



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:00 AM UTC

PDB ID : 6VNO / pdb_00006vno
EMDB ID : EMD-21250
Title : Cryo-EM structure of the C-terminal half of the Parkinson's Disease-linked protein Leucine Rich Repeat Kinase 2 (LRRK2)
Authors : Leschziner, A.; Deniston, C.; Lahiri, I.
Deposited on : 2020-01-29
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

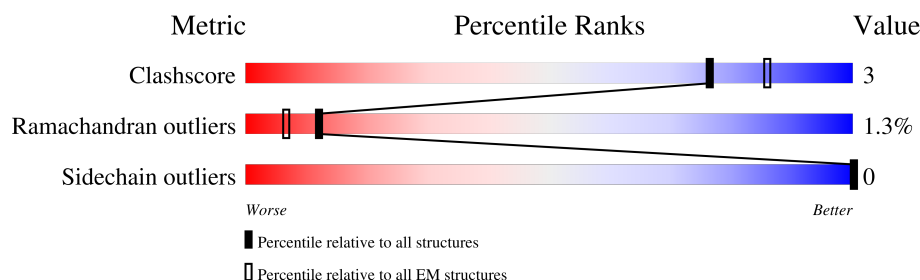
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-A	1201	81% 8% • 10%
1	10-A	1201	83% 7% • 10%
1	2-A	1201	81% 8% • 10%
1	3-A	1201	81% 8% • 10%
1	4-A	1201	81% 8% • 10%
1	5-A	1201	82% 7% • 10%
1	6-A	1201	82% 7% • 10%
1	7-A	1201	81% 8% • 10%
1	8-A	1201	81% 8% • 10%

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Mol	Chain	Length	Quality of chain
1	9-A	1201	81% 8% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 85600 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	2-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	3-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	4-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	5-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	6-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	7-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	8-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	9-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		
1	10-A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	1-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	2-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	3-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	4-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	5-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	6-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	7-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	8-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	9-A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	10-A	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	1-A	1	Total	Mg	0
			1	1	
3	2-A	1	Total	Mg	0
			1	1	

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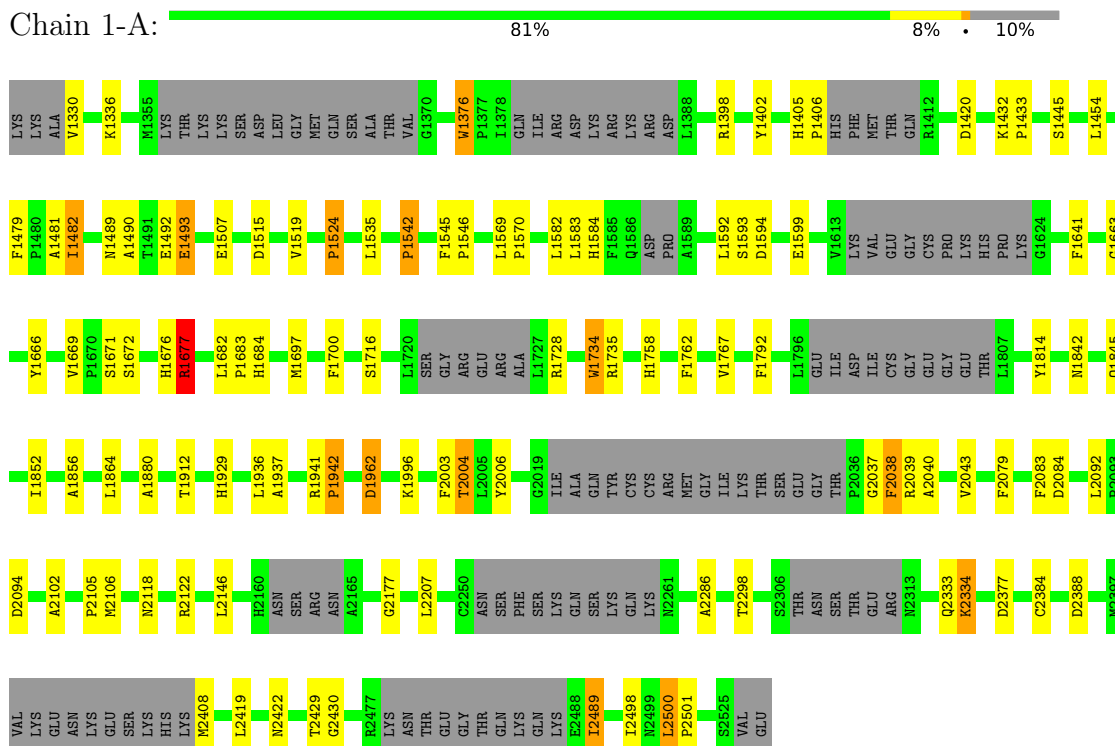
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Mol	Chain	Residues	Atoms		AltConf
3	3-A	1	Total 1	Mg 1	0
3	4-A	1	Total 1	Mg 1	0
3	5-A	1	Total 1	Mg 1	0
3	6-A	1	Total 1	Mg 1	0
3	7-A	1	Total 1	Mg 1	0
3	8-A	1	Total 1	Mg 1	0
3	9-A	1	Total 1	Mg 1	0
3	10-A	1	Total 1	Mg 1	0

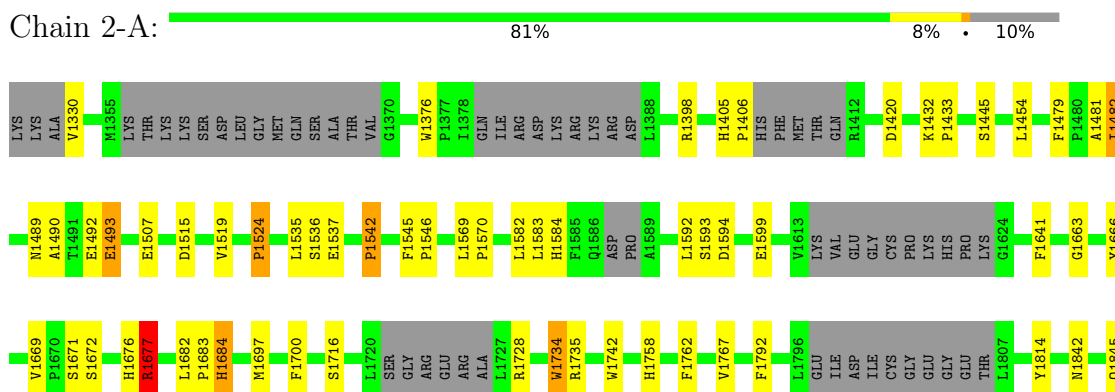
3 Residue-property plots

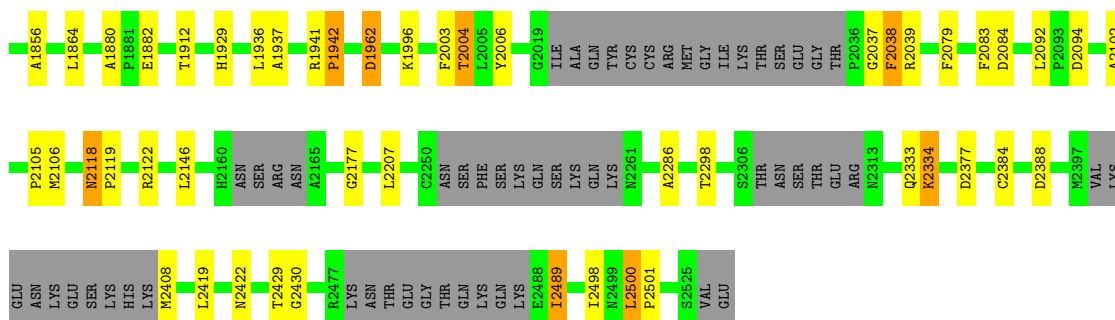
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



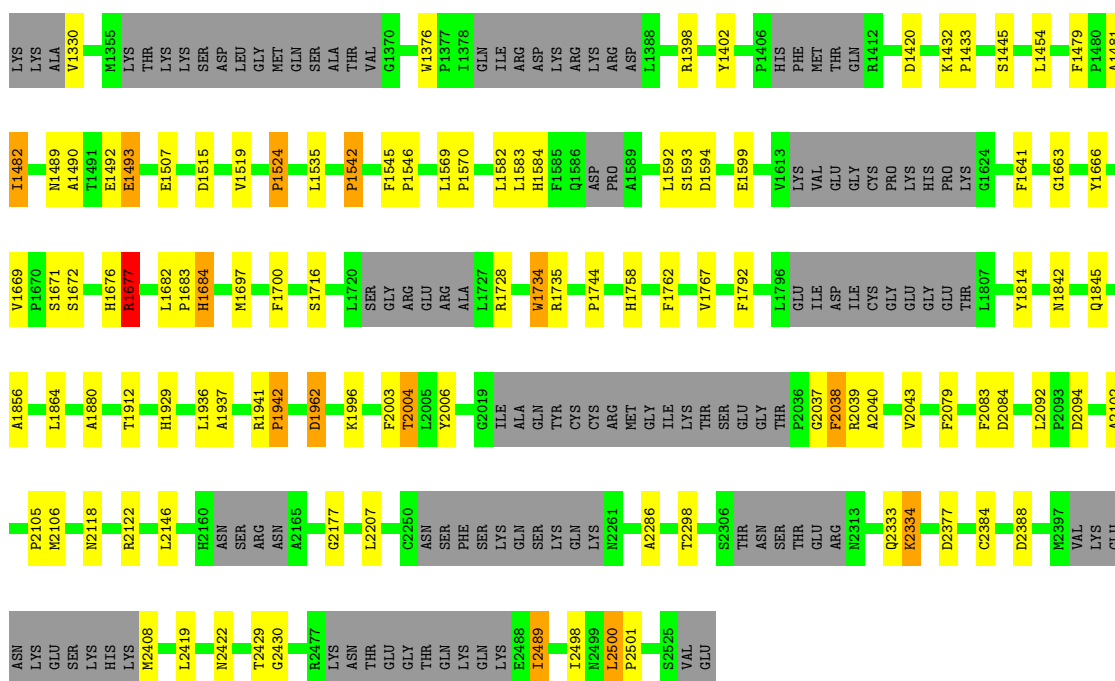
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2





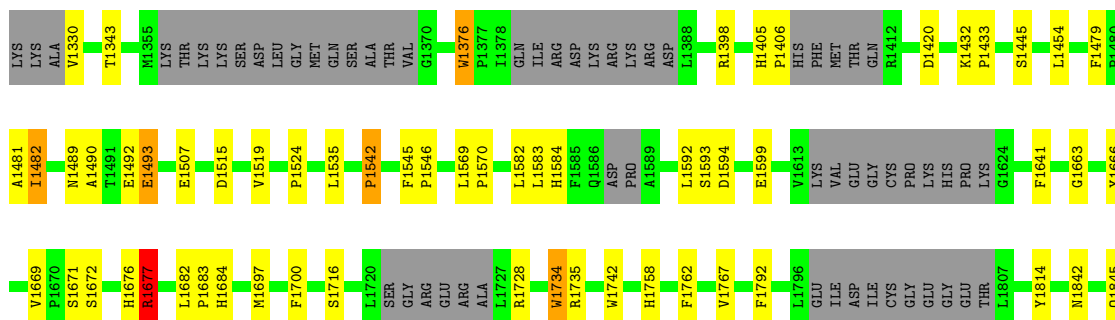
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

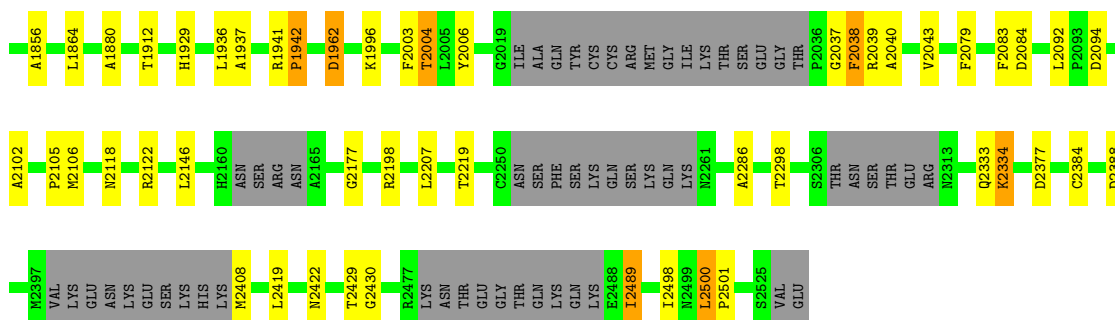
Chain 3-A: 81% 8% 10%



- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

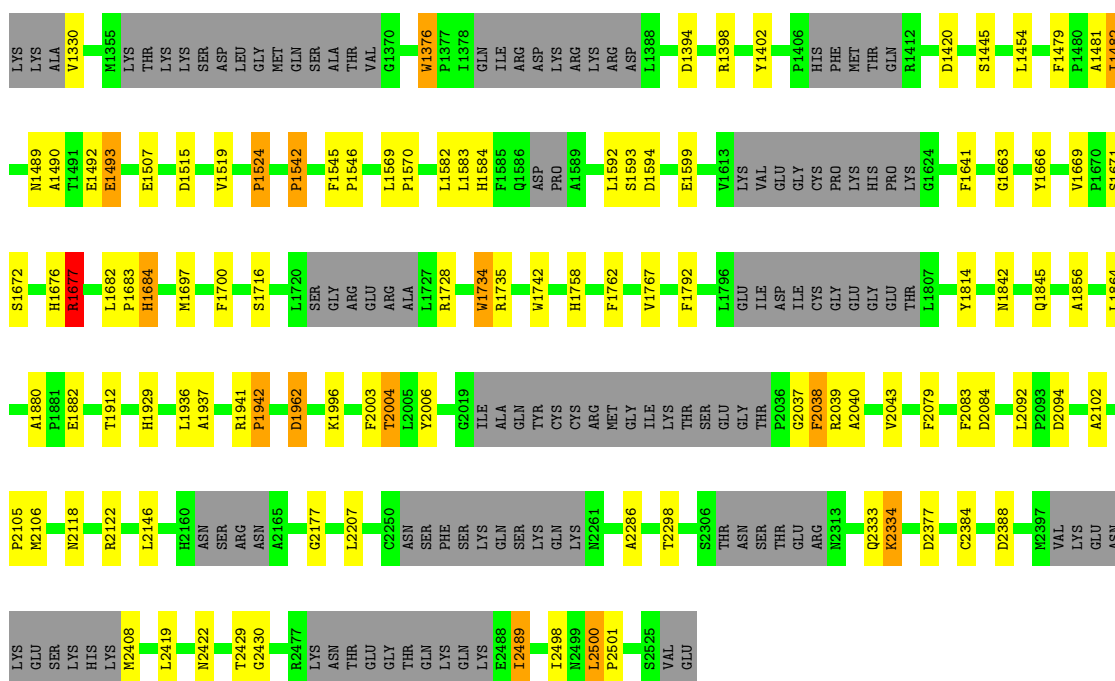
Chain 4-A: 81% 8% 10%





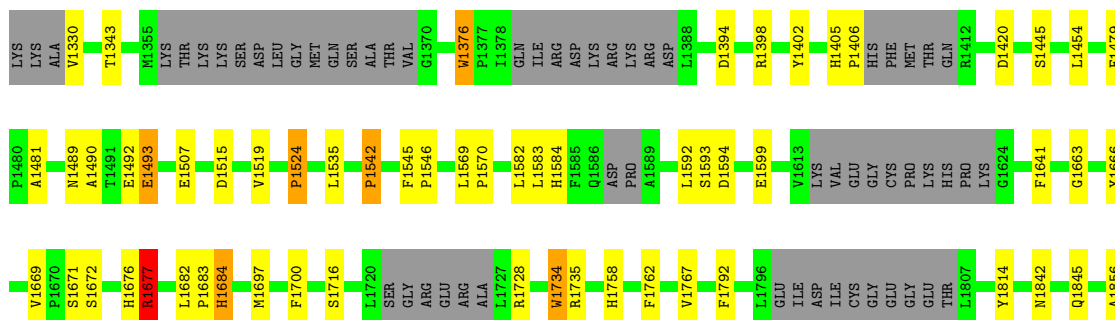
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

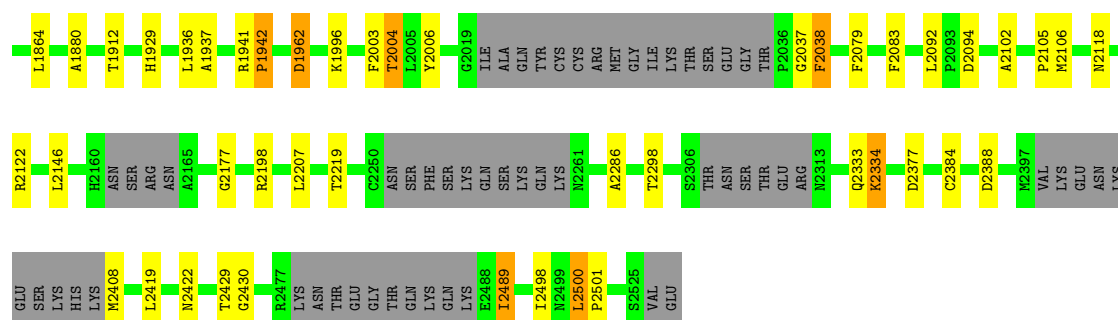
Chain 5-A: 82% 7% 10%



- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

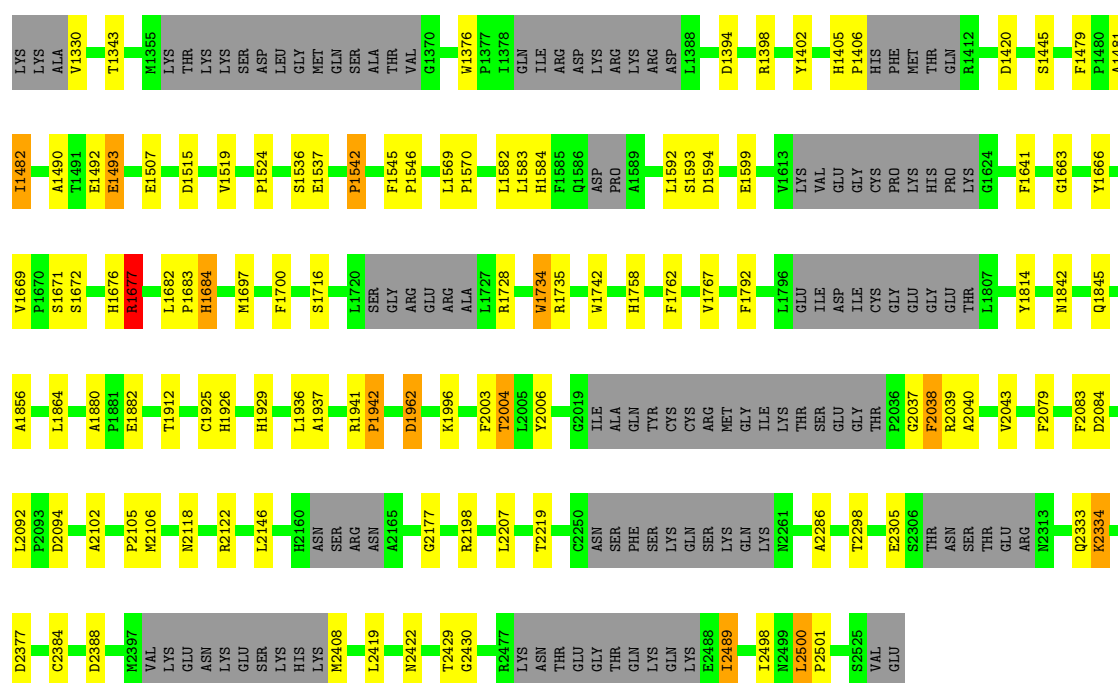
Chain 6-A: 82% 7% 10%





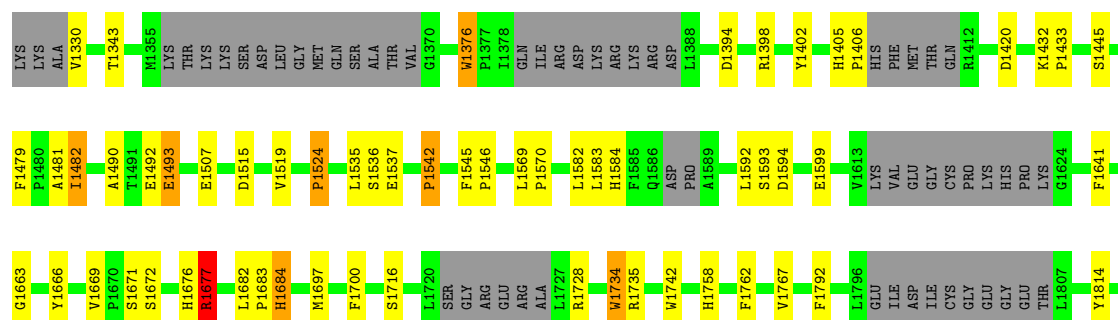
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

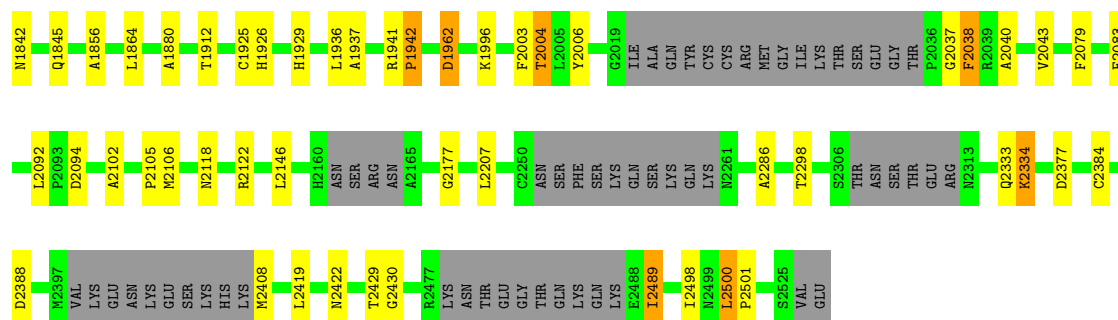
Chain 7-A: 81% 8% 10%



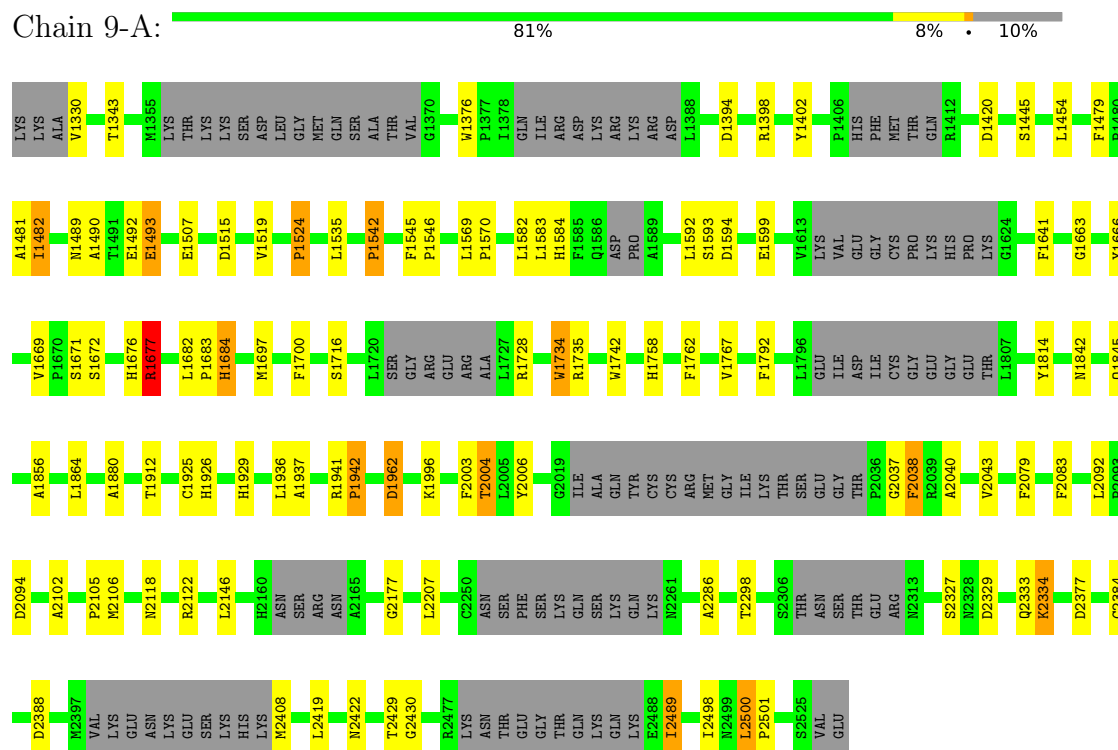
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

Chain 8-A: 81% 8% 10%

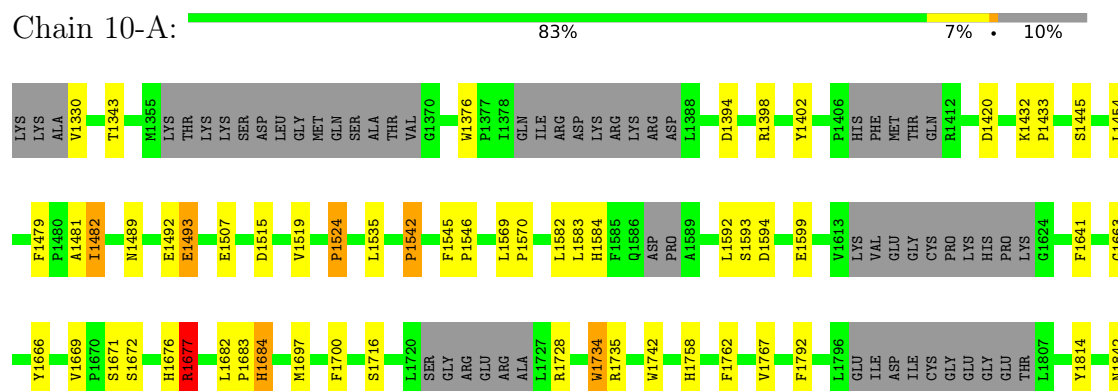




- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	70953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Per-particle CTF values	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: MG, TPO, GDP

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-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	2-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	3-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	4-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	5-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	6-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	7-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	8-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	9-A	0.76	0/8682	1.05	82/11746 (0.7%)
1	10-A	0.76	0/8627	1.05	82/11669 (0.7%)
All	All	0.76	0/86765	1.05	820/117383 (0.7%)

There are no bond length outliers.

All (820) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	1-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	2-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	2-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	3-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	3-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	4-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	4-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	5-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	5-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	6-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	6-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	7-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	7-A	2079	PHE	C-N-CA	8.54	128.27	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	8-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	9-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	9-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	10-A	2079	PHE	CA-C-N	8.54	128.27	119.56
1	10-A	2079	PHE	C-N-CA	8.54	128.27	119.56
1	1-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	1-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	2-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	2-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	3-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	3-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	4-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	4-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	5-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	5-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	6-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	6-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	7-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	7-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	8-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	8-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	9-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	9-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	10-A	1845	GLN	CA-C-N	8.46	129.28	119.47
1	10-A	1845	GLN	C-N-CA	8.46	129.28	119.47
1	1-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	1-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	2-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	2-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	3-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	3-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	4-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	4-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	5-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	5-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	6-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	6-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	7-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	7-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	8-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	8-A	2298	THR	C-N-CA	8.45	128.39	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	9-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	10-A	2298	THR	CA-C-N	8.45	128.39	119.85
1	10-A	2298	THR	C-N-CA	8.45	128.39	119.85
1	1-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	1-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	2-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	2-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	3-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	3-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	4-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	4-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	5-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	5-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	6-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	6-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	7-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	7-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	8-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	8-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	9-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	9-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	10-A	2122	ARG	CA-C-N	8.22	128.24	119.78
1	10-A	2122	ARG	C-N-CA	8.22	128.24	119.78
1	1-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	1-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	2-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	2-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	3-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	3-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	4-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	4-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	5-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	5-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	6-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	6-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	7-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	7-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	8-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	8-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	9-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	9-A	1677	ARG	C-N-CA	8.05	128.11	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	1677	ARG	CA-C-N	8.05	128.11	119.89
1	10-A	1677	ARG	C-N-CA	8.05	128.11	119.89
1	1-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	1-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	2-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	2-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	3-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	3-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	4-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	4-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	5-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	5-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	6-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	6-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	7-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	7-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	8-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	8-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	9-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	9-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	10-A	1880	ALA	CA-C-N	7.83	128.25	119.32
1	10-A	1880	ALA	C-N-CA	7.83	128.25	119.32
1	1-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	1-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	2-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	2-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	3-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	3-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	4-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	4-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	5-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	5-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	6-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	6-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	7-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	7-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	8-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	8-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	9-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	9-A	2102	ALA	C-N-CA	7.64	127.68	119.89
1	10-A	2102	ALA	CA-C-N	7.64	127.68	119.89
1	10-A	2102	ALA	C-N-CA	7.64	127.68	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	1-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	2-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	2-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	3-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	3-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	4-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	4-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	5-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	5-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	6-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	6-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	7-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	7-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	8-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	8-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	9-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	9-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	10-A	1728	ARG	CA-C-N	7.52	127.44	119.85
1	10-A	1728	ARG	C-N-CA	7.52	127.44	119.85
1	1-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	1-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	2-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	2-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	3-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	3-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	4-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	4-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	5-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	5-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	6-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	6-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	7-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	7-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	8-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	8-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	9-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	9-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	10-A	1599	GLU	CA-C-N	7.51	127.88	119.32
1	10-A	1599	GLU	C-N-CA	7.51	127.88	119.32
1	1-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	1-A	1856	ALA	C-N-CA	7.44	128.38	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	2-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	3-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	3-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	4-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	4-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	5-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	5-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	6-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	6-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	7-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	7-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	8-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	8-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	9-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	9-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	10-A	1856	ALA	CA-C-N	7.44	128.38	120.12
1	10-A	1856	ALA	C-N-CA	7.44	128.38	120.12
1	1-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	1-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	2-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	2-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	3-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	3-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	4-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	4-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	5-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	5-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	6-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	6-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	7-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	7-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	8-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	8-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	9-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	9-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	10-A	2118	ASN	CA-C-N	7.43	128.09	119.47
1	10-A	2118	ASN	C-N-CA	7.43	128.09	119.47
1	1-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	1-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	2-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	2-A	2006	TYR	C-N-CA	7.37	127.72	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	3-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	4-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	4-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	5-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	5-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	6-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	6-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	7-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	7-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	8-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	8-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	9-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	9-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	10-A	2006	TYR	CA-C-N	7.37	127.72	119.32
1	10-A	2006	TYR	C-N-CA	7.37	127.72	119.32
1	1-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	2-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	3-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	4-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	5-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	6-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	7-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	8-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	9-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	10-A	1734	TRP	CB-CA-C	-7.34	97.77	110.17
1	1-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	1-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	2-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	2-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	3-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	3-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	4-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	4-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	5-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	5-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	6-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	6-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	7-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	7-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	8-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	8-A	1716	SER	C-N-CA	7.27	127.43	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	9-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	10-A	1716	SER	CA-C-N	7.27	127.43	119.87
1	10-A	1716	SER	C-N-CA	7.27	127.43	119.87
1	1-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	2-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	3-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	4-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	5-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	6-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	7-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	8-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	9-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	10-A	1542	PRO	N-CA-CB	7.18	110.79	103.25
1	1-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	1-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	2-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	2-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	3-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	3-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	4-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	4-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	5-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	5-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	6-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	6-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	7-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	7-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	8-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	8-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	9-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	9-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	10-A	2092	LEU	CA-C-N	7.17	127.33	120.31
1	10-A	2092	LEU	C-N-CA	7.17	127.33	120.31
1	1-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	1-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	2-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	2-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	3-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	3-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	4-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	4-A	2286	ALA	C-N-CA	7.10	127.06	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	5-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	6-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	6-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	7-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	7-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	8-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	8-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	9-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	9-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	10-A	2286	ALA	CA-C-N	7.10	127.06	120.03
1	10-A	2286	ALA	C-N-CA	7.10	127.06	120.03
1	1-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	1-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	2-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	2-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	3-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	3-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	4-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	4-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	5-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	5-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	6-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	6-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	7-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	7-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	8-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	8-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	9-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	9-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	10-A	2207	LEU	CA-C-N	7.08	126.78	119.56
1	10-A	2207	LEU	C-N-CA	7.08	126.78	119.56
1	1-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	2-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	3-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	4-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	5-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	6-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	7-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	8-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	9-A	1524	PRO	N-CA-CB	6.98	110.58	103.25
1	10-A	1524	PRO	N-CA-CB	6.98	110.58	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	1-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	2-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	2-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	3-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	3-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	4-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	4-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	5-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	5-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	6-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	6-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	7-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	7-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	8-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	8-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	9-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	9-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	10-A	1842	ASN	CA-C-N	6.85	126.55	119.56
1	10-A	1842	ASN	C-N-CA	6.85	126.55	119.56
1	1-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	1-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	2-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	2-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	3-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	3-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	4-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	4-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	5-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	5-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	6-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	6-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	7-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	7-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	8-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	8-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	9-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	9-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	10-A	1996	LYS	CA-C-N	6.75	128.28	119.84
1	10-A	1996	LYS	C-N-CA	6.75	128.28	119.84
1	1-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	1-A	2094	ASP	C-N-CA	6.68	126.38	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	2-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	3-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	3-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	4-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	4-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	5-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	5-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	6-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	6-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	7-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	7-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	8-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	8-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	9-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	9-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	10-A	2094	ASP	CA-C-N	6.68	126.38	119.56
1	10-A	2094	ASP	C-N-CA	6.68	126.38	119.56
1	1-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	1-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	2-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	2-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	3-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	3-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	4-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	4-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	5-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	5-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	6-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	6-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	7-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	7-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	8-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	8-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	9-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	9-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	10-A	1700	PHE	CA-C-N	6.64	126.62	119.78
1	10-A	1700	PHE	C-N-CA	6.64	126.62	119.78
1	1-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	1-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	2-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	2-A	1479	PHE	C-N-CA	6.57	128.05	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	3-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	4-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	4-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	5-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	5-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	6-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	6-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	7-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	7-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	8-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	8-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	9-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	9-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	10-A	1479	PHE	CA-C-N	6.57	128.05	119.84
1	10-A	1479	PHE	C-N-CA	6.57	128.05	119.84
1	1-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	1-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	2-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	2-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	3-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	3-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	4-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	4-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	5-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	5-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	6-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	6-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	7-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	7-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	8-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	8-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	9-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	9-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	10-A	1864	LEU	CA-C-N	6.48	126.46	119.78
1	10-A	1864	LEU	C-N-CA	6.48	126.46	119.78
1	1-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	1-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	2-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	2-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	3-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	3-A	1330	VAL	C-N-CA	6.44	127.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	4-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	5-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	5-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	6-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	6-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	7-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	7-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	8-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	8-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	9-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	9-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	10-A	1330	VAL	CA-C-N	6.44	127.89	119.84
1	10-A	1330	VAL	C-N-CA	6.44	127.89	119.84
1	1-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	1-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	2-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	2-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	3-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	3-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	4-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	4-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	5-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	5-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	6-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	6-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	7-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	7-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	8-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	8-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	9-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	9-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	10-A	1445	SER	CA-C-N	6.39	126.89	119.99
1	10-A	1445	SER	C-N-CA	6.39	126.89	119.99
1	1-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	1-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	2-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	2-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	3-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	3-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	4-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	4-A	1641	PHE	C-N-CA	6.34	126.29	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	5-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	6-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	6-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	7-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	7-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	8-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	8-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	9-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	9-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	10-A	1641	PHE	CA-C-N	6.34	126.29	119.76
1	10-A	1641	PHE	C-N-CA	6.34	126.29	119.76
1	1-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	1-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	2-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	2-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	3-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	3-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	4-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	4-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	5-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	5-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	6-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	6-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	7-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	7-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	8-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	8-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	9-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	9-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	10-A	1758	HIS	CA-C-N	6.32	127.74	119.84
1	10-A	1758	HIS	C-N-CA	6.32	127.74	119.84
1	1-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	1-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	2-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	2-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	3-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	3-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	4-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	4-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	5-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	5-A	1792	PHE	C-N-CA	6.31	126.22	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	6-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	7-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	7-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	8-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	8-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	9-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	9-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	10-A	1792	PHE	CA-C-N	6.31	126.22	119.85
1	10-A	1792	PHE	C-N-CA	6.31	126.22	119.85
1	1-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	1-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	2-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	2-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	3-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	3-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	4-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	4-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	5-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	5-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	6-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	6-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	7-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	7-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	8-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	8-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	9-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	9-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	10-A	1697	MET	CA-C-N	6.27	125.97	119.64
1	10-A	1697	MET	C-N-CA	6.27	125.97	119.64
1	1-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	1-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	2-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	2-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	3-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	3-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	4-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	4-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	5-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	5-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	6-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	6-A	1929	HIS	C-N-CA	6.22	126.68	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	7-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	8-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	8-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	9-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	9-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	10-A	1929	HIS	CA-C-N	6.22	126.68	119.47
1	10-A	1929	HIS	C-N-CA	6.22	126.68	119.47
1	1-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	1-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	2-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	2-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	3-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	3-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	4-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	4-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	5-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	5-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	6-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	6-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	7-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	7-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	8-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	8-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	9-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	9-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	10-A	1669	VAL	CA-C-N	6.22	127.61	119.84
1	10-A	1669	VAL	C-N-CA	6.22	127.61	119.84
1	1-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	2-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	3-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	4-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	5-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	6-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	7-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	8-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	9-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	10-A	1762	PHE	N-CA-C	6.20	117.96	108.42
1	1-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	1-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	2-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	2-A	1376	TRP	C-N-CA	6.16	126.48	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	3-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	4-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	4-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	5-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	5-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	6-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	6-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	7-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	7-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	8-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	8-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	9-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	9-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	10-A	1376	TRP	CA-C-N	6.16	126.48	119.83
1	10-A	1376	TRP	C-N-CA	6.16	126.48	119.83
1	1-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	1-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	2-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	2-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	3-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	3-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	4-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	4-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	5-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	5-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	6-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	6-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	7-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	7-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	8-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	8-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	9-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	9-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	10-A	2146	LEU	CA-C-N	6.12	126.06	119.76
1	10-A	2146	LEU	C-N-CA	6.12	126.06	119.76
1	1-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	1-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	2-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	2-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	3-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	3-A	2038	PHE	C-N-CA	5.96	131.28	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	4-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	5-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	5-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	6-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	6-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	7-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	7-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	8-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	8-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	9-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	9-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	10-A	2038	PHE	CA-C-N	5.96	131.28	121.39
1	10-A	2038	PHE	C-N-CA	5.96	131.28	121.39
1	1-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	1-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	2-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	2-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	3-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	3-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	4-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	4-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	5-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	5-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	6-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	6-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	7-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	7-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	8-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	8-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	9-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	9-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	10-A	1767	VAL	CA-C-N	5.95	126.45	120.14
1	10-A	1767	VAL	C-N-CA	5.95	126.45	120.14
1	1-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	2-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	3-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	4-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	5-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	6-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	7-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	8-A	1663	GLY	N-CA-C	-5.84	103.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	10-A	1663	GLY	N-CA-C	-5.84	103.66	112.60
1	1-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	1-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	2-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	2-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	3-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	3-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	4-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	4-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	5-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	5-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	6-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	6-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	7-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	7-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	8-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	8-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	9-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	9-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	10-A	1682	LEU	CA-C-N	5.78	125.68	119.85
1	10-A	1682	LEU	C-N-CA	5.78	125.68	119.85
1	1-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	1-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	2-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	2-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	3-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	3-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	4-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	4-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	5-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	5-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	6-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	6-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	7-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	7-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	8-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	8-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	9-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	9-A	2500	LEU	C-N-CA	5.61	125.71	119.32
1	10-A	2500	LEU	CA-C-N	5.61	125.71	119.32
1	10-A	2500	LEU	C-N-CA	5.61	125.71	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	1-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	2-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	2-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	3-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	3-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	4-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	4-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	5-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	5-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	6-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	6-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	7-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	7-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	8-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	8-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	9-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	9-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	10-A	1545	PHE	CA-C-N	5.48	126.69	119.84
1	10-A	1545	PHE	C-N-CA	5.48	126.69	119.84
1	1-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	2-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	3-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	4-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	5-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	6-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	7-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	8-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	9-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	10-A	1583	LEU	N-CA-C	5.20	118.13	107.69
1	1-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	2-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	3-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	4-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	5-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	6-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	7-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	8-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	9-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	10-A	1962	ASP	N-CA-C	5.03	116.81	107.60
1	1-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	2-A	1666	TYR	N-CA-C	5.00	116.98	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	4-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	5-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	6-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	7-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	8-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	9-A	1666	TYR	N-CA-C	5.00	116.98	109.23
1	10-A	1666	TYR	N-CA-C	5.00	116.98	109.23

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-A	8531	0	8567	50	0
1	2-A	8531	0	8567	51	0
1	3-A	8531	0	8567	48	0
1	4-A	8531	0	8567	52	0
1	5-A	8531	0	8567	49	0
1	6-A	8531	0	8567	50	0
1	7-A	8531	0	8567	56	0
1	8-A	8531	0	8567	51	0
1	9-A	8531	0	8567	48	0
1	10-A	8531	0	5030	37	0
2	1-A	28	0	12	1	0
2	2-A	28	0	12	2	0
2	3-A	28	0	12	1	0
2	4-A	28	0	12	1	0
2	5-A	28	0	12	1	0
2	6-A	28	0	12	2	0
2	7-A	28	0	12	1	0
2	8-A	28	0	12	1	0
2	9-A	28	0	12	1	0
2	10-A	28	0	0	0	0
3	1-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-A	1	0	0	0	0
3	3-A	1	0	0	0	0
3	4-A	1	0	0	0	0
3	5-A	1	0	0	0	0
3	6-A	1	0	0	0	0
3	7-A	1	0	0	0	0
3	8-A	1	0	0	0	0
3	9-A	1	0	0	0	0
3	10-A	1	0	0	0	0
All	All	85600	0	82241	492	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 3.

All (492) 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:A:1490:ALA:HA	2:A:2601:GDP:O6	1.37	1.21
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.39	1.20
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.42	1.17
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.46	1.14
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.46	1.12
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.48	1.10
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.52	1.10
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.52	1.09
1:A:1490:ALA:HA	2:A:2601:GDP:O6	1.57	1.05
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.40	0.74
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.40	0.74
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.41	0.74
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.41	0.73
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.42	0.72
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.45	0.70
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.90	0.69
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.91	0.69
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.74	0.69
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.74	0.69
1:A:1343:TPO:HG21	1:A:1343:TPO:O3P	1.93	0.69
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.92	0.69
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.92	0.67
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.76	0.67
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.93	0.67
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.93	0.67
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.94	0.66
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.94	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.77	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.93	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.94	0.66
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.94	0.65
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.78	0.65
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.94	0.65
1:A:1398:ARG:O	1:A:1398:ARG:HG3	1.96	0.64
1:A:2408:MET:O	1:A:2408:MET:SD	2.57	0.62
1:A:2408:MET:O	1:A:2408:MET:SD	2.58	0.62
1:A:2408:MET:O	1:A:2408:MET:SD	2.59	0.61
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.54	0.61
1:A:2305:GLU:HA	1:A:2305:GLU:OE1	2.01	0.61
1:A:2408:MET:O	1:A:2408:MET:SD	2.59	0.61
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.26	0.60
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.83	0.59
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.04	0.58
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.03	0.58
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.29	0.57
1:A:2408:MET:O	1:A:2408:MET:SD	2.63	0.57
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.30	0.57
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.04	0.57
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.29	0.57
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.30	0.56
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.29	0.56
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.06	0.56
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.06	0.56
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.06	0.56
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.31	0.56
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.07	0.55
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.32	0.55
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.30	0.55
1:A:1912:THR:HG22	1:A:1912:THR:O	2.06	0.55
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.31	0.55
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.32	0.55
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.07	0.55
1:A:1912:THR:HG22	1:A:1912:THR:O	2.06	0.55
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.08	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.08	0.54
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.08	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.08	0.54
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.53
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.53
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.09	0.53
1:A:1912:THR:HG22	1:A:1912:THR:O	2.08	0.53
1:A:2489:ILE:O	1:A:2489:ILE:HG22	2.08	0.53
1:A:2327:SER:OG	1:A:2329:ASP:OD1	2.26	0.53
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.09	0.53
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.91	0.53
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.91	0.52
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.10	0.52
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.10	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.52
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.93	0.51
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1882:GLU:OE1	1:A:1882:GLU:N	2.37	0.51
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.10	0.51
1:A:1882:GLU:OE1	1:A:1882:GLU:N	2.37	0.51
1:A:2305:GLU:OE1	1:A:2305:GLU:CA	2.59	0.51
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.35	0.51
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.92	0.50
1:A:1882:GLU:OE1	1:A:1882:GLU:N	2.37	0.50
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.93	0.50
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.94	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.92	0.50
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.94	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.50
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.50
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.10	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.94	0.49
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.94	0.49
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.36	0.49
1:A:1490:ALA:HA	2:A:2601:GDP:C6	2.35	0.49
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.49
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.10	0.49
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.37	0.49
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.49
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.37	0.49
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.37	0.49
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.37	0.48
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.86	0.48
1:A:1343:TPO:HG21	1:A:1343:TPO:O1P	2.12	0.48
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.38	0.48
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.94	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.56	0.48
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.72	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.56	0.48
1:A:1343:TPO:HG21	1:A:1343:TPO:O1P	2.13	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.56	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.56	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.56	0.48
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.96	0.48
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.72	0.48
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.57	0.47
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.72	0.47
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.96	0.47
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.13	0.47
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.13	0.47
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.57	0.47
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.13	0.47
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.13	0.47
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.68	0.47
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.60	0.47
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.97	0.47
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.72	0.47
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.95	0.47
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.73	0.47
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.73	0.46
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.60	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.74	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.74	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.74	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:2037:GLY:O	1:A:2083:PHE:CE2	2.69	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.46
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.63	0.46
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.64	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.94	0.46
1:A:1481:ALA:O	1:A:1482:ILE:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.46
1:A:1481:ALA:O	1:A:1482:ILE:C	2.59	0.46
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.46
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.46
1:A:1677:ARG:O	1:A:1677:ARG:CG	2.61	0.46
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.94	0.46
1:A:1481:ALA:O	1:A:1482:ILE:C	2.59	0.46
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.94	0.45
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.75	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.16	0.45
1:A:1481:ALA:O	1:A:1482:ILE:C	2.59	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.16	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.57	0.45
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.94	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.57	0.45
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.64	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.57	0.45
1:A:1925:CYS:O	1:A:1926:HIS:HB2	2.17	0.45
1:A:1925:CYS:O	1:A:1926:HIS:HB2	2.17	0.45
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.64	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.57	0.45
1:A:1925:CYS:O	1:A:1926:HIS:HB2	2.17	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1925:CYS:O	1:A:1926:HIS:HB2	2.17	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:1405:HIS:N	1:A:1406:PRO:CD	2.79	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:1405:HIS:N	1:A:1406:PRO:CD	2.80	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.95	0.45
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.61	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.61	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.16	0.44
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.44
1:A:1515:ASP:O	1:A:1519:VAL:N	2.51	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.16	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.61	0.44
1:A:1405:HIS:N	1:A:1406:PRO:CD	2.80	0.44
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.18	0.44
1:A:1515:ASP:O	1:A:1519:VAL:N	2.51	0.44
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.18	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1343:TPO:HG21	1:A:1343:TPO:O1P	2.17	0.44
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.61	0.44
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.65	0.44
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.65	0.44
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.18	0.44
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.18	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.18	0.44
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.18	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.17	0.44
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.65	0.44
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.44
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.65	0.44
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.44
1:A:1343:TPO:HG21	1:A:1343:TPO:O1P	2.17	0.44
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.44
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.43	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.43	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.95	0.43
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.00	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.43	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.95	0.43
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.43
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	2.00	0.43
1:A:1593:SER:OG	1:A:1594:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.43	0.43
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.00	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:2198:ARG:C	1:A:2219:THR:HG1	2.22	0.43
1:A:1481:ALA:O	1:A:1482:ILE:C	2.61	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1481:ALA:O	1:A:1482:ILE:C	2.61	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.00	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1481:ALA:O	1:A:1482:ILE:C	2.61	0.43
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.18	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1481:ALA:O	1:A:1482:ILE:C	2.61	0.43
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.19	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.66	0.43
1:A:1536:SER:OG	1:A:1537:GLU:N	2.52	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.66	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1536:SER:OG	1:A:1537:GLU:N	2.52	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.96	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.19	0.43
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.39	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.43
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.59	0.43
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.63	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.34	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1481:ALA:O	1:A:1482:ILE:C	2.61	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.43
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.43
1:A:1593:SER:OG	1:A:1594:ASP:N	2.52	0.43
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.63	0.43
1:A:1593:SER:OG	1:A:1594:ASP:N	2.51	0.43
1:A:1814:TYR:CD2	1:A:1814:TYR:C	2.96	0.43
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.96	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.52	0.42
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.97	0.42
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.01	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.50	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.51	0.42
1:A:1676:HIS:O	1:A:1677:ARG:C	2.61	0.42
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.96	0.42
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.01	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.51	0.42
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.18	0.42
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.42
1:A:1676:HIS:O	1:A:1677:ARG:C	2.62	0.42
1:A:1398:ARG:O	1:A:1398:ARG:CG	2.64	0.42
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.19	0.42
1:A:1676:HIS:O	1:A:1677:ARG:C	2.62	0.42
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.57	0.42
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.19	0.42
1:A:1592:LEU:HD23	1:A:1592:LEU:C	2.44	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.96	0.42
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.19	0.42
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.59	0.42
1:A:1343:TPO:HG21	1:A:1343:TPO:O1P	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.39	0.42
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.20	0.42
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.19	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.19	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:1962:ASP:OD1	1:A:1962:ASP:C	2.59	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.19	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.19	0.42
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.38	0.42
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.19	0.42
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.42
1:A:2422:ASN:OD1	1:A:2422:ASN:C	2.58	0.42
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.02	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.20	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.52	0.42
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.98	0.42
1:A:2198:ARG:C	1:A:2219:THR:HG1	2.25	0.42
1:A:1402:TYR:CD1	1:A:1402:TYR:C	2.98	0.42
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.01	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.01	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.19	0.41
1:A:2198:ARG:C	1:A:2219:THR:HG1	2.25	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:1593:SER:OG	1:A:1594:ASP:N	2.52	0.41
1:A:1593:SER:OG	1:A:1594:ASP:N	2.52	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.20	0.41
1:A:2118:ASN:HA	1:A:2119:PRO:HD3	1.94	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.44	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.44	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.19	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.61	0.41
1:A:1536:SER:OG	1:A:1537:GLU:N	2.53	0.41
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.02	0.41
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.01	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.20	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.44	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.01	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.20	0.41
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.39	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.44	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.44	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.93	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.02	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.01	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.20	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.20	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.20	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.20	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.61	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.21	0.41
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.40	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.20	0.41
1:A:2003:PHE:O	1:A:2004:THR:HB	2.20	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.61	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	2.01	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.61	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.21	0.41
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.45	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.62	0.41
1:A:2429:THR:OG1	1:A:2430:GLY:N	2.53	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.21	0.41
1:A:1592:LEU:O	1:A:1592:LEU:CD2	2.69	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.36	0.41
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.63	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.61	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.64	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.62	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.36	0.41
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.62	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.41
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.20	0.41
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.21	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.03	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.62	0.40
1:A:1376:TRP:CD1	1:A:1376:TRP:C	2.95	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:1925:CYS:O	1:A:1926:HIS:CB	2.68	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.03	0.40
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.36	0.40
1:A:1420:ASP:OD1	1:A:1420:ASP:C	2.62	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.45	0.40
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	2.03	0.40
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.64	0.40
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.93	0.40
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.64	0.40
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.94	0.40
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.45	0.40
1:A:1925:CYS:O	1:A:1926:HIS:CB	2.68	0.40
1:A:1925:CYS:O	1:A:1926:HIS:CB	2.68	0.40
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.64	0.40
1:A:2388:ASP:OD1	1:A:2388:ASP:C	2.63	0.40
1:A:1582:LEU:C	1:A:1582:LEU:CD1	2.94	0.40
1:A:1394:ASP:OD1	1:A:1394:ASP:C	2.64	0.40
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.36	0.40
1:A:1925:CYS:O	1:A:1926:HIS:CB	2.68	0.40
1:A:1405:HIS:N	1:A:1406:PRO:HD3	2.36	0.40
1:A:1336:LYS:HE2	1:A:1336:LYS:HB2	1.84	0.40
1:A:1490:ALA:HA	2:A:2601:GDP:C6	2.45	0.40
1:A:2419:LEU:HD23	1:A:2419:LEU:C	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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-A	1055/1201 (88%)	974 (92%)	68 (6%)	13 (1%)	10	41
1	2-A	1055/1201 (88%)	976 (92%)	65 (6%)	14 (1%)	9	39
1	3-A	1055/1201 (88%)	974 (92%)	67 (6%)	14 (1%)	9	39
1	4-A	1055/1201 (88%)	976 (92%)	67 (6%)	12 (1%)	11	43
1	5-A	1055/1201 (88%)	974 (92%)	67 (6%)	14 (1%)	9	39
1	6-A	1055/1201 (88%)	977 (93%)	65 (6%)	13 (1%)	10	41
1	7-A	1055/1201 (88%)	970 (92%)	72 (7%)	13 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-A	1055/1201 (88%)	972 (92%)	69 (6%)	14 (1%)	9	39
1	9-A	1055/1201 (88%)	972 (92%)	69 (6%)	14 (1%)	9	39
1	10-A	1047/1201 (87%)	965 (92%)	68 (6%)	14 (1%)	9	39
All	All	10542/12010 (88%)	9730 (92%)	677 (6%)	135 (1%)	12	39

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	1493	GLU
1	1-A	2004	THR
1	2-A	1493	GLU
1	2-A	2004	THR
1	3-A	1493	GLU
1	3-A	2004	THR
1	4-A	1493	GLU
1	4-A	2004	THR
1	5-A	1493	GLU
1	5-A	2004	THR
1	6-A	1493	GLU
1	6-A	2004	THR
1	7-A	1493	GLU
1	7-A	2004	THR
1	8-A	1493	GLU
1	8-A	2004	THR
1	9-A	1493	GLU
1	9-A	2004	THR
1	10-A	1493	GLU
1	10-A	2004	THR
1	1-A	1546	PRO
1	1-A	2334	LYS
1	1-A	2489	ILE
1	2-A	2334	LYS
1	2-A	2489	ILE
1	3-A	2334	LYS
1	4-A	2334	LYS
1	5-A	1546	PRO
1	5-A	2334	LYS
1	6-A	1481	ALA
1	6-A	1546	PRO
1	6-A	2334	LYS
1	6-A	2489	ILE

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Mol	Chain	Res	Type
1	7-A	2177	GLY
1	7-A	2334	LYS
1	7-A	2489	ILE
1	8-A	1546	PRO
1	8-A	2334	LYS
1	8-A	2489	ILE
1	9-A	1524	PRO
1	9-A	2177	GLY
1	9-A	2334	LYS
1	9-A	2489	ILE
1	10-A	2334	LYS
1	1-A	1482	ILE
1	1-A	1524	PRO
1	1-A	1542	PRO
1	1-A	1942	PRO
1	1-A	2177	GLY
1	2-A	1524	PRO
1	2-A	1542	PRO
1	2-A	1942	PRO
1	2-A	2177	GLY
1	3-A	1482	ILE
1	3-A	1524	PRO
1	3-A	1542	PRO
1	3-A	1744	PRO
1	3-A	1942	PRO
1	3-A	2177	GLY
1	4-A	1542	PRO
1	4-A	1942	PRO
1	4-A	2177	GLY
1	5-A	1524	PRO
1	5-A	1542	PRO
1	5-A	1742	TRP
1	5-A	1942	PRO
1	5-A	2177	GLY
1	6-A	1524	PRO
1	6-A	1542	PRO
1	6-A	1942	PRO
1	6-A	2177	GLY
1	7-A	1482	ILE
1	7-A	1542	PRO
1	7-A	1942	PRO
1	8-A	1524	PRO

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Mol	Chain	Res	Type
1	8-A	1542	PRO
1	8-A	1742	TRP
1	8-A	1942	PRO
1	8-A	2177	GLY
1	9-A	1542	PRO
1	9-A	1942	PRO
1	10-A	1482	ILE
1	10-A	1524	PRO
1	10-A	1542	PRO
1	10-A	1942	PRO
1	10-A	2177	GLY
1	10-A	2489	ILE
1	1-A	2038	PHE
1	2-A	1482	ILE
1	2-A	1742	TRP
1	2-A	2038	PHE
1	3-A	2038	PHE
1	4-A	1482	ILE
1	4-A	1742	TRP
1	4-A	2038	PHE
1	5-A	1482	ILE
1	5-A	2038	PHE
1	6-A	2038	PHE
1	7-A	2038	PHE
1	8-A	1482	ILE
1	8-A	2038	PHE
1	9-A	1482	ILE
1	9-A	2038	PHE
1	10-A	2038	PHE
1	1-A	1852	ILE
1	3-A	1684	HIS
1	4-A	2489	ILE
1	5-A	1684	HIS
1	5-A	2489	ILE
1	7-A	1742	TRP
1	9-A	1742	TRP
1	10-A	1742	TRP
1	2-A	1684	HIS
1	6-A	1684	HIS
1	7-A	1684	HIS
1	8-A	1684	HIS
1	9-A	1684	HIS

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Mol	Chain	Res	Type
1	10-A	1684	HIS
1	1-A	1677	ARG
1	2-A	1546	PRO
1	2-A	1677	ARG
1	3-A	1677	ARG
1	4-A	1677	ARG
1	5-A	1677	ARG
1	6-A	1677	ARG
1	7-A	1677	ARG
1	8-A	1677	ARG
1	9-A	1546	PRO
1	9-A	1677	ARG
1	10-A	1677	ARG
1	3-A	1546	PRO
1	4-A	1546	PRO
1	7-A	1546	PRO
1	10-A	1546	PRO
1	3-A	2489	ILE

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 PDB entries followed by that with respect to all EM entries.

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-A	926/1073 (86%)	926 (100%)	0	100	100
1	2-A	926/1073 (86%)	926 (100%)	0	100	100
1	3-A	926/1073 (86%)	926 (100%)	0	100	100
1	4-A	926/1073 (86%)	926 (100%)	0	100	100
1	5-A	926/1073 (86%)	926 (100%)	0	100	100
1	6-A	926/1073 (86%)	926 (100%)	0	100	100
1	7-A	926/1073 (86%)	926 (100%)	0	100	100
1	8-A	926/1073 (86%)	926 (100%)	0	100	100
1	9-A	926/1073 (86%)	926 (100%)	0	100	100
1	10-A	920/1073 (86%)	920 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9254/10730 (86%)	9254 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	1333	ASN
1	1-A	1657	GLN
1	1-A	1676	HIS
1	1-A	1822	HIS
1	1-A	2089	GLN
1	1-A	2333	GLN
1	2-A	1405	HIS
1	2-A	1657	GLN
1	2-A	1676	HIS
1	2-A	1822	HIS
1	2-A	2089	GLN
1	2-A	2333	GLN
1	2-A	2468	ASN
1	3-A	1333	ASN
1	3-A	1657	GLN
1	3-A	1822	HIS
1	3-A	2089	GLN
1	3-A	2333	GLN
1	3-A	2468	ASN
1	4-A	1333	ASN
1	4-A	1405	HIS
1	4-A	1609	GLN
1	4-A	1657	GLN
1	4-A	1676	HIS
1	4-A	1822	HIS
1	4-A	2089	GLN
1	4-A	2333	GLN
1	4-A	2342	GLN
1	4-A	2468	ASN
1	5-A	1657	GLN
1	5-A	1822	HIS
1	5-A	2089	GLN
1	6-A	1333	ASN
1	6-A	1657	GLN
1	6-A	1676	HIS

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Mol	Chain	Res	Type
1	6-A	1822	HIS
1	6-A	2089	GLN
1	6-A	2333	GLN
1	6-A	2468	ASN
1	7-A	1333	ASN
1	7-A	1657	GLN
1	7-A	1676	HIS
1	7-A	1822	HIS
1	7-A	2089	GLN
1	7-A	2333	GLN
1	8-A	1333	ASN
1	8-A	1657	GLN
1	8-A	1822	HIS
1	8-A	2089	GLN
1	8-A	2333	GLN
1	8-A	2468	ASN
1	9-A	1333	ASN
1	9-A	1657	GLN
1	9-A	1676	HIS
1	9-A	1822	HIS
1	9-A	2089	GLN
1	9-A	2342	GLN
1	9-A	2468	ASN
1	10-A	1333	ASN
1	10-A	1657	GLN
1	10-A	1676	HIS
1	10-A	1822	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	9-A	1343	1	8,10,11	0.94	0	10,14,16	0.88	0
1	TPO	5-A	1343	1	8,10,11	0.88	0	10,14,16	0.86	0
1	TPO	2-A	1343	1	8,10,11	0.86	0	10,14,16	0.86	0
1	TPO	7-A	1343	1	8,10,11	0.88	0	10,14,16	0.88	0
1	TPO	10-A	1343	1	8,10,11	0.87	0	10,14,16	0.88	0
1	TPO	4-A	1343	1	8,10,11	0.88	0	10,14,16	0.87	0
1	TPO	8-A	1343	1	8,10,11	0.88	0	10,14,16	0.88	0
1	TPO	6-A	1343	1	8,10,11	0.88	0	10,14,16	0.86	0
1	TPO	3-A	1343	1	8,10,11	0.87	0	10,14,16	0.87	0
1	TPO	1-A	1343	1	8,10,11	0.87	0	10,14,16	0.87	0

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
1	TPO	9-A	1343	1	-	3/9/11/13	-
1	TPO	5-A	1343	1	-	0/9/11/13	-
1	TPO	2-A	1343	1	-	1/9/11/13	-
1	TPO	7-A	1343	1	-	1/9/11/13	-
1	TPO	10-A	1343	1	-	1/9/11/13	-
1	TPO	4-A	1343	1	-	1/9/11/13	-
1	TPO	8-A	1343	1	-	0/9/11/13	-
1	TPO	6-A	1343	1	-	1/9/11/13	-
1	TPO	3-A	1343	1	-	0/9/11/13	-
1	TPO	1-A	1343	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2-A	1343	TPO	CB-OG1-P-O3P
1	9-A	1343	TPO	CB-OG1-P-O2P
1	9-A	1343	TPO	CB-OG1-P-O1P
1	4-A	1343	TPO	CB-OG1-P-O3P

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Mol	Chain	Res	Type	Atoms
1	6-A	1343	TPO	CB-OG1-P-O3P
1	7-A	1343	TPO	CB-OG1-P-O3P
1	9-A	1343	TPO	CB-OG1-P-O3P
1	10-A	1343	TPO	CB-OG1-P-O3P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	1343	TPO	1	0
1	7-A	1343	TPO	1	0
1	10-A	1343	TPO	1	0
1	4-A	1343	TPO	1	0
1	8-A	1343	TPO	1	0
1	6-A	1343	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
2	GDP	3-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	1-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	7-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	4-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	5-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	2-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	6-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	8-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	10-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)
2	GDP	9-A	2601	3	29,30,30	1.51	4 (13%)	45,47,47	1.87	10 (22%)

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
2	GDP	3-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	1-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	7-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	4-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	5-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	2-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	6-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	8-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	10-A	2601	3	-	4/16/32/32	0/3/3/3
2	GDP	9-A	2601	3	-	4/16/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	2-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	3-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	4-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	5-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	6-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	7-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	8-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	9-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	10-A	2601	GDP	PA-O3A	-4.62	1.54	1.59
2	1-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	2-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	3-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	4-A	2601	GDP	C5-C4	3.49	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	6-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	7-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	8-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	9-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	10-A	2601	GDP	C5-C4	3.49	1.48	1.38
2	1-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	2-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	3-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	4-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	5-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	6-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	7-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	8-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	9-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	10-A	2601	GDP	C4-N9	-2.70	1.31	1.38
2	1-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	2-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	3-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	4-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	5-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	6-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	7-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	8-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	9-A	2601	GDP	C5-N7	-2.14	1.34	1.39
2	10-A	2601	GDP	C5-N7	-2.14	1.34	1.39

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	2-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	3-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	4-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	5-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	6-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	7-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	8-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	9-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	10-A	2601	GDP	C5-C4-N3	-4.51	121.20	128.39
2	1-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	2-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	4-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	5-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	6-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	7-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	8-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	9-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	10-A	2601	GDP	C2-N3-C4	4.00	119.19	112.30
2	1-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	2-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	3-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	4-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	5-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	6-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	7-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	8-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	9-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	10-A	2601	GDP	N9-C4-N3	3.98	133.92	125.95
2	1-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	2-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	3-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	4-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	5-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	6-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	7-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	8-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	9-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	10-A	2601	GDP	C1'-N9-C8	-3.86	115.77	126.73
2	1-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	2-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	3-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	4-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	5-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	6-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	7-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	8-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	9-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	10-A	2601	GDP	O2A-PA-O3A	3.54	116.84	107.27
2	1-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	2-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	3-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	4-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	6-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	7-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	8-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	9-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	10-A	2601	GDP	C6-C5-N7	3.15	136.03	130.29
2	1-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	2-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	3-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	4-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	5-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	6-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	7-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	8-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	9-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	10-A	2601	GDP	O4'-C1'-C2'	-2.46	101.36	106.62
2	1-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	2-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	3-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	4-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	5-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	6-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	7-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	8-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	9-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	10-A	2601	GDP	O3A-PA-O1A	-2.24	103.95	110.70
2	1-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	2-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	3-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	4-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	5-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	6-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	7-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	8-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	9-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	10-A	2601	GDP	O2A-PA-O1A	2.16	122.51	112.44
2	1-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	2-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	3-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	4-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	5-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	6-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	8-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	9-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	10-A	2601	GDP	O6-C6-C5	-2.16	120.83	126.53

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	2601	GDP	C3'-C4'-C5'-O5'
2	2-A	2601	GDP	C3'-C4'-C5'-O5'
2	3-A	2601	GDP	C3'-C4'-C5'-O5'
2	4-A	2601	GDP	C3'-C4'-C5'-O5'
2	5-A	2601	GDP	C3'-C4'-C5'-O5'
2	6-A	2601	GDP	C3'-C4'-C5'-O5'
2	7-A	2601	GDP	C3'-C4'-C5'-O5'
2	8-A	2601	GDP	C3'-C4'-C5'-O5'
2	9-A	2601	GDP	C3'-C4'-C5'-O5'
2	10-A	2601	GDP	C3'-C4'-C5'-O5'
2	1-A	2601	GDP	C5'-O5'-PA-O1A
2	2-A	2601	GDP	C5'-O5'-PA-O1A
2	3-A	2601	GDP	C5'-O5'-PA-O1A
2	4-A	2601	GDP	C5'-O5'-PA-O1A
2	5-A	2601	GDP	C5'-O5'-PA-O1A
2	6-A	2601	GDP	C5'-O5'-PA-O1A
2	7-A	2601	GDP	C5'-O5'-PA-O1A
2	8-A	2601	GDP	C5'-O5'-PA-O1A
2	9-A	2601	GDP	C5'-O5'-PA-O1A
2	10-A	2601	GDP	C5'-O5'-PA-O1A
2	1-A	2601	GDP	PB-O3A-PA-O1A
2	2-A	2601	GDP	PB-O3A-PA-O1A
2	3-A	2601	GDP	PB-O3A-PA-O1A
2	4-A	2601	GDP	PB-O3A-PA-O1A
2	5-A	2601	GDP	PB-O3A-PA-O1A
2	6-A	2601	GDP	PB-O3A-PA-O1A
2	7-A	2601	GDP	PB-O3A-PA-O1A
2	8-A	2601	GDP	PB-O3A-PA-O1A
2	9-A	2601	GDP	PB-O3A-PA-O1A
2	10-A	2601	GDP	PB-O3A-PA-O1A
2	1-A	2601	GDP	O4'-C4'-C5'-O5'
2	2-A	2601	GDP	O4'-C4'-C5'-O5'
2	3-A	2601	GDP	O4'-C4'-C5'-O5'

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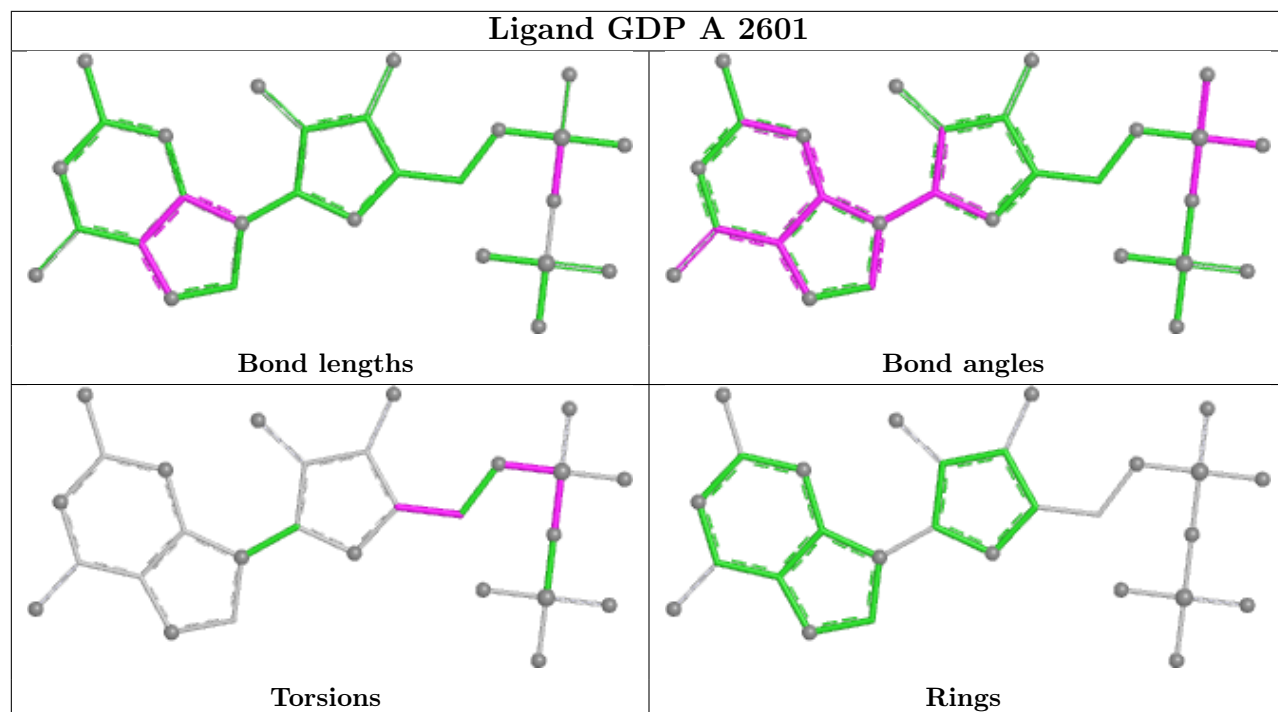
Mol	Chain	Res	Type	Atoms
2	4-A	2601	GDP	O4'-C4'-C5'-O5'
2	5-A	2601	GDP	O4'-C4'-C5'-O5'
2	6-A	2601	GDP	O4'-C4'-C5'-O5'
2	7-A	2601	GDP	O4'-C4'-C5'-O5'
2	8-A	2601	GDP	O4'-C4'-C5'-O5'
2	9-A	2601	GDP	O4'-C4'-C5'-O5'
2	10-A	2601	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3-A	2601	GDP	1	0
2	1-A	2601	GDP	1	0
2	7-A	2601	GDP	1	0
2	4-A	2601	GDP	1	0
2	5-A	2601	GDP	1	0
2	2-A	2601	GDP	2	0
2	6-A	2601	GDP	2	0
2	8-A	2601	GDP	1	0
2	9-A	2601	GDP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21250. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.