



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 AM UTC

PDB ID : 1MEC / pdb_00001mec
Title : CONFORMATIONAL VARIABILITY OF A PICORNAVIRUS CAPSID: PH-DEPENDENT STRUCTURAL CHANGES OF MENO VIRUS RELATED TO ITS HOST RECEPTOR ATTACHMENT SITE AND DISASSEMBLY
Authors : Rossmann, M.G.
Deposited on : 1992-01-17
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

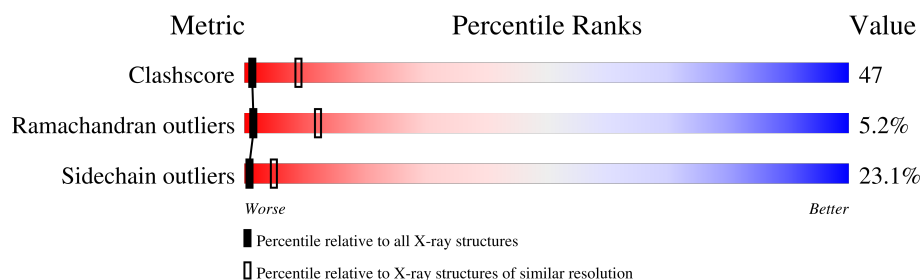
1 Overall quality at a glance

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	274	29% 39% 25% 7%
2	2	256	34% 35% 20% 11%
3	3	231	38% 37% 22% .
4	4	70	24% 19% 26% 20% 11%

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	PO4	2	309	-	X	-	-
5	PO4	2	825	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6710 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 MENO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	274	Total	C	N	O	S	0	0	0
			2139	1375	354	403	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	45	ARG	ALA	conflict	UNP P12296

- Molecule 2 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	256	Total	C	N	O	S	0	0	0
			2031	1279	358	388	6			

- Molecule 3 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	231	Total	C	N	O	S	0	0	0
			1773	1153	283	326	11			

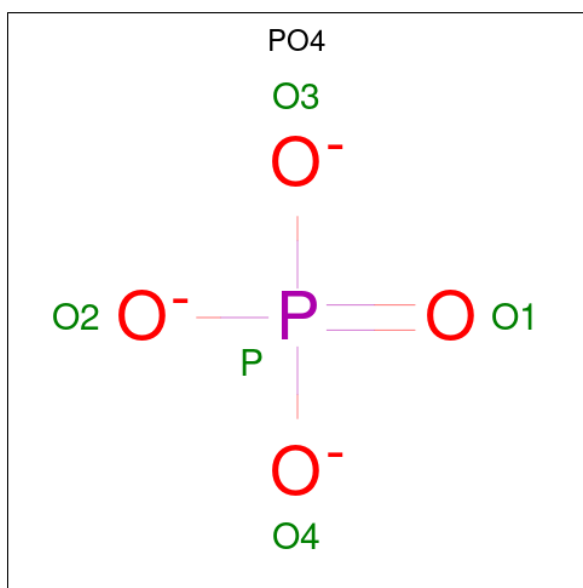
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	58	MET	VAL	conflict	UNP P12296

- Molecule 4 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	62	Total	C	N	O	S	0	0	0
			461	284	77	99	1			

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	2	1	Total	O	P	0	0
			5	4	1		
5	2	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

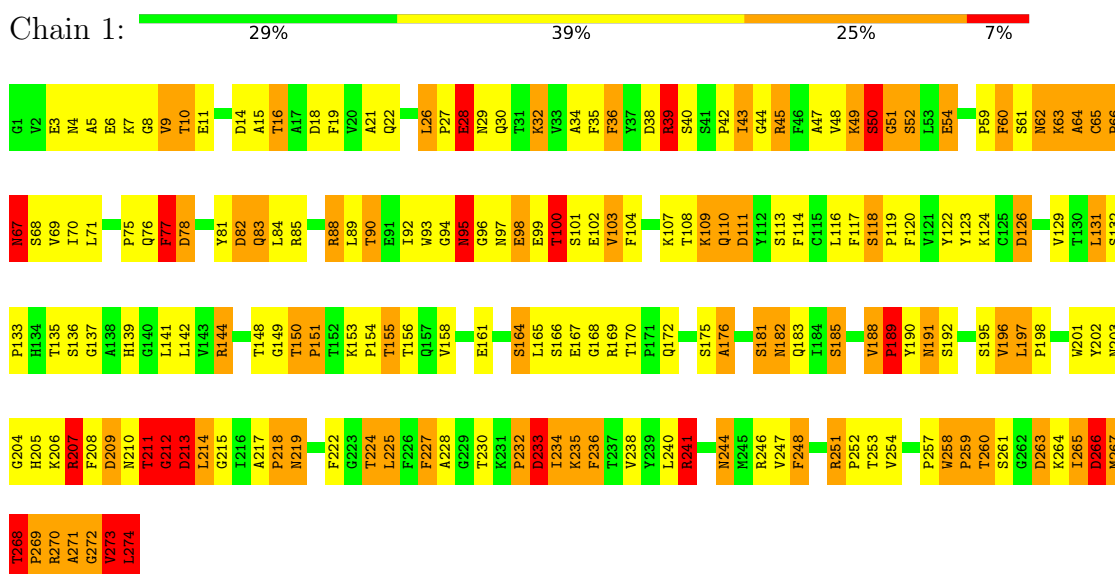
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	114	Total	O	0	0
			114	114		
6	2	122	Total	O	0	0
			122	122		
6	3	50	Total	O	0	0
			50	50		
6	4	10	Total	O	0	0
			10	10		

3 Residue-property plots

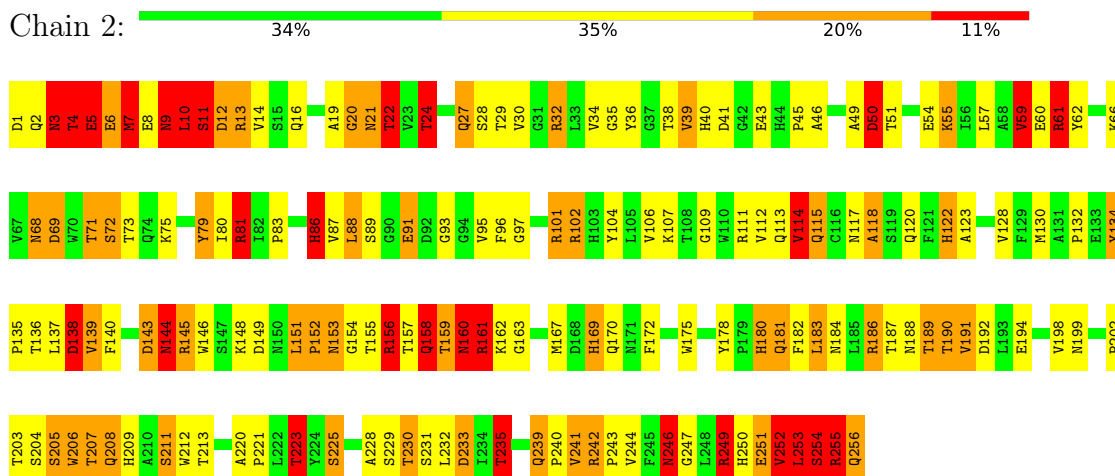
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

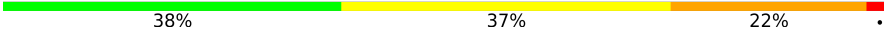
• Molecule 1: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

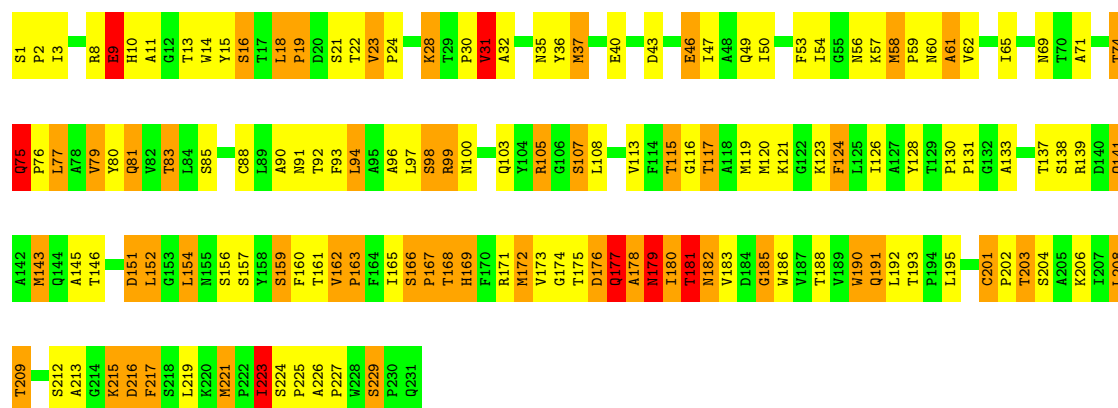


• Molecule 2: MENGO VIRUS COAT PROTEIN (SUBUNIT VP2)



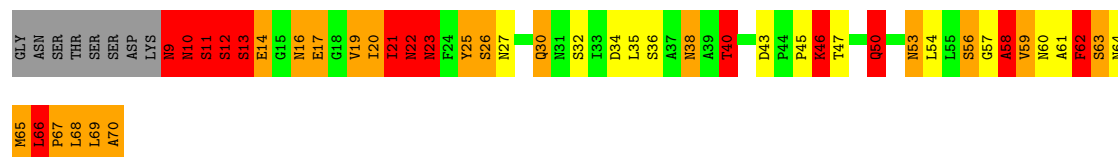
• Molecule 3: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

Chain 3: 



• Molecule 4: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

Chain 4: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	439.80Å 426.90Å 421.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6710	wwPDB-VP
Average B, all atoms (Å ²)	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: PO4

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	1.60	33/2208 (1.5%)	2.58	153/3018 (5.1%)
2	2	1.77	45/2086 (2.2%)	2.61	137/2854 (4.8%)
3	3	1.36	20/1830 (1.1%)	2.27	98/2512 (3.9%)
4	4	2.36	8/469 (1.7%)	4.57	37/638 (5.8%)
All	All	1.66	106/6593 (1.6%)	2.70	425/9022 (4.7%)

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	1
2	2	0	3
4	4	0	3
All	All	0	7

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	58	ALA	C-N	39.73	1.87	1.33
2	2	12	ASP	C-N	-27.35	0.95	1.33
3	3	186	TRP	CA-CB	-17.24	1.25	1.53
1	1	273	VAL	CA-CB	15.00	1.74	1.54
1	1	274	LEU	N-CA	14.21	1.73	1.46
2	2	242	ARG	N-CA	14.02	1.56	1.46
2	2	4	THR	C-N	13.83	1.53	1.33
1	1	268	THR	N-CA	13.78	1.65	1.46
2	2	3	ASN	CA-C	13.14	1.72	1.53
1	1	273	VAL	N-CA	-12.59	1.30	1.46
1	1	266	ASP	C-N	12.23	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	255	ARG	C-N	-11.94	1.16	1.33
2	2	6	GLU	CA-CB	11.83	1.69	1.53
1	1	270	ARG	CA-CB	-11.53	1.33	1.53
2	2	5	GLU	N-CA	10.79	1.60	1.46
1	1	267	MET	CA-C	10.56	1.67	1.52
2	2	151	LEU	CA-C	-10.09	1.38	1.52
2	2	255	ARG	CA-C	-9.83	1.41	1.52
1	1	274	LEU	CA-C	9.42	1.72	1.52
2	2	242	ARG	C-O	8.99	1.28	1.23
1	1	269	PRO	CA-C	8.96	1.63	1.52
2	2	252	VAL	C-N	-8.90	1.22	1.33
2	2	253	LEU	N-CA	-8.67	1.36	1.46
2	2	241	VAL	CA-C	8.52	1.62	1.52
2	2	9	ASN	CA-CB	8.42	1.67	1.53
2	2	4	THR	CA-C	8.38	1.64	1.52
1	1	270	ARG	N-CA	8.37	1.56	1.46
2	2	6	GLU	CA-C	8.32	1.63	1.53
2	2	251	GLU	CA-C	8.28	1.56	1.52
2	2	160	ASN	N-CA	8.20	1.56	1.46
4	4	12	SER	CA-C	-8.15	1.42	1.52
2	2	5	GLU	C-O	-8.02	1.13	1.24
4	4	11	SER	N-CA	7.92	1.55	1.45
1	1	234	ILE	C-O	-7.88	1.15	1.24
3	3	173	VAL	C-O	-7.81	1.14	1.24
1	1	10	THR	C-O	-7.79	1.14	1.23
3	3	182	ASN	CA-CB	-7.76	1.43	1.53
3	3	81	GLN	C-N	-7.75	1.26	1.33
1	1	50	SER	C-N	-7.66	1.25	1.33
3	3	59	PRO	C-N	-7.58	1.23	1.33
2	2	10	LEU	N-CA	7.52	1.54	1.45
3	3	181	THR	C-N	-7.47	1.24	1.33
3	3	176	ASP	C-N	-7.40	1.23	1.33
1	1	267	MET	C-O	-7.35	1.14	1.24
2	2	256	GLN	N-CA	-7.33	1.32	1.46
1	1	51	GLY	CA-C	-7.28	1.44	1.51
2	2	6	GLU	CG-CD	7.20	1.70	1.52
3	3	83	THR	C-N	-7.17	1.23	1.33
2	2	6	GLU	C-N	7.15	1.43	1.33
2	2	152	PRO	N-CD	6.96	1.57	1.47
2	2	151	LEU	CB-CG	-6.96	1.39	1.53
3	3	81	GLN	N-CA	6.80	1.54	1.46
2	2	208	GLN	CA-C	6.70	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	9	VAL	C-O	6.65	1.31	1.23
2	2	252	VAL	N-CA	6.64	1.54	1.46
1	1	271	ALA	N-CA	-6.58	1.37	1.46
3	3	179	ASN	CA-CB	6.52	1.62	1.53
1	1	129	VAL	CA-CB	6.52	1.62	1.54
4	4	12	SER	N-CA	-6.46	1.38	1.46
1	1	273	VAL	C-O	-6.42	1.16	1.24
4	4	11	SER	C-N	-6.39	1.25	1.33
2	2	255	ARG	NE-CZ	6.29	1.40	1.33
3	3	58	MET	CA-C	-6.26	1.47	1.53
1	1	268	THR	CA-C	6.22	1.60	1.52
4	4	10	ASN	CA-C	6.06	1.60	1.52
1	1	10	THR	CA-C	-6.01	1.45	1.52
2	2	253	LEU	C-N	-5.99	1.25	1.33
1	1	214	LEU	N-CA	-5.99	1.39	1.46
1	1	51	GLY	C-N	-5.98	1.25	1.34
4	4	11	SER	CA-C	-5.96	1.45	1.52
2	2	206	TRP	C-N	-5.95	1.25	1.33
2	2	159	THR	C-N	5.90	1.42	1.33
1	1	267	MET	N-CA	5.89	1.53	1.46
1	1	269	PRO	N-CA	5.81	1.54	1.47
3	3	177	GLN	C-N	-5.77	1.25	1.33
3	3	209	THR	CA-CB	5.76	1.62	1.53
2	2	9	ASN	CA-C	5.76	1.60	1.52
1	1	269	PRO	C-O	5.75	1.30	1.23
1	1	265	ILE	C-N	-5.74	1.25	1.33
2	2	140	PHE	N-CA	5.74	1.53	1.46
1	1	270	ARG	NE-CZ	5.72	1.39	1.33
3	3	80	TYR	C-N	5.70	1.41	1.33
3	3	60	ASN	N-CA	-5.69	1.39	1.46
4	4	58	ALA	C-O	5.57	1.30	1.24
3	3	3	ILE	N-CA	5.51	1.50	1.46
3	3	186	TRP	NE1-CE2	-5.51	1.31	1.37
2	2	241	VAL	N-CA	5.49	1.52	1.46
3	3	81	GLN	CA-C	-5.48	1.45	1.52
2	2	2	GLN	N-CA	5.47	1.52	1.45
2	2	207	THR	C-O	-5.46	1.17	1.24
2	2	212	TRP	NE1-CE2	-5.41	1.31	1.37
2	2	6	GLU	CB-CG	5.39	1.68	1.52
2	2	206	TRP	NE1-CE2	-5.39	1.31	1.37
2	2	151	LEU	CA-CB	-5.38	1.45	1.53
2	2	8	GLU	C-N	-5.37	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	178	ALA	CA-C	5.29	1.60	1.53
2	2	146	TRP	NE1-CE2	-5.28	1.31	1.37
1	1	263	ASP	N-CA	-5.20	1.40	1.46
3	3	175	THR	C-N	-5.16	1.26	1.33
1	1	271	ALA	CA-C	5.14	1.59	1.52
1	1	270	ARG	CD-NE	5.09	1.53	1.46
1	1	10	THR	CA-CB	-5.07	1.44	1.53
2	2	11	SER	N-CA	5.07	1.52	1.46
1	1	10	THR	N-CA	-5.02	1.40	1.46
2	2	208	GLN	CA-CB	-5.02	1.46	1.53
2	2	256	GLN	C-O	5.01	1.33	1.23

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	58	ALA	O-C-N	-67.68	32.58	122.59
4	4	9	ASN	O-C-N	-52.56	38.90	123.00
4	4	12	SER	O-C-N	31.40	161.20	122.89
1	1	265	ILE	O-C-N	27.48	146.88	122.97
2	2	12	ASP	CA-C-N	21.46	162.53	121.54
2	2	12	ASP	C-N-CA	21.46	162.53	121.54
2	2	152	PRO	CA-N-CD	-18.06	86.22	111.50
1	1	66	PRO	CA-C-N	17.45	145.06	120.29
1	1	66	PRO	C-N-CA	17.45	145.06	120.29
2	2	246	ASN	CA-CB-CG	16.22	128.82	112.60
1	1	273	VAL	O-C-N	-16.16	102.36	122.57
2	2	252	VAL	O-C-N	15.38	141.80	122.57
1	1	95	ASN	CA-CB-CG	-15.31	97.29	112.60
1	1	51	GLY	O-C-N	14.30	134.09	122.51
4	4	11	SER	CA-C-N	-14.13	100.80	120.87
4	4	11	SER	C-N-CA	-14.13	100.80	120.87
3	3	179	ASN	CA-CB-CG	13.85	126.45	112.60
4	4	9	ASN	CA-C-N	-13.75	95.27	121.54
4	4	9	ASN	C-N-CA	-13.75	95.27	121.54
2	2	12	ASP	O-C-N	-13.70	99.61	121.53
1	1	269	PRO	O-C-N	13.68	138.74	123.01
2	2	5	GLU	CB-CA-C	-13.57	83.42	110.42
2	2	49	ALA	CA-C-N	13.53	139.90	120.95
2	2	49	ALA	C-N-CA	13.53	139.90	120.95
3	3	178	ALA	N-CA-CB	-13.48	91.08	110.36
4	4	12	SER	N-CA-C	13.37	130.06	110.28
3	3	215	LYS	CA-C-N	13.30	140.53	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	215	LYS	C-N-CA	13.30	140.53	120.31
2	2	6	GLU	N-CA-CB	13.06	131.33	111.35
1	1	273	VAL	CB-CA-C	13.06	132.70	111.29
1	1	168	GLY	N-CA-C	12.93	124.65	111.21
2	2	6	GLU	CA-C-N	12.76	145.91	121.54
2	2	6	GLU	C-N-CA	12.76	145.91	121.54
2	2	151	LEU	CB-CA-C	-12.37	91.81	108.76
1	1	269	PRO	CA-C-N	11.91	144.29	121.54
1	1	269	PRO	C-N-CA	11.91	144.29	121.54
2	2	35	GLY	N-CA-C	11.78	128.93	113.27
2	2	152	PRO	N-CA-CB	11.68	115.45	102.60
3	3	178	ALA	CB-CA-C	11.68	133.63	109.68
1	1	266	ASP	CB-CA-C	-11.62	87.29	110.42
1	1	270	ARG	O-C-N	11.50	137.88	122.59
2	2	3	ASN	O-C-N	11.47	137.74	122.82
2	2	4	THR	N-CA-CB	-11.44	91.16	110.49
1	1	265	ILE	CA-C-N	11.34	143.20	121.54
1	1	265	ILE	C-N-CA	11.34	143.20	121.54
1	1	234	ILE	CB-CA-C	11.24	126.13	110.84
3	3	156	SER	N-CA-C	11.24	123.54	111.28
1	1	49	LYS	O-C-N	-11.20	109.85	122.84
2	2	8	GLU	CA-C-N	11.19	142.92	121.54
2	2	8	GLU	C-N-CA	11.19	142.92	121.54
4	4	12	SER	CA-C-N	11.10	142.74	121.54
4	4	12	SER	C-N-CA	11.10	142.74	121.54
1	1	219	ASN	CA-CB-CG	11.01	123.61	112.60
1	1	273	VAL	CA-C-N	-10.95	101.99	121.70
1	1	273	VAL	C-N-CA	-10.95	101.99	121.70
2	2	6	GLU	CB-CG-CD	10.95	131.22	112.60
2	2	255	ARG	O-C-N	10.69	132.86	121.85
1	1	270	ARG	CA-CB-CG	-10.61	92.88	114.10
3	3	185	GLY	O-C-N	10.49	131.59	122.88
1	1	39	ARG	NE-CZ-NH2	10.26	128.43	119.20
2	2	4	THR	N-CA-C	10.17	132.46	110.80
2	2	10	LEU	O-C-N	10.15	134.82	121.83
1	1	273	VAL	CA-CB-CG2	10.12	127.61	110.40
2	2	21	ASN	CA-C-N	9.94	137.00	122.99
2	2	21	ASN	C-N-CA	9.94	137.00	122.99
1	1	270	ARG	N-CA-C	9.82	131.72	110.80
2	2	252	VAL	CB-CA-C	-9.73	95.33	111.29
1	1	189	PRO	CA-C-N	9.67	136.10	121.40
1	1	189	PRO	C-N-CA	9.67	136.10	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	177	GLN	N-CA-C	-9.62	94.66	109.95
1	1	64	ALA	N-CA-C	-9.48	101.01	112.58
2	2	145	ARG	CD-NE-CZ	9.46	137.64	124.40
2	2	3	ASN	N-CA-C	9.44	125.65	107.71
4	4	38	ASN	OD1-CG-ND2	9.42	132.02	122.60
2	2	246	ASN	OD1-CG-ND2	9.38	131.98	122.60
1	1	266	ASP	N-CA-C	9.34	130.69	110.80
2	2	252	VAL	CA-C-N	9.26	135.47	121.40
2	2	252	VAL	C-N-CA	9.26	135.47	121.40
2	2	151	LEU	O-C-N	-9.23	109.80	121.70
2	2	50	ASP	N-CA-CB	-9.10	96.29	109.85
4	4	38	ASN	CA-CB-CG	-9.09	103.51	112.60
4	4	34	ASP	CA-CB-CG	-9.06	103.54	112.60
2	2	39	VAL	N-CA-CB	-9.03	101.77	112.07
3	3	186	TRP	CB-CA-C	-9.02	93.62	109.86
4	4	65	MET	O-C-N	8.98	133.90	123.12
2	2	251	GLU	O-C-N	8.94	128.76	120.71
2	2	6	GLU	O-C-N	8.94	133.12	122.75
1	1	44	GLY	CA-C-N	8.74	134.78	122.72
1	1	44	GLY	C-N-CA	8.74	134.78	122.72
3	3	50	ILE	CA-C-O	-8.68	114.26	119.12
1	1	241	ARG	NE-CZ-NH1	8.68	130.18	121.50
1	1	211	THR	O-C-N	8.67	134.38	122.41
2	2	86	HIS	CA-CB-CG	-8.67	105.13	113.80
1	1	62	ASN	CA-CB-CG	-8.61	103.99	112.60
4	4	53	ASN	N-CA-C	-8.59	96.34	110.17
1	1	244	ASN	CA-CB-CG	8.53	121.13	112.60
1	1	36	PHE	CA-CB-CG	8.52	122.32	113.80
2	2	30	VAL	N-CA-C	-8.48	104.91	113.47
3	3	100	ASN	OD1-CG-ND2	8.46	131.06	122.60
1	1	137	GLY	N-CA-C	-8.43	98.56	111.12
2	2	10	LEU	N-CA-C	8.34	122.79	109.86
1	1	266	ASP	O-C-N	8.33	133.67	122.59
2	2	153	ASN	N-CA-C	8.33	123.01	113.02
1	1	265	ILE	N-CA-C	8.24	119.25	107.88
2	2	35	GLY	CA-C-O	-8.19	112.10	120.45
1	1	191	ASN	CA-CB-CG	8.17	120.77	112.60
2	2	9	ASN	N-CA-CB	-8.15	96.71	110.49
1	1	212	GLY	O-C-N	8.15	133.29	122.70
2	2	151	LEU	CA-C-N	8.14	146.54	127.00
2	2	151	LEU	C-N-CA	8.14	146.54	127.00
2	2	3	ASN	CB-CA-C	-8.14	99.80	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	74	THR	CA-CB-OG1	-8.11	97.43	109.60
1	1	241	ARG	NH1-CZ-NH2	-8.11	108.76	119.30
1	1	45	ARG	NE-CZ-NH2	8.10	126.49	119.20
3	3	91	ASN	CA-CB-CG	8.08	120.68	112.60
3	3	53	PHE	N-CA-C	8.06	122.85	109.46
3	3	100	ASN	CA-CB-CG	-8.06	104.54	112.60
2	2	153	ASN	OD1-CG-ND2	-8.03	114.57	122.60
4	4	66	LEU	O-C-N	-8.03	112.08	121.32
2	2	152	PRO	N-CD-CG	8.01	113.41	103.80
1	1	155	THR	CA-CB-OG1	-7.99	97.61	109.60
2	2	102	ARG	CD-NE-CZ	-7.98	113.23	124.40
2	2	10	LEU	CA-C-N	7.96	136.74	121.54
2	2	10	LEU	C-N-CA	7.96	136.74	121.54
3	3	105	ARG	NE-CZ-NH2	7.95	126.36	119.20
2	2	3	ASN	CA-C-N	7.88	136.60	121.54
2	2	3	ASN	C-N-CA	7.88	136.60	121.54
4	4	12	SER	N-CA-CB	7.88	121.56	109.97
3	3	162	VAL	O-C-N	7.86	127.59	121.46
1	1	155	THR	N-CA-C	7.84	123.17	112.90
1	1	233	ASP	CA-CB-CG	-7.80	104.80	112.60
2	2	223	THR	CA-CB-OG1	-7.75	97.97	109.60
2	2	5	GLU	N-CA-C	7.75	127.31	110.80
2	2	143	ASP	CA-C-N	7.71	130.60	120.28
2	2	143	ASP	C-N-CA	7.71	130.60	120.28
3	3	168	THR	CB-CA-C	7.69	122.81	109.65
2	2	59	VAL	N-CA-CB	-7.68	101.76	112.35
3	3	116	GLY	CA-C-N	7.66	131.59	120.71
3	3	116	GLY	C-N-CA	7.66	131.59	120.71
3	3	49	GLN	CG-CD-NE2	-7.64	104.93	116.40
2	2	36	TYR	N-CA-C	-7.62	101.50	111.71
2	2	21	ASN	CA-C-O	7.57	128.41	119.48
4	4	11	SER	N-CA-C	-7.56	97.99	110.17
1	1	39	ARG	NE-CZ-NH1	-7.54	113.96	121.50
1	1	60	PHE	N-CA-CB	-7.54	99.87	111.56
1	1	234	ILE	N-CA-CB	-7.53	101.96	110.99
3	3	179	ASN	CB-CA-C	7.52	129.18	112.78
3	3	182	ASN	CB-CA-C	-7.51	99.45	111.39
1	1	82	ASP	CA-CB-CG	-7.50	105.10	112.60
1	1	188	VAL	N-CA-CB	-7.48	100.74	111.21
3	3	40	GLU	CA-CB-CG	7.44	128.99	114.10
1	1	268	THR	CA-C-N	7.43	127.86	119.83
1	1	268	THR	C-N-CA	7.43	127.86	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	137	GLY	CA-C-O	-7.42	113.23	121.31
4	4	22	ASN	CB-CA-C	-7.39	99.51	110.16
3	3	50	ILE	O-C-N	7.38	126.79	121.55
2	2	5	GLU	CA-C-N	-7.38	109.49	122.84
2	2	5	GLU	C-N-CA	-7.38	109.49	122.84
1	1	190	TYR	N-CA-C	-7.29	94.81	107.49
1	1	29	ASN	CA-CB-CG	-7.27	105.33	112.60
3	3	176	ASP	CA-CB-CG	-7.27	105.33	112.60
1	1	118	SER	CA-CB-OG	7.25	125.60	111.10
2	2	34	VAL	N-CA-C	-7.25	97.03	107.98
4	4	53	ASN	OD1-CG-ND2	-7.21	115.39	122.60
3	3	1	SER	O-C-N	-7.20	111.49	123.00
3	3	19	PRO	CA-C-O	-7.18	116.00	121.31
3	3	40	GLU	CB-CG-CD	7.18	124.81	112.60
1	1	270	ARG	NE-CZ-NH2	7.16	125.64	119.20
2	2	149	ASP	CB-CA-C	-7.14	99.12	109.84
2	2	254	SER	O-C-N	-7.14	113.09	122.59
1	1	136	SER	N-CA-C	-7.14	101.09	111.30
1	1	260	THR	O-C-N	7.09	132.78	122.43
3	3	37	MET	N-CA-C	7.08	120.76	110.28
2	2	181	GLN	CA-CB-CG	7.08	128.25	114.10
2	2	8	GLU	CA-CB-CG	7.05	128.21	114.10
3	3	162	VAL	CB-CA-C	7.02	118.85	110.78
3	3	179	ASN	N-CA-CB	-7.01	100.03	110.97
3	3	193	THR	N-CA-C	-7.00	101.22	110.40
2	2	144	ASN	OD1-CG-ND2	6.97	129.57	122.60
1	1	209	ASP	CA-CB-CG	6.97	119.57	112.60
4	4	21	ILE	CB-CA-C	-6.94	100.71	111.26
2	2	181	GLN	CB-CA-C	6.88	120.80	109.72
2	2	32	ARG	NE-CZ-NH2	6.86	125.38	119.20
1	1	155	THR	N-CA-CB	-6.85	100.05	110.33
2	2	156	ARG	NE-CZ-NH2	6.84	125.36	119.20
2	2	182	PHE	CA-CB-CG	6.84	120.64	113.80
3	3	2	PRO	N-CA-C	-6.81	100.39	111.21
1	1	222	PHE	CA-CB-CG	6.80	120.60	113.80
4	4	53	ASN	CB-CG-OD1	6.80	134.40	120.80
3	3	69	ASN	N-CA-C	-6.79	104.98	112.72
3	3	173	VAL	CA-C-N	-6.77	116.43	122.73
3	3	173	VAL	C-N-CA	-6.77	116.43	122.73
2	2	156	ARG	CB-CA-C	6.76	121.88	109.71
1	1	28	GLU	CG-CD-OE2	6.76	133.94	118.40
4	4	70	ALA	CB-CA-C	-6.75	100.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	9	VAL	O-C-N	6.74	130.91	123.09
1	1	190	TYR	CB-CA-C	6.73	119.56	110.94
3	3	59	PRO	CB-CA-C	-6.73	95.18	112.00
4	4	17	GLU	CB-CG-CD	6.72	124.03	112.60
3	3	177	GLN	CB-CA-C	6.72	121.67	109.37
2	2	6	GLU	N-CA-C	6.71	116.72	107.73
2	2	253	LEU	O-C-N	-6.69	115.33	123.36
1	1	68	SER	CA-C-O	-6.68	113.74	121.49
1	1	85	ARG	CA-C-O	-6.67	113.48	119.75
2	2	253	LEU	N-CA-C	-6.66	95.90	107.49
3	3	69	ASN	N-CA-CB	6.63	120.58	110.70
2	2	113	GLN	N-CA-CB	6.62	121.57	110.77
3	3	160	PHE	CA-CB-CG	6.62	120.42	113.80
1	1	150	THR	CB-CA-C	6.60	119.12	109.48
4	4	27	ASN	CA-CB-CG	-6.60	106.00	112.60
3	3	28	LYS	N-CA-CB	-6.55	102.09	112.63
4	4	53	ASN	CA-CB-CG	-6.55	106.05	112.60
2	2	109	GLY	N-CA-C	-6.54	101.22	110.96
1	1	11	GLU	N-CA-C	6.52	119.81	110.10
1	1	269	PRO	N-CA-C	6.51	121.06	111.03
2	2	220	ALA	O-C-N	6.48	126.82	121.44
3	3	192	LEU	N-CA-C	-6.47	102.90	111.24
3	3	92	THR	N-CA-C	-6.45	100.97	110.52
4	4	43	ASP	CA-CB-CG	-6.44	106.16	112.60
2	2	117	ASN	CB-CA-C	-6.43	99.19	109.80
1	1	267	MET	N-CA-C	-6.43	97.10	110.80
1	1	274	LEU	N-CA-C	6.42	128.96	111.00
4	4	67	PRO	N-CA-C	-6.41	105.71	113.98
1	1	258	TRP	O-C-N	6.41	127.22	121.19
1	1	59	PRO	CA-C-O	-6.40	114.12	121.36
3	3	23	VAL	N-CA-C	6.38	114.12	108.63
3	3	105	ARG	CD-NE-CZ	6.36	133.30	124.40
1	1	218	PRO	O-C-N	6.31	130.26	123.01
3	3	169	HIS	N-CA-CB	6.30	119.93	110.22
1	1	164	SER	N-CA-C	-6.28	105.58	113.18
3	3	77	LEU	N-CA-C	-6.28	106.26	114.04
2	2	178	TYR	CA-C-O	-6.28	114.95	120.60
2	2	230	THR	CA-CB-OG1	-6.26	100.21	109.60
1	1	103	VAL	CA-C-O	-6.24	114.12	121.05
3	3	32	ALA	O-C-N	6.23	127.08	121.35
1	1	191	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	1	104	PHE	CA-CB-CG	6.22	120.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	134	TYR	CB-CA-C	6.19	119.30	109.52
3	3	88	CYS	CA-C-O	-6.16	114.35	120.70
4	4	21	ILE	O-C-N	6.16	129.33	122.61
1	1	201	TRP	CA-CB-CG	6.16	125.31	113.60
3	3	168	THR	CA-CB-CG2	6.16	120.97	110.50
4	4	25	TYR	CA-C-O	-6.14	114.47	121.72
2	2	101	ARG	NE-CZ-NH1	-6.13	115.36	121.50
2	2	255	ARG	CD-NE-CZ	6.12	132.97	124.40
2	2	233	ASP	CA-CB-CG	6.12	118.72	112.60
1	1	189	PRO	O-C-N	-6.09	114.42	122.64
2	2	6	GLU	CB-CA-C	-6.05	99.68	112.82
1	1	98	GLU	N-CA-C	6.05	118.35	108.55
4	4	12	SER	CB-CA-C	-6.04	99.32	109.65
1	1	144	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	1	155	THR	OG1-CB-CG2	6.00	121.31	109.30
1	1	267	MET	O-C-N	-6.00	114.61	122.59
2	2	21	ASN	CB-CG-ND2	6.00	125.40	116.40
2	2	117	ASN	CA-CB-CG	5.99	118.58	112.60
2	2	117	ASN	OD1-CG-ND2	5.99	128.59	122.60
2	2	114	VAL	CB-CA-C	5.98	119.90	110.81
1	1	183	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	1	207	ARG	CB-CG-CD	5.97	125.04	111.30
2	2	112	VAL	N-CA-CB	-5.95	101.48	112.43
3	3	186	TRP	N-CA-C	5.95	118.19	108.55
3	3	190	TRP	CA-CB-CG	5.95	124.89	113.60
1	1	192	SER	O-C-N	5.94	128.08	121.43
3	3	71	ALA	CA-C-O	-5.92	115.44	122.13
2	2	49	ALA	CA-C-O	5.91	126.18	119.27
2	2	198	VAL	CA-C-O	-5.90	114.27	120.76
1	1	43	ILE	CB-CA-C	5.86	117.27	110.88
3	3	182	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	1	109	LYS	CA-CB-CG	5.84	125.79	114.10
3	3	217	PHE	CA-CB-CG	5.84	119.64	113.80
1	1	168	GLY	CA-C-N	5.83	132.67	121.54
1	1	168	GLY	C-N-CA	5.83	132.67	121.54
2	2	35	GLY	O-C-N	-5.83	116.19	122.19
3	3	3	ILE	N-CA-C	5.82	113.63	107.76
1	1	126	ASP	N-CA-C	-5.80	100.73	109.95
1	1	67	ASN	CB-CA-C	-5.80	100.99	110.85
1	1	60	PHE	CA-CB-CG	5.79	119.59	113.80
3	3	203	THR	CA-CB-OG1	-5.79	100.92	109.60
1	1	18	ASP	CA-CB-CG	-5.78	106.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	81	GLN	N-CA-CB	5.76	118.77	110.06
1	1	260	THR	N-CA-C	-5.75	106.22	113.18
2	2	51	THR	N-CA-C	-5.75	102.40	110.50
2	2	144	ASN	CA-CB-CG	-5.74	106.86	112.60
2	2	21	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	2	241	VAL	CA-C-N	5.72	129.01	122.83
2	2	241	VAL	C-N-CA	5.72	129.01	122.83
3	3	139	ARG	N-CA-C	-5.72	105.19	111.82
3	3	126	ILE	CA-C-O	-5.71	114.39	120.39
1	1	77	PHE	CA-C-O	-5.69	112.37	120.51
2	2	244	VAL	CB-CA-C	5.67	119.24	110.96
3	3	168	THR	N-CA-CB	-5.67	101.64	109.97
1	1	219	ASN	CB-CA-C	-5.67	104.27	111.86
1	1	42	PRO	CA-C-O	-5.66	114.76	121.67
1	1	85	ARG	CA-CB-CG	5.66	125.42	114.10
2	2	39	VAL	CA-C-O	-5.65	117.21	121.68
1	1	51	GLY	CA-C-N	5.65	128.90	120.31
1	1	51	GLY	C-N-CA	5.65	128.90	120.31
2	2	24	THR	N-CA-CB	-5.65	101.60	110.69
2	2	22	THR	CA-CB-OG1	-5.64	101.14	109.60
3	3	94	LEU	O-C-N	5.62	127.94	122.09
3	3	167	PRO	CA-C-N	5.62	128.85	120.87
3	3	167	PRO	C-N-CA	5.62	128.85	120.87
1	1	272	GLY	CA-C-N	-5.62	111.86	121.97
1	1	272	GLY	C-N-CA	-5.62	111.86	121.97
2	2	4	THR	CB-CA-C	5.61	121.59	110.42
2	2	254	SER	CA-C-N	-5.60	111.57	120.70
2	2	254	SER	C-N-CA	-5.60	111.57	120.70
3	3	182	ASN	N-CA-C	5.60	119.72	111.04
1	1	8	GLY	N-CA-C	-5.59	107.60	115.32
4	4	19	VAL	CB-CA-C	5.58	119.15	110.83
2	2	154	GLY	CA-C-O	-5.57	117.44	122.57
3	3	161	THR	CA-C-N	-5.57	117.22	123.02
3	3	161	THR	C-N-CA	-5.57	117.22	123.02
2	2	55	LYS	N-CA-C	5.56	119.37	112.47
1	1	188	VAL	CB-CA-C	5.55	121.47	111.36
1	1	232	PRO	CA-C-N	-5.55	113.39	122.54
1	1	232	PRO	C-N-CA	-5.55	113.39	122.54
1	1	66	PRO	CA-C-O	5.55	129.47	122.15
3	3	105	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	1	32	LYS	N-CA-CB	5.53	118.10	109.97
3	3	138	SER	O-C-N	5.52	129.06	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	132	SER	CA-C-N	5.51	125.44	119.76
1	1	132	SER	C-N-CA	5.51	125.44	119.76
2	2	79	TYR	N-CA-CB	-5.50	102.71	111.62
2	2	138	ASP	O-C-N	5.50	127.81	122.09
3	3	146	THR	CA-C-O	-5.49	114.21	120.58
2	2	30	VAL	N-CA-CB	5.49	118.86	112.33
1	1	224	THR	N-CA-C	-5.48	101.60	110.32
3	3	166	SER	N-CA-C	5.48	115.19	108.11
1	1	211	THR	CA-C-N	5.48	132.15	121.41
1	1	211	THR	C-N-CA	5.48	132.15	121.41
3	3	35	ASN	CA-C-O	-5.47	112.91	119.15
1	1	241	ARG	CA-CB-CG	5.46	125.03	114.10
3	3	13	THR	CA-CB-OG1	-5.46	101.41	109.60
3	3	22	THR	CA-CB-OG1	-5.46	101.42	109.60
1	1	6	GLU	CB-CG-CD	5.44	121.85	112.60
3	3	31	VAL	O-C-N	-5.44	115.77	122.57
1	1	49	LYS	CA-C-O	5.43	128.79	121.89
1	1	85	ARG	N-CA-CB	-5.43	100.01	109.73
2	2	205	SER	O-C-N	5.43	129.38	122.65
2	2	10	LEU	CB-CA-C	-5.42	100.25	113.15
2	2	155	THR	CB-CA-C	-5.41	102.12	110.78
3	3	201	CYS	N-CA-CB	-5.41	101.20	110.72
1	1	26	LEU	CA-C-N	5.40	125.71	119.93
1	1	26	LEU	C-N-CA	5.40	125.71	119.93
1	1	123	TYR	CA-C-N	5.39	131.43	121.94
1	1	123	TYR	C-N-CA	5.39	131.43	121.94
1	1	274	LEU	N-CA-CB	-5.37	101.37	110.50
3	3	75	GLN	CB-CA-C	-5.37	104.21	110.17
3	3	54	ILE	N-CA-CB	5.36	117.96	110.56
3	3	31	VAL	N-CA-CB	-5.36	102.39	111.23
3	3	182	ASN	O-C-N	5.36	128.43	122.11
2	2	115	GLN	N-CA-C	5.34	118.17	109.24
2	2	68	ASN	OD1-CG-ND2	5.33	127.93	122.60
1	1	98	GLU	CA-C-O	5.33	126.72	120.43
3	3	58	MET	N-CA-C	-5.33	103.48	109.60
2	2	163	GLY	O-C-N	5.32	127.09	121.77
2	2	50	ASP	CB-CA-C	5.31	118.39	109.89
2	2	139	VAL	N-CA-CB	-5.31	102.47	111.23
4	4	36	SER	CA-CB-OG	-5.29	100.51	111.10
1	1	227	PHE	CA-CB-CG	5.29	119.09	113.80
4	4	26	SER	CA-CB-OG	-5.29	100.53	111.10
1	1	10	THR	O-C-N	5.28	130.58	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	229	SER	CB-CA-C	5.28	116.52	109.65
1	1	263	ASP	N-CA-CB	-5.28	101.50	111.43
2	2	255	ARG	NH1-CZ-NH2	-5.28	112.44	119.30
3	3	179	ASN	O-C-N	-5.27	116.66	122.72
1	1	54	GLU	CG-CD-OE2	5.26	130.50	118.40
1	1	126	ASP	CA-C-O	-5.26	115.22	121.16
1	1	144	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
2	2	109	GLY	CA-C-O	-5.25	116.01	121.63
4	4	40	THR	CA-CB-OG1	-5.25	101.73	109.60
1	1	168	GLY	CA-C-O	5.25	128.24	120.89
1	1	165	LEU	CA-C-O	5.24	125.98	119.79
1	1	170	THR	CA-CB-OG1	-5.24	101.74	109.60
1	1	144	ARG	CD-NE-CZ	-5.24	117.07	124.40
3	3	219	LEU	N-CA-CB	-5.23	101.66	111.13
3	3	98	SER	CA-C-O	5.22	126.27	120.63
2	2	252	VAL	N-CA-CB	5.22	119.85	111.23
3	3	156	SER	CA-C-O	-5.22	115.02	120.55
1	1	52	SER	N-CA-CB	-5.21	102.20	110.28
3	3	159	SER	CA-C-O	-5.21	114.88	120.46
2	2	81	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	3	15	TYR	CA-C-N	5.20	127.25	120.28
3	3	15	TYR	C-N-CA	5.20	127.25	120.28
1	1	39	ARG	CD-NE-CZ	-5.20	117.12	124.40
2	2	249	ARG	CD-NE-CZ	-5.20	117.12	124.40
2	2	161	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	3	83	THR	O-C-N	5.18	129.33	123.42
1	1	265	ILE	CB-CA-C	-5.18	104.60	111.80
3	3	151	ASP	CA-CB-CG	-5.18	107.42	112.60
1	1	100	THR	OG1-CB-CG2	5.16	119.61	109.30
2	2	229	SER	CA-C-N	5.16	129.45	120.68
2	2	229	SER	C-N-CA	5.16	129.45	120.68
1	1	118	SER	N-CA-CB	5.15	119.13	110.99
2	2	20	GLY	N-CA-C	-5.15	100.97	113.18
1	1	65	CYS	O-C-N	5.15	126.00	121.32
2	2	169	HIS	CA-CB-CG	5.14	118.94	113.80
1	1	103	VAL	CB-CA-C	5.13	118.74	112.02
3	3	9	GLU	CB-CG-CD	5.13	121.32	112.60
3	3	9	GLU	N-CA-C	5.13	116.87	111.28
1	1	222	PHE	O-C-N	5.13	128.44	122.24
2	2	235	THR	N-CA-CB	-5.12	102.04	111.37
1	1	181	SER	O-C-N	5.11	128.47	122.34
4	4	46	LYS	CB-CA-C	-5.11	100.26	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	50	GLN	CA-C-O	-5.10	113.71	119.78
2	2	61	ARG	CD-NE-CZ	5.09	131.53	124.40
3	3	130	PRO	O-C-N	5.09	123.65	121.31
1	1	60	PHE	N-CA-C	5.09	116.58	108.79
3	3	9	GLU	CB-CA-C	-5.08	102.36	110.79
2	2	198	VAL	O-C-N	5.08	128.68	123.05
3	3	219	LEU	CB-CA-C	5.07	119.71	109.68
1	1	236	PHE	CA-C-O	-5.06	115.19	121.06
1	1	29	ASN	OD1-CG-ND2	5.05	127.65	122.60
2	2	183	LEU	CA-C-N	5.05	129.12	122.30
2	2	183	LEU	C-N-CA	5.05	129.12	122.30
3	3	163	PRO	CA-C-O	-5.04	115.60	121.34
1	1	90	THR	CA-CB-CG2	5.03	119.05	110.50
2	2	180	HIS	CA-CB-CG	-5.02	108.78	113.80
1	1	100	THR	CA-CB-OG1	-5.01	102.08	109.60
1	1	16	THR	CA-CB-OG1	-5.01	102.08	109.60
1	1	111	ASP	CA-CB-CG	-5.01	107.59	112.60
1	1	19	PHE	N-CA-C	5.01	117.50	110.14
2	2	7	MET	CA-CB-CG	-5.00	104.09	114.10
2	2	122	HIS	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	273	VAL	Peptide
2	2	12	ASP	Peptide,Mainchain
2	2	5	GLU	Peptide
4	4	11	SER	Peptide
4	4	9	ASN	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2139	0	2065	247	0
2	2	2031	0	1949	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	1773	0	1761	112	0
4	4	461	0	425	93	0
5	2	10	0	0	6	0
6	1	114	0	0	11	0
6	2	122	0	0	13	0
6	3	50	0	0	8	0
6	4	10	0	0	2	0
All	All	6710	0	6200	587	0

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 47.

All (587) 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)
1:1:273:VAL:CB	1:1:273:VAL:CA	1.74	1.62
1:1:268:THR:HG21	1:1:274:LEU:CD1	1.33	1.53
1:1:274:LEU:N	1:1:274:LEU:CA	1.73	1.50
1:1:268:THR:CG2	1:1:274:LEU:HD12	1.43	1.48
1:1:45:ARG:CZ	1:1:235:LYS:HG3	1.39	1.46
2:2:5:GLU:HG2	2:2:10:LEU:CB	1.45	1.46
1:1:45:ARG:NH1	1:1:235:LYS:HD2	1.33	1.42
1:1:45:ARG:CZ	1:1:235:LYS:CG	2.00	1.37
1:1:45:ARG:CZ	1:1:235:LYS:HD2	1.57	1.33
1:1:45:ARG:CZ	1:1:235:LYS:CD	2.07	1.30
2:2:7:MET:CE	2:2:120:GLN:HE22	1.47	1.28
1:1:45:ARG:NH2	1:1:235:LYS:HG3	1.51	1.24
1:1:246:ARG:HG2	4:4:11:SER:CB	1.72	1.20
1:1:246:ARG:HA	4:4:11:SER:OG	1.38	1.19
4:4:60:ASN:ND2	4:4:61:ALA:H	1.42	1.16
1:1:45:ARG:NE	1:1:235:LYS:HG3	1.63	1.13
1:1:246:ARG:HG2	4:4:11:SER:HB2	1.29	1.12
4:4:9:ASN:HD22	4:4:10:ASN:HB2	0.95	1.11
1:1:45:ARG:NH1	1:1:235:LYS:CD	2.12	1.11
2:2:7:MET:HE2	2:2:7:MET:HA	1.20	1.10
2:2:10:LEU:CG	2:2:11:SER:H	1.58	1.09
2:2:7:MET:CE	2:2:7:MET:HA	1.81	1.09
2:2:158:GLN:HE21	2:2:158:GLN:HA	1.17	1.08
2:2:161:ARG:HG3	2:2:161:ARG:HH11	1.00	1.08
1:1:268:THR:CG2	1:1:274:LEU:HA	1.70	1.08
2:2:5:GLU:CG	2:2:10:LEU:CB	2.31	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:34:ALA:HB2	4:4:11:SER:O	1.54	1.07
1:1:99:GLU:O	1:1:100:THR:HB	1.46	1.06
1:1:45:ARG:NE	1:1:235:LYS:CG	2.17	1.05
1:1:273:VAL:CB	1:1:273:VAL:HA	1.86	1.05
2:2:10:LEU:CD1	2:2:11:SER:H	1.70	1.04
1:1:265:ILE:HG13	1:1:266:ASP:HB2	1.38	1.04
2:2:5:GLU:HG2	2:2:10:LEU:HB3	1.37	1.04
1:1:268:THR:HG21	1:1:274:LEU:HD13	1.41	1.03
1:1:268:THR:O	1:1:268:THR:HG23	1.59	1.02
2:2:251:GLU:O	2:2:252:VAL:HG23	1.59	1.02
2:2:7:MET:SD	2:2:120:GLN:NE2	2.31	1.01
2:2:7:MET:CE	2:2:120:GLN:NE2	2.22	1.01
4:4:12:SER:OG	4:4:13:SER:N	1.83	1.01
4:4:10:ASN:ND2	4:4:13:SER:HA	1.76	1.01
1:1:218:PRO:HB3	3:3:179:ASN:HD22	1.21	1.01
2:2:5:GLU:CG	2:2:10:LEU:HB2	1.89	1.00
1:1:36:PHE:O	1:1:39:ARG:HD2	1.62	1.00
4:4:9:ASN:ND2	4:4:10:ASN:HB2	1.74	1.00
2:2:5:GLU:HG2	2:2:10:LEU:HB2	1.03	1.00
1:1:246:ARG:CG	4:4:11:SER:HB2	1.91	1.00
3:3:31:VAL:HG12	6:3:425:HOH:O	1.61	0.99
1:1:270:ARG:NH2	1:1:271:ALA:O	1.96	0.98
4:4:69:LEU:O	4:4:70:ALA:CB	2.07	0.98
2:2:5:GLU:CG	2:2:10:LEU:HB3	1.91	0.97
2:2:7:MET:HE1	2:2:120:GLN:HE22	1.27	0.97
2:2:10:LEU:HD12	2:2:11:SER:N	1.80	0.97
2:2:3:ASN:C	2:2:4:THR:OG1	2.06	0.97
4:4:60:ASN:CG	4:4:61:ALA:H	1.70	0.96
2:2:181:GLN:HG2	2:2:191:VAL:HG22	1.48	0.96
2:2:10:LEU:O	2:2:13:ARG:HB2	1.65	0.95
1:1:218:PRO:CB	3:3:179:ASN:ND2	2.29	0.95
4:4:60:ASN:ND2	4:4:61:ALA:N	2.14	0.94
1:1:265:ILE:HG13	1:1:266:ASP:CB	1.96	0.94
1:1:265:ILE:CG1	1:1:266:ASP:N	2.29	0.94
1:1:246:ARG:CA	4:4:11:SER:OG	2.15	0.94
3:3:18:LEU:HD22	3:3:19:PRO:HD2	1.48	0.93
2:2:22:THR:HG21	2:2:62:TYR:H	1.32	0.93
2:2:161:ARG:HG3	2:2:161:ARG:NH1	1.80	0.92
1:1:218:PRO:HB3	3:3:179:ASN:ND2	1.84	0.92
2:2:24:THR:HG21	6:2:841:HOH:O	1.70	0.92
2:2:71:THR:HG23	2:2:73:THR:H	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:5:GLU:O	2:2:6:GLU:HG2	1.70	0.91
4:4:50:GLN:HA	6:4:78:HOH:O	1.68	0.91
1:1:273:VAL:C	1:1:274:LEU:CA	2.43	0.91
2:2:158:GLN:HA	2:2:158:GLN:NE2	1.78	0.91
3:3:79:VAL:HB	3:3:188:THR:HG22	1.53	0.90
1:1:268:THR:CG2	1:1:268:THR:O	2.18	0.90
1:1:268:THR:CG2	1:1:274:LEU:CD1	2.19	0.90
2:2:50:ASP:OD2	2:2:246:ASN:HB2	1.70	0.90
1:1:273:VAL:CA	1:1:273:VAL:HB	2.01	0.89
2:2:71:THR:CG2	2:2:73:THR:H	1.86	0.88
1:1:45:ARG:NH2	1:1:235:LYS:CG	2.22	0.88
2:2:161:ARG:HH11	2:2:161:ARG:CG	1.87	0.88
3:3:180:ILE:HB	6:3:393:HOH:O	1.74	0.88
3:3:120:MET:HE2	3:3:195:LEU:HD21	1.56	0.87
4:4:10:ASN:HD21	4:4:13:SER:HA	1.35	0.87
4:4:16:ASN:O	4:4:17:GLU:HG2	1.75	0.86
1:1:63:LYS:HD3	1:1:235:LYS:HZ1	1.41	0.86
1:1:61:SER:OG	1:1:82:ASP:HB2	1.75	0.86
1:1:218:PRO:CB	3:3:179:ASN:HD22	1.87	0.86
4:4:69:LEU:O	4:4:70:ALA:HB3	1.75	0.86
1:1:14:ASP:OD1	1:1:16:THR:HB	1.74	0.86
1:1:45:ARG:HH11	1:1:235:LYS:HD2	1.35	0.86
1:1:99:GLU:O	1:1:100:THR:CB	2.23	0.86
1:1:203:ASN:O	2:2:209:HIS:HD2	1.59	0.85
2:2:10:LEU:HD12	2:2:11:SER:H	1.34	0.85
2:2:71:THR:CG2	2:2:73:THR:HB	2.06	0.85
4:4:62:PHE:CD1	4:4:62:PHE:C	2.53	0.85
4:4:63:SER:OG	4:4:64:ASN:N	2.07	0.85
2:2:83:PRO:O	2:2:87:VAL:HG23	1.77	0.85
1:1:273:VAL:O	1:1:274:LEU:CA	2.26	0.83
4:4:62:PHE:HD1	4:4:63:SER:N	1.75	0.83
3:3:56:ASN:O	3:3:61:ALA:HA	1.78	0.83
3:3:36:TYR:CE2	3:3:37:MET:HE3	2.14	0.83
1:1:273:VAL:O	1:1:274:LEU:HD13	1.79	0.82
2:2:10:LEU:CG	2:2:11:SER:N	2.39	0.82
3:3:81:GLN:NE2	3:3:183:VAL:HG11	1.94	0.82
1:1:45:ARG:NE	1:1:235:LYS:CD	2.41	0.82
1:1:268:THR:HG21	1:1:274:LEU:CA	2.09	0.82
1:1:169:ARG:HD2	3:3:223:ILE:O	1.79	0.81
1:1:266:ASP:CG	1:1:267:MET:H	1.66	0.81
2:2:10:LEU:HG	2:2:11:SER:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:181:THR:HA	6:3:432:HOH:O	1.81	0.81
1:1:265:ILE:HG13	1:1:266:ASP:N	1.95	0.81
1:1:268:THR:HG21	1:1:274:LEU:HD12	0.82	0.80
1:1:246:ARG:HG2	4:4:11:SER:OG	1.79	0.80
4:4:45:PRO:HA	4:4:46:LYS:HE3	1.62	0.80
1:1:135:THR:HB	1:1:234:ILE:HG21	1.63	0.79
1:1:93:TRP:HA	2:2:160:ASN:HD21	1.47	0.79
1:1:63:LYS:HD3	1:1:235:LYS:NZ	1.97	0.79
2:2:254:SER:HB3	3:3:133:ALA:HB1	1.65	0.79
1:1:268:THR:N	1:1:269:PRO:HD3	1.99	0.78
1:1:45:ARG:NE	1:1:235:LYS:HD2	1.97	0.78
2:2:40:HIS:O	2:2:242:ARG:NH1	2.17	0.78
1:1:185:SER:HB2	3:3:10:HIS:HB3	1.66	0.78
3:3:143:MET:O	3:3:143:MET:HG2	1.82	0.77
1:1:218:PRO:HB2	3:3:179:ASN:ND2	1.98	0.77
1:1:270:ARG:HE	1:1:270:ARG:HA	1.49	0.77
4:4:12:SER:OG	4:4:13:SER:HB2	1.84	0.77
1:1:95:ASN:OD1	1:1:107:LYS:HE3	1.84	0.77
1:1:93:TRP:HB2	1:1:108:THR:HG23	1.65	0.77
1:1:208:PHE:CE2	3:3:131:PRO:CB	2.68	0.77
2:2:81:ARG:HD3	2:2:143:ASP:OD2	1.84	0.76
1:1:208:PHE:CD2	3:3:131:PRO:HB2	2.21	0.76
2:2:69:ASP:HA	2:2:233:ASP:HA	1.68	0.76
1:1:45:ARG:HH12	1:1:235:LYS:HZ2	1.30	0.76
1:1:45:ARG:NH1	1:1:235:LYS:NZ	2.34	0.75
1:1:208:PHE:CE2	3:3:131:PRO:HB2	2.21	0.75
1:1:61:SER:H	1:1:83:GLN:NE2	1.85	0.75
1:1:70:ILE:H	1:1:76:GLN:HE22	1.32	0.75
2:2:158:GLN:HE21	2:2:158:GLN:CA	1.95	0.75
1:1:3:GLU:HG2	1:1:10:THR:HG23	1.68	0.75
2:2:162:LYS:HA	5:2:825:PO4:O4	1.86	0.75
1:1:4:ASN:HB2	6:2:857:HOH:O	1.87	0.75
2:2:13:ARG:O	2:2:29:THR:HG22	1.87	0.74
2:2:72:SER:HB2	6:2:942:HOH:O	1.85	0.74
1:1:7:LYS:HE3	1:1:9:VAL:O	1.86	0.74
1:1:274:LEU:N	1:1:274:LEU:CB	2.50	0.74
4:4:46:LYS:HG2	4:4:47:THR:HG22	1.69	0.74
4:4:60:ASN:CG	4:4:61:ALA:N	2.45	0.74
3:3:182:ASN:HB3	3:3:183:VAL:HG23	1.69	0.74
1:1:268:THR:N	1:1:269:PRO:CD	2.51	0.73
4:4:62:PHE:CD1	4:4:63:SER:N	2.56	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:PHE:CD1	1:1:253:THR:HG21	2.22	0.73
1:1:246:ARG:CG	4:4:11:SER:CB	2.57	0.73
1:1:268:THR:CG2	1:1:274:LEU:CA	2.60	0.73
1:1:144:ARG:NH1	1:1:167:GLU:O	2.19	0.73
1:1:148:THR:H	1:1:191:ASN:ND2	1.88	0.72
1:1:273:VAL:HA	1:1:273:VAL:HB	1.64	0.72
1:1:268:THR:HG21	1:1:274:LEU:HA	1.42	0.72
2:2:188:ASN:ND2	2:2:190:THR:O	2.22	0.72
3:3:36:TYR:HE2	3:3:37:MET:HE3	1.54	0.72
4:4:13:SER:O	4:4:14:GLU:HB3	1.89	0.72
4:4:69:LEU:O	4:4:70:ALA:HB2	1.89	0.72
4:4:61:ALA:O	4:4:62:PHE:HB3	1.89	0.71
6:1:307:HOH:O	3:3:180:ILE:HG21	1.89	0.71
2:2:111:ARG:HD2	2:2:194:GLU:OE1	1.90	0.71
4:4:12:SER:OG	4:4:13:SER:CA	2.38	0.71
4:4:59:VAL:HG13	4:4:60:ASN:N	2.05	0.71
1:1:30:GLN:HG2	1:1:35:PHE:CE2	2.25	0.71
1:1:122:TYR:HB3	1:1:196:VAL:HG13	1.71	0.71
2:2:10:LEU:CD1	2:2:11:SER:N	2.43	0.71
2:2:5:GLU:HG3	2:2:10:LEU:HB3	1.73	0.70
2:2:71:THR:HG22	2:2:73:THR:HB	1.72	0.70
2:2:256:GLN:C	6:2:903:HOH:O	2.33	0.70
1:1:149:GLY:HA3	3:3:172:MET:HE2	1.73	0.69
1:1:172:GLN:HG3	6:1:362:HOH:O	1.92	0.69
2:2:60:GLU:HG2	6:2:906:HOH:O	1.93	0.69
3:3:120:MET:HE3	3:3:202:PRO:O	1.92	0.69
2:2:202:PRO:HG3	3:3:169:HIS:CE1	2.28	0.68
1:1:268:THR:HG22	1:1:274:LEU:HD12	1.66	0.68
4:4:66:LEU:C	4:4:68:LEU:H	2.01	0.68
1:1:266:ASP:CG	1:1:267:MET:N	2.39	0.68
3:3:123:LYS:NZ	3:3:151:ASP:OD1	2.27	0.68
4:4:45:PRO:CA	4:4:46:LYS:HE3	2.23	0.68
1:1:273:VAL:O	1:1:274:LEU:HA	1.93	0.68
2:2:79:TYR:CD1	2:2:79:TYR:C	2.72	0.68
4:4:9:ASN:HD22	4:4:10:ASN:CB	1.90	0.68
3:3:113:VAL:HB	3:3:208:LEU:HB2	1.76	0.68
3:3:120:MET:HE1	3:3:204:SER:O	1.94	0.67
2:2:13:ARG:C	2:2:29:THR:HG22	2.20	0.67
4:4:59:VAL:HG13	4:4:60:ASN:H	1.58	0.67
1:1:34:ALA:CB	4:4:11:SER:O	2.39	0.67
2:2:80:ILE:HG23	2:2:143:ASP:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:ARG:HE	1:1:235:LYS:HG3	1.59	0.67
1:1:45:ARG:HH12	1:1:235:LYS:NZ	1.92	0.66
1:1:63:LYS:O	1:1:64:ALA:HB3	1.95	0.66
1:1:209:ASP:HB3	1:1:211:THR:OG1	1.94	0.66
2:2:122:HIS:CE1	2:2:228:ALA:HB1	2.31	0.66
4:4:13:SER:O	4:4:14:GLU:CB	2.42	0.66
4:4:66:LEU:C	4:4:68:LEU:N	2.50	0.66
2:2:254:SER:HB3	3:3:133:ALA:CB	2.25	0.66
2:2:22:THR:HG21	2:2:62:TYR:N	2.08	0.66
3:3:65:ILE:HG23	3:3:209:THR:HG21	1.78	0.66
1:1:268:THR:CB	1:1:274:LEU:HD12	2.25	0.66
2:2:71:THR:CG2	2:2:73:THR:CB	2.73	0.65
2:2:252:VAL:HB	2:2:253:LEU:C	2.16	0.65
2:2:162:LYS:HA	5:2:825:PO4:P	2.37	0.65
4:4:12:SER:OG	4:4:13:SER:CB	2.43	0.65
1:1:38:ASP:HB3	4:4:16:ASN:HB2	1.78	0.65
2:2:249:ARG:HG3	2:2:250:HIS:N	2.10	0.65
2:2:254:SER:O	2:2:255:ARG:NE	2.29	0.65
4:4:46:LYS:N	4:4:46:LYS:CE	2.60	0.65
2:2:199:ASN:ND2	2:2:204:SER:HB2	2.12	0.64
4:4:45:PRO:C	4:4:46:LYS:HD2	2.21	0.64
6:1:307:HOH:O	3:3:180:ILE:HG12	1.98	0.64
3:3:81:GLN:HE21	3:3:183:VAL:HG11	1.60	0.64
2:2:123:ALA:HB3	2:2:223:THR:HG22	1.78	0.64
2:2:252:VAL:HB	2:2:253:LEU:O	1.98	0.63
1:1:28:GLU:HG2	1:1:30:GLN:H	1.61	0.63
2:2:7:MET:HE2	2:2:120:GLN:HE22	1.54	0.63
1:1:273:VAL:CA	1:1:273:VAL:CG1	2.72	0.63
4:4:60:ASN:HD22	4:4:61:ALA:N	1.93	0.63
2:2:240:PRO:HB2	2:2:243:PRO:HG3	1.81	0.63
1:1:218:PRO:HB2	3:3:179:ASN:HD21	1.62	0.63
3:3:124:PHE:HE1	3:3:152:LEU:HD13	1.62	0.63
4:4:62:PHE:C	4:4:62:PHE:HD1	2.02	0.62
1:1:45:ARG:NH1	1:1:235:LYS:CE	2.61	0.62
4:4:61:ALA:O	4:4:62:PHE:CB	2.48	0.62
2:2:21:ASN:OD1	2:2:61:ARG:NH1	2.32	0.62
3:3:137:THR:OG1	3:3:141:GLN:NE2	2.32	0.62
1:1:95:ASN:HB3	1:1:102:GLU:O	2.00	0.62
1:1:142:LEU:HD11	6:1:362:HOH:O	1.98	0.62
4:4:23:ASN:ND2	4:4:30:GLN:HE22	1.96	0.62
1:1:139:HIS:HE1	1:1:141:LEU:HD22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:13:ARG:HA	2:2:29:THR:HG22	1.82	0.62
3:3:171:ARG:NH1	6:3:432:HOH:O	2.33	0.62
1:1:51:GLY:HA2	6:1:334:HOH:O	1.99	0.61
1:1:45:ARG:HH21	1:1:235:LYS:HG3	1.53	0.61
3:3:99:ARG:HG3	3:3:225:PRO:HB3	1.80	0.61
3:3:94:LEU:HD13	3:3:213:ALA:HB2	1.82	0.61
2:2:5:GLU:HB2	2:2:6:GLU:HA	1.83	0.61
1:1:191:ASN:HA	3:3:221:MET:HE1	1.82	0.61
1:1:265:ILE:HG12	1:1:266:ASP:N	2.13	0.61
4:4:23:ASN:HD21	4:4:30:GLN:HE22	1.48	0.61
2:2:158:GLN:NE2	2:2:158:GLN:CA	2.56	0.60
3:3:117:THR:CG2	3:3:119:MET:HB2	2.31	0.60
2:2:250:HIS:HE1	3:3:133:ALA:O	1.85	0.60
1:1:49:LYS:HG2	1:1:50:SER:N	2.15	0.60
1:1:71:LEU:HD11	1:1:225:LEU:HD13	1.82	0.60
2:2:104:TYR:CZ	3:3:131:PRO:HG2	2.36	0.60
2:2:19:ALA:HB1	2:2:61:ARG:HA	1.83	0.60
2:2:22:THR:CG2	2:2:62:TYR:HB2	2.32	0.60
1:1:77:PHE:O	1:1:78:ASP:CB	2.50	0.60
1:1:77:PHE:O	1:1:78:ASP:HB3	2.01	0.59
4:4:45:PRO:O	4:4:47:THR:N	2.35	0.59
3:3:62:VAL:CG2	6:3:399:HOH:O	2.50	0.59
1:1:172:GLN:O	3:3:16:SER:HB3	2.01	0.59
1:1:270:ARG:HA	1:1:270:ARG:NE	2.11	0.59
2:2:38:THR:HG22	2:2:39:VAL:N	2.18	0.59
2:2:180:HIS:C	2:2:180:HIS:CD2	2.80	0.59
1:1:246:ARG:HG3	4:4:11:SER:HB2	1.80	0.59
2:2:186:ARG:NH1	2:2:187:THR:OG1	2.36	0.59
3:3:107:SER:H	3:3:216:ASP:HB3	1.68	0.59
1:1:98:GLU:HA	2:2:161:ARG:HH11	1.68	0.58
3:3:177:GLN:O	3:3:182:ASN:ND2	2.36	0.58
1:1:214:LEU:HD11	2:2:138:ASP:HA	1.83	0.58
1:1:268:THR:HG21	1:1:273:VAL:O	2.04	0.58
4:4:57:GLY:O	4:4:58:ALA:C	2.46	0.58
2:2:1:ASP:OD1	2:2:1:ASP:O	2.21	0.58
3:3:154:LEU:O	3:3:154:LEU:HG	2.03	0.58
1:1:49:LYS:HG2	1:1:50:SER:H	1.69	0.58
1:1:96:GLY:HA3	1:1:101:SER:HB3	1.85	0.57
1:1:273:VAL:CB	1:1:273:VAL:N	2.57	0.57
1:1:82:ASP:OD1	1:1:82:ASP:N	2.27	0.57
4:4:38:ASN:ND2	4:4:40:THR:HB	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:LEU:HD12	1:1:238:VAL:HG22	1.87	0.57
2:2:66:LYS:HE3	2:2:233:ASP:HB2	1.84	0.57
2:2:186:ARG:NH1	2:2:186:ARG:HG3	2.19	0.57
1:1:154:PRO:O	1:1:164:SER:OG	2.20	0.57
2:2:241:VAL:CG1	2:2:242:ARG:NH1	2.68	0.57
3:3:117:THR:CG2	3:3:119:MET:H	2.17	0.57
4:4:46:LYS:N	4:4:46:LYS:CD	2.67	0.57
3:3:131:PRO:HD3	3:3:185:GLY:N	2.19	0.57
1:1:61:SER:HB3	1:1:82:ASP:O	2.04	0.57
2:2:162:LYS:HA	5:2:825:PO4:O3	2.05	0.57
2:2:10:LEU:HG	2:2:11:SER:N	2.13	0.57
2:2:152:PRO:HD2	2:2:153:ASN:H	1.70	0.57
1:1:258:TRP:O	1:1:259:PRO:C	2.48	0.57
1:1:268:THR:CG2	1:1:273:VAL:O	2.52	0.57
1:1:122:TYR:HB3	1:1:196:VAL:CG1	2.35	0.56
2:2:50:ASP:OD2	2:2:246:ASN:CB	2.47	0.56
2:2:181:GLN:CG	2:2:191:VAL:HG22	2.28	0.56
1:1:191:ASN:HA	3:3:221:MET:CE	2.35	0.56
3:3:28:LYS:O	3:3:30:PRO:HD3	2.05	0.56
2:2:251:GLU:O	2:2:252:VAL:CG2	2.46	0.56
2:2:71:THR:HG21	2:2:73:THR:HB	1.84	0.56
2:2:241:VAL:HG12	2:2:242:ARG:NH1	2.19	0.56
3:3:137:THR:H	3:3:141:GLN:NE2	2.02	0.56
1:1:267:MET:C	1:1:269:PRO:HD3	2.30	0.56
2:2:162:LYS:CA	5:2:825:PO4:O4	2.52	0.56
3:3:117:THR:HG23	3:3:119:MET:H	1.70	0.56
1:1:230:THR:O	1:1:232:PRO:HD3	2.06	0.56
2:2:118:ALA:HB2	2:2:232:LEU:HD13	1.88	0.56
1:1:148:THR:H	1:1:191:ASN:HD21	1.51	0.56
2:2:241:VAL:CG1	2:2:242:ARG:HH12	2.19	0.56
2:2:205:SER:OG	2:2:208:GLN:OE1	2.23	0.55
3:3:18:LEU:HD22	3:3:19:PRO:CD	2.29	0.55
3:3:18:LEU:CD2	3:3:19:PRO:HD2	2.31	0.55
4:4:16:ASN:C	4:4:17:GLU:HG2	2.31	0.55
3:3:117:THR:HG22	3:3:120:MET:H	1.71	0.55
1:1:98:GLU:HA	2:2:161:ARG:HG3	1.88	0.55
4:4:59:VAL:HG22	4:4:60:ASN:H	1.72	0.55
2:2:106:VAL:HG12	2:2:206:TRP:HB3	1.89	0.55
1:1:94:GLY:O	1:1:96:GLY:N	2.40	0.55
4:4:46:LYS:HD2	4:4:47:THR:H	1.70	0.55
4:4:9:ASN:HD22	4:4:9:ASN:C	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:ARG:CD	1:1:235:LYS:HD2	2.36	0.54
1:1:142:LEU:CD1	6:1:362:HOH:O	2.54	0.54
4:4:22:ASN:O	4:4:23:ASN:C	2.50	0.54
1:1:111:ASP:HB3	1:1:114:PHE:HB3	1.90	0.54
2:2:186:ARG:HG3	2:2:186:ARG:HH11	1.73	0.54
2:2:252:VAL:O	2:2:253:LEU:HD23	2.08	0.54
1:1:45:ARG:NE	1:1:235:LYS:CB	2.71	0.54
4:4:21:ILE:O	4:4:21:ILE:HG22	2.06	0.54
2:2:7:MET:HE2	2:2:120:GLN:NE2	2.15	0.53
3:3:94:LEU:CD1	3:3:213:ALA:HB2	2.38	0.53
3:3:81:GLN:NE2	3:3:183:VAL:CG1	2.68	0.53
4:4:60:ASN:O	4:4:61:ALA:HB3	2.07	0.53
1:1:244:ASN:ND2	4:4:9:ASN:O	2.40	0.53
4:4:38:ASN:HD21	4:4:40:THR:HB	1.74	0.53
4:4:11:SER:O	4:4:12:SER:C	2.51	0.53
2:2:199:ASN:HD22	2:2:204:SER:HB2	1.71	0.53
1:1:273:VAL:C	1:1:274:LEU:CB	2.82	0.52
1:1:3:GLU:CG	1:1:10:THR:HG23	2.37	0.52
4:4:46:LYS:CG	4:4:47:THR:HG22	2.39	0.52
1:1:175:SER:O	1:1:176:ALA:HB2	2.09	0.52
2:2:22:THR:HG21	2:2:62:TYR:HB2	1.92	0.52
2:2:186:ARG:HH11	2:2:186:ARG:CG	2.22	0.52
1:1:76:GLN:O	1:1:77:PHE:CB	2.57	0.52
1:1:32:LYS:HB3	4:4:12:SER:O	2.09	0.52
1:1:93:TRP:HA	2:2:160:ASN:ND2	2.22	0.52
3:3:103:GLN:HE21	3:3:172:MET:HE1	1.73	0.52
3:3:107:SER:OG	3:3:216:ASP:HB2	2.09	0.52
3:3:83:THR:HG23	3:3:83:THR:O	2.09	0.52
1:1:203:ASN:O	2:2:209:HIS:CD2	2.51	0.52
1:1:205:HIS:HD2	1:1:210:ASN:OD1	1.93	0.52
2:2:156:ARG:HG3	2:2:160:ASN:HB3	1.92	0.52
4:4:23:ASN:CG	4:4:30:GLN:HE22	2.18	0.52
1:1:150:THR:HB	3:3:223:ILE:HD13	1.92	0.52
1:1:181:SER:HB2	3:3:9:GLU:O	2.10	0.51
1:1:98:GLU:HA	2:2:161:ARG:NH1	2.25	0.51
1:1:212:GLY:O	1:1:213:ASP:HB2	2.09	0.51
2:2:88:LEU:O	2:2:93:GLY:HA3	2.11	0.51
3:3:81:GLN:HE21	3:3:183:VAL:CG1	2.23	0.51
1:1:202:TYR:HB3	1:1:215:GLY:O	2.11	0.51
1:1:263:ASP:OD1	1:1:263:ASP:O	2.28	0.51
4:4:46:LYS:HE3	4:4:46:LYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:209:ASP:CB	1:1:211:THR:OG1	2.58	0.51
3:3:94:LEU:HD21	3:3:108:LEU:HD22	1.92	0.51
3:3:9:GLU:C	3:3:11:ALA:H	2.18	0.51
1:1:265:ILE:HG13	1:1:266:ASP:CA	2.41	0.50
2:2:203:THR:HG23	3:3:167:PRO:HA	1.93	0.50
3:3:75:GLN:HG3	3:3:76:PRO:O	2.11	0.50
1:1:45:ARG:NH1	1:1:235:LYS:HZ2	1.97	0.50
1:1:218:PRO:HG2	3:3:180:ILE:CG1	2.41	0.50
2:2:14:VAL:HG22	2:2:27:GLN:HG3	1.93	0.50
4:4:66:LEU:O	4:4:67:PRO:C	2.52	0.50
2:2:4:THR:C	2:2:5:GLU:HG3	2.36	0.50
2:2:128:VAL:HB	2:2:191:VAL:HG11	1.94	0.50
2:2:132:PRO:HA	2:2:211:SER:O	2.10	0.50
2:2:206:TRP:CE3	2:2:207:THR:HA	2.47	0.50
3:3:14:TRP:CH2	3:3:16:SER:HB2	2.47	0.50
4:4:57:GLY:O	4:4:59:VAL:N	2.43	0.50
2:2:41:ASP:OD1	2:2:41:ASP:N	2.42	0.50
4:4:9:ASN:ND2	4:4:9:ASN:C	2.67	0.50
2:2:135:PRO:HB2	6:2:914:HOH:O	2.11	0.50
1:1:191:ASN:HB3	3:3:221:MET:HE2	1.93	0.49
2:2:81:ARG:HH11	2:2:143:ASP:CG	2.20	0.49
2:2:114:VAL:HG11	2:2:128:VAL:HG11	1.94	0.49
6:1:307:HOH:O	3:3:180:ILE:CG2	2.56	0.49
2:2:181:GLN:NE2	6:2:884:HOH:O	2.44	0.49
2:2:13:ARG:CA	2:2:29:THR:HG22	2.41	0.49
2:2:181:GLN:HE21	2:2:191:VAL:HA	1.76	0.49
4:4:38:ASN:ND2	4:4:40:THR:H	2.11	0.49
1:1:38:ASP:OD1	1:1:241:ARG:HD2	2.13	0.49
1:1:43:ILE:HG21	1:1:240:LEU:HG	1.95	0.49
1:1:98:GLU:O	1:1:101:SER:N	2.31	0.49
1:1:96:GLY:HA3	1:1:101:SER:CB	2.43	0.49
1:1:207:ARG:HH21	1:1:211:THR:HB	1.77	0.49
1:1:108:THR:OG1	1:1:110:GLN:NE2	2.45	0.49
2:2:161:ARG:NH1	2:2:161:ARG:CG	2.52	0.49
1:1:205:HIS:CE1	1:1:214:LEU:CD2	2.96	0.49
1:1:208:PHE:CE1	3:3:180:ILE:HA	2.48	0.49
1:1:265:ILE:CG1	1:1:266:ASP:CB	2.81	0.49
1:1:126:ASP:HA	1:1:189:PRO:O	2.13	0.49
1:1:208:PHE:CD2	3:3:131:PRO:CB	2.95	0.49
3:3:105:ARG:O	3:3:217:PHE:HA	2.13	0.49
1:1:274:LEU:N	1:1:274:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:257:PRO:HG2	1:1:270:ARG:HD2	1.95	0.48
1:1:97:ASN:O	2:2:161:ARG:NH1	2.46	0.48
1:1:135:THR:HB	1:1:234:ILE:HD13	1.95	0.48
2:2:59:VAL:HG22	2:2:96:PHE:HA	1.95	0.48
4:4:56:SER:C	4:4:58:ALA:H	2.20	0.48
1:1:45:ARG:CD	1:1:235:LYS:CD	2.92	0.48
1:1:101:SER:O	2:2:162:LYS:NZ	2.47	0.48
1:1:182:ASN:HB3	6:1:282:HOH:O	2.13	0.48
4:4:9:ASN:ND2	4:4:10:ASN:CB	2.63	0.48
1:1:76:GLN:O	1:1:77:PHE:HB2	2.13	0.48
2:2:7:MET:CE	2:2:7:MET:CA	2.66	0.48
1:1:47:ALA:HB3	1:1:65:CYS:O	2.13	0.48
1:1:273:VAL:O	1:1:274:LEU:CD1	2.56	0.48
2:2:122:HIS:HE1	2:2:228:ALA:HB1	1.78	0.48
1:1:43:ILE:HD11	1:1:69:VAL:HG21	1.96	0.48
2:2:114:VAL:C	2:2:115:GLN:HG3	2.34	0.48
2:2:183:LEU:C	2:2:183:LEU:HD23	2.38	0.48
2:2:249:ARG:CG	2:2:249:ARG:HH11	2.27	0.48
1:1:117:PHE:CE1	1:1:253:THR:HG21	2.48	0.48
4:4:20:ILE:HD12	4:4:20:ILE:HA	1.59	0.48
1:1:96:GLY:C	1:1:97:ASN:HD22	2.22	0.47
2:2:71:THR:CG2	2:2:73:THR:N	2.67	0.47
4:4:50:GLN:NE2	6:4:76:HOH:O	2.46	0.47
1:1:90:THR:O	2:2:167:MET:HG2	2.14	0.47
4:4:45:PRO:C	4:4:46:LYS:HE3	2.39	0.47
1:1:182:ASN:HD22	1:1:182:ASN:HA	1.44	0.47
2:2:86:HIS:H	2:2:86:HIS:CD2	2.31	0.47
2:2:156:ARG:CG	2:2:160:ASN:HB3	2.44	0.47
1:1:268:THR:HG23	1:1:274:LEU:HA	1.82	0.47
1:1:218:PRO:HG2	3:3:180:ILE:HG13	1.96	0.47
2:2:162:LYS:C	5:2:825:PO4:O4	2.56	0.47
3:3:83:THR:C	3:3:85:SER:H	2.21	0.47
3:3:117:THR:O	3:3:120:MET:HB2	2.15	0.47
4:4:57:GLY:C	4:4:59:VAL:N	2.73	0.47
1:1:148:THR:N	1:1:191:ASN:ND2	2.61	0.47
2:2:71:THR:HG22	2:2:73:THR:H	1.71	0.47
3:3:178:ALA:O	3:3:179:ASN:HB3	2.14	0.47
4:4:38:ASN:HD22	4:4:40:THR:H	1.63	0.47
2:2:249:ARG:CG	2:2:250:HIS:N	2.78	0.47
2:2:59:VAL:HG23	2:2:95:VAL:HG12	1.97	0.46
1:1:150:THR:HB	1:1:151:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:56:SER:C	4:4:58:ALA:N	2.74	0.46
1:1:131:LEU:O	1:1:133:PRO:HD3	2.16	0.46
2:2:32:ARG:HD2	6:2:845:HOH:O	2.15	0.46
2:2:249:ARG:HG3	2:2:250:HIS:H	1.79	0.46
2:2:61:ARG:O	2:2:239:GLN:HB2	2.15	0.46
4:4:10:ASN:HD22	4:4:13:SER:HA	1.70	0.46
1:1:48:VAL:HG23	1:1:236:PHE:HE1	1.81	0.46
1:1:270:ARG:NE	1:1:270:ARG:CA	2.78	0.46
2:2:83:PRO:HB3	2:2:136:THR:HG21	1.98	0.46
3:3:8:ARG:NH1	3:3:9:GLU:OE2	2.49	0.46
1:1:95:ASN:HA	1:1:107:LYS:HG2	1.98	0.46
2:2:28:SER:OG	2:2:189:THR:HB	2.16	0.46
1:1:45:ARG:HD3	1:1:65:CYS:SG	2.56	0.46
1:1:32:LYS:CB	4:4:12:SER:O	2.64	0.45
2:2:152:PRO:HD2	2:2:153:ASN:N	2.28	0.45
1:1:26:LEU:HA	1:1:27:PRO:HD2	1.74	0.45
1:1:92:ILE:HG23	1:1:110:GLN:NE2	2.31	0.45
2:2:115:GLN:HB2	2:2:235:THR:HG23	1.97	0.45
1:1:120:PHE:CG	1:1:247:VAL:HB	2.51	0.45
1:1:270:ARG:HE	1:1:271:ALA:N	2.15	0.45
2:2:101:ARG:NH1	2:2:251:GLU:OE2	2.49	0.45
1:1:98:GLU:O	1:1:99:GLU:C	2.59	0.45
1:1:258:TRP:HA	1:1:259:PRO:HD2	1.76	0.45
3:3:128:TYR:O	3:3:145:ALA:HB1	2.16	0.45
1:1:15:ALA:O	1:1:21:ALA:HB3	2.17	0.45
1:1:141:LEU:HD12	1:1:228:ALA:O	2.16	0.45
1:1:205:HIS:CD2	1:1:210:ASN:HA	2.52	0.45
1:1:233:ASP:N	1:1:233:ASP:OD1	2.49	0.45
2:2:157:THR:O	2:2:160:ASN:N	2.49	0.45
2:2:101:ARG:HB2	2:2:251:GLU:HG3	1.98	0.45
2:2:104:TYR:CE1	3:3:131:PRO:HG2	2.52	0.45
3:3:9:GLU:H	3:3:9:GLU:HG3	1.29	0.45
1:1:45:ARG:NE	1:1:235:LYS:HB2	2.32	0.45
3:3:178:ALA:O	3:3:179:ASN:CB	2.64	0.45
2:2:22:THR:HG23	2:2:62:TYR:HB2	1.98	0.45
2:2:86:HIS:NE2	2:2:206:TRP:O	2.49	0.45
2:2:111:ARG:NH1	2:2:194:GLU:OE1	2.49	0.45
2:2:134:TYR:OH	2:2:175:TRP:CZ2	2.69	0.45
3:3:83:THR:C	3:3:85:SER:N	2.74	0.45
2:2:54:GLU:OE2	2:2:55:LYS:HE3	2.17	0.45
2:2:97:GLY:O	2:2:101:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:241:ARG:HH12	4:4:16:ASN:HB3	1.82	0.45
4:4:23:ASN:OD1	4:4:30:GLN:NE2	2.50	0.45
4:4:46:LYS:N	4:4:46:LYS:HD2	2.30	0.45
2:2:79:TYR:CE2	2:2:151:LEU:HD11	2.52	0.44
1:1:246:ARG:CG	4:4:11:SER:OG	2.58	0.44
2:2:40:HIS:NE2	2:2:107:LYS:NZ	2.45	0.44
2:2:19:ALA:CB	2:2:61:ARG:HA	2.48	0.44
2:2:223:THR:HG21	6:2:869:HOH:O	2.17	0.44
3:3:23:VAL:HA	3:3:24:PRO:HD3	1.72	0.44
1:1:45:ARG:HD3	1:1:235:LYS:CD	2.47	0.44
1:1:251:ARG:HB2	1:1:252:PRO:HD2	1.98	0.44
2:2:5:GLU:O	2:2:5:GLU:CD	2.61	0.44
3:3:62:VAL:HG21	6:3:399:HOH:O	2.15	0.44
3:3:115:THR:HB	3:3:206:LYS:O	2.17	0.44
2:2:81:ARG:HB3	2:2:213:THR:CG2	2.48	0.44
2:2:169:HIS:O	2:2:170:GLN:HG2	2.18	0.44
3:3:117:THR:HG21	3:3:201:CYS:SG	2.57	0.44
2:2:21:ASN:OD1	2:2:21:ASN:C	2.60	0.44
2:2:46:ALA:O	3:3:105:ARG:NH2	2.51	0.44
1:1:62:ASN:C	1:1:63:LYS:CG	2.90	0.44
1:1:133:PRO:HA	1:1:236:PHE:HB3	2.00	0.44
6:1:307:HOH:O	3:3:180:ILE:CG1	2.59	0.44
2:2:156:ARG:NH2	5:2:825:PO4:O4	2.45	0.44
1:1:191:ASN:CB	3:3:221:MET:HE2	2.48	0.44
2:2:7:MET:HG3	2:2:7:MET:O	2.17	0.44
2:2:254:SER:CB	3:3:133:ALA:CB	2.94	0.44
1:1:95:ASN:CB	1:1:102:GLU:O	2.65	0.44
2:2:144:ASN:HD22	2:2:144:ASN:HA	1.36	0.44
2:2:249:ARG:CG	2:2:249:ARG:NH1	2.79	0.44
3:3:81:GLN:HE22	3:3:183:VAL:HG11	1.81	0.44
1:1:81:TYR:HB3	1:1:84:LEU:HD12	1.99	0.43
3:3:163:PRO:HG2	3:3:165:ILE:CD1	2.48	0.43
1:1:197:LEU:HA	1:1:198:PRO:HD3	1.93	0.43
2:2:91:GLU:C	2:2:93:GLY:H	2.26	0.43
2:2:104:TYR:HB3	2:2:247:GLY:HA3	2.00	0.43
3:3:75:GLN:HE21	3:3:75:GLN:HB2	1.51	0.43
3:3:124:PHE:HE1	3:3:152:LEU:CD1	2.30	0.43
1:1:208:PHE:CE2	3:3:131:PRO:HB3	2.52	0.43
2:2:186:ARG:NH1	2:2:186:ARG:CG	2.80	0.43
3:3:163:PRO:HG2	3:3:165:ILE:HD11	2.01	0.43
3:3:191:GLN:HE21	3:3:191:GLN:HB3	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:47:THR:HG23	4:4:47:THR:O	2.18	0.43
1:1:60:PHE:HB3	1:1:67:ASN:CG	2.44	0.43
1:1:69:VAL:HG12	1:1:227:PHE:CZ	2.54	0.43
2:2:5:GLU:CB	2:2:10:LEU:HB2	2.45	0.43
1:1:119:PRO:HB3	1:1:253:THR:HG23	2.01	0.43
2:2:13:ARG:HA	2:2:29:THR:CG2	2.48	0.43
1:1:70:ILE:HD13	1:1:88:ARG:HG2	2.01	0.43
1:1:167:GLU:HG2	6:1:298:HOH:O	2.19	0.43
1:1:208:PHE:CD1	1:1:208:PHE:N	2.85	0.43
2:2:9:ASN:HB3	2:2:27:GLN:O	2.19	0.43
2:2:104:TYR:HA	2:2:249:ARG:HH21	1.84	0.43
1:1:254:VAL:HG23	2:2:169:HIS:CE1	2.54	0.42
1:1:259:PRO:C	1:1:261:SER:H	2.18	0.42
1:1:60:PHE:O	1:1:66:PRO:HA	2.20	0.42
1:1:82:ASP:C	1:1:83:GLN:OE1	2.62	0.42
1:1:208:PHE:HE1	6:3:393:HOH:O	2.02	0.42
1:1:268:THR:HG22	1:1:274:LEU:CD1	2.36	0.42
2:2:136:THR:CG2	2:2:213:THR:OG1	2.68	0.42
2:2:101:ARG:NH2	6:2:843:HOH:O	2.52	0.42
1:1:202:TYR:CG	1:1:217:ALA:HB2	2.54	0.42
2:2:45:PRO:HB3	2:2:203:THR:HB	2.01	0.42
3:3:43:ASP:O	3:3:46:GLU:HB2	2.20	0.42
4:4:23:ASN:HD22	4:4:25:TYR:H	1.68	0.42
1:1:268:THR:HG23	1:1:273:VAL:O	2.20	0.42
1:1:75:PRO:HA	1:1:110:GLN:HB3	2.01	0.42
3:3:85:SER:OG	3:3:174:GLY:HA2	2.20	0.42
4:4:46:LYS:HD2	4:4:47:THR:N	2.35	0.42
4:4:64:ASN:O	4:4:67:PRO:HD2	2.20	0.42
1:1:263:ASP:O	1:1:264:LYS:HB3	2.19	0.42
2:2:157:THR:HG22	2:2:159:THR:H	1.85	0.42
3:3:93:PHE:HA	3:3:96:ALA:HB3	2.01	0.42
1:1:67:ASN:O	1:1:227:PHE:CD2	2.73	0.41
2:2:54:GLU:HG2	6:2:936:HOH:O	2.20	0.41
3:3:94:LEU:O	3:3:98:SER:HB2	2.20	0.41
1:1:43:ILE:CG2	1:1:240:LEU:HG	2.49	0.41
1:1:265:ILE:CG1	1:1:266:ASP:CA	2.97	0.41
4:4:66:LEU:O	4:4:68:LEU:N	2.52	0.41
1:1:101:SER:C	2:2:162:LYS:NZ	2.79	0.41
1:1:204:GLY:O	1:1:214:LEU:HA	2.20	0.41
1:1:218:PRO:O	1:1:219:ASN:HB2	2.20	0.41
1:1:251:ARG:NH2	6:2:831:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:181:GLN:NE2	2:2:192:ASP:H	2.18	0.41
1:1:224:THR:HG22	1:1:225:LEU:N	2.34	0.41
2:2:102:ARG:HH11	2:2:102:ARG:HD2	1.48	0.41
2:2:111:ARG:HD2	2:2:194:GLU:CD	2.45	0.41
1:1:61:SER:HA	1:1:66:PRO:HA	2.01	0.41
2:2:5:GLU:O	2:2:6:GLU:CG	2.55	0.41
2:2:151:LEU:HA	2:2:151:LEU:HD23	1.85	0.41
3:3:47:ILE:HD11	3:3:93:PHE:CZ	2.56	0.41
3:3:107:SER:OG	3:3:216:ASP:CB	2.69	0.41
3:3:226:ALA:HA	3:3:227:PRO:HD3	1.86	0.41
1:1:49:LYS:CG	1:1:50:SER:N	2.82	0.41
1:1:62:ASN:C	1:1:63:LYS:HG3	2.45	0.41
2:2:225:SER:HB2	6:2:871:HOH:O	2.21	0.41
3:3:208:LEU:HD12	3:3:208:LEU:HA	1.93	0.41
2:2:101:ARG:HH11	2:2:101:ARG:HD2	1.50	0.41
1:1:77:PHE:HD1	1:1:77:PHE:HA	1.81	0.40
1:1:230:THR:O	1:1:232:PRO:CD	2.69	0.40
2:2:6:GLU:OE2	2:2:13:ARG:NH1	2.54	0.40
2:2:114:VAL:CG1	2:2:128:VAL:HG11	2.50	0.40
2:2:38:THR:CG2	2:2:39:VAL:N	2.84	0.40
3:3:76:PRO:HA	3:3:190:TRP:CE3	2.57	0.40
1:1:248:PHE:CD1	1:1:248:PHE:N	2.88	0.40
2:2:256:GLN:O	2:2:256:GLN:HG2	2.22	0.40
3:3:168:THR:CG2	6:3:432:HOH:O	2.69	0.40
1:1:15:ALA:HA	6:1:284:HOH:O	2.21	0.40
1:1:45:ARG:HD3	1:1:235:LYS:HD2	2.03	0.40
4:4:16:ASN:C	4:4:17:GLU:CG	2.93	0.40
4:4:59:VAL:HG22	4:4:60:ASN:N	2.35	0.40

There are no symmetry-related clashes.

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	272/274 (99%)	222 (82%)	37 (14%)	13 (5%)	2	14
2	2	254/256 (99%)	214 (84%)	27 (11%)	13 (5%)	1	13
3	3	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	9	40
4	4	60/70 (86%)	39 (65%)	8 (13%)	13 (22%)	0	0
All	All	815/831 (98%)	680 (83%)	93 (11%)	42 (5%)	1	12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	PHE
1	1	95	ASN
1	1	176	ALA
1	1	189	PRO
1	1	213	ASP
1	1	266	ASP
2	2	5	GLU
2	2	11	SER
2	2	13	ARG
2	2	252	VAL
4	4	10	ASN
4	4	46	LYS
4	4	58	ALA
4	4	62	PHE
4	4	66	LEU
4	4	69	LEU
1	1	100	THR
1	1	212	GLY
2	2	7	MET
2	2	86	HIS
3	3	90	ALA
4	4	63	SER
2	2	9	ASN
2	2	118	ALA
3	3	61	ALA
4	4	23	ASN
4	4	68	LEU
1	1	78	ASP
2	2	4	THR
2	2	158	GLN
2	2	160	ASN
4	4	59	VAL
3	3	223	ILE

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Mol	Chain	Res	Type
4	4	13	SER
4	4	14	GLU
4	4	32	SER
1	1	5	ALA
2	2	20	GLY
2	2	172	PHE
1	1	151	PRO
1	1	259	PRO
1	1	272	GLY

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	238/238 (100%)	191 (80%)	47 (20%)	1	8
2	2	224/224 (100%)	170 (76%)	54 (24%)	1	4
3	3	195/195 (100%)	152 (78%)	43 (22%)	1	5
4	4	52/59 (88%)	32 (62%)	20 (38%)	0	0
All	All	709/716 (99%)	545 (77%)	164 (23%)	1	5

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	22	GLN
1	1	28	GLU
1	1	39	ARG
1	1	40	SER
1	1	50	SER
1	1	52	SER
1	1	54	GLU
1	1	63	LYS
1	1	67	ASN
1	1	83	GLN
1	1	88	ARG
1	1	89	LEU

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Mol	Chain	Res	Type
1	1	100	THR
1	1	103	VAL
1	1	109	LYS
1	1	110	GLN
1	1	113	SER
1	1	116	LEU
1	1	118	SER
1	1	124	LYS
1	1	131	LEU
1	1	153	LYS
1	1	155	THR
1	1	156	THR
1	1	158	VAL
1	1	161	GLU
1	1	166	SER
1	1	182	ASN
1	1	185	SER
1	1	188	VAL
1	1	195	SER
1	1	196	VAL
1	1	197	LEU
1	1	206	LYS
1	1	207	ARG
1	1	211	THR
1	1	213	ASP
1	1	225	LEU
1	1	233	ASP
1	1	235	LYS
1	1	241	ARG
1	1	248	PHE
1	1	251	ARG
1	1	260	THR
1	1	268	THR
1	1	273	VAL
1	1	274	LEU
2	2	3	ASN
2	2	4	THR
2	2	5	GLU
2	2	7	MET
2	2	10	LEU
2	2	16	GLN
2	2	22	THR

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Mol	Chain	Res	Type
2	2	24	THR
2	2	27	GLN
2	2	43	GLU
2	2	50	ASP
2	2	57	LEU
2	2	59	VAL
2	2	61	ARG
2	2	68	ASN
2	2	69	ASP
2	2	71	THR
2	2	72	SER
2	2	75	LYS
2	2	81	ARG
2	2	88	LEU
2	2	89	SER
2	2	91	GLU
2	2	114	VAL
2	2	130	MET
2	2	137	LEU
2	2	138	ASP
2	2	139	VAL
2	2	144	ASN
2	2	145	ARG
2	2	148	LYS
2	2	156	ARG
2	2	158	GLN
2	2	160	ASN
2	2	161	ARG
2	2	184	ASN
2	2	186	ARG
2	2	189	THR
2	2	190	THR
2	2	191	VAL
2	2	211	SER
2	2	221	PRO
2	2	223	THR
2	2	225	SER
2	2	230	THR
2	2	231	SER
2	2	235	THR
2	2	239	GLN
2	2	246	ASN

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Mol	Chain	Res	Type
2	2	249	ARG
2	2	252	VAL
2	2	253	LEU
2	2	254	SER
2	2	255	ARG
3	3	9	GLU
3	3	16	SER
3	3	18	LEU
3	3	21	SER
3	3	31	VAL
3	3	46	GLU
3	3	57	LYS
3	3	58	MET
3	3	74	THR
3	3	75	GLN
3	3	77	LEU
3	3	79	VAL
3	3	97	LEU
3	3	99	ARG
3	3	107	SER
3	3	115	THR
3	3	117	THR
3	3	121	LYS
3	3	124	PHE
3	3	141	GLN
3	3	143	MET
3	3	152	LEU
3	3	154	LEU
3	3	157	SER
3	3	159	SER
3	3	162	VAL
3	3	166	SER
3	3	172	MET
3	3	176	ASP
3	3	177	GLN
3	3	179	ASN
3	3	180	ILE
3	3	181	THR
3	3	191	GLN
3	3	203	THR
3	3	208	LEU
3	3	212	SER

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Mol	Chain	Res	Type
3	3	215	LYS
3	3	216	ASP
3	3	221	MET
3	3	223	ILE
3	3	224	SER
3	3	229	SER
4	4	12	SER
4	4	13	SER
4	4	16	ASN
4	4	19	VAL
4	4	20	ILE
4	4	21	ILE
4	4	22	ASN
4	4	23	ASN
4	4	26	SER
4	4	30	GLN
4	4	35	LEU
4	4	40	THR
4	4	46	LYS
4	4	50	GLN
4	4	53	ASN
4	4	54	LEU
4	4	56	SER
4	4	62	PHE
4	4	65	MET
4	4	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	ASN
1	1	76	GLN
1	1	97	ASN
1	1	110	GLN
1	1	139	HIS
1	1	157	GLN
1	1	172	GLN
1	1	182	ASN
1	1	191	ASN
1	1	205	HIS
2	2	2	GLN
2	2	27	GLN

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Mol	Chain	Res	Type
2	2	120	GLN
2	2	144	ASN
2	2	150	ASN
2	2	158	GLN
2	2	160	ASN
2	2	181	GLN
2	2	184	ASN
2	2	209	HIS
2	2	250	HIS
3	3	10	HIS
3	3	75	GLN
3	3	81	GLN
3	3	103	GLN
3	3	141	GLN
3	3	144	GLN
3	3	169	HIS
3	3	177	GLN
3	3	179	ASN
3	3	182	ASN
4	4	9	ASN
4	4	10	ASN
4	4	16	ASN
4	4	23	ASN
4	4	27	ASN
4	4	28	GLN
4	4	30	GLN
4	4	31	ASN
4	4	38	ASN
4	4	50	GLN
4	4	53	ASN
4	4	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	PO4	2	309	-	4,4,4	2.94	4 (100%)	6,6,6	0.31	0
5	PO4	2	825	-	4,4,4	2.93	4 (100%)	6,6,6	0.42	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	825	PO4	P-O3	-3.18	1.45	1.54
5	2	309	PO4	P-O4	-3.16	1.45	1.54
5	2	825	PO4	P-O2	-3.16	1.45	1.54
5	2	309	PO4	P-O2	-3.15	1.45	1.54
5	2	309	PO4	P-O3	-3.11	1.45	1.54
5	2	825	PO4	P-O4	-3.07	1.45	1.54
5	2	309	PO4	P-O1	-2.23	1.45	1.50
5	2	825	PO4	P-O1	-2.18	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	825	PO4	6	0

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
2	2	2
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	58:ALA	C	59:VAL	N	1.87
1	2	255:ARG	C	256:GLN	N	1.16
1	2	12:ASP	C	13:ARG	N	0.95

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.