80
1	1	49	ASP	CA-CB-CG	-8.21	104.39	112.60
1	1	35	ASP	CA-C-O	-8.19	112.34	121.51
3	3	32	LYS	O-C-N	8.18	132.33	122.68
1	1	252	ARG	O-C-N	8.18	127.93	121.55
1	1	86	TYR	CB-CA-C	8.16	122.74	109.02
2	2	28	VAL	CA-CB-CG1	8.16	124.28	110.40
2	2	83	PRO	CB-CA-C	8.16	125.89	112.26
2	2	147	THR	O-C-N	8.16	131.96	122.25
1	1	59	SER	N-CA-CB	-8.16	96.70	110.49
3	3	206	THR	N-CA-C	-8.14	96.64	109.50
3	3	95	ALA	CA-C-O	-8.11	108.91	120.51
1	1	270	GLU	N-CA-CB	8.10	122.68	109.88
2	2	31	ALA	N-CA-CB	8.08	123.85	111.56
2	2	218	ASN	CB-CG-ND2	8.02	128.44	116.40
1	1	12	ASN	OD1-CG-ND2	-8.01	114.59	122.60
2	2	203	VAL	N-CA-CB	-8.00	100.01	111.21
1	1	217	MET	CA-C-O	-7.98	109.78	119.59
2	2	257	ARG	NE-CZ-NH2	-7.96	112.04	119.20
1	1	25	HIS	O-C-N	7.95	131.91	122.85
3	3	227	THR	N-CA-C	7.93	120.82	110.43
2	2	91	ILE	N-CA-CB	7.93	124.31	111.23
1	1	100	LYS	CA-C-N	7.92	132.25	120.69
1	1	100	LYS	C-N-CA	7.92	132.25	120.69
1	1	5	ASN	CA-CB-CG	7.92	120.52	112.60
2	2	160	ARG	N-CA-CB	-7.90	98.30	111.57
2	2	183	LEU	O-C-N	7.88	132.99	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	251	PRO	CA-C-O	7.88	130.70	121.56
3	3	90	THR	N-CA-CB	7.86	122.94	111.54
2	2	50	ILE	CA-CB-CG2	7.86	123.86	110.50
2	2	161	ASP	O-C-N	7.86	132.69	122.95
2	2	188	HIS	N-CA-C	7.86	118.61	108.24
3	3	50	ASP	CA-C-O	7.86	129.60	120.49
1	1	234	VAL	CA-C-O	7.83	128.97	120.43
3	3	36	ILE	N-CA-CB	7.83	122.16	111.21
1	1	28	SER	N-CA-C	7.80	122.11	109.40
2	2	156	VAL	CA-C-N	7.80	136.43	121.54
2	2	156	VAL	C-N-CA	7.80	136.43	121.54
3	3	199	VAL	O-C-N	7.80	129.99	121.10
2	2	156	VAL	CA-C-O	7.79	130.51	120.78
1	1	13	GLU	CA-C-O	-7.78	112.66	119.97
4	4	38	SER	CA-C-O	-7.78	109.39	120.51
1	1	168	ASN	CA-C-N	-7.76	112.29	123.00
1	1	168	ASN	C-N-CA	-7.76	112.29	123.00
3	3	233	SER	CA-C-O	7.76	131.29	122.37
2	2	29	ALA	N-CA-CB	7.75	123.48	110.69
3	3	42	ASN	OD1-CG-ND2	7.74	130.34	122.60
4	4	43	LEU	N-CA-C	7.69	122.57	112.72
2	2	119	GLN	OE1-CD-NE2	7.69	130.29	122.60
1	1	255	ARG	CA-C-O	-7.68	111.86	120.54
1	1	196	PHE	CA-C-O	-7.65	113.25	121.36
1	1	285	THR	CA-C-O	-7.62	111.48	120.10
2	2	72	ASN	CA-CB-CG	-7.62	104.98	112.60
3	3	55	VAL	CB-CA-C	7.61	123.78	111.29
1	1	122	ASP	CA-CB-CG	-7.60	105.00	112.60
1	1	227	GLU	CG-CD-OE1	7.60	135.87	118.40
3	3	168	PRO	CA-C-N	-7.59	112.97	122.84
3	3	168	PRO	C-N-CA	-7.59	112.97	122.84
2	2	161	ASP	CA-CB-CG	-7.59	105.01	112.60
3	3	35	SER	CA-C-O	-7.59	112.08	120.81
2	2	160	ARG	N-CA-C	7.59	119.67	108.14
1	1	275	THR	OG1-CB-CG2	7.58	124.45	109.30
1	1	44	ASN	CA-CB-CG	-7.57	105.03	112.60
1	1	134	ARG	NH1-CZ-NH2	-7.57	109.46	119.30
2	2	32	VAL	O-C-N	7.57	131.45	123.05
4	4	42	ARG	CA-C-N	-7.55	108.88	122.46
4	4	42	ARG	C-N-CA	-7.55	108.88	122.46
2	2	12	ARG	CG-CD-NE	7.54	128.58	112.00
1	1	38	GLU	CB-CG-CD	7.53	125.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	111	GLN	CB-CG-CD	7.53	125.40	112.60
2	2	182	ASN	O-C-N	7.51	131.06	122.20
3	3	200	PRO	N-CA-C	-7.48	101.57	110.70
1	1	202	GLY	CA-C-N	7.48	135.99	121.18
1	1	202	GLY	C-N-CA	7.48	135.99	121.18
4	4	32	PHE	CA-C-N	7.47	131.17	120.79
4	4	32	PHE	C-N-CA	7.47	131.17	120.79
2	2	169	ASP	N-CA-C	-7.46	104.15	113.18
2	2	224	ILE	CB-CA-C	7.45	120.48	110.42
1	1	34	LEU	CA-C-O	-7.45	112.80	120.54
2	2	233	GLU	CA-C-O	7.42	127.23	119.51
1	1	181	ARG	CG-CD-NE	7.41	128.30	112.00
1	1	70	PHE	O-C-N	7.41	133.17	122.28
3	3	57	ASN	CA-CB-CG	-7.40	105.20	112.60
1	1	159	ASN	CA-C-O	-7.40	112.41	121.58
1	1	49	ASP	N-CA-C	7.39	119.12	111.14
1	1	215	ASN	O-C-N	7.38	131.94	122.87
1	1	104	GLN	CA-C-O	-7.37	112.03	121.17
3	3	160	GLN	OE1-CD-NE2	-7.37	115.23	122.60
1	1	226	THR	N-CA-C	7.36	126.48	110.80
1	1	111	ARG	CD-NE-CZ	7.36	134.70	124.40
3	3	185	MET	N-CA-CB	7.34	121.02	109.71
1	1	271	THR	CA-CB-OG1	-7.33	98.61	109.60
3	3	89	ILE	CB-CA-C	-7.33	99.28	111.29
1	1	213	VAL	O-C-N	7.31	129.06	121.89
2	2	70	HIS	CA-C-N	-7.31	112.73	123.11
2	2	70	HIS	C-N-CA	-7.31	112.73	123.11
1	1	147	TYR	CA-C-O	-7.31	112.28	120.32
2	2	233	GLU	CG-CD-OE1	7.30	135.19	118.40
2	2	126	MET	CA-CB-CG	-7.29	99.52	114.10
3	3	163	ILE	N-CA-C	-7.29	97.98	108.48
1	1	31	ALA	O-C-N	7.28	128.20	120.85
2	2	86	LEU	CA-C-O	7.28	129.35	120.55
3	3	50	ASP	CA-CB-CG	7.26	119.86	112.60
1	1	5	ASN	N-CA-CB	7.26	122.84	110.50
1	1	158	ARG	CD-NE-CZ	7.25	134.56	124.40
1	1	8	ASP	CA-CB-CG	-7.25	105.35	112.60
2	2	155	ASP	CA-CB-CG	7.24	119.84	112.60
1	1	173	TRP	CA-CB-CG	7.22	127.32	113.60
1	1	189	ILE	CA-C-N	7.22	134.41	122.07
1	1	189	ILE	C-N-CA	7.22	134.41	122.07
3	3	201	PRO	N-CA-C	7.21	127.31	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	16	VAL	CB-CA-C	7.20	122.19	111.31
2	2	52	LYS	CG-CD-CE	7.19	127.84	111.30
3	3	123	ALA	CA-C-O	-7.19	111.86	120.56
3	3	67	MET	CA-C-N	7.18	133.52	122.24
3	3	67	MET	C-N-CA	7.18	133.52	122.24
3	3	161	SER	CA-C-N	-7.18	111.68	122.74
3	3	161	SER	C-N-CA	-7.18	111.68	122.74
2	2	78	TRP	CA-CB-CG	7.17	127.23	113.60
3	3	218	ASP	CA-C-N	7.17	135.22	121.54
3	3	218	ASP	C-N-CA	7.17	135.22	121.54
1	1	23	SER	CA-C-O	7.16	129.88	121.58
1	1	55	TYR	O-C-N	7.14	132.09	122.59
3	3	161	SER	CB-CA-C	-7.14	96.21	110.42
1	1	164	GLN	CG-CD-OE1	7.14	135.07	120.80
1	1	231	LEU	CA-CB-CG	7.14	141.28	116.30
2	2	130	HIS	O-C-N	7.13	132.17	122.83
2	2	220	TRP	CA-C-N	7.12	133.71	122.74
2	2	220	TRP	C-N-CA	7.12	133.71	122.74
1	1	231	LEU	CB-CA-C	7.12	121.45	109.84
1	1	233	VAL	CB-CA-C	-7.12	99.61	111.29
3	3	114	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	1	163	TRP	N-CA-C	-7.10	104.62	112.72
3	3	70	VAL	CA-C-N	-7.10	112.18	122.19
3	3	70	VAL	C-N-CA	-7.10	112.18	122.19
1	1	145	TYR	N-CA-CB	7.10	122.25	110.47
3	3	216	CYS	CA-C-O	-7.08	113.16	121.44
2	2	147	THR	N-CA-C	-7.07	103.76	112.88
2	2	176	ASP	N-CA-C	-7.07	104.30	114.12
2	2	114	ALA	CA-C-O	-7.05	110.42	120.51
1	1	124	GLU	CA-C-O	7.05	127.84	120.30
2	2	256	ALA	CA-C-O	-7.04	113.88	121.56
3	3	237	GLU	CA-C-O	7.04	130.58	120.51
1	1	82	ILE	CB-CA-C	-7.04	99.75	111.29
3	3	218	ASP	CA-C-O	7.01	127.92	120.70
2	2	127	ILE	O-C-N	7.01	129.09	121.10
1	1	217	MET	CB-CA-C	-7.00	98.69	110.81
2	2	205	TYR	CA-C-O	-6.99	113.10	120.58
2	2	52	LYS	CA-CB-CG	6.98	128.07	114.10
3	3	101	GLU	CA-C-O	6.98	128.02	120.20
1	1	134	ARG	CD-NE-CZ	6.98	134.17	124.40
2	2	134	SER	CA-C-O	6.96	128.93	120.92
2	2	168	SER	CA-C-O	6.96	128.23	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	61	THR	CB-CA-C	6.95	121.25	109.50
4	4	28	ASN	CA-C-N	-6.94	109.48	121.97
4	4	28	ASN	C-N-CA	-6.94	109.48	121.97
3	3	210	LEU	CA-C-O	-6.94	113.09	121.28
2	2	190	PHE	CA-CB-CG	6.93	120.73	113.80
1	1	246	THR	N-CA-C	6.93	120.74	110.48
3	3	201	PRO	CA-C-N	-6.93	112.17	122.36
3	3	201	PRO	C-N-CA	-6.93	112.17	122.36
2	2	67	GLU	CA-C-O	-6.92	113.16	121.05
1	1	224	ILE	CB-CG1-CD1	-6.92	99.28	113.80
2	2	82	LEU	N-CA-C	6.92	125.09	109.81
2	2	237	SER	CB-CA-C	6.89	123.54	109.55
4	4	43	LEU	O-C-N	6.89	130.56	122.09
1	1	41	HIS	CA-C-N	-6.88	111.78	122.87
1	1	41	HIS	C-N-CA	-6.88	111.78	122.87
1	1	283	THR	O-C-N	6.88	131.25	123.27
3	3	160	GLN	O-C-N	6.88	131.74	122.59
3	3	70	VAL	O-C-N	6.88	129.16	122.97
1	1	215	ASN	OD1-CG-ND2	6.87	129.47	122.60
2	2	126	MET	CA-C-O	-6.87	113.25	121.56
4	4	29	ILE	O-C-N	6.86	131.15	122.57
1	1	8	ASP	CA-C-N	6.84	133.75	121.92
1	1	8	ASP	C-N-CA	6.84	133.75	121.92
1	1	138	ILE	N-CA-C	6.84	122.37	113.07
1	1	243	ALA	CA-C-O	6.83	127.65	120.54
1	1	71	LEU	CA-C-O	-6.83	112.29	120.56
1	1	152	ALA	N-CA-CB	-6.83	103.93	111.10
1	1	287	ALA	CA-C-O	-6.83	109.19	120.80
2	2	70	HIS	CA-CB-CG	-6.82	106.98	113.80
1	1	147	TYR	O-C-N	6.81	131.31	123.27
3	3	160	GLN	N-CA-CB	6.81	121.99	110.49
2	2	87	LYS	CB-CG-CD	6.80	126.94	111.30
3	3	146	ASP	CB-CG-OD2	-6.80	102.77	118.40
3	3	15	THR	CB-CA-C	6.79	123.44	110.27
1	1	248	ALA	CA-C-N	6.78	133.12	122.94
1	1	248	ALA	C-N-CA	6.78	133.12	122.94
3	3	225	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	1	217	MET	O-C-N	6.78	131.04	122.37
1	1	78	HIS	CA-CB-CG	-6.77	107.03	113.80
3	3	89	ILE	CA-C-O	-6.77	112.32	120.78
1	1	179	PHE	O-C-N	6.76	126.92	121.38
3	3	234	GLY	O-C-N	6.75	128.52	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	119	GLN	CB-CA-C	6.75	121.47	109.65
3	3	65	VAL	N-CA-CB	6.74	120.18	110.68
2	2	80	TRP	N-CA-CB	6.74	123.19	111.00
3	3	58	VAL	CA-C-O	6.73	127.62	120.48
2	2	171	SER	CA-C-N	6.71	131.44	120.63
2	2	171	SER	C-N-CA	6.71	131.44	120.63
1	1	64	GLU	CA-CB-CG	6.71	127.52	114.10
2	2	31	ALA	O-C-N	6.71	130.10	123.46
1	1	275	THR	CA-CB-OG1	-6.70	99.55	109.60
2	2	198	SER	CB-CA-C	-6.69	97.33	113.19
1	1	45	VAL	O-C-N	6.69	130.13	122.97
1	1	55	TYR	CA-C-N	-6.69	113.48	122.98
1	1	55	TYR	C-N-CA	-6.69	113.48	122.98
3	3	90	THR	N-CA-C	-6.68	102.34	111.56
1	1	215	ASN	N-CA-C	6.67	120.17	107.75
1	1	63	ASP	CA-C-O	-6.67	114.03	120.90
2	2	158	GLN	CB-CG-CD	-6.67	101.26	112.60
2	2	83	PRO	CA-C-N	6.67	135.84	121.64
2	2	83	PRO	C-N-CA	6.67	135.84	121.64
3	3	203	THR	N-CA-C	-6.67	97.55	108.82
1	1	53	THR	N-CA-CB	-6.66	101.25	110.38
1	1	268	MET	O-C-N	6.64	128.96	121.32
3	3	206	THR	CA-CB-OG1	-6.64	99.64	109.60
1	1	164	GLN	N-CA-C	-6.63	104.21	112.90
2	2	177	GLY	CA-C-N	6.63	131.77	121.76
2	2	177	GLY	C-N-CA	6.63	131.77	121.76
1	1	223	ARG	NE-CZ-NH2	6.63	125.17	119.20
3	3	71	GLN	OE1-CD-NE2	6.62	129.22	122.60
3	3	147	ALA	CA-C-N	6.62	131.19	120.60
3	3	147	ALA	C-N-CA	6.62	131.19	120.60
1	1	100	LYS	CA-C-O	6.61	127.41	120.54
2	2	155	ASP	N-CA-CB	6.61	121.66	110.49
1	1	190	ALA	CA-C-O	-6.60	113.44	121.36
3	3	128	LYS	CB-CA-C	-6.58	102.80	111.42
2	2	150	GLY	O-C-N	6.57	131.24	122.70
3	3	94	LEU	CA-C-O	-6.55	111.14	120.51
2	2	168	SER	CA-C-N	6.55	134.35	121.58
2	2	168	SER	C-N-CA	6.55	134.35	121.58
3	3	87	VAL	N-CA-C	6.54	121.20	112.04
1	1	62	ARG	N-CA-C	-6.54	103.63	112.26
3	3	169	TRP	CB-CA-C	6.54	121.24	110.78
1	1	270	GLU	O-C-N	6.53	131.37	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	130	HIS	CA-C-O	-6.53	113.76	122.51
1	1	52	GLU	O-C-N	6.53	130.68	122.84
2	2	232	SER	N-CA-CB	6.53	121.62	110.65
3	3	88	ASP	CA-CB-CG	6.53	119.13	112.60
3	3	10	SER	CB-CA-C	6.53	120.08	109.90
2	2	202	ILE	CA-C-O	-6.52	113.37	120.67
1	1	150	PRO	CA-C-O	6.52	128.77	121.34
2	2	161	ASP	CB-CA-C	-6.51	99.75	109.90
2	2	68	SER	CA-CB-OG	6.50	124.11	111.10
1	1	281	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	1	223	ARG	CA-C-O	6.50	128.75	121.40
1	1	280	ARG	NH1-CZ-NH2	6.50	127.75	119.30
3	3	15	THR	N-CA-CB	-6.50	98.98	110.42
3	3	165	LEU	O-C-N	6.50	130.96	123.29
3	3	70	VAL	CA-C-O	-6.49	114.44	120.22
2	2	180	LEU	CA-C-O	-6.48	113.90	120.96
1	1	52	GLU	CA-C-N	6.48	133.24	121.06
1	1	52	GLU	C-N-CA	6.48	133.24	121.06
3	3	56	ASN	CA-CB-CG	-6.46	106.14	112.60
1	1	175	HIS	N-CA-CB	-6.46	99.58	110.49
1	1	234	VAL	CB-CA-C	6.45	120.47	110.28
3	3	16	THR	CA-CB-CG2	6.43	121.44	110.50
3	3	64	ASN	CB-CG-ND2	-6.43	106.76	116.40
3	3	206	THR	OG1-CB-CG2	6.43	122.16	109.30
1	1	201	ASP	CA-C-N	6.43	129.69	120.56
1	1	201	ASP	C-N-CA	6.43	129.69	120.56
1	1	223	ARG	CA-CB-CG	6.42	126.95	114.10
1	1	180	PRO	CB-CA-C	6.42	119.90	110.85
3	3	106	TYR	CA-C-O	-6.42	113.93	121.44
1	1	132	ALA	CA-C-O	6.42	127.61	120.43
3	3	72	LEU	N-CA-C	-6.41	98.76	108.96
1	1	204	ASN	N-CA-CB	6.41	119.64	109.51
2	2	54	THR	N-CA-CB	6.41	120.73	110.16
2	2	206	VAL	CB-CA-C	6.40	120.36	110.83
2	2	50	ILE	CB-CA-C	6.39	121.77	111.29
2	2	103	ARG	CD-NE-CZ	6.39	133.34	124.40
2	2	91	ILE	CA-C-O	-6.38	112.80	120.78
1	1	195	MET	N-CA-C	-6.38	104.76	112.54
1	1	66	SER	O-C-N	6.37	130.88	123.30
1	1	263	HIS	O-C-N	6.37	129.96	122.00
2	2	152	ALA	N-CA-CB	-6.37	100.08	110.14
1	1	104	GLN	OE1-CD-NE2	-6.36	116.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	201	ASP	O-C-N	6.36	129.40	122.15
1	1	214	THR	N-CA-C	6.36	121.29	111.56
2	2	176	ASP	CB-CA-C	6.35	120.06	109.38
3	3	226	ASP	OD1-CG-OD2	-6.35	107.65	122.90
2	2	157	SER	CA-C-N	-6.35	112.14	122.81
2	2	157	SER	C-N-CA	-6.35	112.14	122.81
4	4	42	ARG	NE-CZ-NH1	6.35	127.85	121.50
2	2	228	SER	CA-C-N	6.35	126.37	119.90
2	2	228	SER	C-N-CA	6.35	126.37	119.90
1	1	94	ILE	O-C-N	6.34	130.23	123.00
1	1	285	THR	CA-CB-OG1	-6.33	100.10	109.60
3	3	27	TRP	CA-C-N	-6.33	114.27	123.00
3	3	27	TRP	C-N-CA	-6.33	114.27	123.00
2	2	228	SER	O-C-N	6.33	128.38	121.36
1	1	49	ASP	CA-C-N	6.32	131.43	120.68
1	1	49	ASP	C-N-CA	6.32	131.43	120.68
1	1	5	ASN	O-C-N	6.32	133.11	123.00
2	2	183	LEU	CA-C-O	-6.32	111.61	119.38
2	2	238	ASN	O-C-N	6.32	130.51	122.93
2	2	68	SER	N-CA-CB	6.32	120.02	110.42
4	4	40	ALA	N-CA-CB	6.32	119.37	109.83
2	2	183	LEU	N-CA-C	-6.31	104.84	112.54
1	1	47	PRO	CB-CA-C	6.31	121.97	111.56
1	1	174	GLN	CB-CG-CD	6.31	123.33	112.60
1	1	20	ILE	O-C-N	6.30	132.03	122.76
1	1	201	ASP	CA-C-O	-6.30	113.74	120.42
1	1	39	THR	O-C-N	6.30	131.16	122.46
3	3	235	PRO	CA-C-O	6.30	135.32	120.20
3	3	100	GLY	O-C-N	6.29	128.36	122.13
1	1	268	MET	CA-CB-CG	-6.29	101.52	114.10
3	3	77	GLY	CA-C-O	6.29	130.74	122.75
2	2	56	PRO	CA-C-O	6.28	128.19	121.03
1	1	19	ASN	CA-CB-CG	-6.28	106.32	112.60
2	2	81	LYS	CA-CB-CG	6.28	126.66	114.10
2	2	233	GLU	CG-CD-OE2	-6.27	103.98	118.40
1	1	216	ASP	CB-CA-C	6.25	121.89	111.51
3	3	148	MET	CG-SD-CE	6.25	114.66	100.90
1	1	66	SER	CA-CB-OG	-6.24	98.61	111.10
3	3	234	GLY	N-CA-C	-6.24	99.62	112.34
1	1	117	THR	CB-CA-C	-6.22	101.06	110.90
3	3	8	PRO	CA-C-N	6.22	133.60	121.41
3	3	8	PRO	C-N-CA	6.22	133.60	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	114	GLU	CB-CG-CD	6.22	123.17	112.60
4	4	30	ASN	CB-CA-C	6.22	122.79	110.42
1	1	155	PRO	CA-C-N	6.20	128.59	120.28
1	1	155	PRO	C-N-CA	6.20	128.59	120.28
1	1	205	THR	OG1-CB-CG2	6.20	121.70	109.30
2	2	95	ASN	N-CA-C	-6.20	105.58	113.01
2	2	212	ASP	CA-C-N	6.19	130.70	121.72
2	2	212	ASP	C-N-CA	6.19	130.70	121.72
2	2	262	LYS	CB-CA-C	6.19	122.36	109.68
1	1	154	ILE	N-CA-C	-6.19	100.75	108.05
3	3	181	ASN	O-C-N	6.18	130.92	123.26
2	2	95	ASN	OD1-CG-ND2	6.18	128.78	122.60
4	4	44	ASP	CA-C-O	6.18	131.30	120.80
1	1	19	ASN	CB-CG-OD1	-6.18	108.45	120.80
1	1	235	ILE	CA-C-O	6.17	127.75	120.72
2	2	56	PRO	N-CA-C	-6.16	101.50	110.80
1	1	69	SER	N-CA-C	-6.15	105.42	113.17
2	2	196	ASN	N-CA-C	6.15	117.97	110.41
3	3	123	ALA	O-C-N	6.14	129.39	122.32
2	2	128	PRO	CB-CA-C	6.12	119.00	110.98
2	2	39	PRO	CB-CA-C	-6.12	103.57	111.46
2	2	221	CYS	CA-C-O	6.11	127.11	120.32
1	1	106	MET	CA-C-O	-6.11	112.55	120.25
1	1	161	PHE	N-CA-C	-6.11	97.79	110.80
3	3	134	THR	CB-CA-C	6.11	115.94	110.44
2	2	228	SER	N-CA-CB	6.09	118.91	110.01
1	1	117	THR	N-CA-CB	6.08	118.89	110.07
1	1	45	VAL	CA-C-O	-6.08	114.58	121.75
3	3	26	PRO	N-CA-CB	6.07	108.97	103.33
1	1	104	GLN	O-C-N	6.06	130.15	121.97
2	2	27	ASP	CA-C-O	-6.06	113.28	120.43
1	1	60	GLN	N-CA-C	-6.04	99.06	108.90
2	2	70	HIS	CB-CA-C	-6.04	99.57	109.53
1	1	131	ILE	N-CA-C	6.03	116.38	107.15
2	2	236	SER	CA-C-N	6.02	132.26	121.66
2	2	236	SER	C-N-CA	6.02	132.26	121.66
1	1	223	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	1	94	ILE	N-CA-C	6.01	118.55	108.81
1	1	87	THR	CA-C-O	6.01	127.31	121.00
1	1	189	ILE	CA-C-O	6.01	127.30	119.85
1	1	276	THR	O-C-N	6.01	130.44	123.17
3	3	4	VAL	O-C-N	6.00	129.39	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	71	GLN	O-C-N	6.00	130.06	123.22
3	3	228	ASP	CB-CA-C	-6.00	99.58	110.56
1	1	286	THR	CA-C-O	-5.99	113.67	120.32
1	1	237	THR	CA-CB-OG1	-5.98	100.62	109.60
2	2	116	LYS	CB-CA-C	-5.98	99.30	110.36
2	2	161	ASP	CA-C-N	-5.97	112.68	122.54
2	2	161	ASP	C-N-CA	-5.97	112.68	122.54
2	2	173	LEU	CB-CA-C	5.97	120.06	110.09
3	3	89	ILE	CA-CB-CG2	5.97	120.65	110.50
1	1	211	SER	CA-C-N	-5.95	111.25	121.97
1	1	211	SER	C-N-CA	-5.95	111.25	121.97
4	4	32	PHE	CA-CB-CG	-5.95	107.85	113.80
1	1	236	THR	CB-CA-C	5.95	120.33	111.17
1	1	233	VAL	CA-C-O	5.95	128.21	120.78
3	3	194	GLN	N-CA-C	-5.94	103.49	112.04
1	1	62	ARG	O-C-N	5.93	129.80	122.20
2	2	155	ASP	O-C-N	5.93	130.48	122.59
3	3	56	ASN	OD1-CG-ND2	5.92	128.53	122.60
1	1	274	VAL	O-C-N	5.92	129.47	122.66
2	2	61	ASN	CA-C-N	5.92	131.84	122.36
2	2	61	ASN	C-N-CA	5.92	131.84	122.36
1	1	227	GLU	OE1-CD-OE2	-5.92	108.70	122.90
2	2	225	ILE	CA-C-O	5.91	123.01	119.94
2	2	71	TRP	CA-C-O	5.89	126.77	120.46
2	2	114	ALA	N-CA-C	-5.89	98.24	110.80
3	3	75	GLN	CA-C-N	5.89	128.10	120.44
3	3	75	GLN	C-N-CA	5.89	128.10	120.44
3	3	178	THR	N-CA-CB	5.88	119.36	110.30
1	1	273	ASP	CA-C-O	-5.88	115.31	121.55
2	2	209	VAL	CA-C-N	5.88	126.29	119.47
2	2	209	VAL	C-N-CA	5.88	126.29	119.47
2	2	215	LEU	CA-C-O	-5.88	111.90	120.13
3	3	73	GLY	N-CA-C	5.88	121.00	112.60
3	3	181	ASN	OD1-CG-ND2	5.88	128.47	122.60
2	2	238	ASN	N-CA-CB	5.87	119.55	110.21
2	2	12	ARG	CB-CA-C	-5.86	99.97	110.70
2	2	94	GLU	CA-C-O	5.85	127.31	119.47
4	4	40	ALA	CA-C-O	-5.85	114.75	121.19
2	2	59	SER	CA-C-O	5.85	126.57	119.38
1	1	122	ASP	N-CA-C	-5.84	100.15	109.96
1	1	163	TRP	CB-CA-C	5.84	120.57	110.94
3	3	198	VAL	O-C-N	5.83	129.09	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	81	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	2	38	TRP	CA-C-N	5.82	125.76	119.76
2	2	38	TRP	C-N-CA	5.82	125.76	119.76
3	3	92	THR	N-CA-C	-5.82	96.94	109.81
1	1	90	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	1	181	ARG	NE-CZ-NH2	5.82	124.44	119.20
3	3	161	SER	O-C-N	5.82	130.33	122.59
2	2	239	ILE	CB-CA-C	5.82	119.50	110.83
1	1	205	THR	CA-CB-OG1	-5.81	100.89	109.60
1	1	283	THR	CA-CB-OG1	-5.81	100.89	109.60
1	1	63	ASP	O-C-N	5.81	128.30	122.03
2	2	197	ASN	CA-C-N	5.81	131.91	122.39
2	2	197	ASN	C-N-CA	5.81	131.91	122.39
4	4	42	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
3	3	191	CYS	O-C-N	5.80	130.35	123.33
1	1	10	VAL	N-CA-CB	-5.80	101.15	112.75
3	3	180	ASP	CA-C-O	5.80	126.33	120.88
2	2	155	ASP	CB-CG-OD1	-5.80	105.07	118.40
1	1	273	ASP	CA-CB-CG	-5.79	106.81	112.60
2	2	14	MET	CA-C-O	5.79	127.78	121.06
1	1	204	ASN	CB-CG-ND2	5.79	125.09	116.40
1	1	210	GLY	CA-C-O	5.79	126.26	121.05
2	2	28	VAL	CB-CA-C	-5.79	101.80	111.29
1	1	260	THR	O-C-N	5.78	130.42	123.26
1	1	36	ALA	CA-C-N	5.77	132.56	121.54
1	1	36	ALA	C-N-CA	5.77	132.56	121.54
2	2	175	PHE	CA-CB-CG	5.76	119.56	113.80
3	3	222	ARG	NH1-CZ-NH2	-5.76	111.81	119.30
3	3	57	ASN	OD1-CG-ND2	5.76	128.36	122.60
3	3	165	LEU	CA-C-O	-5.76	114.10	120.38
1	1	282	ASN	CA-C-O	5.75	126.63	120.70
2	2	154	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	1	68	GLU	CA-C-O	5.74	125.46	119.14
1	1	68	GLU	CA-CB-CG	5.74	125.57	114.10
1	1	143	MET	CA-C-O	-5.74	114.41	121.06
3	3	24	ALA	N-CA-CB	-5.72	102.08	110.26
1	1	171	ILE	CB-CA-C	5.71	119.04	110.98
1	1	259	TYR	CB-CA-C	-5.71	100.42	113.33
2	2	154	ARG	CG-CD-NE	5.71	124.56	112.00
2	2	241	PRO	O-C-N	-5.71	114.94	122.64
2	2	157	SER	O-C-N	5.70	130.16	122.59
2	2	62	ARG	NE-CZ-NH1	5.69	127.19	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	71	GLN	N-CA-CB	5.69	119.54	110.16
3	3	120	CYS	CA-CB-SG	-5.69	101.32	114.40
3	3	96	THR	N-CA-C	5.68	122.90	110.80
2	2	227	ILE	N-CA-CB	5.67	120.59	111.23
1	1	37	ALA	N-CA-CB	-5.67	100.91	110.49
1	1	90	ASN	CB-CA-C	5.67	121.70	110.42
2	2	74	SER	O-C-N	5.67	128.89	122.20
3	3	180	ASP	CB-CA-C	5.67	116.77	109.80
1	1	120	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	2	90	GLY	CA-C-O	5.67	130.43	120.57
1	1	173	TRP	O-C-N	5.66	130.27	123.36
1	1	266	ASN	O-C-N	5.66	130.12	122.59
2	2	67	GLU	OE1-CD-OE2	5.66	136.49	122.90
2	2	176	ASP	CA-CB-CG	-5.66	106.94	112.60
3	3	185	MET	O-C-N	5.65	130.08	122.96
1	1	43	SER	CA-C-O	5.65	128.08	121.87
3	3	126	THR	O-C-N	5.65	129.71	123.33
3	3	162	THR	CB-CA-C	5.65	119.92	109.70
3	3	27	TRP	CA-C-O	-5.65	113.98	120.98
2	2	96	MET	CA-C-O	5.64	126.50	120.24
1	1	162	SER	CA-C-N	-5.64	113.65	122.73
1	1	162	SER	C-N-CA	-5.64	113.65	122.73
1	1	150	PRO	CB-CA-C	5.64	118.73	111.46
1	1	246	THR	N-CA-CB	-5.63	101.73	110.29
2	2	12	ARG	CA-C-O	-5.63	113.99	120.24
3	3	155	TRP	O-C-N	5.63	129.80	123.27
1	1	158	ARG	NE-CZ-NH1	5.63	127.13	121.50
3	3	156	ASP	CA-CB-CG	5.63	118.23	112.60
3	3	135	PRO	CA-C-O	5.62	128.72	120.56
1	1	276	THR	CA-CB-OG1	-5.61	101.18	109.60
3	3	81	LYS	N-CA-C	5.61	119.25	110.32
2	2	84	ASP	CA-C-O	-5.61	113.16	120.00
1	1	281	ARG	N-CA-CB	-5.61	101.88	110.85
3	3	112	SER	CA-C-N	5.61	131.77	121.85
3	3	112	SER	C-N-CA	5.61	131.77	121.85
3	3	204	PRO	CA-C-O	-5.60	114.95	121.95
3	3	172	ALA	N-CA-C	-5.60	103.00	111.56
1	1	72	GLY	CA-C-N	5.59	130.69	121.86
1	1	72	GLY	C-N-CA	5.59	130.69	121.86
2	2	160	ARG	CG-CD-NE	5.59	124.29	112.00
2	2	56	PRO	CA-C-N	-5.58	114.84	122.93
2	2	56	PRO	C-N-CA	-5.58	114.84	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	41	TYR	O-C-N	5.58	129.26	122.96
1	1	250	CYS	CA-C-N	5.57	125.52	119.78
1	1	250	CYS	C-N-CA	5.57	125.52	119.78
1	1	105	GLU	CG-CD-OE2	-5.57	105.59	118.40
1	1	153	PRO	N-CD-CG	-5.56	94.86	103.20
3	3	146	ASP	N-CA-CB	5.56	119.89	110.49
1	1	71	LEU	CB-CA-C	5.56	121.43	111.03
2	2	263	GLN	OE1-CD-NE2	5.56	128.16	122.60
2	2	135	ALA	N-CA-CB	-5.55	100.88	110.32
1	1	104	GLN	CB-CG-CD	-5.55	103.16	112.60
1	1	282	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	1	84	VAL	O-C-N	5.55	127.53	122.65
3	3	46	MET	CA-C-O	5.54	126.36	120.10
1	1	108	GLN	N-CA-C	5.54	122.60	110.80
1	1	286	THR	O-C-N	5.53	129.78	123.31
2	2	158	GLN	CA-C-N	5.53	130.89	122.65
2	2	158	GLN	C-N-CA	5.53	130.89	122.65
3	3	66	SER	CA-C-O	5.53	128.41	120.51
1	1	275	THR	CA-C-O	5.52	126.56	120.71
2	2	75	SER	O-C-N	5.52	129.38	122.86
3	3	89	ILE	N-CA-C	5.51	120.81	109.34
3	3	55	VAL	O-C-N	5.51	129.46	122.57
3	3	67	MET	O-C-N	-5.51	115.26	122.59
3	3	224	ALA	CA-C-O	5.51	127.33	121.16
2	2	43	THR	CA-C-N	5.50	126.71	119.84
2	2	43	THR	C-N-CA	5.50	126.71	119.84
1	1	10	VAL	N-CA-C	-5.49	107.47	112.96
2	2	73	GLY	N-CA-C	-5.49	106.22	115.62
3	3	89	ILE	CB-CG1-CD1	-5.49	102.27	113.80
1	1	76	CYS	CA-C-O	-5.49	114.66	120.92
2	2	131	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	1	251	PRO	N-CA-CB	5.48	108.12	103.35
1	1	186	PHE	CB-CA-C	5.48	118.48	110.26
1	1	70	PHE	N-CA-CB	5.48	118.42	110.26
1	1	183	SER	CA-CB-OG	5.48	122.06	111.10
1	1	17	VAL	CA-C-N	5.48	126.24	120.11
1	1	17	VAL	C-N-CA	5.48	126.24	120.11
2	2	261	ILE	O-C-N	5.47	129.23	123.00
1	1	42	THR	O-C-N	5.47	130.05	123.16
1	1	270	GLU	CB-CA-C	-5.47	102.13	110.88
3	3	227	THR	OG1-CB-CG2	5.47	120.23	109.30
2	2	31	ALA	N-CA-C	-5.46	100.01	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	142	ALA	CA-C-N	5.46	127.52	120.64
2	2	142	ALA	C-N-CA	5.46	127.52	120.64
2	2	106	TYR	N-CA-C	5.46	117.70	109.41
3	3	167	VAL	N-CA-CB	5.46	118.85	111.21
1	1	157	LYS	CA-C-O	5.46	126.47	120.31
1	1	134	ARG	CA-C-O	5.45	125.81	119.32
2	2	150	GLY	CA-C-O	-5.45	111.09	120.57
1	1	82	ILE	N-CA-CB	5.44	120.21	111.23
1	1	89	TYR	CA-C-N	-5.44	111.16	121.54
1	1	89	TYR	C-N-CA	-5.44	111.16	121.54
2	2	94	GLU	CG-CD-OE2	-5.44	105.89	118.40
3	3	33	GLU	CG-CD-OE2	-5.44	105.90	118.40
2	2	30	ASN	N-CA-CB	-5.43	101.31	110.49
3	3	28	TYR	CB-CG-CD1	5.43	128.95	120.80
1	1	27	THR	CA-CB-OG1	-5.43	101.45	109.60
1	1	222	SER	CA-C-O	5.43	126.83	120.80
3	3	124	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	1	86	TYR	N-CA-C	-5.43	107.31	114.31
1	1	90	ASN	CB-CG-ND2	5.42	124.54	116.40
1	1	191	SER	N-CA-C	5.42	118.99	112.38
2	2	139	SER	N-CA-CB	-5.42	102.04	110.98
2	2	227	ILE	CA-C-N	-5.42	113.38	121.83
2	2	227	ILE	C-N-CA	-5.42	113.38	121.83
2	2	256	ALA	O-C-N	5.42	129.25	122.86
1	1	51	ILE	CA-CB-CG2	5.41	119.70	110.50
2	2	72	ASN	N-CA-C	5.41	118.53	110.52
2	2	237	SER	CA-CB-OG	5.41	121.92	111.10
3	3	152	HIS	O-C-N	5.41	128.77	122.99
1	1	172	PHE	O-C-N	5.40	129.73	123.30
4	4	27	PHE	CA-C-O	5.39	128.22	120.51
1	1	279	VAL	CB-CA-C	5.39	118.93	111.38
3	3	131	LEU	O-C-N	5.39	129.95	123.16
3	3	235	PRO	N-CD-CG	-5.38	97.34	103.80
3	3	235	PRO	CB-CA-C	-5.38	98.56	112.00
2	2	86	LEU	O-C-N	-5.37	115.32	122.20
1	1	168	ASN	O-C-N	5.37	130.29	122.94
1	1	76	CYS	CB-CA-C	5.37	118.27	109.90
1	1	175	HIS	CA-C-O	5.37	128.18	120.51
2	2	141	THR	O-C-N	5.37	128.95	122.94
3	3	226	ASP	CB-CA-C	5.36	118.59	109.53
1	1	208	LYS	O-C-N	5.36	129.01	122.96
3	3	182	LYS	O-C-N	5.36	127.80	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	ASP	CB-CG-OD2	5.36	130.72	118.40
3	3	5	TYR	CA-C-N	5.36	129.07	122.37
3	3	5	TYR	C-N-CA	5.36	129.07	122.37
2	2	24	SER	CA-C-N	5.35	128.82	121.33
2	2	24	SER	C-N-CA	5.35	128.82	121.33
1	1	40	GLY	N-CA-C	-5.35	108.34	115.40
3	3	114	ARG	N-CA-CB	-5.34	102.31	110.65
1	1	255	ARG	CA-C-N	-5.34	113.96	122.29
1	1	255	ARG	C-N-CA	-5.34	113.96	122.29
1	1	274	VAL	CA-CB-CG1	5.34	119.47	110.40
2	2	201	LEU	CA-C-N	5.33	130.35	122.94
2	2	201	LEU	C-N-CA	5.33	130.35	122.94
2	2	219	ASN	CB-CA-C	5.32	119.73	110.79
1	1	192	ALA	N-CA-CB	-5.32	102.78	111.66
2	2	87	LYS	CB-CA-C	5.32	121.00	110.42
2	2	134	SER	N-CA-CB	5.32	118.85	110.23
2	2	223	VAL	N-CA-CB	-5.32	102.72	111.44
1	1	193	TYR	N-CA-CB	5.31	118.19	109.95
2	2	127	ILE	CA-C-O	-5.31	112.83	119.95
2	2	35	TYR	N-CA-CB	-5.31	104.18	112.41
1	1	110	ARG	NE-CZ-NH1	5.31	126.81	121.50
2	2	190	PHE	O-C-N	5.31	130.35	122.81
1	1	88	ASP	CA-CB-CG	5.31	117.91	112.60
1	1	89	TYR	N-CA-C	-5.30	101.05	109.59
2	2	108	VAL	CB-CA-C	5.30	118.56	111.19
3	3	201	PRO	N-CA-CB	-5.30	97.68	103.25
1	1	247	LYS	CB-CA-C	-5.29	98.33	109.38
2	2	144	TYR	CA-C-N	5.29	131.64	121.54
2	2	144	TYR	C-N-CA	5.29	131.64	121.54
1	1	201	ASP	CA-CB-CG	-5.28	107.32	112.60
3	3	57	ASN	N-CA-CB	-5.28	101.57	110.49
1	1	261	HIS	CA-CB-CG	-5.28	108.52	113.80
3	3	77	GLY	N-CA-C	-5.27	103.44	112.30
2	2	81	LYS	CA-C-O	-5.27	114.53	120.32
3	3	165	LEU	CA-C-N	-5.26	114.16	122.64
3	3	165	LEU	C-N-CA	-5.26	114.16	122.64
2	2	63	PHE	CA-CB-CG	-5.26	108.54	113.80
1	1	69	SER	CB-CA-C	5.26	118.87	110.09
3	3	228	ASP	CB-CG-OD2	-5.26	106.31	118.40
2	2	141	THR	CA-C-O	-5.26	115.52	121.72
1	1	232	SER	N-CA-CB	5.25	117.44	110.29
1	1	45	VAL	N-CA-C	-5.25	100.80	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	82	ILE	O-C-N	5.24	129.12	122.57
1	1	204	ASN	N-CA-C	-5.24	102.15	109.96
1	1	236	THR	CA-CB-CG2	5.24	119.41	110.50
2	2	45	GLN	N-CA-CB	5.24	119.65	110.27
2	2	37	VAL	O-C-N	5.24	128.84	123.18
1	1	214	THR	CB-CA-C	-5.24	101.24	111.03
1	1	154	ILE	N-CA-CB	5.23	117.86	111.21
3	3	157	VAL	CA-C-N	-5.23	113.30	120.57
3	3	157	VAL	C-N-CA	-5.23	113.30	120.57
2	2	157	SER	N-CA-CB	5.23	119.33	110.49
2	2	202	ILE	O-C-N	5.23	128.69	123.10
2	2	224	ILE	CA-CB-CG2	5.23	119.39	110.50
3	3	154	VAL	N-CA-C	-5.22	102.11	109.21
2	2	45	GLN	O-C-N	5.22	128.35	122.19
3	3	127	LEU	N-CA-CB	-5.22	102.80	111.57
4	4	42	ARG	CA-C-O	-5.22	113.90	120.84
1	1	111	ARG	CA-C-O	5.22	127.12	121.02
2	2	20	ASP	CA-CB-CG	5.22	117.82	112.60
4	4	42	ARG	N-CA-C	5.21	116.71	109.31
1	1	108	GLN	CB-CG-CD	5.21	121.46	112.60
2	2	96	MET	N-CA-CB	-5.21	102.43	110.20
3	3	141	PRO	CA-C-N	5.21	129.54	120.68
3	3	141	PRO	C-N-CA	5.21	129.54	120.68
2	2	165	ARG	N-CA-C	-5.21	99.71	110.80
3	3	142	THR	N-CA-CB	-5.20	102.29	110.30
3	3	15	THR	N-CA-C	-5.20	107.01	113.19
1	1	101	ILE	CB-CA-C	5.19	119.91	111.71
1	1	242	LYS	CA-C-O	5.19	126.62	120.66
2	2	76	LYS	CA-CB-CG	-5.18	103.73	114.10
2	2	166	GLN	N-CA-CB	-5.18	102.65	110.32
3	3	66	SER	CA-C-N	5.18	131.44	121.54
3	3	66	SER	C-N-CA	5.18	131.44	121.54
2	2	62	ARG	NE-CZ-NH2	5.17	123.86	119.20
2	2	79	TRP	CA-C-N	5.17	131.11	122.73
2	2	79	TRP	C-N-CA	5.17	131.11	122.73
2	2	97	TYR	N-CA-CB	-5.17	102.38	110.44
1	1	86	TYR	CA-C-O	5.17	124.51	118.77
2	2	194	ARG	NH1-CZ-NH2	5.17	126.02	119.30
1	1	262	SER	O-C-N	5.17	130.03	123.11
2	2	186	PHE	N-CA-C	-5.17	102.64	110.39
1	1	119	VAL	CA-C-O	-5.16	116.29	121.45
3	3	39	GLU	CB-CG-CD	5.16	121.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	79	ALA	O-C-N	5.16	131.54	122.09
3	3	160	GLN	CG-CD-NE2	5.16	124.14	116.40
2	2	182	ASN	CA-CB-CG	5.16	117.76	112.60
4	4	29	ILE	CB-CA-C	5.15	119.74	111.29
2	2	146	LEU	N-CA-CB	5.15	118.22	110.65
2	2	171	SER	N-CA-C	5.15	119.44	111.56
1	1	226	THR	CA-CB-OG1	-5.14	101.89	109.60
3	3	163	ILE	N-CA-CB	5.14	120.34	111.39
1	1	43	SER	N-CA-CB	5.14	117.61	110.26
1	1	18	PRO	O-C-N	5.14	128.88	122.71
2	2	111	GLN	CB-CA-C	5.14	118.11	109.48
4	4	30	ASN	O-C-N	5.14	129.42	122.59
2	2	252	GLU	CG-CD-OE2	-5.13	106.61	118.40
2	2	257	ARG	O-C-N	5.13	129.41	122.59
2	2	68	SER	O-C-N	5.12	128.67	122.68
2	2	12	ARG	CA-CB-CG	-5.12	103.87	114.10
2	2	160	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	1	106	MET	O-C-N	5.11	129.78	123.14
3	3	97	THR	N-CA-CB	5.10	117.80	109.69
3	3	149	LEU	N-CA-CB	-5.10	102.37	110.22
3	3	183	TYR	CB-CG-CD1	5.10	128.45	120.80
3	3	184	SER	CA-C-N	5.10	128.58	121.24
3	3	184	SER	C-N-CA	5.10	128.58	121.24
1	1	219	THR	N-CA-CB	-5.09	102.83	111.69
1	1	237	THR	OG1-CB-CG2	5.09	119.48	109.30
2	2	20	ASP	CA-C-N	5.09	130.31	122.93
2	2	20	ASP	C-N-CA	5.09	130.31	122.93
2	2	160	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	2	152	ALA	N-CA-C	5.09	118.26	111.75
2	2	215	LEU	O-C-N	5.09	128.85	122.19
3	3	122	THR	N-CA-CB	5.09	118.55	110.87
3	3	167	VAL	O-C-N	5.08	126.90	121.10
1	1	283	THR	N-CA-CB	-5.07	102.09	111.53
3	3	12	GLN	CA-C-N	5.07	130.72	121.89
3	3	12	GLN	C-N-CA	5.07	130.72	121.89
3	3	76	THR	N-CA-CB	5.07	117.36	110.01
2	2	219	ASN	CA-C-O	5.07	125.97	120.55
1	1	228	LYS	CD-CE-NZ	5.07	128.11	111.90
1	1	102	THR	O-C-N	5.06	129.32	122.59
3	3	200	PRO	O-C-N	5.06	127.43	121.46
2	2	79	TRP	CA-CB-CG	5.06	123.22	113.60
3	3	140	GLU	CB-CA-C	5.06	117.56	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	83	LYS	N-CA-C	-5.06	99.09	107.99
1	1	70	PHE	CA-C-N	-5.06	112.56	121.81
1	1	70	PHE	C-N-CA	-5.06	112.56	121.81
1	1	62	ARG	CD-NE-CZ	-5.05	117.33	124.40
4	4	26	TYR	N-CA-CB	5.05	119.08	110.50
3	3	177	LEU	N-CA-CB	-5.04	102.19	110.41
1	1	18	PRO	CA-C-N	-5.04	114.02	123.05
1	1	18	PRO	C-N-CA	-5.04	114.02	123.05
2	2	11	ASP	O-C-N	5.04	131.07	123.00
3	3	148	MET	CA-C-O	5.04	125.59	119.49
1	1	175	HIS	CB-CA-C	5.04	120.45	110.42
3	3	111	GLY	CA-C-O	5.04	128.99	122.59
4	4	33	LYS	N-CA-C	5.03	117.16	111.02
2	2	94	GLU	N-CA-C	-5.03	106.49	113.18
2	2	31	ALA	CA-C-N	-5.03	115.47	122.71
2	2	31	ALA	C-N-CA	-5.03	115.47	122.71
3	3	189	ILE	CA-C-O	-5.03	115.23	120.76
1	1	192	ALA	O-C-N	-5.02	117.52	123.25
3	3	84	SER	CA-C-N	5.02	129.09	122.51
3	3	84	SER	C-N-CA	5.02	129.09	122.51
3	3	114	ARG	O-C-N	5.02	129.09	123.27
1	1	170	SER	CB-CA-C	5.01	117.86	110.14
2	2	15	GLN	CA-C-N	-5.01	115.49	122.71
2	2	15	GLN	C-N-CA	-5.01	115.49	122.71
2	2	121	THR	N-CA-CB	-5.01	102.32	110.59
2	2	14	MET	O-C-N	-5.01	117.46	123.27
1	1	124	GLU	CB-CG-CD	5.00	121.11	112.60
3	3	222	ARG	N-CA-C	5.00	115.75	108.14
3	3	125	THR	CB-CA-C	-5.00	99.42	109.68

There are no chirality outliers.

There are no planarity outliers.

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	2194	348	1
2	2	1979	0	1922	223	1
3	3	1831	0	1810	238	0
4	4	151	0	136	18	0
5	A	23	0	19	30	0
All	All	6246	0	6081	739	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (739) 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)
1:1:102:THR:CA	5:A:2:FRU:H61	1.09	1.55
1:1:102:THR:HA	5:A:2:FRU:C6	0.95	1.41
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.21
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
2:2:18:ARG:HH12	2:2:249:MET:HE2	1.06	1.13
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.13
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.12
1:1:102:THR:C	5:A:2:FRU:H61	1.78	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
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
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:HD2	3:3:211:CYS:HB3	1.25	1.01
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.90	1.01
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	1.00
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.00
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.00
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
1:1:102:THR:HA	5:A:2:FRU:O6	1.60	0.99
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	0.99
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.93	0.98
1:1:215:ASN:CG	5:A:2:FRU:O3	2.07	0.97
3:3:117:PHE:CD2	3:3:211:CYS:HB3	2.00	0.97
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:113:PHE:O	1:1:115:LEU:N	1.99	0.95
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
3:3:24:ALA:O	3:3:25:LEU:HB2	1.72	0.90
1:1:96:PHE:CE1	1:1:157:LYS:HA	2.06	0.90
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.90
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.09	0.88
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.88
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
2:2:159:GLU:C	2:2:160:ARG:HG2	1.97	0.88
1:1:97:THR:HG23	1:1:222:SER:HB3	1.55	0.87
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.87
1:1:197:TYR:CE1	1:1:214:THR:HG23	2.08	0.87
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.86
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	0.86
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.86
1:1:102:THR:CA	5:A:2:FRU:C6	1.90	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.38	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.13	0.84
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.84
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.83
1:1:204:ASN:C	1:1:206:SER:H	1.82	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
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.82
1:1:119:VAL:CG1	1:1:121:PHE:HE2	1.93	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:215:ASN:H	1:1:215:ASN:ND2	1.77	0.81
1:1:197:TYR:H	2:2:131:GLN:HE21	1.28	0.80
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.67	0.77
3:3:55:VAL:C	3:3:57:ASN:H	1.93	0.77
1:1:103:LEU:N	5:A:2:FRU:H61	1.99	0.76
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.75
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.74
2:2:65:THR:OG1	2:2:245:SER:OG	2.05	0.74
4:4:26:TYR:CD2	4:4:29:ILE:HD11	2.22	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.52	0.74
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.74
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.00	0.73
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.73
1:1:119:VAL:HG13	1:1:121:PHE:CE2	2.24	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
1:1:223:ARG:HH11	1:1:223:ARG:HG2	1.53	0.73
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.73
1:1:197:TYR:CD1	1:1:214:THR:HG23	2.24	0.73
1:1:210:GLY:O	1:1:213:VAL:HG23	1.89	0.72
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
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:LEU:HD12	2:2:186:PHE:HD1	1.52	0.72
1:1:101:ILE:O	5:A:2:FRU:O6	2.08	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.72
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.06	0.71
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.71
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71
1:1:123:SER:HB3	1:1:241:HIS:NE2	2.05	0.71
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.71
1:1:124:GLU:OE2	1:1:181:ARG:HD3	1.91	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.70
1:1:104:GLN:HB3	1:1:110:ARG:HG3	1.72	0.70
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:102:THR:OG1	5:A:2:FRU:H5	1.91	0.70
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
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
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.71	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.93	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.69
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.69
1:1:127:LEU:O	1:1:180:PRO:HD2	1.92	0.69
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.69
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.69
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.68
1:1:160:ASP:H	1:1:163:TRP:CD1	2.10	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.94	0.68
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:215:ASN:ND2	1:1:215:ASN:N	2.42	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.68
1:1:260:THR:C	1:1:261:HIS:CD2	2.71	0.67
2:2:174:ASN:C	2:2:175:PHE:HD2	2.02	0.67
2:2:171:SER:HA	2:2:175:PHE:CE2	2.28	0.67
1:1:260:THR:C	1:1:261:HIS:HD2	2.02	0.67
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.77	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.67
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67
2:2:107:THR:OG1	2:2:249:MET:HE3	1.95	0.66
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.66
2:2:91:ILE:O	2:2:92:PHE:C	2.38	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
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.65
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.65
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.62	0.65
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.65
1:1:186:PHE:HE2	3:3:31:THR:HG22	1.62	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.64
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.63
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.63
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.98	0.63
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.62
1:1:148:VAL:HG12	1:1:152:ALA:HB3	1.82	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:215:ASN:CB	5:A:2:FRU:O3	2.47	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	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
2:2:235:THR:C	2:2:237:SER:H	2.06	0.62
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.62
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.62
3:3:145:LYS:O	3:3:148:MET:HE3	1.98	0.62
1:1:141:ILE:HA	1:1:226:THR:HG21	1.80	0.62
5:A:1:GLC:H5	5:A:2:FRU:H62	1.80	0.62
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.61
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:150:PRO:HG3	1:1:218:GLY:N	2.15	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
1:1:223:ARG:HG2	1:1:223:ARG:NH1	2.16	0.61
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61
2:2:183:LEU:HD12	2:2:186:PHE:CD1	2.34	0.61
1:1:103:LEU:HG	5:A:1:GLC:H61	1.83	0.61
1:1:94:ILE:HD12	1:1:94:ILE:N	2.16	0.61
1:1:105:GLU:O	1:1:106:MET:HG3	2.01	0.61
1:1:108:GLN:HB3	1:1:109:ILE:HG22	1.83	0.61
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.60
1:1:200:TYR:CD1	1:1:209:TYR:HB2	2.37	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.60
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.60
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.60
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.35	0.60
1:1:102:THR:HA	5:A:2:FRU:C5	2.15	0.60
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.29	0.60
2:2:84:ASP:OD2	2:2:87:LYS:HE2	2.02	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
2:2:159:GLU:C	2:2:160:ARG:CG	2.71	0.60
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.59
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.67	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59

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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	0.59
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.59
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.59
1:1:127:LEU:CB	1:1:180:PRO:HG2	2.33	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
1:1:102:THR:CB	5:A:2:FRU:C6	2.78	0.59
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.59
2:2:14:MET:HE1	2:2:31:ALA:HB2	1.83	0.58
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.76	0.58
2:2:174:ASN:C	2:2:175:PHE:CD2	2.82	0.58
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.86	0.58
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
1:1:197:TYR:HD2	1:1:198:ASP:H	1.52	0.58
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.58
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.58
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:85:ASP:OD2	1:1:86:TYR:N	2.36	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
1:1:99:TRP:CZ3	1:1:101:ILE:HA	2.39	0.57
1:1:89:TYR:HE1	1:1:227:GLU:C	2.12	0.57
1:1:110:ARG:O	1:1:114:GLU:HG3	2.04	0.57
1:1:163:TRP:CD2	1:1:223:ARG:HD3	2.39	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.57
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
1:1:195:MET:HE1	5:A:2:FRU:H11	1.86	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
1:1:145:TYR:CD2	1:1:145:TYR:N	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:104:GLN:OE1	1:1:263:HIS:ND1	2.32	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.56
1:1:129:PRO:HG2	1:1:173:TRP:CZ2	2.41	0.56
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.56
1:1:102:THR:CB	5:A:2:FRU:H5	2.35	0.56
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.20	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:103:LEU:N	5:A:2:FRU:C6	2.67	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.56
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.56
1:1:124:GLU:O	1:1:124:GLU:HG3	2.06	0.56
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.56
1:1:261:HIS:H	3:3:237:GLU:H	1.52	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.56
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.87	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:92:GLN:N	1:1:94:ILE:CD1	2.68	0.55
1:1:119:VAL:HG11	1:1:121:PHE:HE2	1.69	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.55
2:2:154:ARG:HD3	2:2:155:ASP:H	1.71	0.55
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.55
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
1:1:217:MET:SD	5:A:1:GLC:O3	2.55	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	0.55
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.55
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.55
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.88	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.54
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.23	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.88	0.54
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.07	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
3:3:107:THR:HG21	3:3:223:MET:HE2	1.89	0.54
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
1:1:195:MET:CE	5:A:2:FRU:H11	2.37	0.54
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.54
2:2:174:ASN:HB3	2:2:176:ASP:OD1	2.08	0.54
1:1:103:LEU:CG	5:A:1:GLC:H61	2.38	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
1:1:215:ASN:H	1:1:215:ASN:HD22	1.51	0.54
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.54
1:1:96:PHE:HE1	1:1:157:LYS:HA	1.70	0.53
1:1:106:MET:O	1:1:107:ALA:O	2.27	0.53
3:3:14:MET:C	3:3:16:THR:H	2.16	0.53
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	0.53
1:1:103:LEU:H	5:A:2:FRU:C5	2.21	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.53
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:197:TYR:H	2:2:131:GLN:NE2	2.04	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.53
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.53
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.52
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.52
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
3:3:43:LEU:CD2	3:3:46:MET:HE2	2.39	0.52
1:1:263:HIS:CE1	5:A:2:FRU:O4	2.61	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
4:4:26:TYR:CD2	4:4:29:ILE:CD1	2.91	0.52
1:1:261:HIS:CD2	1:1:261:HIS:N	2.74	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
1:1:200:TYR:CE1	1:1:209:TYR:HB2	2.44	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.52
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.52
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.52
1:1:119:VAL:CG1	1:1:121:PHE:CE2	2.79	0.51
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
1:1:124:GLU:CD	1:1:181:ARG:HH11	2.18	0.51
1:1:197:TYR:CD1	1:1:214:THR:CG2	2.94	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.51
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51
1:1:103:LEU:H	5:A:2:FRU:C6	2.24	0.51
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.45	0.51
1:1:143:MET:HG2	1:1:145:TYR:CE2	2.45	0.51
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.50
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.50
2:2:175:PHE:CD2	2:2:175:PHE:N	2.79	0.50
3:3:72:LEU:HD12	3:3:72:LEU:N	2.26	0.50
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.50
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.50
1:1:146:MET:HE3	1:1:168:ASN:CB	2.42	0.50
1:1:184:ILE:HG22	1:1:185:PRO:O	2.12	0.50
1:1:102:THR:CA	5:A:2:FRU:C5	2.85	0.50
1:1:244:LYS:CE	4:4:38:SER:O	2.60	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.50
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.49
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD1	2.48	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.49
1:1:127:LEU:HD12	1:1:239:ILE:HG12	1.95	0.49
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.49
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:186:PHE:CE2	3:3:31:THR:HG22	2.45	0.49
1:1:244:LYS:HZ1	4:4:38:SER:H	1.61	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
3:3:117:PHE:CE1	3:3:131:LEU:HG	2.47	0.49
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.49
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.49
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:MET:HE3	2:2:126:MET:HA	1.94	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.49
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.49
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.49
1:1:215:ASN:CG	5:A:2:FRU:HO3	2.12	0.49
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.49
1:1:103:LEU:HG	5:A:1:GLC:C6	2.42	0.48
1:1:261:HIS:H	3:3:237:GLU:N	2.11	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.48
1:1:191:SER:CB	3:3:34:ILE:HG12	2.43	0.48
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.48
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.48
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.48
1:1:197:TYR:HD2	1:1:198:ASP:N	2.11	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.48
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.48
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.48
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.48
1:1:197:TYR:N	2:2:131:GLN:HE21	2.05	0.48
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.48
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.48
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.48
1:1:197:TYR:CD2	1:1:198:ASP:N	2.81	0.48
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.48
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.48
3:3:82:VAL:HG12	3:3:83:PHE:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.47
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.47
1:1:271:THR:O	1:1:272:GLY:C	2.57	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD2	2.49	0.47
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.47
1:1:119:VAL:HG13	1:1:121:PHE:CD2	2.49	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.47
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.47
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.47
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
3:3:216:CYS:C	3:3:218:ASP:H	2.23	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
1:1:102:THR:CA	5:A:2:FRU:O6	2.35	0.47
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.47
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.47
3:3:43:LEU:HD23	3:3:46:MET:HE2	1.97	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
1:1:38:GLU:C	1:1:40:GLY:N	2.73	0.47
1:1:215:ASN:HB2	5:A:2:FRU:O3	2.15	0.47
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
1:1:89:TYR:HD2	1:1:89:TYR:HA	1.49	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46

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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	0.46
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.46
1:1:129:PRO:HA	1:1:237:THR:HA	1.98	0.46
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.31	0.46
1:1:190:ALA:C	3:3:31:THR:HG21	2.38	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.14	0.46
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.46
1:1:197:TYR:CE1	1:1:214:THR:CG2	2.91	0.46
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
3:3:91:SER:C	3:3:92:THR:O	2.58	0.46
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.46
1:1:184:ILE:HD13	1:1:184:ILE:HG21	1.63	0.46
1:1:197:TYR:HE2	2:2:217:HIS:CG	2.34	0.46
3:3:14:MET:C	3:3:16:THR:N	2.74	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	0.46
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.46
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.46
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.45
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.97	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
1:1:101:ILE:C	5:A:2:FRU:O6	2.58	0.45
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:124:GLU:OE1	1:1:181:ARG:NH1	2.49	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
1:1:165:SER:C	1:1:167:THR:N	2.74	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:240:VAL:HA	2:2:241:PRO:HD2	1.88	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
2:2:228:SER:HA	2:2:229:PRO:HD2	1.69	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:90: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
1:1:39:THR:C	1:1:41:HIS:H	2.24	0.45
1:1:97:THR:O	1:1:221:CYS:HA	2.16	0.45
1:1:75:GLY:N	1:1:240:TYR:HD2	2.15	0.45
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.45
3:3:42:ASN:CG	3:3:44:ILE:HG22	2.38	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
2:2:144:TYR:C	2:2:146:LEU:H	2.25	0.45
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.45
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.50	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE2	2.17	0.44
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.58	0.44
2:2:18:ARG:HD3	2:2:18:ARG:HA	1.57	0.44
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.44
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.44
1:1:90:ASN:HD22	1:1:90:ASN:N	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
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.44
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.44
2:2:83:PRO:CG	2:2:218:ASN:HA	2.31	0.44
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.44
3:3:65:VAL:C	3:3:67:MET:N	2.74	0.44
1:1:262:SER:O	1:1:263:HIS:HB2	2.18	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.44
1:1:61:THR:CG2	1:1:63:ASP:CG	2.91	0.43
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.43
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:120:ARG:C	1:1:121:PHE:CD2	2.96	0.43
1:1:149:PRO:HA	1:1:150:PRO:HD3	1.86	0.43
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.43
3:3:88:ASP:OD2	3:3:186:ALA:N	2.39	0.43
3:3:159:LEU:HA	3:3:159:LEU:HD23	1.72	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:104:GLN:HB3	1:1:104:GLN:HE21	1.64	0.43
1:1:104:GLN:O	3:3:236:ILE:HD11	2.18	0.43
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.43
2:2:247:SER:O	2:2:248:PRO:C	2.60	0.43
3:3:102:ILE:C	3:3:104:SER:N	2.76	0.43
2:2:126:MET:HB3	2:2:126:MET:HE2	1.61	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:85:ASP:OD2	1:1:85:ASP:C	2.61	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.51	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.43
1:1:192:ALA:HB3	2:2:208:ALA:HB2	2.01	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
1:1:244:LYS:NZ	4:4:38:SER:O	2.52	0.43
3:3:54:PRO:HA	3:3:68:TYR:CD2	2.54	0.43
4:4:26:TYR:HD2	4:4:29:ILE:HD11	1.78	0.43
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43
1:1:36:ALA:C	1:1:38:GLU:H	2.27	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	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
1:1:260:THR:HB	1:1:261:HIS:CD2	2.53	0.42
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.42
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.42
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.42
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.42
1:1:260:THR:HB	1:1:261:HIS:HD2	1.84	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.42
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:ILE:N	2:2:221:CYS:O	2.53	0.42
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
2:2:178:THR:O	2:2:179:LEU:C	2.62	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
1:1:145:TYR:O	1:1:170:SER:HA	2.19	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.42
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.42
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.42
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:94:LEU:HA	3:3:94:LEU:HD23	1.83	0.42
3:3:158:GLY:C	3:3:160:GLN:N	2.77	0.42
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.42
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:46:MET:HE3	3:3:102:ILE:HD11	2.01	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
1:1:103:LEU:CD2	5:A:1:GLC:H61	2.50	0.41
1:1:110:ARG:NE	1:1:114:GLU:OE1	2.53	0.41
1:1:145:TYR:N	1:1:145:TYR:HD2	2.16	0.41
1:1:261:HIS:HA	3:3:237:GLU:C	2.45	0.41
3:3:143:THR:C	3:3:192:TRP:CH2	2.97	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
1:1:66:SER:O	1:1:67:ILE:C	2.60	0.41
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	0.41
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.56	0.41
3:3:2:LEU:HA	3:3:2:LEU:HD23	1.80	0.41
1:1:136:ASP:O	1:1:137:ASP:CB	2.67	0.41
2:2:61:ASN:HB2	2:2:248:PRO:C	2.45	0.41
2:2:63:PHE:CD2	2:2:247:SER:HB2	2.55	0.41
2:2:94:GLU:C	2:2:96:MET:N	2.76	0.41
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.41
1:1:82:ILE:HD13	1:1:82:ILE:HG21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:199:GLY:C	1:1:200:TYR:CD2	2.98	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.41
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.41
3:3:30:PRO:O	3:3:31:THR:C	2.62	0.41
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	0.41
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.41
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.41
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.41
2:2:155:ASP:C	2:2:157:SER:H	2.29	0.41
3:3:43:LEU:HD23	3:3:43:LEU:HA	1.78	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.41
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.55	0.41
2:2:192:ASN:C	2:2:194:ARG:N	2.79	0.41
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.41
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.41
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.41
1:1:70:PHE:O	1:1:112:LYS:HE2	2.20	0.41
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.20	0.41
1:1:143:MET:HG3	1:1:223:ARG:O	2.20	0.41
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.41
1:1:255:ARG:NH1	1:1:265:THR:O	2.36	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
3:3:43:LEU:HD22	3:3:46:MET:HE2	2.02	0.41
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.41
1:1:97:THR:CG2	1:1:222:SER:HB3	2.39	0.41
1:1:186:PHE:CD2	1:1:186:PHE:C	2.98	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
2:2:51:ASN:H	2:2:51:ASN:ND2	2.15	0.40
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.40
1:1:9:GLU:OE1	4:4:42:ARG:HG3	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:46:GLN:CD	3:3:217:LYS:HG3	2.47	0.40
1:1:146:MET:HE3	1:1:168:ASN:HB3	2.02	0.40
1:1:197:TYR:CE2	2:2:217:HIS:CE1	3.09	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.40
1:1:235:ILE:HG22	1:1:236:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:252:ARG:HB3	1:1:253:PRO:HD2	2.03	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.02	0.40
3:3:145:LYS:O	3:3:146:ASP:C	2.65	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.40
2:2:164:LEU:C	2:2:166:GLN:N	2.80	0.40
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.40
1:1:225:VAL:H	1:1:225:VAL:HG23	1.61	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
2:2:202:ILE:HD13	2:2:249:MET:HE3	2.02	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:114:ARG:NH2	3:3:215:ALA:O	2.55	0.40
3:3:115:PHE:CE2	3:3:167:VAL:HG21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:27:THR:OG1	2:2:18:ARG:NH2[2_655]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	281/287 (98%)	217 (77%)	46 (16%)	18 (6%)	1	8
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1	10
3	3	236/238 (99%)	178 (75%)	38 (16%)	20 (8%)	0	3
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1	10
All	All	785/832 (94%)	605 (77%)	126 (16%)	54 (7%)	1	7

All (54) 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	158	ARG
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	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	159	LEU
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	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE

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Mol	Chain	Res	Type
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
3	3	121	GLY
2	2	44	PRO
3	3	82	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	254/258 (98%)	184 (72%)	70 (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%)	496 (71%)	201 (29%)	0	1

All (201) 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

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Mol	Chain	Res	Type
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	101	ILE
1	1	102	THR
1	1	104	GLN
1	1	105	GLU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
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	148	VAL
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	211	SER
1	1	212	VAL
1	1	215	ASN
1	1	217	MET
1	1	219	THR
1	1	223	ARG
1	1	224	ILE
1	1	226	THR

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	2	86	LEU
2	2	87	LYS
2	2	88	ASP
2	2	91	ILE
2	2	94	GLU
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	119	GLN
2	2	126	MET
2	2	132	LEU
2	2	136	LYS
2	2	139	SER
2	2	140	VAL
2	2	145	LYS
2	2	146	LEU
2	2	151	GLU
2	2	154	ARG
2	2	158	GLN
2	2	159	GLU
2	2	160	ARG
2	2	164	LEU
2	2	170	ASP
2	2	171	SER
2	2	173	LEU
2	2	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	194	ARG
2	2	195	SER
2	2	197	ASN
2	2	198	SER
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	3	182	LYS
3	3	189	ILE
3	3	192	TRP
3	3	194	GLN
3	3	196	ASN
3	3	197	LEU
3	3	201	PRO
3	3	205	GLN
3	3	209	MET
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE
3	3	213	VAL
3	3	216	CYS
3	3	217	LYS
3	3	231	ILE
3	3	236	ILE
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	144	GLN
1	1	159	ASN
1	1	168	ASN
1	1	175	HIS
1	1	204	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

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Mol	Chain	Res	Type
2	2	111	GLN
2	2	131	GLN
2	2	192	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
3	3	12	GLN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN
3	3	75	GLN
3	3	80	GLN
3	3	124	ASN
3	3	194	GLN
3	3	205	GLN
4	4	28	ASN
4	4	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are 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	GLC	A	1	5	11,11,12	2.12	2 (18%)	15,15,17	4.94	8 (53%)
5	FRU	A	2	5	11,12,12	1.09	0	10,18,18	2.26	2 (20%)

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	GLC	A	1	5	1/1/4/5	2/2/19/22	0/1/1/1
5	FRU	A	2	5	-	5/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	GLC	O5-C1	-5.97	1.33	1.43
5	A	1	GLC	C2-C3	-2.63	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	GLC	O3-C3-C2	14.18	139.00	110.05
5	A	1	GLC	C1-O5-C5	7.07	121.67	112.19
5	A	1	GLC	O2-C2-C3	6.27	123.13	110.15
5	A	2	FRU	O2-C2-O5	5.80	120.45	109.33
5	A	1	GLC	O5-C5-C6	5.14	117.67	107.66
5	A	1	GLC	C3-C4-C5	-4.57	101.95	110.23
5	A	2	FRU	C6-C5-C4	-2.90	108.25	115.10
5	A	1	GLC	O2-C2-C1	-2.90	102.58	109.22
5	A	1	GLC	C1-C2-C3	2.57	113.38	109.64
5	A	1	GLC	O4-C4-C5	-2.28	103.70	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1	GLC	C1

All (7) torsion outliers are listed below:

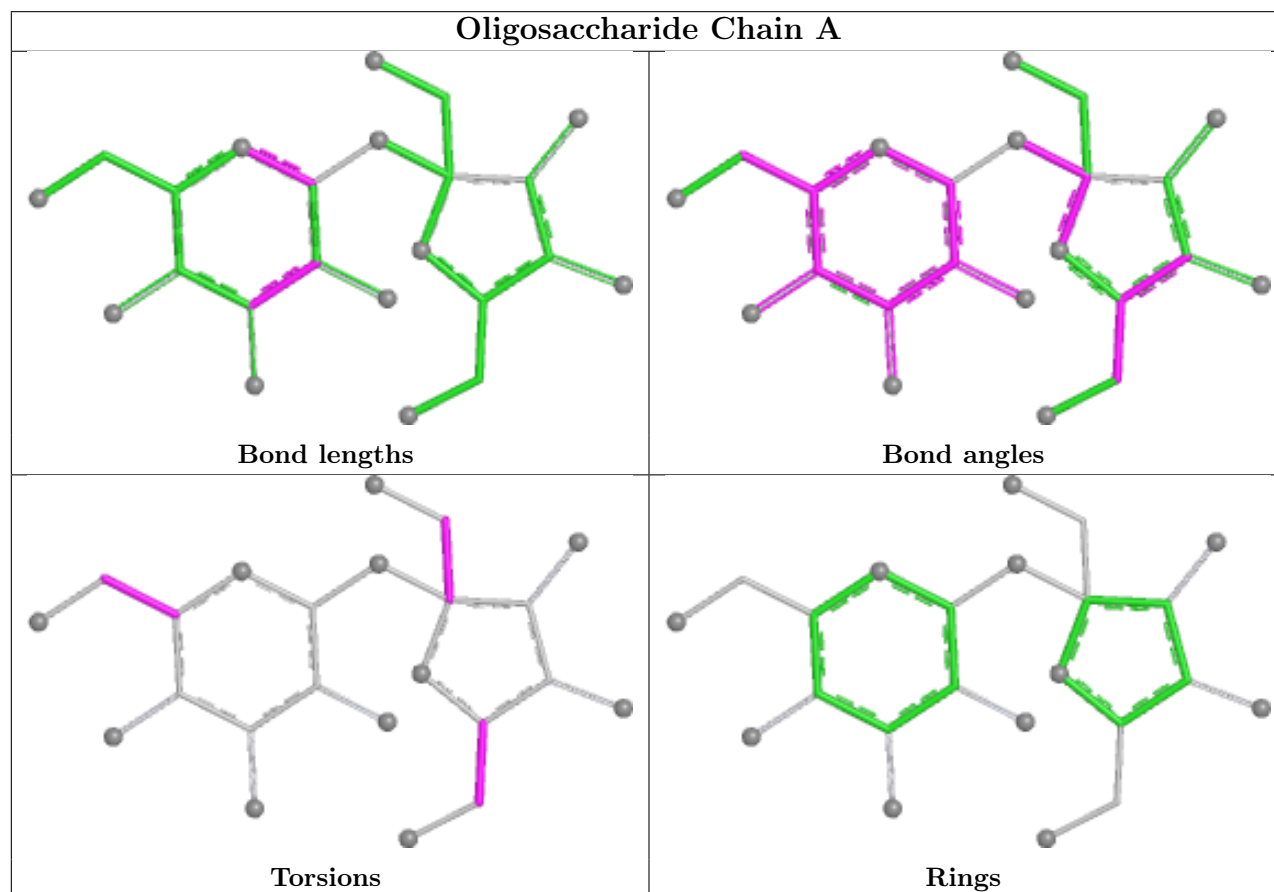
Mol	Chain	Res	Type	Atoms
5	A	2	FRU	O1-C1-C2-C3
5	A	2	FRU	O1-C1-C2-O2
5	A	2	FRU	O5-C5-C6-O6
5	A	1	GLC	O5-C5-C6-O6
5	A	1	GLC	C4-C5-C6-O6
5	A	2	FRU	O1-C1-C2-O5
5	A	2	FRU	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	FRU	25	0
5	A	1	GLC	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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.