



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:43 AM UTC

PDB ID : 1AFC / pdb_00001afc
Title : STRUCTURAL STUDIES OF THE BINDING OF THE ANTI-ULCER
DRUG SUCROSE OCTASULFATE TO ACIDIC FIBROBLAST GROWTH
FACTOR
Authors : Zhu, X.; Hsu, B.T.; Rees, D.C.
Deposited on : 1993-07-13
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

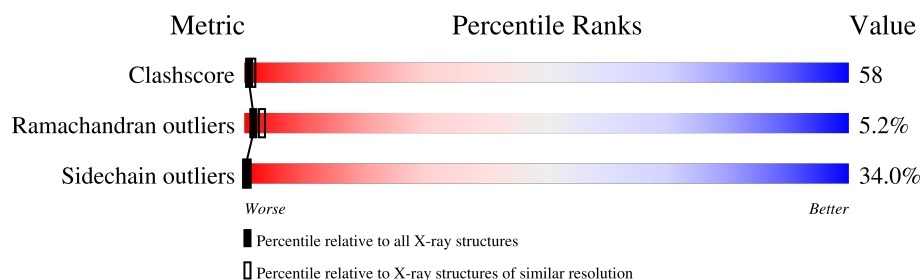
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	140	9% 31% 31% 20% 9%
1	B	140	7% 36% 30% 18% 9%
1	C	140	11% 25% 34% 21% 9%
1	D	140	16% 27% 36% 11% 9%
1	E	140	14% 24% 31% 22% 9%
1	F	140	11% 25% 31% 23% 9%
1	G	140	9% 32% 31% 18% 9%
1	H	140	11% 24% 29% 26% 9%

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	P	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GU4	I	1	-	-	X	-
2	YYJ	I	2	-	-	X	-
2	GU4	K	1	-	-	X	-
2	YYJ	K	2	-	-	X	-
2	YYJ	L	2	-	-	X	-
2	GU4	M	1	-	-	X	-
2	YYJ	M	2	-	-	X	-
2	YYJ	N	2	-	-	X	-
2	GU4	O	1	-	-	X	-
2	YYJ	O	2	-	-	X	-
2	GU4	P	1	-	-	X	-
2	YYJ	P	2	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

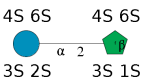
- Molecule 1 is a protein called ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	B	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	C	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	D	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	E	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	F	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	G	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			
1	H	127	Total	C	N	O	S	0	0	0
			983	630	168	182	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP P03968
B	47	ALA	CYS	conflict	UNP P03968
C	47	ALA	CYS	conflict	UNP P03968
D	47	ALA	CYS	conflict	UNP P03968
E	47	ALA	CYS	conflict	UNP P03968
F	47	ALA	CYS	conflict	UNP P03968
G	47	ALA	CYS	conflict	UNP P03968
H	47	ALA	CYS	conflict	UNP P03968

- Molecule 2 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose.



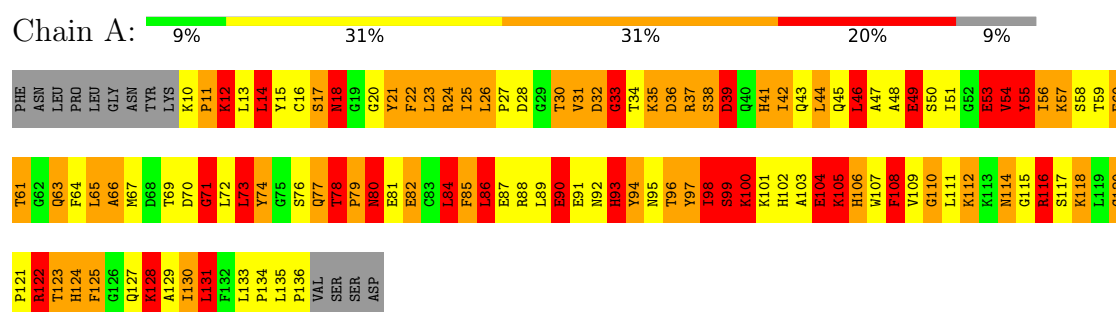
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	J	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	K	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	L	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	M	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	N	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	O	2	Total	C	O	S	0	0	0
			55	12	35	8			
2	P	2	Total	C	O	S	0	0	0
			55	12	35	8			

3 Residue-property plots

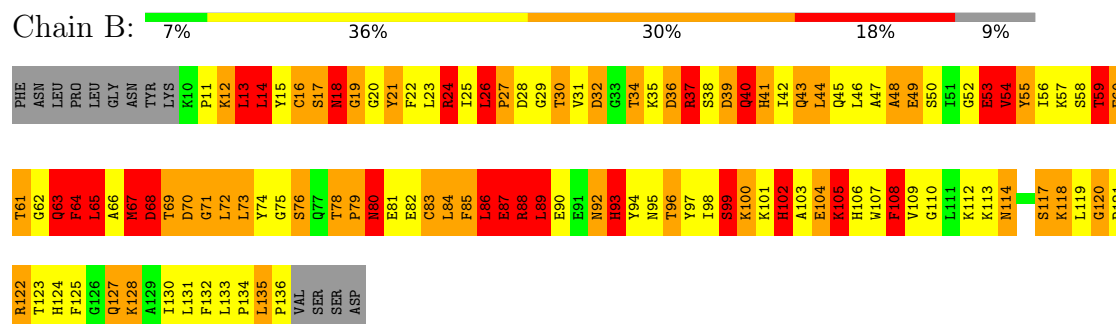
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

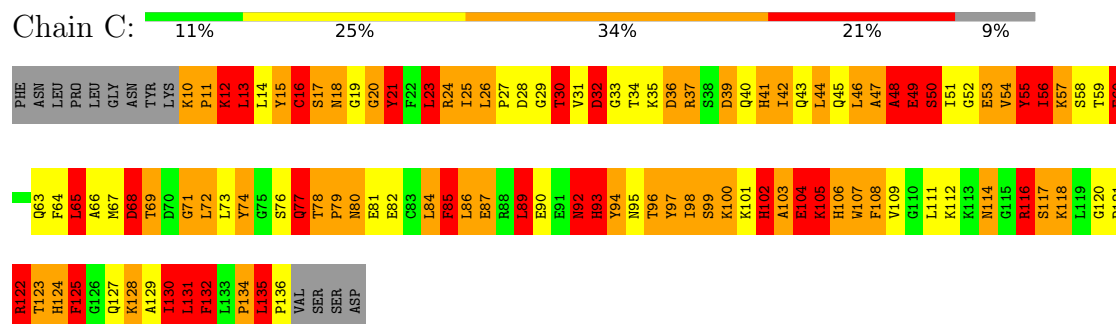
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

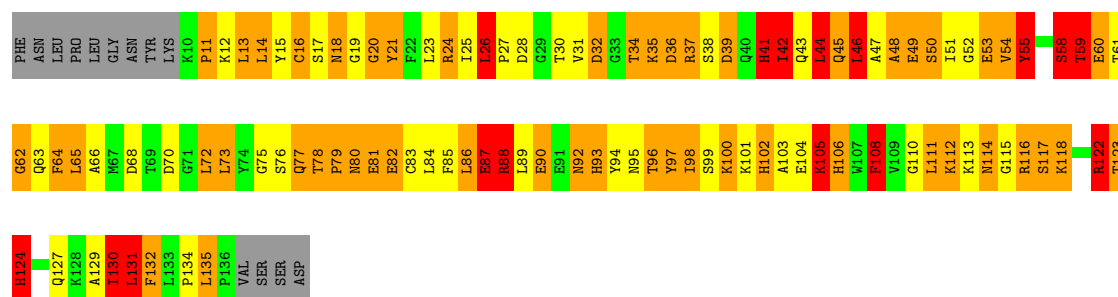


• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



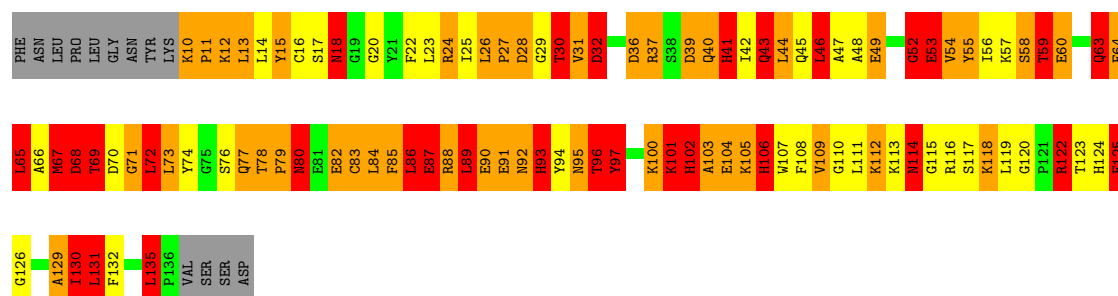
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain D: 

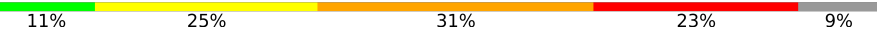


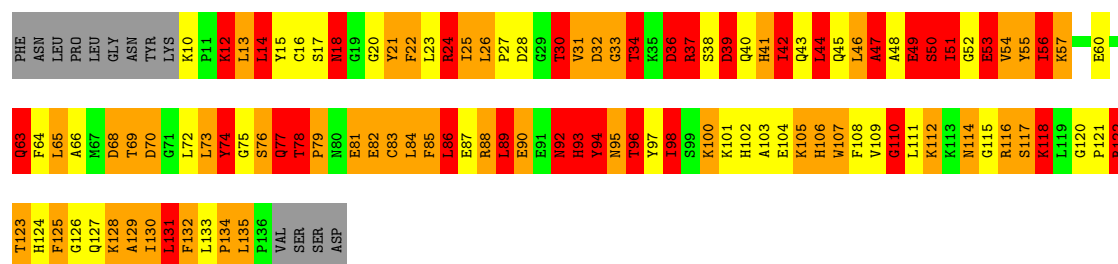
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain E: 



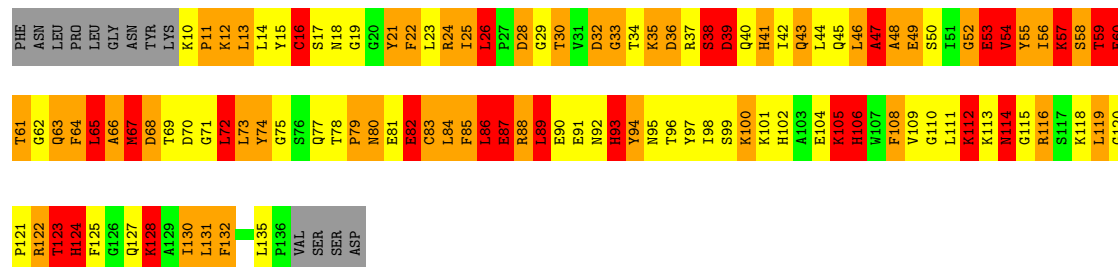
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain F: 



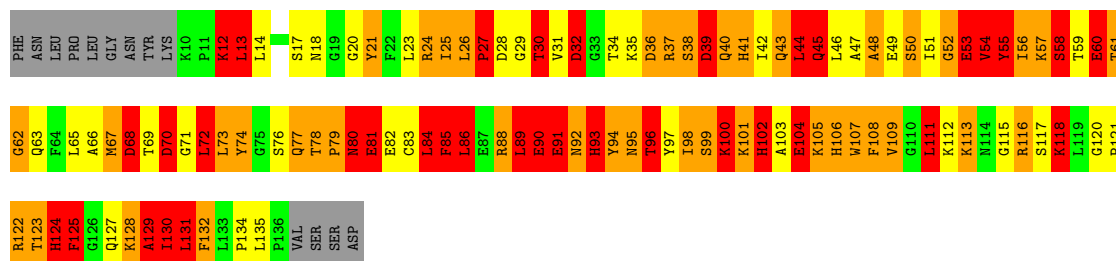
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain G: 



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain H: 



- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain I: 

GU41
YYJ2

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain J: 

GU41
YYJ2

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain K: 

GU41
YYJ2

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain L: 

GU41
YYJ2

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain M: 

GU41
YYJ2

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain N:  100%

CH01
YY02

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain O:  100%

CH01
YY02

- Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain P:  100%

CH01
YY02

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.60Å 110.60Å 172.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8304	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YYJ, GU4

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	A	1.20	3/1007 (0.3%)	2.06	35/1363 (2.6%)
1	B	1.25	5/1007 (0.5%)	2.04	31/1363 (2.3%)
1	C	1.23	8/1007 (0.8%)	2.05	41/1363 (3.0%)
1	D	1.23	6/1007 (0.6%)	1.92	21/1363 (1.5%)
1	E	1.26	4/1007 (0.4%)	2.00	32/1363 (2.3%)
1	F	1.28	5/1007 (0.5%)	2.04	35/1363 (2.6%)
1	G	1.21	5/1007 (0.5%)	2.01	33/1363 (2.4%)
1	H	1.23	6/1007 (0.6%)	2.04	37/1363 (2.7%)
All	All	1.24	42/8056 (0.5%)	2.02	265/10904 (2.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	89
1	B	0	77
1	C	0	76
1	D	0	76
1	E	0	74
1	F	0	78
1	G	0	67
1	H	0	83
All	All	0	620

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	106	HIS	CD2-NE2	-7.23	1.29	1.37
1	F	106	HIS	CD2-NE2	-6.91	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	HIS	CD2-NE2	-6.86	1.30	1.37
1	D	106	HIS	CD2-NE2	-6.85	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.74	1.30	1.37
1	E	102	HIS	CD2-NE2	-6.42	1.30	1.37
1	G	106	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	93	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	106	HIS	CD2-NE2	-6.09	1.31	1.37
1	F	102	HIS	CD2-NE2	-6.08	1.31	1.37
1	C	41	HIS	CD2-NE2	-6.07	1.31	1.37
1	D	93	HIS	CD2-NE2	-5.99	1.31	1.37
1	F	41	HIS	CD2-NE2	-5.90	1.31	1.37
1	G	93	HIS	CD2-NE2	-5.79	1.31	1.37
1	H	102	HIS	CD2-NE2	-5.78	1.31	1.37
1	F	102	HIS	CG-ND1	-5.78	1.31	1.38
1	B	41	HIS	CG-ND1	-5.76	1.31	1.38
1	C	124	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	93	HIS	CD2-NE2	-5.74	1.31	1.37
1	H	41	HIS	CD2-NE2	-5.72	1.31	1.37
1	F	93	HIS	CD2-NE2	-5.72	1.31	1.37
1	G	124	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	41	HIS	CD2-NE2	-5.66	1.31	1.37
1	B	102	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	93	HIS	CD2-NE2	-5.63	1.31	1.37
1	D	124	HIS	CG-ND1	-5.51	1.32	1.38
1	D	124	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	106	HIS	CD2-NE2	-5.47	1.31	1.37
1	E	41	HIS	CD2-NE2	-5.46	1.31	1.37
1	C	41	HIS	CG-ND1	-5.40	1.32	1.38
1	C	56	ILE	CA-C	-5.36	1.48	1.53
1	D	41	HIS	CD2-NE2	-5.36	1.31	1.37
1	H	93	HIS	CD2-NE2	-5.34	1.31	1.37
1	H	124	HIS	CD2-NE2	-5.30	1.32	1.37
1	G	41	HIS	CG-ND1	-5.21	1.32	1.38
1	C	102	HIS	CG-ND1	-5.18	1.32	1.38
1	G	93	HIS	CG-ND1	-5.18	1.32	1.38
1	C	102	HIS	CD2-NE2	-5.17	1.32	1.37
1	H	41	HIS	CG-ND1	-5.12	1.32	1.38
1	E	93	HIS	CD2-NE2	-5.04	1.32	1.37
1	D	102	HIS	CD2-NE2	-5.03	1.32	1.37
1	H	106	HIS	CD2-NE2	-5.03	1.32	1.37

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	PHE	CA-CB-CG	-11.62	102.18	113.80
1	C	36	ASP	CA-CB-CG	11.40	124.00	112.60
1	G	33	GLY	O-C-N	-10.21	114.71	123.60
1	H	125	PHE	CA-CB-CG	-9.88	103.92	113.80
1	D	32	ASP	CA-C-N	-9.31	114.44	121.61
1	D	32	ASP	C-N-CA	-9.31	114.44	121.61
1	F	114	ASN	CA-CB-CG	8.87	121.47	112.60
1	A	21	TYR	O-C-N	-8.67	110.91	122.97
1	H	54	VAL	N-CA-C	8.62	121.15	108.65
1	A	32	ASP	CA-C-N	-8.42	116.19	122.33
1	A	32	ASP	C-N-CA	-8.42	116.19	122.33
1	F	42	ILE	O-C-N	-7.99	114.39	122.14
1	E	105	LYS	N-CA-C	-7.94	103.04	112.89
1	E	69	THR	N-CA-C	-7.75	103.97	113.50
1	G	86	LEU	CA-C-N	-7.60	112.27	122.99
1	G	86	LEU	C-N-CA	-7.60	112.27	122.99
1	B	55	TYR	CA-C-N	-7.55	113.53	122.22
1	B	55	TYR	C-N-CA	-7.55	113.53	122.22
1	A	54	VAL	N-CA-C	7.53	119.98	109.29
1	F	85	PHE	CA-C-N	-7.36	110.97	121.50
1	F	85	PHE	C-N-CA	-7.36	110.97	121.50
1	C	54	VAL	N-CA-C	7.29	120.49	109.20
1	G	54	VAL	N-CA-C	7.26	117.67	108.82
1	C	33	GLY	O-C-N	-7.23	117.71	123.49
1	G	124	HIS	CA-C-N	-7.05	111.42	121.50
1	G	124	HIS	C-N-CA	-7.05	111.42	121.50
1	H	93	HIS	CA-CB-CG	-7.02	106.78	113.80
1	H	131	LEU	O-C-N	-6.97	115.39	123.27
1	C	85	PHE	CA-C-N	-6.92	111.61	121.50
1	C	85	PHE	C-N-CA	-6.92	111.61	121.50
1	H	54	VAL	CA-C-O	6.91	128.41	121.64
1	C	16	CYS	O-C-N	-6.85	115.53	123.27
1	F	36	ASP	CA-CB-CG	6.83	119.43	112.60
1	E	52	GLY	N-CA-C	-6.82	105.81	115.30
1	C	92	ASN	CA-CB-CG	6.80	119.40	112.60
1	B	36	ASP	CA-CB-CG	6.73	119.33	112.60
1	D	122	ARG	CD-NE-CZ	-6.72	114.99	124.40
1	F	129	ALA	CA-C-N	6.69	129.63	120.46
1	F	129	ALA	C-N-CA	6.69	129.63	120.46
1	A	33	GLY	O-C-N	-6.67	117.21	123.48
1	A	54	VAL	N-CA-CB	-6.65	104.76	112.34
1	G	109	VAL	O-C-N	-6.64	115.44	122.81
1	F	85	PHE	O-C-N	-6.63	115.41	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	89	LEU	CA-C-N	-6.62	111.53	122.39
1	G	89	LEU	C-N-CA	-6.62	111.53	122.39
1	G	19	GLY	O-C-N	-6.62	117.42	122.71
1	A	97	TYR	O-C-N	-6.58	115.83	123.27
1	E	36	ASP	O-C-N	-6.58	114.93	123.02
1	A	108	PHE	CA-CB-CG	6.56	120.36	113.80
1	B	99	SER	CA-C-N	-6.55	109.38	120.58
1	B	99	SER	C-N-CA	-6.55	109.38	120.58
1	G	86	LEU	O-C-N	-6.53	115.59	123.29
1	G	73	LEU	O-C-N	-6.49	115.35	123.01
1	E	36	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	18	ASN	CA-CB-CG	-6.47	106.13	112.60
1	F	70	ASP	CA-CB-CG	6.46	119.06	112.60
1	C	18	ASN	CA-C-N	-6.43	108.81	121.41
1	C	18	ASN	C-N-CA	-6.43	108.81	121.41
1	H	27	PRO	O-C-N	-6.43	113.96	122.64
1	H	41	HIS	N-CA-C	6.42	120.82	112.92
1	C	132	PHE	O-C-N	-6.42	114.05	122.97
1	A	99	SER	N-CA-C	-6.40	100.81	110.28
1	A	55	TYR	CB-CA-C	-6.36	101.33	110.62
1	F	53	GLU	O-C-N	-6.35	115.13	123.13
1	A	18	ASN	CA-CB-CG	-6.32	106.28	112.60
1	C	20	GLY	N-CA-C	-6.29	105.21	114.90
1	E	124	HIS	CA-C-N	-6.27	111.96	120.87
1	E	124	HIS	C-N-CA	-6.27	111.96	120.87
1	D	81	GLU	N-CA-C	-6.24	105.83	113.50
1	A	85	PHE	CA-C-N	-6.23	114.12	122.72
1	A	85	PHE	C-N-CA	-6.23	114.12	122.72
1	E	92	ASN	N-CA-C	-6.21	105.75	113.15
1	F	74	TYR	O-C-N	-6.20	116.19	123.25
1	C	13	LEU	CA-C-N	-6.18	114.20	122.42
1	C	13	LEU	C-N-CA	-6.18	114.20	122.42
1	E	78	THR	N-CA-CB	-6.18	99.38	110.37
1	H	131	LEU	N-CA-C	6.15	119.26	109.24
1	D	62	GLY	CA-C-N	-6.12	110.65	121.29
1	D	62	GLY	C-N-CA	-6.12	110.65	121.29
1	C	21	TYR	CA-C-O	-6.11	115.60	122.01
1	G	94	TYR	N-CA-C	-6.09	101.18	110.14
1	E	32	ASP	CA-C-N	-6.08	116.93	121.61
1	E	32	ASP	C-N-CA	-6.08	116.93	121.61
1	H	96	THR	CA-C-N	-6.08	114.61	123.00
1	H	96	THR	C-N-CA	-6.08	114.61	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	32	ASP	CA-CB-CG	6.07	118.67	112.60
1	H	36	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	124	HIS	CA-C-N	-6.03	112.51	120.95
1	B	124	HIS	C-N-CA	-6.03	112.51	120.95
1	A	53	GLU	CA-C-O	-5.97	113.91	120.24
1	D	55	TYR	O-C-N	-5.96	116.30	123.27
1	G	124	HIS	O-C-N	-5.95	117.57	123.46
1	B	63	GLN	CA-C-O	-5.94	115.11	121.94
1	G	123	THR	O-C-N	-5.93	115.81	122.75
1	H	55	TYR	CA-C-O	-5.93	113.92	120.33
1	C	30	THR	O-C-N	-5.93	116.31	123.13
1	C	32	ASP	CA-C-N	-5.92	117.62	121.65
1	C	32	ASP	C-N-CA	-5.92	117.62	121.65
1	G	16	CYS	O-C-N	-5.91	116.27	123.19
1	G	72	LEU	O-C-N	-5.91	116.60	123.27
1	F	131	LEU	N-CA-C	5.89	118.27	109.25
1	G	88	ARG	O-C-N	-5.87	116.36	123.10
1	E	46	LEU	O-C-N	-5.86	116.11	122.79
1	E	130	ILE	N-CA-C	5.83	116.48	110.36
1	D	105	LYS	N-CA-C	-5.83	106.02	113.01
1	C	18	ASN	O-C-N	-5.82	114.84	122.59
1	F	18	ASN	O-C-N	-5.82	114.85	122.59
1	F	44	LEU	CA-C-N	-5.82	115.03	122.77
1	F	44	LEU	C-N-CA	-5.82	115.03	122.77
1	G	47	ALA	O-C-N	-5.82	116.59	123.22
1	C	15	TYR	O-C-N	-5.81	116.59	123.22
1	D	23	LEU	CA-C-N	-5.81	114.50	122.93
1	D	23	LEU	C-N-CA	-5.81	114.50	122.93
1	A	109	VAL	CA-C-N	-5.81	114.29	121.38
1	A	109	VAL	C-N-CA	-5.81	114.29	121.38
1	A	110	GLY	O-C-N	-5.80	118.53	123.23
1	A	125	PHE	O-C-N	-5.80	115.76	122.95
1	C	94	TYR	CA-C-O	-5.80	114.54	121.56
1	C	50	SER	N-CA-C	5.78	115.91	108.34
1	A	71	GLY	O-C-N	-5.78	115.43	122.30
1	F	56	ILE	CA-C-O	-5.77	113.57	120.78
1	C	56	ILE	CA-C-O	-5.73	115.01	121.09
1	A	128	LYS	N-CA-C	-5.72	106.26	113.18
1	C	49	GLU	O-C-N	-5.70	115.01	122.59
1	F	77	GLN	O-C-N	-5.69	115.35	122.35
1	G	114	ASN	CA-CB-CG	5.69	118.29	112.60
1	E	30	THR	CA-C-N	-5.69	115.51	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	THR	C-N-CA	-5.69	115.51	123.13
1	F	134	PRO	O-C-N	-5.67	118.70	122.73
1	F	12	LYS	CA-C-O	-5.65	115.26	121.31
1	E	122	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	G	87	GLU	O-C-N	-5.64	116.59	123.30
1	D	108	PHE	CA-C-O	-5.63	115.47	121.94
1	F	63	GLN	CA-C-O	-5.62	115.02	121.82
1	B	99	SER	O-C-N	-5.61	116.13	122.97
1	A	36	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	125	PHE	CA-CB-CG	-5.58	108.22	113.80
1	G	50	SER	CA-C-N	-5.57	115.87	123.12
1	G	50	SER	C-N-CA	-5.57	115.87	123.12
1	G	109	VAL	CA-C-N	-5.57	113.91	121.27
1	G	109	VAL	C-N-CA	-5.57	113.91	121.27
1	C	89	LEU	N-CA-C	-5.57	103.18	110.53
1	G	48	ALA	N-CA-C	5.56	118.30	109.24
1	H	69	THR	N-CA-C	-5.56	106.50	113.28
1	B	34	THR	O-C-N	-5.52	115.25	122.59
1	E	87	GLU	CA-C-N	-5.52	113.03	121.26
1	E	87	GLU	C-N-CA	-5.52	113.03	121.26
1	D	13	LEU	N-CA-C	-5.52	100.69	109.96
1	H	122	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	F	107	TRP	CD1-CG-CD2	5.50	115.11	106.30
1	C	59	THR	O-C-N	-5.50	115.18	122.33
1	F	107	TRP	CG-CD1-NE1	-5.50	103.06	110.20
1	B	64	PHE	CA-CB-CG	5.49	119.29	113.80
1	B	108	PHE	O-C-N	-5.49	115.18	122.59
1	A	30	THR	O-C-N	-5.48	116.54	123.01
1	D	93	HIS	N-CA-C	5.47	122.46	110.80
1	H	85	PHE	O-C-N	-5.47	115.53	122.43
1	B	40	GLN	CA-C-N	-5.47	113.16	122.56
1	B	40	GLN	C-N-CA	-5.47	113.16	122.56
1	H	111	LEU	O-C-N	-5.46	116.92	123.31
1	E	67	MET	N-CA-C	5.45	117.30	108.26
1	H	30	THR	CA-CB-OG1	-5.45	101.43	109.60
1	H	72	LEU	N-CA-C	5.44	117.39	108.52
1	B	86	LEU	O-C-N	-5.44	116.31	123.16
1	D	11	PRO	CA-N-CD	-5.44	104.39	112.00
1	C	96	THR	CA-C-N	-5.43	114.38	122.74
1	C	96	THR	C-N-CA	-5.43	114.38	122.74
1	B	40	GLN	O-C-N	-5.43	115.87	122.22
1	F	32	ASP	CA-CB-CG	5.42	118.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	GLU	CA-C-N	-5.41	113.76	121.33
1	B	87	GLU	C-N-CA	-5.41	113.76	121.33
1	C	125	PHE	O-C-N	-5.41	116.37	122.97
1	F	76	SER	O-C-N	-5.40	116.17	123.19
1	H	107	TRP	CE2-CD2-CE3	5.38	124.17	118.80
1	F	130	ILE	CB-CG1-CD1	-5.37	102.53	113.80
1	A	116	ARG	O-C-N	-5.37	116.23	122.89
1	E	18	ASN	CA-CB-CG	-5.37	107.23	112.60
1	H	90	GLU	N-CA-C	5.37	122.23	110.80
1	C	114	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	21	TYR	O-C-N	-5.36	116.94	122.94
1	B	54	VAL	N-CA-C	5.36	115.35	108.82
1	A	99	SER	CA-C-O	-5.35	115.16	121.16
1	G	88	ARG	CA-C-O	-5.35	114.96	121.28
1	E	41	HIS	O-C-N	-5.33	115.50	122.59
1	C	55	TYR	CA-C-N	-5.31	117.91	122.96
1	C	55	TYR	C-N-CA	-5.31	117.91	122.96
1	A	73	LEU	O-C-N	-5.30	116.83	123.04
1	F	110	GLY	O-C-N	-5.30	118.63	123.56
1	F	34	THR	CA-C-N	-5.30	114.67	122.83
1	F	34	THR	C-N-CA	-5.30	114.67	122.83
1	H	78	THR	CA-C-N	-5.29	115.32	120.98
1	H	78	THR	C-N-CA	-5.29	115.32	120.98
1	B	75	GLY	O-C-N	-5.28	120.02	123.35
1	E	125	PHE	N-CA-CB	5.28	117.73	109.97
1	H	48	ALA	N-CA-C	5.27	117.34	110.43
1	E	77	GLN	CB-CA-C	-5.27	101.39	110.72
1	F	107	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	E	131	LEU	N-CA-C	5.26	117.80	109.96
1	H	92	ASN	CA-CB-CG	5.26	117.86	112.60
1	D	58	SER	O-C-N	-5.25	116.34	122.96
1	G	48	ALA	CA-C-N	-5.24	114.42	121.71
1	G	48	ALA	C-N-CA	-5.24	114.42	121.71
1	G	123	THR	CA-CB-OG1	-5.23	101.75	109.60
1	H	122	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	H	25	ILE	CA-C-N	-5.21	113.68	120.67
1	H	25	ILE	C-N-CA	-5.21	113.68	120.67
1	C	106	HIS	ND1-CG-CD2	5.21	111.31	106.10
1	C	130	ILE	CA-C-N	-5.21	114.29	122.73
1	C	130	ILE	C-N-CA	-5.21	114.29	122.73
1	B	70	ASP	N-CA-C	-5.18	106.81	112.72
1	G	54	VAL	CB-CA-C	-5.18	104.09	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	130	ILE	O-C-N	-5.18	116.10	122.57
1	E	59	THR	CA-C-O	-5.17	115.04	120.63
1	F	21	TYR	O-C-N	-5.17	116.65	123.16
1	D	20	GLY	N-CA-C	-5.16	106.61	115.08
1	A	38	SER	CA-C-N	-5.16	115.44	122.93
1	A	38	SER	C-N-CA	-5.16	115.44	122.93
1	C	124	HIS	ND1-CG-CD2	5.15	111.25	106.10
1	D	93	HIS	CA-CB-CG	-5.15	108.65	113.80
1	H	52	GLY	N-CA-C	-5.15	100.97	113.18
1	F	39	ASP	O-C-N	-5.14	116.89	123.06
1	A	78	THR	N-CA-CB	-5.13	102.51	110.01
1	B	93	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	C	48	ALA	CB-CA-C	-5.13	104.78	111.40
1	B	59	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	120	GLY	CA-C-O	-5.10	116.48	119.69
1	A	85	PHE	CA-CB-CG	-5.09	108.70	113.80
1	A	54	VAL	O-C-N	-5.09	117.95	122.69
1	B	89	LEU	CA-C-O	-5.09	114.84	120.70
1	G	130	ILE	N-CA-CB	-5.09	106.61	112.21
1	H	130	ILE	N-CA-CB	-5.09	102.83	111.23
1	B	78	THR	N-CA-CB	-5.08	101.77	110.72
1	F	47	ALA	CA-C-O	-5.08	114.73	120.32
1	H	68	ASP	CB-CA-C	-5.08	100.31	110.42
1	B	134	PRO	O-C-N	-5.08	117.29	123.03
1	E	109	VAL	CA-C-N	-5.08	116.12	121.35
1	E	109	VAL	C-N-CA	-5.08	116.12	121.35
1	D	87	GLU	O-C-N	-5.08	115.84	122.59
1	C	116	ARG	O-C-N	-5.07	116.70	122.89
1	F	41	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	94	TYR	N-CA-C	-5.06	102.29	110.14
1	C	117	SER	O-C-N	-5.06	117.02	122.79
1	B	88	ARG	O-C-N	-5.06	118.46	123.62
1	F	77	GLN	CA-C-O	5.06	125.80	119.78
1	A	107	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	55	TYR	CA-C-O	-5.05	113.89	120.25
1	G	34	THR	O-C-N	-5.04	117.73	123.48
1	E	15	TYR	CA-C-N	-5.04	115.08	122.19
1	E	15	TYR	C-N-CA	-5.04	115.08	122.19
1	C	104	GLU	N-CA-C	-5.03	107.20	113.19
1	E	114	ASN	O-C-N	-5.03	114.94	122.39
1	H	48	ALA	O-C-N	-5.03	116.86	122.75
1	H	129	ALA	CA-C-N	5.03	131.02	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	129	ALA	C-N-CA	5.03	131.02	121.97
1	D	45	GLN	O-C-N	-5.02	117.37	123.29
1	H	129	ALA	CA-C-O	-5.01	115.55	121.07
1	E	129	ALA	CA-C-N	5.01	127.06	120.60
1	E	129	ALA	C-N-CA	5.01	127.06	120.60
1	A	98	ILE	CB-CA-C	-5.01	102.89	110.95
1	D	85	PHE	CA-C-N	-5.01	115.13	122.19
1	D	85	PHE	C-N-CA	-5.01	115.13	122.19
1	B	85	PHE	O-C-N	-5.01	116.64	123.15
1	F	94	TYR	CA-C-O	-5.00	115.76	121.82
1	C	74	TYR	O-C-N	-5.00	118.07	123.42
1	H	128	LYS	N-CA-C	-5.00	107.03	113.23

There are no chirality outliers.

All (620) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	100	LYS	Mainchain
1	A	103	ALA	Mainchain
1	A	104	GLU	Mainchain
1	A	105	LYS	Mainchain
1	A	108	PHE	Mainchain
1	A	11	PRO	Mainchain
1	A	110	GLY	Mainchain
1	A	114	ASN	Mainchain
1	A	115	GLY	Mainchain
1	A	116	ARG	Mainchain
1	A	12	LYS	Mainchain
1	A	120	GLY	Mainchain
1	A	122	ARG	Mainchain
1	A	123	THR	Mainchain
1	A	124	HIS	Mainchain
1	A	125	PHE	Sidechain,Mainchain
1	A	128	LYS	Mainchain
1	A	129	ALA	Mainchain
1	A	131	LEU	Mainchain
1	A	134	PRO	Mainchain
1	A	14	LEU	Mainchain
1	A	15	TYR	Sidechain
1	A	16	CYS	Mainchain
1	A	18	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	20	GLY	Mainchain
1	A	21	TYR	Mainchain
1	A	22	PHE	Mainchain
1	A	24	ARG	Sidechain,Mainchain
1	A	28	ASP	Mainchain
1	A	30	THR	Mainchain
1	A	31	VAL	Mainchain
1	A	33	GLY	Mainchain
1	A	35	LYS	Mainchain
1	A	36	ASP	Mainchain
1	A	38	SER	Mainchain
1	A	39	ASP	Sidechain,Mainchain
1	A	41	HIS	Mainchain
1	A	42	ILE	Mainchain
1	A	43	GLN	Mainchain
1	A	45	GLN	Mainchain
1	A	46	LEU	Mainchain
1	A	47	ALA	Mainchain
1	A	48	ALA	Mainchain
1	A	49	GLU	Mainchain
1	A	50	SER	Mainchain
1	A	51	ILE	Mainchain
1	A	53	GLU	Mainchain
1	A	54	VAL	Mainchain
1	A	55	TYR	Sidechain,Mainchain
1	A	56	ILE	Mainchain
1	A	58	SER	Mainchain
1	A	59	THR	Mainchain
1	A	60	GLU	Mainchain
1	A	61	THR	Mainchain
1	A	63	GLN	Mainchain
1	A	64	PHE	Mainchain
1	A	65	LEU	Mainchain
1	A	66	ALA	Mainchain
1	A	67	MET	Mainchain
1	A	69	THR	Mainchain
1	A	70	ASP	Mainchain
1	A	71	GLY	Mainchain
1	A	73	LEU	Mainchain
1	A	74	TYR	Sidechain,Mainchain
1	A	76	SER	Mainchain
1	A	77	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	79	PRO	Mainchain
1	A	80	ASN	Mainchain
1	A	82	GLU	Mainchain
1	A	84	LEU	Mainchain
1	A	86	LEU	Mainchain
1	A	87	GLU	Mainchain
1	A	88	ARG	Mainchain
1	A	90	GLU	Mainchain
1	A	91	GLU	Mainchain
1	A	92	ASN	Mainchain
1	A	93	HIS	Mainchain
1	A	95	ASN	Mainchain
1	A	96	THR	Mainchain
1	A	97	TYR	Sidechain,Mainchain
1	A	98	ILE	Mainchain
1	A	99	SER	Mainchain
1	B	102	HIS	Mainchain
1	B	103	ALA	Mainchain
1	B	105	LYS	Mainchain
1	B	108	PHE	Mainchain
1	B	11	PRO	Mainchain
1	B	110	GLY	Mainchain
1	B	113	LYS	Mainchain
1	B	114	ASN	Mainchain
1	B	117	SER	Mainchain
1	B	118	LYS	Mainchain
1	B	12	LYS	Mainchain
1	B	122	ARG	Sidechain
1	B	123	THR	Mainchain
1	B	13	LEU	Mainchain
1	B	14	LEU	Mainchain
1	B	16	CYS	Mainchain
1	B	17	SER	Mainchain
1	B	18	ASN	Mainchain
1	B	19	GLY	Mainchain
1	B	21	TYR	Mainchain
1	B	24	ARG	Sidechain,Mainchain
1	B	25	ILE	Mainchain
1	B	26	LEU	Mainchain
1	B	27	PRO	Mainchain
1	B	29	GLY	Mainchain
1	B	32	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	B	34	THR	Mainchain
1	B	36	ASP	Mainchain
1	B	37	ARG	Mainchain
1	B	38	SER	Mainchain
1	B	39	ASP	Sidechain,Mainchain
1	B	40	GLN	Mainchain
1	B	41	HIS	Mainchain
1	B	43	GLN	Mainchain
1	B	45	GLN	Mainchain
1	B	46	LEU	Mainchain
1	B	48	ALA	Mainchain
1	B	52	GLY	Mainchain
1	B	53	GLU	Mainchain
1	B	54	VAL	Mainchain
1	B	55	TYR	Sidechain,Mainchain
1	B	58	SER	Mainchain
1	B	59	THR	Mainchain
1	B	60	GLU	Mainchain
1	B	62	GLY	Mainchain
1	B	63	GLN	Mainchain
1	B	64	PHE	Mainchain
1	B	65	LEU	Mainchain
1	B	66	ALA	Mainchain
1	B	67	MET	Mainchain
1	B	68	ASP	Sidechain,Mainchain
1	B	69	THR	Mainchain
1	B	70	ASP	Sidechain
1	B	71	GLY	Mainchain
1	B	74	TYR	Sidechain,Mainchain
1	B	76	SER	Mainchain
1	B	79	PRO	Mainchain
1	B	80	ASN	Mainchain
1	B	83	CYS	Mainchain
1	B	84	LEU	Mainchain
1	B	85	PHE	Sidechain
1	B	86	LEU	Mainchain
1	B	87	GLU	Sidechain,Mainchain
1	B	88	ARG	Mainchain
1	B	89	LEU	Mainchain
1	B	92	ASN	Mainchain
1	B	93	HIS	Sidechain,Mainchain
1	B	95	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	B	97	TYR	Mainchain
1	B	99	SER	Mainchain
1	C	10	LYS	Mainchain
1	C	102	HIS	Mainchain
1	C	103	ALA	Mainchain
1	C	104	GLU	Mainchain
1	C	105	LYS	Mainchain
1	C	106	HIS	Mainchain
1	C	107	TRP	Mainchain
1	C	108	PHE	Sidechain
1	C	11	PRO	Mainchain
1	C	116	ARG	Sidechain,Mainchain
1	C	118	LYS	Mainchain
1	C	12	LYS	Mainchain
1	C	122	ARG	Mainchain
1	C	123	THR	Mainchain
1	C	125	PHE	Mainchain
1	C	129	ALA	Mainchain
1	C	13	LEU	Mainchain
1	C	131	LEU	Mainchain
1	C	132	PHE	Mainchain
1	C	134	PRO	Mainchain
1	C	135	LEU	Mainchain
1	C	15	TYR	Sidechain,Mainchain
1	C	16	CYS	Mainchain
1	C	20	GLY	Mainchain
1	C	21	TYR	Sidechain,Mainchain
1	C	23	LEU	Mainchain
1	C	25	ILE	Mainchain
1	C	27	PRO	Mainchain
1	C	29	GLY	Mainchain
1	C	30	THR	Mainchain
1	C	32	ASP	Sidechain,Mainchain
1	C	35	LYS	Mainchain
1	C	36	ASP	Sidechain,Mainchain
1	C	37	ARG	Mainchain
1	C	39	ASP	Sidechain,Mainchain
1	C	40	GLN	Mainchain
1	C	41	HIS	Mainchain
1	C	42	ILE	Mainchain
1	C	47	ALA	Mainchain
1	C	48	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	C	50	SER	Mainchain
1	C	52	GLY	Mainchain
1	C	53	GLU	Mainchain
1	C	55	TYR	Mainchain
1	C	56	ILE	Mainchain
1	C	57	LYS	Mainchain
1	C	58	SER	Mainchain
1	C	60	GLU	Mainchain
1	C	63	GLN	Mainchain
1	C	65	LEU	Mainchain
1	C	66	ALA	Mainchain
1	C	68	ASP	Sidechain
1	C	69	THR	Mainchain
1	C	71	GLY	Mainchain
1	C	74	TYR	Sidechain,Mainchain
1	C	77	GLN	Mainchain
1	C	79	PRO	Mainchain
1	C	80	ASN	Mainchain
1	C	82	GLU	Mainchain
1	C	84	LEU	Mainchain
1	C	85	PHE	Sidechain,Mainchain
1	C	87	GLU	Mainchain
1	C	92	ASN	Mainchain
1	C	93	HIS	Mainchain
1	C	94	TYR	Mainchain
1	C	95	ASN	Mainchain
1	C	97	TYR	Sidechain
1	C	99	SER	Mainchain
1	D	100	LYS	Mainchain
1	D	101	LYS	Mainchain
1	D	104	GLU	Mainchain
1	D	105	LYS	Mainchain
1	D	108	PHE	Mainchain
1	D	11	PRO	Mainchain
1	D	110	GLY	Mainchain
1	D	111	LEU	Mainchain
1	D	113	LYS	Mainchain
1	D	114	ASN	Mainchain
1	D	115	GLY	Mainchain
1	D	117	SER	Mainchain
1	D	12	LYS	Mainchain
1	D	122	ARG	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	D	123	THR	Mainchain
1	D	124	HIS	Sidechain
1	D	130	ILE	Mainchain
1	D	131	LEU	Mainchain
1	D	132	PHE	Mainchain
1	D	134	PRO	Mainchain
1	D	135	LEU	Mainchain
1	D	16	CYS	Mainchain
1	D	17	SER	Mainchain
1	D	21	TYR	Mainchain
1	D	24	ARG	Sidechain
1	D	26	LEU	Mainchain
1	D	27	PRO	Mainchain
1	D	28	ASP	Mainchain
1	D	30	THR	Mainchain
1	D	31	VAL	Mainchain
1	D	32	ASP	Mainchain
1	D	34	THR	Mainchain
1	D	35	LYS	Mainchain
1	D	36	ASP	Sidechain,Mainchain
1	D	37	ARG	Sidechain,Mainchain
1	D	39	ASP	Mainchain
1	D	41	HIS	Mainchain
1	D	42	ILE	Mainchain
1	D	43	GLN	Mainchain
1	D	44	LEU	Mainchain
1	D	46	LEU	Mainchain
1	D	48	ALA	Mainchain
1	D	49	GLU	Mainchain
1	D	50	SER	Mainchain
1	D	51	ILE	Mainchain
1	D	52	GLY	Mainchain
1	D	53	GLU	Sidechain,Mainchain
1	D	54	VAL	Mainchain
1	D	55	TYR	Mainchain
1	D	58	SER	Mainchain
1	D	59	THR	Mainchain
1	D	61	THR	Mainchain
1	D	64	PHE	Sidechain,Mainchain
1	D	65	LEU	Mainchain
1	D	70	ASP	Sidechain
1	D	72	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	75	GLY	Mainchain
1	D	76	SER	Mainchain
1	D	79	PRO	Mainchain
1	D	80	ASN	Mainchain
1	D	82	GLU	Mainchain
1	D	87	GLU	Sidechain,Mainchain
1	D	88	ARG	Mainchain
1	D	90	GLU	Mainchain
1	D	92	ASN	Mainchain
1	D	95	ASN	Mainchain
1	D	96	THR	Mainchain
1	D	97	TYR	Sidechain,Mainchain
1	D	99	SER	Mainchain
1	E	10	LYS	Mainchain
1	E	102	HIS	Mainchain
1	E	103	ALA	Mainchain
1	E	104	GLU	Sidechain,Mainchain
1	E	106	HIS	Mainchain
1	E	107	TRP	Mainchain
1	E	108	PHE	Mainchain
1	E	11	PRO	Mainchain
1	E	110	GLY	Mainchain
1	E	111	LEU	Mainchain
1	E	113	LYS	Mainchain
1	E	114	ASN	Mainchain
1	E	115	GLY	Mainchain
1	E	117	SER	Mainchain
1	E	118	LYS	Mainchain
1	E	12	LYS	Mainchain
1	E	125	PHE	Mainchain
1	E	129	ALA	Mainchain
1	E	13	LEU	Mainchain
1	E	130	ILE	Mainchain
1	E	131	LEU	Mainchain
1	E	135	LEU	Mainchain
1	E	15	TYR	Mainchain
1	E	20	GLY	Mainchain
1	E	22	PHE	Mainchain
1	E	23	LEU	Mainchain
1	E	25	ILE	Mainchain
1	E	26	LEU	Mainchain
1	E	27	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	E	28	ASP	Mainchain
1	E	31	VAL	Mainchain
1	E	32	ASP	Sidechain
1	E	36	ASP	Mainchain
1	E	37	ARG	Sidechain,Mainchain
1	E	39	ASP	Mainchain
1	E	40	GLN	Mainchain
1	E	41	HIS	Mainchain
1	E	43	GLN	Mainchain
1	E	45	GLN	Mainchain
1	E	46	LEU	Mainchain
1	E	47	ALA	Mainchain
1	E	49	GLU	Mainchain
1	E	52	GLY	Mainchain
1	E	53	GLU	Mainchain
1	E	54	VAL	Mainchain
1	E	55	TYR	Mainchain
1	E	58	SER	Mainchain
1	E	59	THR	Mainchain
1	E	63	GLN	Mainchain
1	E	64	PHE	Mainchain
1	E	65	LEU	Mainchain
1	E	67	MET	Mainchain
1	E	68	ASP	Mainchain
1	E	69	THR	Mainchain
1	E	71	GLY	Mainchain
1	E	72	LEU	Mainchain
1	E	74	TYR	Mainchain
1	E	77	GLN	Mainchain
1	E	79	PRO	Mainchain
1	E	80	ASN	Mainchain
1	E	82	GLU	Mainchain
1	E	83	CYS	Mainchain
1	E	85	PHE	Sidechain
1	E	86	LEU	Mainchain
1	E	87	GLU	Sidechain
1	E	88	ARG	Mainchain
1	E	89	LEU	Mainchain
1	E	91	GLU	Mainchain
1	E	92	ASN	Mainchain
1	E	93	HIS	Sidechain
1	E	96	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	E	97	TYR	Sidechain
1	F	10	LYS	Mainchain
1	F	100	LYS	Mainchain
1	F	101	LYS	Mainchain
1	F	103	ALA	Mainchain
1	F	104	GLU	Mainchain
1	F	107	TRP	Mainchain
1	F	108	PHE	Mainchain
1	F	110	GLY	Mainchain
1	F	112	LYS	Mainchain
1	F	115	GLY	Mainchain
1	F	117	SER	Mainchain
1	F	118	LYS	Mainchain
1	F	12	LYS	Mainchain
1	F	121	PRO	Mainchain
1	F	122	ARG	Sidechain
1	F	123	THR	Mainchain
1	F	125	PHE	Sidechain
1	F	128	LYS	Mainchain
1	F	132	PHE	Mainchain
1	F	14	LEU	Mainchain
1	F	15	TYR	Sidechain
1	F	20	GLY	Mainchain
1	F	21	TYR	Mainchain
1	F	22	PHE	Sidechain,Mainchain
1	F	23	LEU	Mainchain
1	F	24	ARG	Mainchain
1	F	25	ILE	Mainchain
1	F	30	THR	Mainchain
1	F	31	VAL	Mainchain
1	F	32	ASP	Sidechain
1	F	33	GLY	Mainchain
1	F	34	THR	Mainchain
1	F	36	ASP	Mainchain
1	F	37	ARG	Mainchain
1	F	40	GLN	Mainchain
1	F	42	ILE	Mainchain
1	F	43	GLN	Mainchain
1	F	44	LEU	Mainchain
1	F	46	LEU	Mainchain
1	F	47	ALA	Mainchain
1	F	48	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	F	49	GLU	Mainchain
1	F	50	SER	Mainchain
1	F	51	ILE	Mainchain
1	F	52	GLY	Mainchain
1	F	53	GLU	Mainchain
1	F	54	VAL	Mainchain
1	F	55	TYR	Sidechain,Mainchain
1	F	56	ILE	Mainchain
1	F	60	GLU	Mainchain
1	F	63	GLN	Mainchain
1	F	65	LEU	Mainchain
1	F	66	ALA	Mainchain
1	F	68	ASP	Mainchain
1	F	70	ASP	Sidechain
1	F	73	LEU	Mainchain
1	F	74	TYR	Mainchain
1	F	75	GLY	Mainchain
1	F	76	SER	Mainchain
1	F	78	THR	Mainchain
1	F	79	PRO	Mainchain
1	F	82	GLU	Mainchain
1	F	83	CYS	Mainchain
1	F	85	PHE	Sidechain,Mainchain
1	F	86	LEU	Mainchain
1	F	87	GLU	Sidechain
1	F	88	ARG	Mainchain
1	F	90	GLU	Mainchain
1	F	92	ASN	Mainchain
1	F	94	TYR	Mainchain
1	F	95	ASN	Mainchain
1	F	96	THR	Mainchain
1	F	97	TYR	Sidechain,Mainchain
1	F	98	ILE	Mainchain
1	G	100	LYS	Mainchain
1	G	105	LYS	Mainchain
1	G	106	HIS	Mainchain
1	G	108	PHE	Mainchain
1	G	11	PRO	Mainchain
1	G	112	LYS	Mainchain
1	G	113	LYS	Mainchain
1	G	114	ASN	Mainchain
1	G	115	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	G	119	LEU	Mainchain
1	G	12	LYS	Mainchain
1	G	121	PRO	Mainchain
1	G	123	THR	Mainchain
1	G	128	LYS	Mainchain
1	G	13	LEU	Mainchain
1	G	132	PHE	Mainchain
1	G	135	LEU	Mainchain
1	G	15	TYR	Sidechain
1	G	16	CYS	Mainchain
1	G	21	TYR	Mainchain
1	G	22	PHE	Mainchain
1	G	24	ARG	Sidechain,Mainchain
1	G	25	ILE	Mainchain
1	G	26	LEU	Mainchain
1	G	29	GLY	Mainchain
1	G	32	ASP	Mainchain
1	G	33	GLY	Mainchain
1	G	36	ASP	Mainchain
1	G	38	SER	Mainchain
1	G	39	ASP	Mainchain
1	G	40	GLN	Mainchain
1	G	45	GLN	Mainchain
1	G	47	ALA	Mainchain
1	G	52	GLY	Mainchain
1	G	53	GLU	Sidechain,Mainchain
1	G	54	VAL	Mainchain
1	G	55	TYR	Mainchain
1	G	57	LYS	Mainchain
1	G	58	SER	Mainchain
1	G	59	THR	Mainchain
1	G	60	GLU	Mainchain
1	G	64	PHE	Sidechain,Mainchain
1	G	67	MET	Mainchain
1	G	69	THR	Mainchain
1	G	70	ASP	Mainchain
1	G	71	GLY	Mainchain
1	G	72	LEU	Mainchain
1	G	74	TYR	Mainchain
1	G	75	GLY	Mainchain
1	G	77	GLN	Mainchain
1	G	79	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	G	82	GLU	Mainchain
1	G	83	CYS	Mainchain
1	G	85	PHE	Mainchain
1	G	86	LEU	Mainchain
1	G	87	GLU	Sidechain,Mainchain
1	G	88	ARG	Mainchain
1	G	92	ASN	Mainchain
1	G	93	HIS	Mainchain
1	G	95	ASN	Mainchain
1	G	97	TYR	Mainchain
1	G	98	ILE	Mainchain
1	G	99	SER	Mainchain
1	H	100	LYS	Mainchain
1	H	102	HIS	Mainchain
1	H	103	ALA	Mainchain
1	H	104	GLU	Mainchain
1	H	105	LYS	Mainchain
1	H	108	PHE	Mainchain
1	H	109	VAL	Mainchain
1	H	111	LEU	Mainchain
1	H	113	LYS	Mainchain
1	H	115	GLY	Mainchain
1	H	116	ARG	Mainchain
1	H	118	LYS	Mainchain
1	H	12	LYS	Mainchain
1	H	123	THR	Mainchain
1	H	124	HIS	Sidechain,Mainchain
1	H	125	PHE	Sidechain,Mainchain
1	H	129	ALA	Mainchain
1	H	13	LEU	Mainchain
1	H	130	ILE	Mainchain
1	H	131	LEU	Mainchain
1	H	132	PHE	Mainchain
1	H	134	PRO	Mainchain
1	H	17	SER	Mainchain
1	H	18	ASN	Mainchain
1	H	20	GLY	Mainchain
1	H	21	TYR	Sidechain,Mainchain
1	H	27	PRO	Mainchain
1	H	28	ASP	Sidechain
1	H	30	THR	Mainchain
1	H	32	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	H	35	LYS	Mainchain
1	H	37	ARG	Mainchain
1	H	38	SER	Mainchain
1	H	39	ASP	Sidechain,Mainchain
1	H	40	GLN	Mainchain
1	H	41	HIS	Mainchain
1	H	43	GLN	Mainchain
1	H	44	LEU	Mainchain
1	H	45	GLN	Mainchain
1	H	47	ALA	Mainchain
1	H	48	ALA	Mainchain
1	H	50	SER	Mainchain
1	H	51	ILE	Mainchain
1	H	52	GLY	Mainchain
1	H	53	GLU	Mainchain
1	H	55	TYR	Sidechain,Mainchain
1	H	56	ILE	Mainchain
1	H	57	LYS	Mainchain
1	H	58	SER	Mainchain
1	H	59	THR	Mainchain
1	H	60	GLU	Mainchain
1	H	61	THR	Mainchain
1	H	62	GLY	Mainchain
1	H	63	GLN	Mainchain
1	H	68	ASP	Mainchain
1	H	70	ASP	Mainchain
1	H	72	LEU	Mainchain
1	H	74	TYR	Sidechain,Mainchain
1	H	76	SER	Mainchain
1	H	77	GLN	Mainchain
1	H	79	PRO	Mainchain
1	H	80	ASN	Mainchain
1	H	81	GLU	Mainchain
1	H	84	LEU	Mainchain
1	H	85	PHE	Sidechain,Mainchain
1	H	86	LEU	Mainchain
1	H	88	ARG	Mainchain
1	H	89	LEU	Mainchain
1	H	90	GLU	Mainchain
1	H	91	GLU	Mainchain
1	H	92	ASN	Mainchain
1	H	93	HIS	Mainchain

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Mol	Chain	Res	Type	Group
1	H	94	TYR	Mainchain
1	H	96	THR	Mainchain
1	H	97	TYR	Mainchain
1	H	99	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	983	0	944	109	0
1	B	983	0	944	98	0
1	C	983	0	944	116	0
1	D	983	0	944	97	0
1	E	983	0	944	92	0
1	F	983	0	944	88	0
1	G	983	0	944	128	0
1	H	983	0	944	123	0
2	I	55	0	6	24	0
2	J	55	0	6	7	0
2	K	55	0	6	13	0
2	L	55	0	6	21	0
2	M	55	0	6	19	0
2	N	55	0	6	14	0
2	O	55	0	6	26	0
2	P	55	0	6	18	0
All	All	8304	0	7600	925	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 58.

All (925) 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:114:ASN:HD21	1:A:116:ARG:NH1	1.43	1.16
1:G:24:ARG:HH11	1:G:26:LEU:HD11	1.01	1.14
1:H:27:PRO:HB3	1:H:61:THR:HG21	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:HD21	1:D:100:LYS:HG3	1.30	1.11
1:F:24:ARG:HD2	1:F:26:LEU:HD11	1.30	1.11
1:B:26:LEU:HB2	1:B:30:THR:HG22	1.22	1.11
1:D:98:ILE:HD11	1:D:106:HIS:HA	1.32	1.11
1:E:26:LEU:HD23	1:E:30:THR:CG2	1.85	1.06
1:E:95:ASN:N	1:E:95:ASN:HD22	1.51	1.05
1:E:26:LEU:HD23	1:E:30:THR:HG22	1.06	1.04
1:B:24:ARG:HD3	1:B:26:LEU:HD13	1.36	1.02
1:H:12:LYS:HB3	1:H:135:LEU:O	1.60	1.02
1:A:24:ARG:HD2	1:A:26:LEU:HD11	1.42	1.00
1:G:102:HIS:HB3	1:G:105:LYS:HG3	1.39	1.00
1:F:112:LYS:HE2	2:N:2:YYJ:S3	2.03	0.99
1:G:24:ARG:NH1	1:G:26:LEU:HD11	1.78	0.99
1:G:26:LEU:HD23	1:G:30:THR:CG2	1.92	0.99
1:C:89:LEU:HD13	1:C:90:GLU:N	1.78	0.98
2:O:1:GU4:H62	2:O:1:GU4:O24	1.63	0.98
1:D:123:THR:O	1:D:124:HIS:HB3	1.60	0.98
1:E:26:LEU:CD2	1:E:30:THR:HG22	1.93	0.98
1:F:92:ASN:O	1:F:93:HIS:HB2	1.64	0.96
1:H:53:GLU:HG2	1:H:84:LEU:HD23	1.47	0.94
1:G:26:LEU:HD23	1:G:30:THR:HG22	1.46	0.94
1:A:90:GLU:HA	1:A:90:GLU:OE1	1.68	0.94
2:O:2:YYJ:O2S4	2:O:2:YYJ:C5	2.16	0.93
1:C:55:TYR:CZ	1:C:84:LEU:HD21	2.05	0.91
1:B:13:LEU:HB2	1:B:135:LEU:O	1.69	0.91
2:P:1:GU4:H62	2:P:2:YYJ:O1S6	1.71	0.91
1:A:89:LEU:HD23	1:A:90:GLU:N	1.85	0.91
1:D:24:ARG:HD3	1:D:26:LEU:HD13	1.50	0.91
1:A:11:PRO:O	1:A:12:LYS:HD3	1.71	0.91
1:C:108:PHE:CE1	1:C:130:ILE:HD11	2.06	0.91
1:C:65:LEU:HD21	1:C:73:LEU:HD23	1.50	0.90
1:A:46:LEU:HD23	1:A:56:ILE:HG12	1.54	0.90
1:G:124:HIS:C	1:G:124:HIS:CD2	2.49	0.90
1:B:16:CYS:HB2	1:B:132:PHE:CE1	2.07	0.90
1:A:26:LEU:N	1:A:26:LEU:HD12	1.88	0.89
1:C:24:ARG:HD3	1:C:26:LEU:HD13	1.53	0.89
1:B:28:ASP:OD1	1:B:30:THR:HB	1.74	0.88
1:H:12:LYS:CB	1:H:135:LEU:O	2.22	0.88
1:B:112:LYS:HE3	2:J:2:YYJ:O2S3	1.73	0.88
1:A:114:ASN:ND2	1:A:116:ARG:NH1	2.22	0.87
1:G:80:ASN:O	1:G:83:CYS:HB2	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:HD21	1:E:100:LYS:CD	2.05	0.86
1:G:24:ARG:HD3	1:G:26:LEU:HD13	1.55	0.86
1:D:98:ILE:HD11	1:D:106:HIS:CA	2.05	0.86
2:I:1:GU4:H61	2:I:2:YYJ:C6	2.06	0.85
1:A:46:LEU:HB3	1:A:56:ILE:HG13	1.58	0.85
1:D:48:ALA:HA	1:D:54:VAL:HG12	1.57	0.85
1:B:56:ILE:HD12	1:B:65:LEU:HD12	1.58	0.85
1:H:112:LYS:CE	2:P:1:GU4:H61	2.07	0.85
1:A:102:HIS:HA	1:A:104:GLU:OE1	1.76	0.84
1:D:96:THR:HG23	1:D:130:ILE:HG23	1.58	0.84
1:G:24:ARG:HH11	1:G:26:LEU:CD1	1.87	0.84
1:A:89:LEU:HD23	1:A:90:GLU:H	1.42	0.84
1:F:124:HIS:C	1:F:130:ILE:HD11	2.03	0.84
1:F:53:GLU:HB3	1:F:84:LEU:HD22	1.60	0.83
1:F:86:LEU:HD21	1:F:100:LYS:HD2	1.61	0.83
1:G:124:HIS:HD2	1:G:124:HIS:O	1.61	0.83
1:D:112:LYS:HZ1	2:L:1:GU4:H61	1.44	0.82
1:G:112:LYS:HE2	2:O:2:YYJ:C6	2.09	0.82
2:M:2:YYJ:C4	2:M:2:YYJ:S6	2.67	0.82
1:G:86:LEU:HD21	1:G:100:LYS:HG3	1.59	0.82
1:D:108:PHE:O	1:D:123:THR:HG21	1.80	0.82
1:D:77:GLN:O	1:D:77:GLN:HG3	1.78	0.82
1:D:112:LYS:NZ	2:L:1:GU4:H61	1.95	0.82
1:H:57:LYS:HG3	1:H:58:SER:N	1.94	0.82
1:B:89:LEU:HD12	1:B:90:GLU:N	1.94	0.82
1:B:102:HIS:HB3	1:B:105:LYS:HG3	1.60	0.82
1:A:26:LEU:N	1:A:26:LEU:CD1	2.43	0.81
1:H:111:LEU:HD23	1:H:117:SER:HA	1.61	0.81
1:C:122:ARG:CD	2:K:2:YYJ:O3S1	2.28	0.81
1:F:89:LEU:HD21	1:F:93:HIS:ND1	1.94	0.81
2:I:1:GU4:H61	2:I:2:YYJ:S6	2.19	0.81
1:C:104:GLU:OE2	1:C:105:LYS:HD3	1.79	0.81
1:B:64:PHE:CZ	1:B:79:PRO:HG3	2.15	0.80
1:G:124:HIS:CD2	1:G:125:PHE:C	2.59	0.80
1:B:94:TYR:CE1	1:B:133:LEU:HB2	2.16	0.80
2:I:1:GU4:C6	2:I:2:YYJ:C6	2.59	0.80
1:C:60:GLU:OE1	1:C:60:GLU:N	2.15	0.80
1:B:39:ASP:O	1:B:42:ILE:HG12	1.80	0.80
1:C:24:ARG:HD2	1:C:32:ASP:OD1	1.81	0.80
1:E:39:ASP:OD1	1:E:41:HIS:HB2	1.81	0.80
1:F:112:LYS:HE2	2:N:2:YYJ:O1S3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LYS:HE2	2:L:2:YYJ:S3	2.23	0.79
1:D:86:LEU:CD2	1:D:100:LYS:HG3	2.10	0.79
1:B:72:LEU:HD23	1:B:119:LEU:HD21	1.63	0.79
1:F:49:GLU:HG3	1:F:84:LEU:HD21	1.63	0.79
1:G:112:LYS:HE2	2:O:2:YYJ:C4	2.13	0.78
1:D:37:ARG:O	1:D:37:ARG:HG2	1.84	0.78
1:B:26:LEU:CB	1:B:30:THR:HG22	2.11	0.78
1:C:131:LEU:HD22	1:C:131:LEU:H	1.49	0.78
1:H:57:LYS:HG3	1:H:58:SER:H	1.49	0.78
1:A:84:LEU:HB2	1:A:100:LYS:CE	2.13	0.77
1:C:12:LYS:HA	1:C:136:PRO:HA	1.65	0.77
1:A:124:HIS:CE1	1:A:127:GLN:NE2	2.53	0.77
1:H:90:GLU:O	1:H:91:GLU:CB	2.30	0.77
1:D:14:LEU:HD22	1:D:44:LEU:HD23	1.67	0.77
1:G:39:ASP:O	1:G:42:ILE:HG12	1.84	0.77
1:G:105:LYS:O	1:G:106:HIS:HB2	1.84	0.77
2:N:1:GU4:O6	2:N:2:YYJ:O1S6	2.02	0.77
1:D:130:ILE:HG22	1:D:131:LEU:HD13	1.66	0.77
1:G:89:LEU:HD22	1:G:90:GLU:H	1.49	0.77
1:A:24:ARG:CD	1:A:26:LEU:HD11	2.14	0.77
1:F:24:ARG:HD2	1:F:26:LEU:CD1	2.13	0.77
1:A:90:GLU:OE1	1:A:90:GLU:CA	2.31	0.76
1:C:122:ARG:HD2	2:K:2:YYJ:O3S1	1.84	0.76
1:A:105:LYS:O	1:A:106:HIS:HB2	1.84	0.76
1:G:124:HIS:C	1:G:124:HIS:HD2	1.90	0.76
1:G:124:HIS:CD2	1:G:124:HIS:O	2.39	0.76
1:C:12:LYS:HB3	1:C:135:LEU:O	1.86	0.76
1:E:84:LEU:O	1:E:100:LYS:HB2	1.86	0.76
1:E:90:GLU:HB2	1:E:94:TYR:O	1.86	0.75
2:K:1:GU4:O11	2:K:2:YYJ:O1S1	2.04	0.75
1:B:94:TYR:HE1	1:B:133:LEU:HB2	1.51	0.75
1:G:61:THR:OG1	1:G:63:GLN:NE2	2.18	0.75
1:C:54:VAL:O	1:C:84:LEU:HD13	1.86	0.75
1:F:89:LEU:HD21	1:F:93:HIS:CE1	2.22	0.75
1:D:112:LYS:HG2	2:L:2:YYJ:O2S3	1.85	0.75
1:C:104:GLU:CD	1:C:104:GLU:H	1.95	0.75
1:F:46:LEU:HD23	1:F:56:ILE:HG13	1.67	0.75
1:G:65:LEU:O	1:G:66:ALA:HB2	1.85	0.75
2:N:1:GU4:O23	2:N:2:YYJ:O2S6	2.05	0.75
1:F:89:LEU:O	1:F:90:GLU:HG2	1.86	0.75
1:G:24:ARG:HD3	1:G:26:LEU:CD1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:GLU:HG3	1:H:86:LEU:HD23	1.69	0.74
1:H:123:THR:O	1:H:124:HIS:HB3	1.88	0.74
1:C:108:PHE:CZ	1:C:130:ILE:HD11	2.23	0.74
1:F:26:LEU:HD13	1:F:26:LEU:N	2.03	0.74
1:H:112:LYS:HE3	2:P:1:GU4:H61	1.67	0.73
1:E:112:LYS:HE2	2:M:2:YYJ:O3S6	1.88	0.73
1:A:112:LYS:HE3	2:I:2:YYJ:O3S4	1.88	0.73
1:D:98:ILE:CD1	1:D:106:HIS:HA	2.15	0.73
1:G:26:LEU:HB2	1:G:30:THR:HG22	1.71	0.73
1:G:87:GLU:O	1:G:87:GLU:HG3	1.87	0.73
1:D:87:GLU:HG3	1:D:97:TYR:CE2	2.23	0.73
2:N:1:GU4:H3	2:N:2:YYJ:O1S1	1.89	0.73
1:C:37:ARG:O	1:C:37:ARG:HG2	1.88	0.72
1:A:23:LEU:HD23	1:A:44:LEU:HD21	1.70	0.72
1:B:56:ILE:CD1	1:B:65:LEU:HD12	2.17	0.72
1:D:96:THR:CG2	1:D:130:ILE:HG23	2.18	0.72
1:D:19:GLY:HA3	1:D:21:TYR:CE2	2.24	0.72
1:G:47:ALA:C	1:G:54:VAL:HG12	2.14	0.72
1:G:124:HIS:HD2	1:G:125:PHE:C	1.97	0.72
1:C:108:PHE:CD1	1:C:130:ILE:HD11	2.25	0.71
1:A:118:LYS:HE2	2:I:2:YYJ:O2S3	1.91	0.71
1:B:86:LEU:HD21	1:B:100:LYS:CG	2.20	0.71
1:B:26:LEU:HB2	1:B:30:THR:CG2	2.13	0.71
1:F:111:LEU:HD23	1:F:117:SER:HA	1.73	0.71
1:E:105:LYS:O	1:E:106:HIS:HB2	1.89	0.71
1:G:16:CYS:HB2	1:G:132:PHE:CE1	2.26	0.71
1:G:112:LYS:HD3	2:O:1:GU4:O23	1.91	0.71
1:C:55:TYR:OH	1:C:84:LEU:HD21	1.90	0.71
1:C:46:LEU:HD22	1:C:56:ILE:HG12	1.73	0.70
1:E:89:LEU:HG	1:E:90:GLU:H	1.57	0.70
1:F:36:ASP:C	1:F:38:SER:H	1.98	0.70
1:C:134:PRO:C	1:C:135:LEU:HD23	2.15	0.70
1:C:16:CYS:HB2	1:C:132:PHE:CE2	2.27	0.70
1:C:89:LEU:O	1:C:90:GLU:HG2	1.92	0.70
2:J:2:YYJ:O3S3	2:J:2:YYJ:O1	2.09	0.70
1:B:92:ASN:O	1:B:93:HIS:HB2	1.91	0.70
2:P:1:GU4:C6	2:P:2:YYJ:O1S6	2.39	0.70
1:G:89:LEU:HD22	1:G:90:GLU:N	2.06	0.69
1:G:112:LYS:CE	2:O:2:YYJ:C4	2.70	0.69
2:P:1:GU4:H62	2:P:2:YYJ:S6	2.31	0.69
1:C:122:ARG:HD3	2:K:2:YYJ:O3S1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:TYR:HB2	1:D:135:LEU:CD1	2.21	0.69
1:E:64:PHE:CE1	1:E:79:PRO:HD3	2.26	0.69
2:O:1:GU4:H3	2:O:2:YYJ:O3	1.91	0.69
1:E:55:TYR:OH	1:E:84:LEU:HD22	1.93	0.69
2:M:2:YYJ:C4	2:M:2:YYJ:O2S6	2.40	0.69
1:A:84:LEU:CB	1:A:100:LYS:CE	2.70	0.69
1:F:39:ASP:HB3	1:F:42:ILE:HG23	1.74	0.69
1:G:49:GLU:HG3	1:G:55:TYR:CE2	2.26	0.69
1:A:85:PHE:HA	1:A:98:ILE:O	1.93	0.69
1:A:114:ASN:HD21	1:A:116:ARG:HH12	1.40	0.69
1:F:26:LEU:HD13	1:F:26:LEU:H	1.56	0.68
1:F:24:ARG:HG3	1:F:34:THR:HG21	1.75	0.68
1:D:15:TYR:HB2	1:D:135:LEU:HD12	1.76	0.68
1:E:43:GLN:HE22	1:E:60:GLU:HG3	1.57	0.68
1:A:112:LYS:NZ	2:I:2:YYJ:O2S3	2.27	0.68
1:C:127:GLN:O	1:C:130:ILE:HG22	1.93	0.68
1:B:72:LEU:HD23	1:B:119:LEU:CD2	2.23	0.68
1:H:79:PRO:O	1:H:80:ASN:HB3	1.92	0.68
1:F:47:ALA:O	1:F:55:TYR:HD2	1.76	0.67
1:H:27:PRO:HB3	1:H:61:THR:CG2	2.19	0.67
2:N:2:YYJ:O1	2:N:2:YYJ:O3S3	2.11	0.67
1:A:84:LEU:HB2	1:A:100:LYS:HD2	1.76	0.67
1:B:64:PHE:CE2	1:B:79:PRO:HG3	2.28	0.67
1:C:131:LEU:O	1:C:131:LEU:HD23	1.94	0.67
1:C:73:LEU:HD21	1:C:109:VAL:HG13	1.76	0.67
1:F:26:LEU:CD1	1:F:26:LEU:N	2.57	0.67
1:F:89:LEU:C	1:F:90:GLU:HG2	2.20	0.67
1:G:26:LEU:CD2	1:G:30:THR:HG22	2.24	0.67
1:A:111:LEU:HD23	1:A:117:SER:HA	1.75	0.67
1:E:26:LEU:HB2	1:E:28:ASP:OD1	1.95	0.67
1:A:80:ASN:HD22	1:A:82:GLU:H	1.41	0.67
1:E:95:ASN:N	1:E:95:ASN:ND2	2.25	0.67
1:A:46:LEU:HA	1:A:55:TYR:O	1.95	0.67
1:C:65:LEU:HD21	1:C:73:LEU:CD2	2.23	0.66
1:C:108:PHE:HB2	1:C:123:THR:HB	1.77	0.66
1:F:124:HIS:O	1:F:130:ILE:HD11	1.94	0.66
1:H:105:LYS:O	1:H:106:HIS:HB2	1.94	0.66
2:M:1:GU4:O11	2:M:2:YYJ:O1S3	2.13	0.66
1:B:49:GLU:OE1	1:B:53:GLU:HB3	1.95	0.66
1:C:128:LYS:HB2	1:C:128:LYS:NZ	2.08	0.66
1:D:87:GLU:O	1:D:88:ARG:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:HA	1:C:55:TYR:O	1.95	0.66
1:F:105:LYS:O	1:F:106:HIS:HB2	1.94	0.66
1:G:49:GLU:HG3	1:G:55:TYR:HE2	1.61	0.66
1:G:66:ALA:HB1	1:G:74:TYR:CE1	2.30	0.66
1:A:94:TYR:CD2	1:A:133:LEU:HB2	2.31	0.66
1:A:54:VAL:HG22	1:A:85:PHE:O	1.96	0.66
1:D:98:ILE:HD12	1:D:103:ALA:HA	1.78	0.66
1:C:12:LYS:HA	1:C:135:LEU:O	1.96	0.66
1:C:98:ILE:HD11	1:C:108:PHE:CE1	2.30	0.66
1:G:57:LYS:HG3	1:G:57:LYS:O	1.95	0.65
2:O:1:GU4:H62	2:O:1:GU4:S4	2.36	0.65
1:H:89:LEU:C	1:H:90:GLU:HG2	2.21	0.65
2:O:1:GU4:H3	2:O:2:YYJ:S3	2.36	0.65
1:B:24:ARG:HD3	1:B:26:LEU:CD1	2.20	0.65
1:B:79:PRO:O	1:B:80:ASN:HB3	1.95	0.65
1:B:86:LEU:HD21	1:B:100:LYS:HG3	1.79	0.65
1:B:24:ARG:HD2	1:B:32:ASP:OD1	1.96	0.65
1:C:64:PHE:CZ	1:C:79:PRO:HG3	2.31	0.65
1:F:12:LYS:HD3	1:F:135:LEU:O	1.96	0.65
1:G:102:HIS:HB3	1:G:105:LYS:CG	2.20	0.65
1:H:104:GLU:OE1	1:H:105:LYS:N	2.29	0.65
1:E:39:ASP:OD1	1:E:39:ASP:C	2.38	0.65
1:E:68:ASP:HB3	1:E:70:ASP:H	1.60	0.65
2:I:1:GU4:O29	2:I:1:GU4:O24	2.15	0.65
1:F:68:ASP:OD1	1:F:72:LEU:HB3	1.96	0.65
1:A:112:LYS:NZ	1:A:112:LYS:HB3	2.11	0.65
1:B:67:MET:HE1	1:B:107:TRP:HB3	1.79	0.65
1:E:80:ASN:ND2	1:E:83:CYS:SG	2.70	0.65
1:C:23:LEU:HD21	1:C:65:LEU:HD11	1.78	0.64
1:G:124:HIS:CD2	1:G:125:PHE:O	2.50	0.64
2:K:1:GU4:H62	2:K:2:YYJ:O1S6	1.97	0.64
1:E:94:TYR:C	1:E:95:ASN:HD22	2.05	0.64
1:H:24:ARG:NE	1:H:26:LEU:HD11	2.13	0.64
1:B:89:LEU:HD12	1:B:89:LEU:C	2.22	0.64
1:C:47:ALA:HB3	1:C:55:TYR:HB2	1.78	0.64
1:D:24:ARG:HD3	1:D:26:LEU:CD1	2.26	0.64
1:A:11:PRO:C	1:A:12:LYS:HD3	2.21	0.64
1:B:68:ASP:HB3	1:B:72:LEU:H	1.62	0.64
1:G:89:LEU:C	1:G:90:GLU:HG2	2.23	0.64
1:C:46:LEU:N	1:C:46:LEU:HD23	2.12	0.64
1:H:46:LEU:HD12	1:H:46:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ARG:HH21	1:F:135:LEU:HD13	1.63	0.64
1:D:64:PHE:HE1	1:D:78:THR:HA	1.62	0.64
1:F:28:ASP:OD1	1:F:28:ASP:C	2.41	0.64
1:G:65:LEU:O	1:G:66:ALA:CB	2.45	0.63
1:A:31:VAL:O	1:A:117:SER:HB3	1.97	0.63
1:C:55:TYR:CZ	1:C:84:LEU:CD2	2.82	0.63
1:G:64:PHE:CE2	1:G:79:PRO:N	2.66	0.63
1:H:24:ARG:HD3	1:H:26:LEU:HD13	1.79	0.63
1:C:103:ALA:C	1:C:105:LYS:H	2.06	0.63
1:E:104:GLU:OE2	1:E:105:LYS:N	2.30	0.63
1:H:57:LYS:CG	1:H:58:SER:N	2.61	0.63
2:J:2:YYJ:O3S3	2:J:2:YYJ:O2	2.17	0.63
1:B:87:GLU:HG3	1:B:88:ARG:N	2.13	0.63
1:D:55:TYR:CE1	1:D:79:PRO:HB3	2.33	0.63
1:D:114:ASN:OD1	1:D:116:ARG:HB2	1.98	0.63
1:H:24:ARG:N	1:H:32:ASP:O	2.28	0.62
1:H:129:ALA:HB3	1:H:130:ILE:HD13	1.81	0.62
2:I:1:GU4:H61	2:I:2:YYJ:O6	1.97	0.62
1:B:89:LEU:HD11	1:B:93:HIS:HA	1.80	0.62
1:E:58:SER:N	1:E:63:GLN:O	2.32	0.62
1:B:19:GLY:O	1:B:35:LYS:HE2	2.00	0.62
1:B:79:PRO:O	1:B:80:ASN:CB	2.47	0.62
1:B:37:ARG:O	1:B:42:ILE:HD11	1.99	0.62
1:C:26:LEU:HD23	1:C:30:THR:HG21	1.80	0.62
1:E:112:LYS:CE	2:M:2:YYJ:O3S6	2.47	0.62
1:F:114:ASN:OD1	1:F:116:ARG:HB2	1.99	0.62
1:D:47:ALA:HB3	1:D:55:TYR:HB2	1.82	0.62
1:E:24:ARG:HD3	1:E:26:LEU:CD1	2.29	0.62
1:H:85:PHE:HA	1:H:98:ILE:O	2.00	0.62
1:H:24:ARG:HD3	1:H:26:LEU:CD1	2.30	0.62
1:B:112:LYS:HA	2:J:1:GU4:O25	1.98	0.62
1:D:118:LYS:NZ	2:L:1:GU4:O24	2.31	0.62
1:A:84:LEU:CB	1:A:100:LYS:HE2	2.29	0.62
1:H:108:PHE:HB2	1:H:123:THR:CB	2.30	0.61
1:A:84:LEU:HB2	1:A:100:LYS:CD	2.29	0.61
1:G:110:GLY:O	1:G:111:LEU:HD23	2.01	0.61
1:C:68:ASP:OD1	1:C:72:LEU:HB3	2.00	0.61
1:C:118:LYS:HE2	2:K:2:YYJ:O2S3	2.00	0.61
1:D:98:ILE:HD11	1:D:106:HIS:C	2.24	0.61
1:E:89:LEU:HG	1:E:90:GLU:N	2.15	0.61
1:E:125:PHE:CD1	1:E:126:GLY:N	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:PHE:HB2	1:H:123:THR:HB	1.83	0.61
1:H:112:LYS:HE2	2:P:1:GU4:H61	1.82	0.61
1:D:16:CYS:HB2	1:D:132:PHE:CE1	2.35	0.61
1:A:84:LEU:HB2	1:A:100:LYS:HE2	1.81	0.61
1:B:86:LEU:HD21	1:B:100:LYS:HG2	1.81	0.61
1:D:92:ASN:CG	1:D:92:ASN:O	2.39	0.61
1:A:131:LEU:HD13	1:A:131:LEU:N	2.16	0.61
1:C:102:HIS:O	1:C:105:LYS:HB2	2.00	0.61
1:D:112:LYS:CE	2:L:2:YYJ:O2S3	2.48	0.61
1:E:28:ASP:OD1	1:E:28:ASP:N	2.34	0.61
1:E:86:LEU:HD21	1:E:100:LYS:HD2	1.83	0.61
1:H:54:VAL:HG12	1:H:55:TYR:H	1.64	0.61
1:C:13:LEU:HD21	1:C:37:ARG:HG3	1.83	0.60
1:C:131:LEU:HD23	1:C:131:LEU:C	2.25	0.60
1:D:78:THR:HG23	1:D:79:PRO:HD2	1.81	0.60
1:E:86:LEU:HD21	1:E:100:LYS:CE	2.30	0.60
1:F:112:LYS:HE2	2:N:2:YYJ:O2S3	2.00	0.60
1:H:53:GLU:HG2	1:H:84:LEU:CD2	2.26	0.60
1:A:112:LYS:HB3	1:A:112:LYS:HZ2	1.65	0.60
1:C:104:GLU:CD	1:C:104:GLU:N	2.58	0.60
1:C:131:LEU:HD22	1:C:131:LEU:N	2.10	0.60
1:D:112:LYS:HA	2:L:1:GU4:O25	2.02	0.60
1:E:39:ASP:O	1:E:42:ILE:HG12	2.01	0.60
1:A:24:ARG:CD	1:A:26:LEU:CD1	2.79	0.60
1:E:112:LYS:NZ	2:M:2:YYJ:O3S6	2.33	0.60
1:D:64:PHE:CZ	1:D:79:PRO:HG3	2.36	0.60
1:D:58:SER:O	1:D:59:THR:C	2.42	0.60
1:A:114:ASN:ND2	1:A:116:ARG:HH12	1.96	0.60
1:B:80:ASN:O	1:B:83:CYS:N	2.33	0.60
2:K:1:GU4:S2	2:K:2:YYJ:O1S1	2.60	0.60
1:G:122:ARG:HD2	2:O:2:YYJ:O1S3	2.01	0.60
1:C:124:HIS:C	1:C:124:HIS:HD1	2.10	0.60
1:F:112:LYS:HG3	1:F:118:LYS:HG3	1.83	0.60
1:E:87:GLU:CG	1:E:88:ARG:N	2.64	0.59
1:A:99:SER:OG	1:A:102:HIS:HD2	1.84	0.59
1:C:60:GLU:N	1:C:60:GLU:CD	2.59	0.59
1:C:107:TRP:CZ2	1:C:121:PRO:HG3	2.37	0.59
1:D:123:THR:HA	1:D:127:GLN:OE1	2.03	0.59
1:G:89:LEU:O	1:G:90:GLU:HG2	2.03	0.59
1:G:104:GLU:HB2	1:G:105:LYS:HE2	1.83	0.59
1:A:99:SER:OG	1:A:102:HIS:CD2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:TYR:CE2	1:C:84:LEU:HD11	2.37	0.59
1:C:111:LEU:HD23	1:C:117:SER:HA	1.83	0.59
1:F:49:GLU:HB2	1:F:84:LEU:HD21	1.84	0.59
1:D:53:GLU:OE1	1:D:100:LYS:HD2	2.01	0.59
1:F:125:PHE:HA	1:F:130:ILE:CD1	2.33	0.59
1:B:22:PHE:O	1:B:23:LEU:C	2.42	0.59
1:G:55:TYR:O	1:G:56:ILE:HG12	2.03	0.59
1:G:66:ALA:HB1	1:G:74:TYR:CZ	2.37	0.59
1:C:64:PHE:CE2	1:C:79:PRO:HD3	2.38	0.59
1:G:47:ALA:O	1:G:54:VAL:HG12	2.02	0.59
1:C:26:LEU:HD23	1:C:30:THR:CG2	2.33	0.58
1:B:80:ASN:C	1:B:82:GLU:N	2.59	0.58
1:E:26:LEU:N	1:E:26:LEU:HD22	2.18	0.58
1:F:49:GLU:CG	1:F:84:LEU:HD21	2.31	0.58
1:G:18:ASN:ND2	1:G:111:LEU:O	2.36	0.58
1:B:48:ALA:HA	1:B:53:GLU:O	2.03	0.58
1:D:102:HIS:O	1:D:106:HIS:N	2.36	0.58
1:H:130:ILE:HG22	1:H:131:LEU:HD13	1.85	0.58
2:J:2:YYJ:O3S3	2:J:2:YYJ:C2	2.51	0.58
1:A:108:PHE:O	1:A:123:THR:HG21	2.03	0.58
1:H:55:TYR:CZ	1:H:84:LEU:CD1	2.87	0.58
1:A:46:LEU:HD23	1:A:56:ILE:CG1	2.31	0.57
1:E:27:PRO:C	1:E:29:GLY:N	2.60	0.57
2:P:2:YYJ:O3S3	2:P:2:YYJ:O1	2.22	0.57
1:C:45:GLN:C	1:C:46:LEU:HD23	2.30	0.57
1:D:112:LYS:NZ	2:L:2:YYJ:O2S3	2.36	0.57
1:D:123:THR:HB	1:D:130:ILE:HD11	1.85	0.57
1:E:87:GLU:HG3	1:E:88:ARG:H	1.69	0.57
1:F:98:ILE:HD11	1:F:106:HIS:HA	1.85	0.57
2:M:1:GU4:S2	2:M:2:YYJ:C1	2.92	0.57
1:A:112:LYS:HG3	1:A:116:ARG:O	2.04	0.57
1:B:89:LEU:HD12	1:B:90:GLU:O	2.03	0.57
1:D:24:ARG:HG2	1:D:25:ILE:N	2.18	0.57
2:M:1:GU4:H61	2:M:1:GU4:S4	2.45	0.57
1:A:24:ARG:HD2	1:A:32:ASP:OD1	2.04	0.57
2:L:2:YYJ:O3S3	2:L:2:YYJ:O1	2.22	0.57
1:B:80:ASN:H	1:B:83:CYS:HB2	1.69	0.57
1:A:12:LYS:HG3	1:A:135:LEU:O	2.04	0.57
1:F:45:GLN:N	1:F:57:LYS:O	2.35	0.56
1:G:48:ALA:HA	1:G:54:VAL:CG1	2.35	0.56
1:G:112:LYS:HE3	2:O:1:GU4:O26	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:ILE:HD11	1:H:108:PHE:CZ	2.40	0.56
1:G:105:LYS:O	1:G:106:HIS:CB	2.52	0.56
1:H:124:HIS:O	1:H:125:PHE:O	2.23	0.56
1:D:39:ASP:OD1	1:D:41:HIS:N	2.36	0.56
1:D:48:ALA:CA	1:D:54:VAL:HG12	2.31	0.56
1:D:111:LEU:HD23	1:D:117:SER:HA	1.88	0.56
1:D:122:ARG:HD2	2:L:2:YYJ:O1	2.06	0.56
1:E:104:GLU:H	1:E:104:GLU:CD	2.13	0.56
1:H:80:ASN:HD22	1:H:80:ASN:C	2.13	0.56
1:E:64:PHE:CZ	1:E:79:PRO:HG3	2.40	0.56
1:G:89:LEU:CD2	1:G:90:GLU:H	2.17	0.56
1:H:37:ARG:C	1:H:42:ILE:HD11	2.30	0.56
1:A:61:THR:OG1	1:A:63:GLN:HG2	2.04	0.56
1:H:37:ARG:O	1:H:42:ILE:HD11	2.05	0.56
2:O:1:GU4:C5	2:O:2:YYJ:O5	2.53	0.56
1:B:26:LEU:HD12	1:B:27:PRO:HD2	1.88	0.56
1:C:12:LYS:CA	1:C:135:LEU:O	2.53	0.56
2:I:2:YYJ:O3S3	2:I:2:YYJ:S1	2.63	0.56
1:D:124:HIS:O	1:D:127:GLN:HG3	2.04	0.56
1:H:54:VAL:HG12	1:H:55:TYR:N	2.21	0.56
1:H:55:TYR:CZ	1:H:84:LEU:HD12	2.41	0.56
1:B:87:GLU:CG	1:B:88:ARG:N	2.68	0.56
1:E:16:CYS:SG	1:E:18:ASN:HB2	2.46	0.56
1:H:112:LYS:HE3	2:P:2:YYJ:O2S3	2.06	0.56
1:C:103:ALA:C	1:C:105:LYS:N	2.57	0.56
1:D:124:HIS:ND1	1:D:124:HIS:C	2.64	0.56
1:F:37:ARG:NH2	1:F:135:LEU:HD13	2.20	0.56
1:A:108:PHE:HB2	1:A:130:ILE:HD12	1.88	0.56
2:L:1:GU4:O3	2:L:1:GU4:S4	2.63	0.56
1:C:12:LYS:CB	1:C:135:LEU:O	2.54	0.55
1:C:104:GLU:OE2	1:C:104:GLU:N	2.38	0.55
2:I:1:GU4:C5	2:I:2:YYJ:C6	2.83	0.55
1:E:52:GLY:O	1:E:86:LEU:HA	2.06	0.55
1:E:112:LYS:HB2	1:E:114:ASN:OD1	2.06	0.55
1:C:16:CYS:HB2	1:C:132:PHE:CD2	2.42	0.55
1:C:125:PHE:HA	1:C:130:ILE:HD12	1.87	0.55
1:G:102:HIS:HA	1:G:105:LYS:HE3	1.88	0.55
1:B:44:LEU:HG	1:B:56:ILE:HG22	1.88	0.55
1:D:92:ASN:C	1:D:93:HIS:CD2	2.85	0.55
1:H:85:PHE:CD2	1:H:109:VAL:HG21	2.42	0.55
1:H:85:PHE:CE2	1:H:109:VAL:CG2	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:HIS:C	1:H:125:PHE:O	2.48	0.55
1:C:19:GLY:HA3	1:C:21:TYR:CD2	2.41	0.55
1:C:131:LEU:C	1:C:131:LEU:CD2	2.79	0.55
1:D:45:GLN:C	1:D:46:LEU:HD23	2.32	0.55
1:G:112:LYS:NZ	2:O:2:YYJ:C4	2.69	0.55
2:I:1:GU4:O22	2:I:2:YYJ:O1S6	2.24	0.55
2:O:2:YYJ:O2S4	2:O:2:YYJ:C1	2.55	0.55
1:C:19:GLY:HA3	1:C:21:TYR:CE2	2.41	0.55
1:D:48:ALA:HA	1:D:54:VAL:CG1	2.33	0.55
1:H:13:LEU:N	1:H:13:LEU:HD13	2.21	0.55
1:B:96:THR:HG23	1:B:108:PHE:HE2	1.72	0.55
1:D:80:ASN:HB2	1:D:83:CYS:SG	2.47	0.55
2:I:2:YYJ:O3S3	2:I:2:YYJ:O1S1	2.25	0.55
2:O:1:GU4:O6	2:O:2:YYJ:C6	2.55	0.55
1:G:52:GLY:O	1:G:86:LEU:HA	2.06	0.55
1:G:102:HIS:O	1:G:105:LYS:HG2	2.06	0.55
1:A:26:LEU:CD1	1:A:26:LEU:H	2.20	0.55
1:C:48:ALA:O	1:C:50:SER:N	2.40	0.55
1:E:27:PRO:C	1:E:29:GLY:H	2.13	0.55
1:E:123:THR:HB	1:E:130:ILE:HD11	1.89	0.55
1:H:89:LEU:CD1	1:H:93:HIS:HA	2.37	0.55
1:H:89:LEU:HD12	1:H:93:HIS:HA	1.89	0.55
2:M:1:GU4:H61	2:M:1:GU4:O24	2.06	0.55
1:A:89:LEU:O	1:A:90:GLU:OE1	2.25	0.54
1:H:71:GLY:HA3	1:H:121:PRO:CD	2.37	0.54
1:A:105:LYS:O	1:A:106:HIS:CB	2.51	0.54
1:A:124:HIS:O	1:A:127:GLN:HG3	2.08	0.54
1:E:122:ARG:HD2	2:M:2:YYJ:O2S3	2.06	0.54
1:H:29:GLY:O	1:H:30:THR:C	2.50	0.54
1:H:112:LYS:CE	2:P:1:GU4:C6	2.82	0.54
2:O:1:GU4:O23	2:O:2:YYJ:C6	2.56	0.54
1:D:37:ARG:O	1:D:37:ARG:CG	2.54	0.54
1:E:12:LYS:HA	1:E:135:LEU:O	2.08	0.54
1:B:15:TYR:HB2	1:B:22:PHE:HE1	1.72	0.54
1:E:24:ARG:HD2	1:E:32:ASP:OD1	2.08	0.54
1:G:112:LYS:CE	2:O:2:YYJ:C6	2.83	0.54
1:H:25:ILE:O	1:H:25:ILE:HG22	2.07	0.54
1:A:123:THR:HB	1:A:130:ILE:HD11	1.90	0.54
1:E:55:TYR:CZ	1:E:84:LEU:HD22	2.43	0.54
1:C:78:THR:HG22	1:C:78:THR:O	2.08	0.53
1:F:49:GLU:CB	1:F:84:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:THR:HG22	1:G:60:GLU:N	2.22	0.53
2:O:1:GU4:H5	2:O:2:YYJ:O5	2.08	0.53
1:D:24:ARG:HH21	1:D:34:THR:HB	1.72	0.53
1:E:55:TYR:CE1	1:E:84:LEU:HD13	2.44	0.53
1:G:122:ARG:C	1:G:123:THR:O	2.47	0.53
1:E:49:GLU:N	1:E:53:GLU:O	2.41	0.53
1:C:89:LEU:HD13	1:C:89:LEU:C	2.32	0.53
2:O:1:GU4:S6	2:O:2:YYJ:C6	2.96	0.53
1:A:86:LEU:HD21	1:A:100:LYS:HB2	1.89	0.53
1:A:102:HIS:CA	1:A:104:GLU:OE1	2.54	0.53
1:F:18:ASN:HD22	1:F:129:ALA:HA	1.73	0.53
1:G:36:ASP:O	1:G:38:SER:N	2.42	0.53
1:G:68:ASP:OD1	1:G:72:LEU:HB3	2.08	0.53
1:A:89:LEU:HD21	1:A:93:HIS:HA	1.90	0.53
1:G:61:THR:OG1	1:G:63:GLN:HG3	2.09	0.53
1:H:123:THR:HB	1:H:130:ILE:HD11	1.91	0.53
1:E:43:GLN:HE22	1:E:60:GLU:CG	2.22	0.52
1:A:49:GLU:HG3	1:A:55:TYR:CE2	2.44	0.52
1:A:131:LEU:N	1:A:131:LEU:CD1	2.72	0.52
1:G:66:ALA:CB	1:G:74:TYR:CE1	2.92	0.52
1:B:68:ASP:HB2	1:B:72:LEU:HB3	1.90	0.52
1:A:14:LEU:HD22	1:A:44:LEU:HD23	1.91	0.52
1:B:87:GLU:HG3	1:B:88:ARG:H	1.73	0.52
1:D:105:LYS:O	1:D:106:HIS:HB2	2.09	0.52
1:F:114:ASN:OD1	1:F:116:ARG:CB	2.58	0.52
1:G:53:GLU:HB3	1:G:86:LEU:HD23	1.91	0.52
1:H:68:ASP:HB2	1:H:72:LEU:H	1.73	0.52
1:H:71:GLY:HA3	1:H:121:PRO:HD2	1.90	0.52
1:G:57:LYS:HD2	1:G:58:SER:C	2.34	0.52
1:H:24:ARG:CD	1:H:26:LEU:CD1	2.87	0.52
2:I:1:GU4:O22	2:I:2:YYJ:O2S6	2.28	0.52
2:L:1:GU4:H5	2:L:2:YYJ:O3	2.09	0.52
1:A:78:THR:HG23	1:A:79:PRO:O	2.09	0.52
1:B:15:TYR:HB2	1:B:22:PHE:CE1	2.44	0.52
1:H:85:PHE:CD2	1:H:109:VAL:CG2	2.93	0.52
1:C:31:VAL:HG11	1:C:73:LEU:HD23	1.91	0.52
1:F:112:LYS:CE	2:N:2:YYJ:O2S3	2.57	0.52
1:G:80:ASN:ND2	1:G:83:CYS:SG	2.83	0.52
1:D:89:LEU:C	1:D:90:GLU:HG2	2.35	0.52
1:G:21:TYR:CE1	1:G:35:LYS:HD3	2.44	0.52
1:A:112:LYS:HB3	2:I:1:GU4:O25	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ARG:HD2	1:G:26:LEU:HD22	1.92	0.51
1:B:118:LYS:NZ	1:B:127:GLN:HE22	2.07	0.51
2:M:1:GU4:O24	2:M:1:GU4:C6	2.59	0.51
2:P:1:GU4:H62	2:P:2:YYJ:O3S6	2.09	0.51
1:C:131:LEU:O	1:C:131:LEU:CD2	2.58	0.51
1:G:131:LEU:HD13	1:G:131:LEU:N	2.24	0.51
1:H:55:TYR:CE1	1:H:84:LEU:HD12	2.46	0.51
1:F:56:ILE:O	1:F:56:ILE:HG22	2.10	0.51
2:L:1:GU4:H3	2:L:2:YYJ:O1S1	2.11	0.51
1:C:45:GLN:O	1:C:56:ILE:HA	2.10	0.51
1:H:44:LEU:HG	1:H:56:ILE:CG2	2.41	0.51
1:B:49:GLU:HG2	1:B:49:GLU:O	2.10	0.51
1:B:102:HIS:CB	1:B:105:LYS:HG3	2.38	0.51
1:C:124:HIS:C	1:C:124:HIS:ND1	2.67	0.51
1:D:15:TYR:HB2	1:D:135:LEU:HD11	1.91	0.51
1:H:95:ASN:HB2	1:H:132:PHE:O	2.11	0.51
1:H:104:GLU:CD	1:H:104:GLU:N	2.67	0.51
1:A:22:PHE:O	1:A:33:GLY:HA2	2.11	0.51
1:G:17:SER:HB3	1:G:94:TYR:CE2	2.46	0.51
1:H:12:LYS:HB2	1:H:135:LEU:O	2.11	0.51
1:H:84:LEU:O	1:H:100:LYS:HB3	2.10	0.51
1:A:39:ASP:OD1	1:A:42:ILE:HG23	2.11	0.51
1:C:71:GLY:O	1:C:120:GLY:N	2.41	0.51
1:F:28:ASP:OD1	1:F:30:THR:OG1	2.28	0.51
1:G:112:LYS:HE2	2:O:2:YYJ:C5	2.40	0.51
2:K:1:GU4:O2	2:K:2:YYJ:C1	2.59	0.51
1:A:80:ASN:HD22	1:A:80:ASN:C	2.20	0.51
1:B:119:LEU:O	1:B:120:GLY:C	2.52	0.51
1:C:84:LEU:O	1:C:100:LYS:HB2	2.10	0.51
2:M:1:GU4:O10	2:M:2:YYJ:C1	2.58	0.51
1:F:36:ASP:C	1:F:38:SER:N	2.66	0.50
1:G:57:LYS:O	1:G:57:LYS:CG	2.58	0.50
2:I:1:GU4:O23	2:I:2:YYJ:O1S6	2.29	0.50
1:D:39:ASP:HB3	1:D:42:ILE:HG23	1.92	0.50
1:E:71:GLY:HA3	1:E:120:GLY:HA3	1.92	0.50
1:F:92:ASN:O	1:F:93:HIS:CB	2.42	0.50
1:A:24:ARG:HB3	1:A:32:ASP:OD1	2.11	0.50
1:E:68:ASP:HB2	1:E:72:LEU:H	1.75	0.50
1:E:87:GLU:CG	1:E:88:ARG:H	2.24	0.50
1:G:37:ARG:O	1:G:37:ARG:HG2	2.11	0.50
1:H:39:ASP:HB3	1:H:42:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HG	1:C:56:ILE:HG22	1.94	0.50
1:E:68:ASP:HB3	1:E:70:ASP:N	2.25	0.50
1:H:105:LYS:O	1:H:106:HIS:CB	2.59	0.50
1:A:112:LYS:HE3	2:I:2:YYJ:O2S6	2.11	0.50
1:B:112:LYS:C	1:B:114:ASN:H	2.20	0.50
1:F:13:LEU:O	1:F:134:PRO:HA	2.11	0.50
1:C:24:ARG:HB3	1:C:32:ASP:O	2.12	0.50
1:C:25:ILE:HG23	1:C:31:VAL:HG22	1.93	0.50
1:G:57:LYS:HA	1:G:64:PHE:HA	1.93	0.50
1:H:49:GLU:HB2	1:H:53:GLU:O	2.12	0.50
1:A:90:GLU:HB2	1:A:94:TYR:O	2.12	0.50
1:E:80:ASN:C	1:E:80:ASN:HD22	2.19	0.50
1:G:39:ASP:O	1:G:42:ILE:CG1	2.57	0.50
2:I:1:GU4:H61	2:I:2:YYJ:O2S6	2.10	0.50
2:M:2:YYJ:O1S4	2:M:2:YYJ:C3	2.60	0.50
2:P:1:GU4:C5	2:P:2:YYJ:O1S6	2.60	0.50
1:B:64:PHE:O	1:B:65:LEU:C	2.55	0.50
1:C:28:ASP:C	1:C:28:ASP:OD1	2.52	0.50
1:E:24:ARG:HD3	1:E:26:LEU:HD13	1.93	0.50
1:B:99:SER:O	1:B:100:LYS:C	2.54	0.49
1:F:49:GLU:O	1:F:50:SER:CB	2.59	0.49
2:M:1:GU4:O24	2:M:1:GU4:C5	2.58	0.49
1:D:24:ARG:NH2	1:D:34:THR:HB	2.27	0.49
1:D:124:HIS:O	1:D:124:HIS:ND1	2.42	0.49
1:E:97:TYR:N	1:E:97:TYR:CD1	2.79	0.49
1:H:38:SER:O	1:H:39:ASP:C	2.52	0.49
1:H:53:GLU:CG	1:H:84:LEU:HD23	2.32	0.49
1:C:28:ASP:OD1	1:C:30:THR:HB	2.13	0.49
1:D:19:GLY:HA3	1:D:21:TYR:HE2	1.76	0.49
1:F:49:GLU:HB2	1:F:84:LEU:CD2	2.43	0.49
1:H:112:LYS:HE3	2:P:1:GU4:C6	2.41	0.49
1:A:89:LEU:C	1:A:90:GLU:OE1	2.56	0.49
1:H:24:ARG:CD	1:H:26:LEU:HD13	2.41	0.49
1:C:64:PHE:N	1:C:76:SER:O	2.38	0.49
1:E:48:ALA:HA	1:E:54:VAL:HG12	1.93	0.49
1:E:91:GLU:C	1:E:93:HIS:H	2.20	0.49
1:G:18:ASN:CG	1:G:18:ASN:O	2.54	0.49
1:A:84:LEU:CB	1:A:100:LYS:HE3	2.43	0.49
1:A:123:THR:CG2	1:A:130:ILE:HD11	2.43	0.49
1:D:64:PHE:CE1	1:D:78:THR:HA	2.46	0.49
1:F:24:ARG:HG3	1:F:34:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:GU4:S6	2:I:2:YYJ:O1S6	2.71	0.49
1:H:112:LYS:NZ	2:P:2:YYJ:O2S6	2.45	0.49
1:D:18:ASN:O	1:D:20:GLY:N	2.46	0.48
1:G:28:ASP:OD1	1:G:30:THR:HB	2.13	0.48
1:H:89:LEU:HD11	1:H:93:HIS:ND1	2.28	0.48
1:C:13:LEU:HD21	1:C:37:ARG:CG	2.43	0.48
1:C:89:LEU:HD13	1:C:90:GLU:H	1.72	0.48
1:H:112:LYS:HA	2:P:1:GU4:O25	2.13	0.48
1:G:81:GLU:CB	1:G:101:LYS:HE3	2.43	0.48
2:M:2:YYJ:O3	2:M:2:YYJ:O1S6	2.31	0.48
1:A:25:ILE:C	1:A:26:LEU:HD12	2.39	0.48
1:A:71:GLY:HA3	1:A:121:PRO:HD3	1.96	0.48
1:A:120:GLY:O	1:A:122:ARG:N	2.47	0.48
1:H:14:LEU:HD12	1:H:23:LEU:HD23	1.95	0.48
1:A:17:SER:O	1:A:18:ASN:C	2.55	0.48
1:H:24:ARG:CD	1:H:32:ASP:OD1	2.61	0.48
1:A:114:ASN:OD1	1:A:116:ARG:HB2	2.14	0.48
1:B:89:LEU:C	1:B:89:LEU:CD1	2.87	0.48
1:D:46:LEU:HD23	1:D:46:LEU:N	2.28	0.48
1:E:11:PRO:O	1:E:12:LYS:CD	2.61	0.48
1:F:22:PHE:O	1:F:33:GLY:HA2	2.14	0.48
1:G:48:ALA:HA	1:G:54:VAL:HG12	1.95	0.48
1:B:14:LEU:HD23	1:B:44:LEU:HD23	1.96	0.48
1:C:112:LYS:CB	2:K:1:GU4:O25	2.61	0.48
1:D:80:ASN:HB3	1:D:82:GLU:H	1.78	0.48
1:E:85:PHE:CE2	1:E:109:VAL:CG2	2.97	0.48
1:F:78:THR:C	1:F:79:PRO:O	2.53	0.48
2:L:1:GU4:O29	2:L:1:GU4:H2	2.13	0.48
1:C:23:LEU:HD21	1:C:65:LEU:CD1	2.43	0.47
1:F:124:HIS:O	1:F:124:HIS:CD2	2.67	0.47
1:G:124:HIS:CD2	1:G:125:PHE:N	2.82	0.47
1:C:89:LEU:C	1:C:90:GLU:HG2	2.40	0.47
1:G:64:PHE:CE2	1:G:79:PRO:CD	2.97	0.47
1:B:61:THR:CB	1:B:63:GLN:HE21	2.27	0.47
1:E:105:LYS:O	1:E:106:HIS:CB	2.57	0.47
1:E:53:GLU:CD	1:E:100:LYS:HE3	2.39	0.47
1:G:68:ASP:OD1	1:G:72:LEU:CB	2.62	0.47
1:G:120:GLY:O	1:G:123:THR:OG1	2.31	0.47
1:A:84:LEU:HB3	1:A:100:LYS:HE2	1.96	0.47
1:F:50:SER:O	1:F:51:ILE:C	2.57	0.47
1:H:80:ASN:C	1:H:82:GLU:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ARG:O	1:H:89:LEU:O	2.32	0.47
1:B:17:SER:OG	1:B:128:LYS:HD3	2.15	0.47
1:C:112:LYS:HG2	2:K:1:GU4:O25	2.14	0.47
1:G:48:ALA:HA	1:G:54:VAL:HG13	1.97	0.47
1:A:89:LEU:CD2	1:A:90:GLU:N	2.69	0.47
1:D:122:ARG:CD	2:L:2:YYJ:O1	2.63	0.47
1:F:130:ILE:HG21	1:F:130:ILE:HD13	1.39	0.47
1:G:108:PHE:HB2	1:G:123:THR:HB	1.97	0.47
1:G:122:ARG:CD	2:O:2:YYJ:O1S3	2.62	0.47
1:B:80:ASN:C	1:B:82:GLU:H	2.22	0.47
1:D:112:LYS:HE2	2:L:2:YYJ:O2S3	2.13	0.47
1:E:44:LEU:HG	1:E:56:ILE:CG2	2.45	0.47
1:F:112:LYS:CE	2:N:2:YYJ:S3	2.91	0.47
1:A:96:THR:HG23	1:A:130:ILE:HG23	1.96	0.47
1:C:31:VAL:HG11	1:C:73:LEU:CD2	2.45	0.47
1:D:58:SER:O	1:D:62:GLY:N	2.45	0.47
1:E:16:CYS:HB2	1:E:132:PHE:CE2	2.50	0.47
1:F:24:ARG:O	1:F:31:VAL:HA	2.14	0.47
1:F:64:PHE:CE2	1:F:79:PRO:HB3	2.50	0.47
2:J:1:GU4:O2	2:J:2:YYJ:O1S1	2.33	0.47
1:A:84:LEU:N	1:A:84:LEU:HD22	2.30	0.46
1:D:18:ASN:O	1:D:19:GLY:C	2.57	0.46
1:B:71:GLY:HA3	1:B:121:PRO:HD3	1.96	0.46
1:B:98:ILE:O	1:B:99:SER:C	2.56	0.46
1:H:80:ASN:O	1:H:81:GLU:C	2.57	0.46
1:H:102:HIS:HB2	1:H:107:TRP:HB2	1.96	0.46
2:M:1:GU4:O24	2:M:1:GU4:H5	2.16	0.46
1:B:71:GLY:C	1:B:120:GLY:H	2.23	0.46
1:B:104:GLU:H	1:B:104:GLU:HG3	1.36	0.46
1:D:98:ILE:CD1	1:D:103:ALA:HA	2.43	0.46
1:E:80:ASN:ND2	1:E:82:GLU:HB2	2.30	0.46
1:G:24:ARG:CD	1:G:26:LEU:HD22	2.45	0.46
1:G:38:SER:O	1:G:39:ASP:C	2.56	0.46
1:H:112:LYS:HE2	1:H:112:LYS:HB3	1.61	0.46
1:B:112:LYS:C	1:B:114:ASN:N	2.74	0.46
1:E:48:ALA:HA	1:E:53:GLU:O	2.15	0.46
1:F:124:HIS:CD2	1:F:127:GLN:HG3	2.51	0.46
1:H:55:TYR:HE1	1:H:83:CYS:HB2	1.80	0.46
1:C:17:SER:HB2	1:C:131:LEU:CD2	2.46	0.46
1:C:122:ARG:HD3	1:C:122:ARG:HH11	1.56	0.46
1:E:85:PHE:HB3	1:E:97:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:PRO:O	1:H:80:ASN:CB	2.58	0.46
1:E:12:LYS:HA	1:E:12:LYS:HD2	1.73	0.46
1:E:125:PHE:CG	1:E:126:GLY:N	2.84	0.46
1:F:105:LYS:O	1:F:106:HIS:CB	2.60	0.46
1:G:116:ARG:NH1	2:O:2:YYJ:O2S6	2.49	0.46
1:A:78:THR:C	1:A:79:PRO:O	2.58	0.46
1:A:123:THR:CB	1:A:130:ILE:HD11	2.46	0.46
1:B:56:ILE:HB	1:B:65:LEU:HB2	1.97	0.46
1:B:61:THR:OG1	1:B:63:GLN:NE2	2.48	0.46
1:D:112:LYS:CG	2:L:2:YYJ:O2S3	2.61	0.46
1:B:17:SER:O	1:B:128:LYS:HD2	2.16	0.46
1:D:127:GLN:C	1:D:129:ALA:N	2.71	0.46
1:E:11:PRO:O	1:E:12:LYS:HD3	2.16	0.46
1:F:118:LYS:NZ	2:N:2:YYJ:O1S1	2.49	0.46
1:B:96:THR:HG23	1:B:108:PHE:CE2	2.51	0.46
1:C:112:LYS:HA	2:K:1:GU4:O25	2.16	0.46
1:E:43:GLN:O	1:E:59:THR:HB	2.15	0.46
1:B:19:GLY:C	1:B:35:LYS:HE2	2.40	0.45
1:B:98:ILE:HG13	1:B:108:PHE:CE2	2.51	0.45
1:C:128:LYS:HB2	1:C:128:LYS:HZ3	1.80	0.45
1:D:78:THR:HG23	1:D:79:PRO:CD	2.46	0.45
1:E:86:LEU:HD21	1:E:100:LYS:HD3	1.94	0.45
1:F:14:LEU:HB3	1:F:132:PHE:HD2	1.81	0.45
1:D:36:ASP:O	1:D:38:SER:N	2.49	0.45
1:F:94:TYR:CE1	1:F:133:LEU:HB2	2.51	0.45
1:F:124:HIS:O	1:F:124:HIS:HD2	1.98	0.45
1:G:26:LEU:HD23	1:G:30:THR:HG21	1.90	0.45
1:H:86:LEU:N	1:H:98:ILE:O	2.50	0.45
1:A:128:LYS:HA	1:A:131:LEU:HD22	1.97	0.45
1:F:112:LYS:HE3	2:N:2:YYJ:O1S4	2.16	0.45
1:G:67:MET:C	1:G:68:ASP:O	2.56	0.45
1:H:118:LYS:HE2	1:H:122:ARG:O	2.17	0.45
1:A:84:LEU:O	1:A:100:LYS:HB3	2.16	0.45
1:D:24:ARG:NH1	1:D:26:LEU:HD21	2.32	0.45
1:D:112:LYS:CE	2:L:2:YYJ:S3	3.00	0.45
1:D:127:GLN:C	1:D:129:ALA:H	2.25	0.45
1:H:27:PRO:CB	1:H:61:THR:HG21	2.22	0.45
1:F:81:GLU:C	1:F:83:CYS:H	2.24	0.45
1:G:53:GLU:HA	1:G:85:PHE:O	2.17	0.45
1:G:124:HIS:NE2	1:G:125:PHE:O	2.50	0.45
1:B:40:GLN:O	1:B:60:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:HIS:C	1:D:124:HIS:HD1	2.19	0.45
1:F:110:GLY:O	1:F:118:LYS:N	2.47	0.45
1:G:89:LEU:CD2	1:G:90:GLU:N	2.77	0.45
1:H:73:LEU:O	1:H:74:TYR:HB3	2.16	0.45
1:H:82:GLU:HG3	1:H:101:LYS:CD	2.47	0.45
1:A:98:ILE:HG22	1:A:99:SER:O	2.17	0.45
1:A:123:THR:HG22	1:A:130:ILE:HD11	1.99	0.45
1:B:24:ARG:HH11	1:B:32:ASP:CG	2.24	0.45
1:E:66:ALA:HB2	1:E:83:CYS:SG	2.57	0.45
1:F:17:SER:O	1:F:18:ASN:O	2.34	0.45
1:G:59:THR:CG2	1:G:60:GLU:N	2.80	0.45
1:G:105:LYS:HG2	1:G:105:LYS:H	1.42	0.45
1:H:80:ASN:ND2	1:H:82:GLU:CB	2.80	0.45
1:A:26:LEU:HD11	1:A:32:ASP:OD1	2.16	0.45
1:B:68:ASP:CB	1:B:72:LEU:CB	2.95	0.45
1:B:89:LEU:CD1	1:B:90:GLU:N	2.75	0.45
1:C:104:GLU:HG2	1:C:105:LYS:CD	2.47	0.45
1:D:68:ASP:OD1	1:D:68:ASP:C	2.57	0.45
2:I:2:YYJ:O1S3	2:I:2:YYJ:O1S4	2.35	0.45
2:M:2:YYJ:O2S3	2:M:2:YYJ:O1S6	2.35	0.45
1:A:37:ARG:O	1:A:37:ARG:HG2	2.17	0.45
1:D:122:ARG:NH2	2:L:2:YYJ:O2S4	2.50	0.45
1:F:118:LYS:HD2	2:N:1:GU4:O25	2.17	0.45
1:G:123:THR:O	1:G:124:HIS:HB3	2.16	0.45
1:H:12:LYS:HD2	1:H:46:LEU:CD1	2.47	0.45
1:H:26:LEU:HD12	1:H:26:LEU:HA	1.72	0.45
1:H:40:GLN:O	1:H:60:GLU:HG3	2.16	0.45
1:H:67:MET:HE1	1:H:120:GLY:CA	2.46	0.45
1:B:68:ASP:OD2	1:B:72:LEU:HB2	2.17	0.44
1:G:26:LEU:O	1:G:28:ASP:N	2.50	0.44
1:A:66:ALA:HB3	1:A:74:TYR:CZ	2.52	0.44
1:G:124:HIS:O	1:G:130:ILE:HD13	2.17	0.44
1:A:37:ARG:O	1:A:42:ILE:HD11	2.18	0.44
1:H:127:GLN:O	1:H:130:ILE:HB	2.17	0.44
1:C:44:LEU:HG	1:C:56:ILE:CG2	2.48	0.44
1:E:119:LEU:O	1:E:120:GLY:C	2.61	0.44
1:F:63:GLN:HE21	1:F:63:GLN:HB2	1.46	0.44
1:H:104:GLU:CD	1:H:104:GLU:H	2.23	0.44
2:P:1:GU4:O2	2:P:2:YYJ:C1	2.65	0.44
1:E:26:LEU:CB	1:E:28:ASP:OD1	2.62	0.44
1:G:102:HIS:CB	1:G:105:LYS:HG3	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:ILE:N	1:E:130:ILE:HD13	2.32	0.44
1:C:135:LEU:HD23	1:C:135:LEU:N	2.31	0.44
1:G:18:ASN:HB2	1:G:128:LYS:C	2.43	0.44
1:H:85:PHE:CA	1:H:98:ILE:O	2.66	0.44
1:H:99:SER:OG	1:H:102:HIS:CD2	2.71	0.44
1:A:84:LEU:HB3	1:A:100:LYS:CE	2.48	0.44
1:B:67:MET:HG2	1:B:73:LEU:CD1	2.47	0.44
1:C:112:LYS:HE3	2:K:1:GU4:O22	2.17	0.44
1:D:130:ILE:HG22	1:D:131:LEU:CD1	2.44	0.44
1:H:12:LYS:HD2	1:H:46:LEU:HD13	1.99	0.44
1:A:98:ILE:HG22	1:A:99:SER:N	2.33	0.43
1:C:28:ASP:OD1	1:C:30:THR:CB	2.65	0.43
1:E:91:GLU:C	1:E:93:HIS:N	2.76	0.43
1:E:100:LYS:O	1:E:101:LYS:C	2.60	0.43
1:F:112:LYS:HG2	2:N:2:YYJ:O2S3	2.18	0.43
1:G:112:LYS:NZ	2:O:2:YYJ:O4	2.51	0.43
1:H:112:LYS:CB	2:P:1:GU4:O25	2.66	0.43
1:B:71:GLY:O	1:B:120:GLY:N	2.46	0.43
1:E:67:MET:HE2	1:E:73:LEU:CD1	2.48	0.43
1:F:88:ARG:C	1:F:89:LEU:O	2.60	0.43
1:F:95:ASN:O	1:F:131:LEU:HD12	2.17	0.43
1:H:21:TYR:HE2	1:H:113:LYS:O	2.01	0.43
1:C:48:ALA:O	1:C:49:GLU:C	2.60	0.43
1:F:120:GLY:C	1:F:122:ARG:H	2.26	0.43
1:G:10:LYS:HA	1:G:11:PRO:HD3	1.77	0.43
1:H:68:ASP:HB3	1:H:70:ASP:H	1.81	0.43
1:E:104:GLU:CD	1:E:104:GLU:N	2.74	0.43
1:G:124:HIS:CD2	1:G:127:GLN:HG3	2.53	0.43
1:H:58:SER:HB3	1:H:62:GLY:H	1.83	0.43
1:A:26:LEU:H	1:A:26:LEU:HD13	1.82	0.43
1:A:118:LYS:HE3	2:I:1:GU4:O24	2.19	0.43
1:B:67:MET:C	1:B:68:ASP:O	2.61	0.43
1:C:64:PHE:HE2	1:C:79:PRO:HD3	1.81	0.43
1:C:104:GLU:HG2	1:C:105:LYS:HD2	1.99	0.43
1:F:26:LEU:HB3	1:F:27:PRO:HD2	2.00	0.43
2:I:2:YYJ:O1S4	2:I:2:YYJ:C3	2.66	0.43
1:B:24:ARG:NH1	1:B:32:ASP:OD2	2.52	0.43
1:F:77:GLN:H	1:F:77:GLN:HG2	1.59	0.43
1:G:36:ASP:C	1:G:38:SER:H	2.26	0.43
1:G:61:THR:HG1	1:G:63:GLN:HE21	1.61	0.43
1:G:112:LYS:CE	2:O:1:GU4:O26	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ASN:ND2	1:H:82:GLU:HB2	2.33	0.43
2:K:1:GU4:O10	2:K:2:YYJ:C1	2.67	0.43
2:M:1:GU4:O2	2:M:2:YYJ:C1	2.67	0.43
1:A:112:LYS:CD	1:A:116:ARG:HB3	2.49	0.43
1:C:16:CYS:C	1:C:18:ASN:N	2.74	0.43
1:C:39:ASP:O	1:C:42:ILE:HG12	2.19	0.43
1:C:86:LEU:HD21	1:C:100:LYS:HG3	2.01	0.43
1:C:130:ILE:HD12	1:C:130:ILE:HG21	1.76	0.43
1:E:100:LYS:O	1:E:103:ALA:N	2.52	0.43
1:C:47:ALA:O	1:C:54:VAL:HA	2.18	0.43
1:C:120:GLY:N	1:C:121:PRO:HD2	2.33	0.43
1:D:15:TYR:CB	1:D:135:LEU:HD11	2.49	0.43
1:D:94:TYR:HB3	1:D:132:PHE:O	2.19	0.43
1:F:120:GLY:C	1:F:122:ARG:N	2.77	0.43
1:H:95:ASN:HD22	1:H:95:ASN:HA	1.41	0.43
2:J:2:YYJ:O2	2:J:2:YYJ:S3	2.77	0.43
1:F:96:THR:OG1	1:F:130:ILE:CG2	2.66	0.43
1:G:84:LEU:HB3	1:G:100:LYS:HD3	2.01	0.43
1:H:31:VAL:HG23	1:H:74:TYR:HA	2.01	0.43
1:H:108:PHE:HB2	1:H:123:THR:OG1	2.18	0.43
1:H:124:HIS:ND1	1:H:127:GLN:HG3	2.33	0.43
1:A:57:LYS:O	1:A:57:LYS:HG2	2.14	0.43
1:F:112:LYS:HZ2	1:F:112:LYS:HB3	1.84	0.43
1:H:24:ARG:HD3	1:H:32:ASP:OD1	2.18	0.43
1:H:24:ARG:HD2	1:H:32:ASP:OD1	2.19	0.43
1:H:55:TYR:CZ	1:H:84:LEU:HD11	2.53	0.43
1:H:112:LYS:NZ	2:P:2:YYJ:S6	2.85	0.43
1:D:89:LEU:HG	1:D:90:GLU:H	1.83	0.42
1:A:24:ARG:HD3	1:A:26:LEU:CD1	2.47	0.42
1:A:27:PRO:HA	1:A:63:GLN:HE22	1.84	0.42
1:A:101:LYS:HD3	1:A:102:HIS:CE1	2.54	0.42
1:B:92:ASN:ND2	1:B:94:TYR:HD2	2.17	0.42
1:H:24:ARG:CZ	1:H:26:LEU:HD11	2.48	0.42
1:H:130:ILE:CD1	1:H:130:ILE:N	2.82	0.42
1:E:122:ARG:HH11	1:E:122:ARG:HD3	1.52	0.42
1:F:49:GLU:HG2	1:F:55:TYR:CE2	2.54	0.42
1:G:21:TYR:CD1	1:G:35:LYS:HD3	2.54	0.42
1:G:80:ASN:OD1	1:G:82:GLU:HG3	2.19	0.42
2:I:1:GU4:O22	2:I:2:YYJ:S6	2.77	0.42
2:N:2:YYJ:O3S3	2:N:2:YYJ:S1	2.77	0.42
1:B:90:GLU:OE2	1:B:125:PHE:CZ	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HE2	1:B:112:LYS:HB3	1.60	0.42
1:C:92:ASN:O	1:C:93:HIS:HB2	2.18	0.42
1:D:96:THR:HG22	1:D:108:PHE:CD1	2.55	0.42
1:E:44:LEU:HD13	1:E:44:LEU:N	2.34	0.42
1:G:102:HIS:C	1:G:105:LYS:HG2	2.45	0.42
1:B:18:ASN:O	1:B:20:GLY:N	2.53	0.42
1:B:43:GLN:C	1:B:44:LEU:HD13	2.44	0.42
1:D:112:LYS:HE2	2:L:2:YYJ:O1S3	2.19	0.42
1:F:68:ASP:HB3	1:F:74:TYR:CD2	2.55	0.42
1:F:123:THR:O	1:F:124:HIS:HB3	2.20	0.42
1:H:36:ASP:O	1:H:39:ASP:HB2	2.20	0.42
1:C:19:GLY:CA	1:C:21:TYR:CD2	3.02	0.42
1:F:39:ASP:OD2	1:F:41:HIS:HB2	2.19	0.42
1:G:32:ASP:C	1:G:32:ASP:OD1	2.58	0.42
1:A:44:LEU:HG	1:A:56:ILE:CG2	2.48	0.42
1:B:108:PHE:HB3	1:B:109:VAL:H	1.68	0.42
1:E:10:LYS:C	1:E:11:PRO:O	2.63	0.42
1:H:71:GLY:HA3	1:H:121:PRO:HD3	2.02	0.42
1:C:98:ILE:HG22	1:C:99:SER:O	2.19	0.42
1:D:97:TYR:CD1	1:D:97:TYR:N	2.87	0.42
1:G:22:PHE:O	1:G:23:LEU:C	2.60	0.42
1:G:91:GLU:C	1:G:93:HIS:H	2.27	0.42
1:A:63:GLN:HG2	1:A:63:GLN:H	1.53	0.42
1:E:26:LEU:O	1:E:29:GLY:N	2.45	0.42
1:G:66:ALA:CB	1:G:74:TYR:CZ	3.02	0.42
1:G:84:LEU:HD13	1:G:84:LEU:HA	1.68	0.42
2:I:1:GU4:H3	2:I:2:YYJ:O3S3	2.19	0.42
1:A:12:LYS:HD2	1:A:136:PRO:HA	2.01	0.42
1:B:89:LEU:CD1	1:B:93:HIS:HA	2.47	0.42
1:C:112:LYS:C	1:C:114:ASN:N	2.77	0.42
1:D:130:ILE:HA	1:D:130:ILE:HD12	1.68	0.42
1:F:86:LEU:CD2	1:F:100:LYS:HD2	2.39	0.42
1:G:39:ASP:OD1	1:G:41:HIS:N	2.53	0.42
1:G:93:HIS:CD2	1:G:93:HIS:N	2.87	0.42
1:B:49:GLU:OE1	1:B:50:SER:N	2.52	0.41
1:G:102:HIS:HA	1:G:105:LYS:CE	2.48	0.41
1:H:21:TYR:CE2	1:H:113:LYS:O	2.73	0.41
1:H:67:MET:HE1	1:H:120:GLY:HA2	2.02	0.41
1:A:94:TYR:CE2	1:A:133:LEU:HB2	2.55	0.41
1:E:130:ILE:HA	1:E:130:ILE:HD12	1.78	0.41
1:G:122:ARG:HH11	1:G:122:ARG:HD3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2:YYJ:C4	2:M:2:YYJ:O1S6	2.68	0.41
1:C:10:LYS:N	1:C:11:PRO:HD3	2.35	0.41
1:E:67:MET:HB2	1:E:73:LEU:HD13	2.02	0.41
1:F:126:GLY:H	1:F:130:ILE:HD12	1.84	0.41
1:G:64:PHE:O	1:G:65:LEU:O	2.39	0.41
1:H:95:ASN:HB3	1:H:96:THR:H	1.59	0.41
1:H:120:GLY:N	1:H:121:PRO:HD2	2.36	0.41
1:E:40:GLN:HA	1:E:43:GLN:OE1	2.20	0.41
1:H:24:ARG:CD	1:H:26:LEU:HD11	2.49	0.41
1:H:66:ALA:O	1:H:73:LEU:HA	2.20	0.41
1:H:99:SER:OG	1:H:102:HIS:HD2	2.03	0.41
2:P:2:YYJ:O3	2:P:2:YYJ:O1S4	2.39	0.41
1:A:53:GLU:HG3	1:A:86:LEU:HD23	2.03	0.41
1:A:112:LYS:HG2	1:A:118:LYS:HG3	2.03	0.41
1:C:54:VAL:O	1:C:84:LEU:HA	2.19	0.41
1:E:31:VAL:HG11	1:E:65:LEU:HD21	2.03	0.41
1:B:61:THR:HB	1:B:63:GLN:HE21	1.84	0.41
1:C:85:PHE:HB3	1:C:97:TYR:HB3	2.03	0.41
1:G:114:ASN:ND2	2:O:2:YYJ:O2S6	2.53	0.41
1:B:56:ILE:HD13	1:B:65:LEU:HD12	2.02	0.41
1:C:77:GLN:H	1:C:77:GLN:HG2	1.23	0.41
1:D:72:LEU:HD23	1:D:73:LEU:O	2.21	0.41
1:D:80:ASN:HB3	1:D:81:GLU:H	1.71	0.41
1:E:100:LYS:O	1:E:102:HIS:N	2.53	0.41
1:F:73:LEU:HD21	1:F:109:VAL:HG13	2.02	0.41
1:G:43:GLN:O	1:G:59:THR:HB	2.21	0.41
1:A:46:LEU:HB3	1:A:56:ILE:CG1	2.40	0.41
1:B:19:GLY:O	1:B:35:LYS:CE	2.67	0.41
1:C:108:PHE:CE2	1:C:130:ILE:HD11	2.54	0.41
1:B:47:ALA:O	1:B:54:VAL:HA	2.21	0.41
1:D:98:ILE:HD13	1:D:98:ILE:HG23	1.82	0.41
1:E:67:MET:HB2	1:E:73:LEU:CD1	2.51	0.41
1:E:104:GLU:OE2	1:E:105:LYS:HD2	2.21	0.41
1:G:58:SER:O	1:G:62:GLY:HA2	2.20	0.41
1:G:112:LYS:C	1:G:114:ASN:H	2.27	0.41
1:H:44:LEU:HB3	1:H:45:GLN:H	1.75	0.41
1:B:135:LEU:HA	1:B:136:PRO:HD3	1.75	0.41
1:F:111:LEU:HD23	1:F:117:SER:CA	2.48	0.41
1:G:124:HIS:O	1:G:130:ILE:CD1	2.69	0.41
1:H:37:ARG:HA	1:H:42:ILE:HD11	2.02	0.41
1:A:84:LEU:N	1:A:84:LEU:CD2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:CG2	1:C:103:ALA:HA	2.51	0.40
1:F:16:CYS:HB2	1:F:132:PHE:CE2	2.56	0.40
1:G:108:PHE:C	1:G:123:THR:HG21	2.45	0.40
2:L:2:YYJ:O3S3	2:L:2:YYJ:S1	2.79	0.40
1:A:31:VAL:HG23	1:A:74:TYR:HA	2.03	0.40
1:B:49:GLU:OE1	1:B:53:GLU:CB	2.68	0.40
1:C:26:LEU:CD2	1:C:30:THR:CG2	2.97	0.40
1:D:66:ALA:O	1:D:73:LEU:HD12	2.21	0.40
1:F:47:ALA:O	1:F:55:TYR:CD2	2.66	0.40
1:G:72:LEU:HD12	1:G:119:LEU:HD21	2.03	0.40
1:H:24:ARG:HB2	1:H:42:ILE:CG2	2.51	0.40
1:A:89:LEU:CD2	1:A:90:GLU:O	2.69	0.40
1:B:18:ASN:HB3	1:B:19:GLY:H	1.54	0.40
1:B:26:LEU:N	1:B:30:THR:O	2.54	0.40
1:C:89:LEU:C	1:C:89:LEU:CD1	2.94	0.40
1:H:122:ARG:HH11	1:H:122:ARG:HD2	1.65	0.40
2:I:2:YYJ:S6	2:I:2:YYJ:C4	3.10	0.40
2:O:1:GU4:O5	2:O:2:YYJ:O5	2.38	0.40
1:D:89:LEU:O	1:D:90:GLU:HG2	2.21	0.40
1:D:123:THR:O	1:D:124:HIS:CB	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/140 (89%)	104 (83%)	17 (14%)	4 (3%)	3	7
1	B	125/140 (89%)	112 (90%)	9 (7%)	4 (3%)	3	7
1	C	125/140 (89%)	103 (82%)	18 (14%)	4 (3%)	3	7
1	D	125/140 (89%)	104 (83%)	16 (13%)	5 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	125/140 (89%)	102 (82%)	16 (13%)	7 (6%)	1	2
1	F	125/140 (89%)	105 (84%)	11 (9%)	9 (7%)	1	1
1	G	125/140 (89%)	105 (84%)	15 (12%)	5 (4%)	2	5
1	H	125/140 (89%)	92 (74%)	19 (15%)	14 (11%)	0	0
All	All	1000/1120 (89%)	827 (83%)	121 (12%)	52 (5%)	1	3

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	81	GLU
1	B	18	ASN
1	B	68	ASP
1	D	18	ASN
1	D	50	SER
1	D	88	ARG
1	D	124	HIS
1	E	18	ASN
1	E	68	ASP
1	F	18	ASN
1	F	37	ARG
1	F	50	SER
1	F	93	HIS
1	G	39	ASP
1	G	66	ALA
1	H	30	THR
1	H	45	GLN
1	H	68	ASP
1	H	89	LEU
1	H	125	PHE
1	B	81	GLU
1	C	81	GLU
1	E	41	HIS
1	E	89	LEU
1	F	51	ILE
1	F	69	THR
1	F	89	LEU
1	G	46	LEU
1	G	60	GLU
1	H	81	GLU
1	H	91	GLU

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Mol	Chain	Res	Type
1	H	94	TYR
1	H	130	ILE
1	A	37	ARG
1	B	93	HIS
1	F	81	GLU
1	H	39	ASP
1	H	44	LEU
1	C	68	ASP
1	D	60	GLU
1	E	96	THR
1	E	101	LYS
1	G	65	LEU
1	H	60	GLU
1	C	49	GLU
1	E	60	GLU
1	A	104	GLU
1	F	135	LEU
1	H	27	PRO
1	H	50	SER
1	C	51	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/122 (83%)	65 (64%)	36 (36%)	0	0
1	B	101/122 (83%)	65 (64%)	36 (36%)	0	0
1	C	101/122 (83%)	63 (62%)	38 (38%)	0	0
1	D	101/122 (83%)	75 (74%)	26 (26%)	0	2
1	E	101/122 (83%)	65 (64%)	36 (36%)	0	0
1	F	101/122 (83%)	70 (69%)	31 (31%)	0	1
1	G	101/122 (83%)	62 (61%)	39 (39%)	0	0
1	H	101/122 (83%)	68 (67%)	33 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	808/976 (83%)	533 (66%)	275 (34%)	0 0

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	LEU
1	A	14	LEU
1	A	17	SER
1	A	23	LEU
1	A	25	ILE
1	A	26	LEU
1	A	34	THR
1	A	35	LYS
1	A	39	ASP
1	A	44	LEU
1	A	46	LEU
1	A	49	GLU
1	A	53	GLU
1	A	57	LYS
1	A	60	GLU
1	A	65	LEU
1	A	72	LEU
1	A	73	LEU
1	A	77	GLN
1	A	78	THR
1	A	80	ASN
1	A	84	LEU
1	A	86	LEU
1	A	90	GLU
1	A	98	ILE
1	A	100	LYS
1	A	104	GLU
1	A	105	LYS
1	A	108	PHE
1	A	112	LYS
1	A	116	ARG
1	A	118	LYS
1	A	122	ARG
1	A	130	ILE
1	A	131	LEU
1	B	12	LYS

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	14	LEU
1	B	24	ARG
1	B	26	LEU
1	B	30	THR
1	B	31	VAL
1	B	37	ARG
1	B	44	LEU
1	B	49	GLU
1	B	53	GLU
1	B	57	LYS
1	B	59	THR
1	B	61	THR
1	B	65	LEU
1	B	67	MET
1	B	69	THR
1	B	72	LEU
1	B	73	LEU
1	B	76	SER
1	B	78	THR
1	B	80	ASN
1	B	84	LEU
1	B	89	LEU
1	B	96	THR
1	B	100	LYS
1	B	101	LYS
1	B	104	GLU
1	B	105	LYS
1	B	117	SER
1	B	122	ARG
1	B	127	GLN
1	B	128	LYS
1	B	130	ILE
1	B	131	LEU
1	B	135	LEU
1	C	12	LYS
1	C	13	LEU
1	C	14	LEU
1	C	17	SER
1	C	23	LEU
1	C	24	ARG
1	C	26	LEU

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Mol	Chain	Res	Type
1	C	30	THR
1	C	34	THR
1	C	43	GLN
1	C	44	LEU
1	C	46	LEU
1	C	53	GLU
1	C	57	LYS
1	C	60	GLU
1	C	65	LEU
1	C	67	MET
1	C	69	THR
1	C	72	LEU
1	C	77	GLN
1	C	78	THR
1	C	80	ASN
1	C	86	LEU
1	C	87	GLU
1	C	89	LEU
1	C	92	ASN
1	C	96	THR
1	C	98	ILE
1	C	100	LYS
1	C	101	LYS
1	C	104	GLU
1	C	105	LYS
1	C	116	ARG
1	C	122	ARG
1	C	128	LYS
1	C	130	ILE
1	C	131	LEU
1	C	135	LEU
1	D	13	LEU
1	D	14	LEU
1	D	26	LEU
1	D	35	LYS
1	D	42	ILE
1	D	44	LEU
1	D	46	LEU
1	D	49	GLU
1	D	59	THR
1	D	60	GLU
1	D	63	GLN

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Mol	Chain	Res	Type
1	D	65	LEU
1	D	73	LEU
1	D	77	GLN
1	D	78	THR
1	D	84	LEU
1	D	86	LEU
1	D	98	ILE
1	D	105	LYS
1	D	112	LYS
1	D	116	ARG
1	D	118	LYS
1	D	122	ARG
1	D	124	HIS
1	D	130	ILE
1	D	131	LEU
1	E	13	LEU
1	E	14	LEU
1	E	17	SER
1	E	24	ARG
1	E	30	THR
1	E	37	ARG
1	E	43	GLN
1	E	44	LEU
1	E	46	LEU
1	E	53	GLU
1	E	57	LYS
1	E	59	THR
1	E	63	GLN
1	E	65	LEU
1	E	67	MET
1	E	69	THR
1	E	72	LEU
1	E	73	LEU
1	E	76	SER
1	E	78	THR
1	E	80	ASN
1	E	84	LEU
1	E	86	LEU
1	E	90	GLU
1	E	95	ASN
1	E	96	THR
1	E	97	TYR

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Mol	Chain	Res	Type
1	E	100	LYS
1	E	101	LYS
1	E	112	LYS
1	E	116	ARG
1	E	118	LYS
1	E	122	ARG
1	E	130	ILE
1	E	131	LEU
1	E	135	LEU
1	F	13	LEU
1	F	14	LEU
1	F	24	ARG
1	F	25	ILE
1	F	26	LEU
1	F	30	THR
1	F	34	THR
1	F	39	ASP
1	F	44	LEU
1	F	49	GLU
1	F	54	VAL
1	F	56	ILE
1	F	57	LYS
1	F	63	GLN
1	F	65	LEU
1	F	69	THR
1	F	77	GLN
1	F	78	THR
1	F	82	GLU
1	F	84	LEU
1	F	86	LEU
1	F	89	LEU
1	F	92	ASN
1	F	96	THR
1	F	98	ILE
1	F	105	LYS
1	F	116	ARG
1	F	118	LYS
1	F	122	ARG
1	F	128	LYS
1	F	131	LEU
1	G	12	LYS
1	G	13	LEU

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Mol	Chain	Res	Type
1	G	14	LEU
1	G	25	ILE
1	G	26	LEU
1	G	28	ASP
1	G	30	THR
1	G	35	LYS
1	G	38	SER
1	G	43	GLN
1	G	44	LEU
1	G	46	LEU
1	G	49	GLU
1	G	53	GLU
1	G	54	VAL
1	G	56	ILE
1	G	57	LYS
1	G	59	THR
1	G	61	THR
1	G	63	GLN
1	G	65	LEU
1	G	67	MET
1	G	68	ASP
1	G	72	LEU
1	G	73	LEU
1	G	78	THR
1	G	80	ASN
1	G	82	GLU
1	G	84	LEU
1	G	89	LEU
1	G	96	THR
1	G	105	LYS
1	G	112	LYS
1	G	116	ARG
1	G	118	LYS
1	G	122	ARG
1	G	124	HIS
1	G	128	LYS
1	G	131	LEU
1	H	12	LYS
1	H	13	LEU
1	H	24	ARG
1	H	26	LEU
1	H	30	THR

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Mol	Chain	Res	Type
1	H	34	THR
1	H	43	GLN
1	H	44	LEU
1	H	53	GLU
1	H	54	VAL
1	H	58	SER
1	H	65	LEU
1	H	67	MET
1	H	70	ASP
1	H	73	LEU
1	H	77	GLN
1	H	78	THR
1	H	80	ASN
1	H	84	LEU
1	H	86	LEU
1	H	89	LEU
1	H	95	ASN
1	H	96	THR
1	H	98	ILE
1	H	100	LYS
1	H	101	LYS
1	H	104	GLU
1	H	116	ARG
1	H	118	LYS
1	H	125	PHE
1	H	128	LYS
1	H	130	ILE
1	H	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	80	ASN
1	A	102	HIS
1	A	124	HIS
1	A	127	GLN
1	B	63	GLN
1	B	80	ASN
1	B	93	HIS
1	B	127	GLN
1	C	102	HIS

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Mol	Chain	Res	Type
1	D	93	HIS
1	E	43	GLN
1	E	63	GLN
1	E	80	ASN
1	E	95	ASN
1	E	102	HIS
1	F	18	ASN
1	F	63	GLN
1	F	124	HIS
1	G	41	HIS
1	G	63	GLN
1	G	80	ASN
1	G	93	HIS
1	G	95	ASN
1	G	106	HIS
1	G	124	HIS
1	G	127	GLN
1	H	41	HIS
1	H	43	GLN
1	H	63	GLN
1	H	80	ASN
1	H	95	ASN
1	H	102	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GU4	I	1	2	27,27,28	1.48	4 (14%)	32,43,45	2.16	7 (21%)
2	YYJ	I	2	2	27,28,28	2.10	6 (22%)	33,46,46	1.52	3 (9%)
2	GU4	J	1	2	27,27,28	1.46	5 (18%)	32,43,45	1.75	7 (21%)
2	YYJ	J	2	2	27,28,28	1.80	5 (18%)	33,46,46	1.28	2 (6%)
2	GU4	K	1	2	27,27,28	1.50	4 (14%)	32,43,45	2.14	7 (21%)
2	YYJ	K	2	2	27,28,28	1.81	4 (14%)	33,46,46	1.56	6 (18%)
2	GU4	L	1	2	27,27,28	1.92	5 (18%)	32,43,45	1.70	4 (12%)
2	YYJ	L	2	2	27,28,28	1.46	5 (18%)	33,46,46	1.29	5 (15%)
2	GU4	M	1	2	27,27,28	1.66	5 (18%)	32,43,45	2.34	11 (34%)
2	YYJ	M	2	2	27,28,28	1.77	4 (14%)	33,46,46	1.19	4 (12%)
2	GU4	N	1	2	27,27,28	1.53	5 (18%)	32,43,45	1.52	5 (15%)
2	YYJ	N	2	2	27,28,28	1.55	4 (14%)	33,46,46	1.44	5 (15%)
2	GU4	O	1	2	27,27,28	1.46	4 (14%)	32,43,45	1.98	10 (31%)
2	YYJ	O	2	2	27,28,28	1.43	4 (14%)	33,46,46	1.34	2 (6%)
2	GU4	P	1	2	27,27,28	1.86	5 (18%)	32,43,45	1.61	5 (15%)
2	YYJ	P	2	2	27,28,28	1.74	5 (18%)	33,46,46	1.72	5 (15%)

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	GU4	I	1	2	-	8/21/38/41	0/1/1/1
2	YYJ	I	2	2	-	7/23/42/42	0/1/1/1
2	GU4	J	1	2	-	12/21/38/41	0/1/1/1
2	YYJ	J	2	2	-	15/23/42/42	0/1/1/1
2	GU4	K	1	2	-	10/21/38/41	0/1/1/1
2	YYJ	K	2	2	-	6/23/42/42	0/1/1/1
2	GU4	L	1	2	-	12/21/38/41	0/1/1/1
2	YYJ	L	2	2	-	8/23/42/42	0/1/1/1
2	GU4	M	1	2	-	13/21/38/41	0/1/1/1
2	YYJ	M	2	2	-	14/23/42/42	0/1/1/1
2	GU4	N	1	2	-	10/21/38/41	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YYJ	N	2	2	-	12/23/42/42	0/1/1/1
2	GU4	O	1	2	-	12/21/38/41	0/1/1/1
2	YYJ	O	2	2	-	13/23/42/42	0/1/1/1
2	GU4	P	1	2	-	9/21/38/41	0/1/1/1
2	YYJ	P	2	2	-	8/23/42/42	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	YYJ	O3-S3	-5.95	1.39	1.57
2	L	1	GU4	O6-S6	-4.95	1.43	1.56
2	J	2	YYJ	O3-S3	-4.89	1.42	1.57
2	P	1	GU4	O4-S4	-4.85	1.42	1.57
2	P	1	GU4	O2-S2	-4.71	1.43	1.57
2	P	2	YYJ	O3-S3	-4.64	1.43	1.57
2	L	1	GU4	O2-S2	-4.55	1.43	1.57
2	K	2	YYJ	O6-S6	-4.53	1.44	1.56
2	I	1	GU4	O4-S4	-4.53	1.43	1.57
2	M	2	YYJ	O1-S1	-4.48	1.44	1.56
2	N	2	YYJ	O3-S3	-4.44	1.44	1.57
2	M	1	GU4	O4-S4	-4.41	1.44	1.57
2	K	2	YYJ	O3-S3	-4.40	1.44	1.57
2	O	2	YYJ	O1-S1	-4.34	1.45	1.56
2	N	1	GU4	O6-S6	-4.34	1.45	1.56
2	J	2	YYJ	O1-S1	-4.31	1.45	1.56
2	K	2	YYJ	O1-S1	-4.31	1.45	1.56
2	M	2	YYJ	O3-S3	-4.27	1.44	1.57
2	L	2	YYJ	O3-S3	-4.26	1.44	1.57
2	P	2	YYJ	O1-S1	-4.26	1.45	1.56
2	O	1	GU4	O6-S6	-4.24	1.45	1.56
2	M	2	YYJ	O6-S6	-4.22	1.45	1.56
2	J	2	YYJ	O6-S6	-4.09	1.45	1.56
2	L	1	GU4	O4-S4	-4.09	1.45	1.57
2	P	1	GU4	O6-S6	-4.08	1.45	1.56
2	N	1	GU4	O4-S4	-4.05	1.45	1.57
2	L	1	GU4	O3-S3	-4.04	1.45	1.57
2	I	2	YYJ	O4-S4	-4.01	1.45	1.57
2	M	1	GU4	O6-S6	-3.97	1.46	1.56
2	K	1	GU4	O4-S4	-3.96	1.45	1.57
2	I	2	YYJ	O3-C3	-3.89	1.40	1.47
2	K	2	YYJ	O4-S4	-3.88	1.45	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	YYJ	O4-S4	-3.84	1.45	1.57
2	I	2	YYJ	O6-S6	-3.81	1.46	1.56
2	I	2	YYJ	O1-S1	-3.75	1.46	1.56
2	M	2	YYJ	O4-S4	-3.69	1.46	1.57
2	J	2	YYJ	O4-S4	-3.68	1.46	1.57
2	J	1	GU4	O6-S6	-3.65	1.47	1.56
2	J	1	GU4	O4-S4	-3.63	1.46	1.57
2	O	1	GU4	O4-S4	-3.55	1.46	1.57
2	I	1	GU4	O6-S6	-3.51	1.47	1.56
2	O	2	YYJ	O6-S6	-3.49	1.47	1.56
2	N	2	YYJ	O1-S1	-3.42	1.47	1.56
2	O	1	GU4	O2-S2	-3.30	1.47	1.57
2	M	1	GU4	O3-S3	-3.29	1.47	1.57
2	K	1	GU4	O6-S6	-3.29	1.48	1.56
2	K	1	GU4	O2-S2	-3.26	1.47	1.57
2	L	2	YYJ	O1-S1	-3.26	1.48	1.56
2	J	1	GU4	O2-S2	-3.24	1.47	1.57
2	P	1	GU4	O3-S3	-3.18	1.47	1.57
2	L	2	YYJ	O6-S6	-3.11	1.48	1.56
2	P	1	GU4	O2-C2	-3.11	1.42	1.47
2	N	2	YYJ	O4-S4	-3.08	1.48	1.57
2	P	2	YYJ	O6-S6	-3.08	1.48	1.56
2	N	2	YYJ	O6-S6	-3.03	1.48	1.56
2	O	2	YYJ	O4-S4	-3.03	1.48	1.57
2	M	1	GU4	C1-C2	2.98	1.56	1.51
2	L	2	YYJ	O4-S4	-2.98	1.48	1.57
2	O	1	GU4	O3-S3	-2.88	1.48	1.57
2	K	1	GU4	O3-S3	-2.86	1.48	1.57
2	L	1	GU4	O2-C2	-2.85	1.43	1.47
2	O	2	YYJ	O3-S3	-2.84	1.48	1.57
2	J	1	GU4	O3-S3	-2.82	1.48	1.57
2	I	1	GU4	O3-S3	-2.77	1.49	1.57
2	N	1	GU4	O2-S2	-2.75	1.49	1.57
2	I	1	GU4	O2-S2	-2.72	1.49	1.57
2	N	1	GU4	O3-S3	-2.59	1.49	1.57
2	P	2	YYJ	O2-C2	2.55	1.45	1.40
2	I	2	YYJ	O2-C2	2.50	1.45	1.40
2	J	2	YYJ	O3-C3	-2.44	1.43	1.47
2	M	1	GU4	O2-S2	-2.35	1.50	1.57
2	N	1	GU4	C3-C4	2.32	1.57	1.52
2	L	2	YYJ	O3-C3	-2.26	1.43	1.47
2	J	1	GU4	C3-C4	2.02	1.56	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GU4	C1-O5-C5	-8.15	101.27	112.19
2	I	1	GU4	O2-C2-C3	6.87	114.26	106.65
2	M	1	GU4	C1-O5-C5	-5.83	104.38	112.19
2	M	1	GU4	O6-C6-C5	5.59	117.53	107.57
2	L	1	GU4	O4-C4-C3	-5.47	96.61	108.56
2	P	2	YYJ	C3-O3-S3	5.33	124.28	117.69
2	J	1	GU4	C1-O5-C5	5.12	119.05	112.19
2	O	1	GU4	C4-O4-S4	5.01	131.05	119.04
2	M	1	GU4	O5-C5-C4	-4.78	101.47	110.06
2	J	2	YYJ	C3-O3-S3	4.44	123.18	117.69
2	I	1	GU4	C1-C2-C3	-4.42	102.78	109.40
2	O	1	GU4	C3-O3-S3	4.40	129.59	119.04
2	O	1	GU4	O2-C2-C3	4.33	111.45	106.65
2	O	2	YYJ	O5-C5-C6	4.27	119.55	109.50
2	J	1	GU4	C3-C4-C5	4.26	119.30	110.58
2	P	1	GU4	C1-O5-C5	-4.12	106.66	112.19
2	L	1	GU4	O24-S4-O4	4.11	115.83	106.37
2	N	1	GU4	C3-C4-C5	4.06	118.89	110.58
2	P	2	YYJ	C4-O4-S4	-4.04	109.35	119.04
2	I	2	YYJ	O3-C3-C4	-4.03	98.12	109.27
2	O	2	YYJ	O2-C2-O5	4.00	117.00	109.33
2	I	1	GU4	O6-C6-C5	3.99	114.67	107.57
2	I	2	YYJ	O6-C6-C5	3.94	114.58	107.57
2	N	1	GU4	O2-C2-C3	3.94	111.01	106.65
2	K	1	GU4	C6-C5-C4	3.73	122.34	113.35
2	M	1	GU4	O5-C5-C6	3.73	115.64	107.59
2	L	1	GU4	C1-O5-C5	-3.68	107.26	112.19
2	I	2	YYJ	C4-O4-S4	-3.67	110.23	119.04
2	M	1	GU4	O5-C1-C2	3.65	116.90	109.51
2	K	1	GU4	O6-C6-C5	3.65	114.06	107.57
2	N	2	YYJ	O4-C4-C3	3.61	116.75	108.91
2	P	1	GU4	C1-C2-C3	3.56	114.73	109.40
2	P	1	GU4	O2-C2-C3	-3.55	102.72	106.65
2	I	1	GU4	C6-C5-C4	3.50	121.78	113.35
2	P	1	GU4	O4-C4-C3	-3.48	100.97	108.56
2	P	2	YYJ	O3-C3-C4	-3.44	99.77	109.27
2	I	1	GU4	O4-C4-C3	-3.38	101.17	108.56
2	K	2	YYJ	O5-C5-C4	3.29	108.88	103.54
2	K	2	YYJ	C6-C5-C4	-3.24	103.57	114.38
2	I	1	GU4	O24-S4-O4	3.13	113.56	106.37
2	K	2	YYJ	O4-C4-C3	3.03	115.50	108.91
2	K	2	YYJ	O1S1-S1-O1	3.03	113.33	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	GU4	C6-C5-C4	2.92	120.39	113.35
2	K	1	GU4	C1-C2-C3	2.92	113.77	109.40
2	J	1	GU4	O6-C6-C5	2.88	112.69	107.57
2	O	1	GU4	O24-S4-O4	2.87	112.98	106.37
2	O	1	GU4	C1-O5-C5	2.85	116.01	112.19
2	N	2	YYJ	O5-C5-C4	2.85	108.15	103.54
2	J	1	GU4	O5-C5-C4	2.79	115.08	110.06
2	J	2	YYJ	O3-C3-C4	-2.75	101.68	109.27
2	M	1	GU4	O10-S2-O2	2.74	112.67	106.37
2	M	1	GU4	O4-C4-C3	2.74	114.53	108.56
2	M	1	GU4	C1-C2-C3	2.70	113.45	109.40
2	M	2	YYJ	O1S6-S6-O6	2.60	112.36	106.37
2	L	2	YYJ	C4-O4-S4	2.60	125.28	119.04
2	N	2	YYJ	O1S3-S3-O3	2.58	112.31	106.37
2	M	2	YYJ	O1S3-S3-O3	2.57	112.28	106.37
2	L	2	YYJ	O1-S1-O3S1	2.55	114.71	106.92
2	N	1	GU4	O24-S4-O4	2.53	112.19	106.37
2	O	1	GU4	O21-S6-O6	2.51	112.15	106.37
2	N	1	GU4	O29-S3-O3	2.50	112.11	106.37
2	O	1	GU4	O6-C6-C5	2.47	111.97	107.57
2	K	1	GU4	C4-O4-S4	2.43	124.86	119.04
2	O	1	GU4	C3-C4-C5	-2.42	105.63	110.58
2	K	1	GU4	O5-C5-C4	-2.40	105.74	110.06
2	J	1	GU4	O21-S6-O6	2.39	111.87	106.37
2	J	1	GU4	O5-C1-C2	2.36	114.29	109.51
2	K	2	YYJ	C4-O4-S4	-2.36	113.38	119.04
2	O	1	GU4	O10-S2-O2	2.35	111.78	106.37
2	K	1	GU4	O5-C5-C6	2.35	112.67	107.59
2	I	1	GU4	O10-S2-O2	2.33	111.72	106.37
2	M	2	YYJ	O1S4-S4-O4	2.26	111.58	106.37
2	P	1	GU4	O21-S6-O6	2.26	111.56	106.37
2	L	2	YYJ	O1S3-S3-O3	2.25	111.53	106.37
2	L	1	GU4	O29-S3-O3	2.24	111.53	106.37
2	P	2	YYJ	C5-C4-C3	2.23	108.66	103.15
2	K	2	YYJ	O6-C6-C5	2.22	111.52	107.57
2	N	2	YYJ	O3-C3-C4	-2.21	103.16	109.27
2	M	1	GU4	C4-O4-S4	2.21	124.33	119.04
2	L	2	YYJ	O5-C5-C4	2.20	107.11	103.54
2	M	1	GU4	O29-S3-O3	2.16	111.34	106.37
2	O	1	GU4	O5-C1-C2	2.16	113.88	109.51
2	N	2	YYJ	C6-C5-C4	-2.15	107.23	114.38
2	P	2	YYJ	O6-C6-C5	2.09	111.29	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	GU4	C3-O3-S3	2.07	124.00	119.04
2	J	1	GU4	O29-S3-O3	2.06	111.12	106.37
2	M	2	YYJ	C4-O4-S4	2.04	123.92	119.04
2	L	2	YYJ	O3S1-S1-O2S1	-2.02	104.45	112.24

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	GU4	C4-C5-C6-O6
2	I	2	YYJ	C2-C1-O1-S1
2	I	2	YYJ	C6-O6-S6-O1S6
2	J	1	GU4	C2-O2-S2-O10
2	J	2	YYJ	C2-C1-O1-S1
2	J	2	YYJ	C2-C3-O3-S3
2	J	2	YYJ	C4-C5-C6-O6
2	J	2	YYJ	O5-C5-C6-O6
2	J	2	YYJ	C5-C6-O6-S6
2	J	2	YYJ	C3-O3-S3-O3S3
2	J	2	YYJ	C4-O4-S4-O3S4
2	K	2	YYJ	O1-C1-C2-C3
2	K	2	YYJ	O1-C1-C2-O2
2	K	2	YYJ	O1-C1-C2-O5
2	K	2	YYJ	C4-O4-S4-O1S4
2	K	2	YYJ	C4-O4-S4-O2S4
2	K	2	YYJ	C4-O4-S4-O3S4
2	L	1	GU4	C6-O6-S6-O21
2	L	1	GU4	C5-C4-O4-S4
2	L	1	GU4	C3-C4-O4-S4
2	L	1	GU4	C2-C3-O3-S3
2	L	2	YYJ	C2-C1-O1-S1
2	L	2	YYJ	C5-C6-O6-S6
2	M	1	GU4	O5-C5-C6-O6
2	M	1	GU4	C4-C5-C6-O6
2	M	1	GU4	C5-C4-O4-S4
2	M	1	GU4	C3-C4-O4-S4
2	M	1	GU4	C3-O3-S3-O29
2	M	2	YYJ	O1-C1-C2-C3
2	M	2	YYJ	O1-C1-C2-O2
2	M	2	YYJ	O1-C1-C2-O5
2	M	2	YYJ	C2-C1-O1-S1
2	M	2	YYJ	C3-C4-O4-S4

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Mol	Chain	Res	Type	Atoms
2	M	2	YYJ	C4-C5-C6-O6
2	N	1	GU4	C3-O3-S3-O27
2	N	2	YYJ	C2-C1-O1-S1
2	N	2	YYJ	C4-C5-C6-O6
2	N	2	YYJ	O5-C5-C6-O6
2	N	2	YYJ	C4-O4-S4-O3S4
2	N	2	YYJ	C6-O6-S6-O1S6
2	O	1	GU4	C6-O6-S6-O21
2	O	1	GU4	C5-C4-O4-S4
2	O	1	GU4	C4-C3-O3-S3
2	O	1	GU4	C2-C3-O3-S3
2	O	1	GU4	C3-O3-S3-O29
2	O	1	GU4	C2-O2-S2-O12
2	O	2	YYJ	C2-C1-O1-S1
2	O	2	YYJ	C5-C4-O4-S4
2	O	2	YYJ	C4-C5-C6-O6
2	O	2	YYJ	C1-O1-S1-O1S1
2	O	2	YYJ	C4-O4-S4-O1S4
2	O	2	YYJ	C4-O4-S4-O2S4
2	P	2	YYJ	C2-C3-O3-S3
2	P	2	YYJ	C4-C5-C6-O6
2	P	2	YYJ	O5-C5-C6-O6
2	P	2	YYJ	C1-O1-S1-O3S1
2	J	2	YYJ	C6-O6-S6-O3S6
2	M	2	YYJ	C6-O6-S6-O2S6
2	O	2	YYJ	C1-O1-S1-O3S1
2	P	2	YYJ	C1-O1-S1-O2S1
2	I	2	YYJ	C6-O6-S6-O3S6
2	K	1	GU4	C6-O6-S6-O23
2	M	1	GU4	C6-O6-S6-O23
2	M	2	YYJ	C6-O6-S6-O3S6
2	N	2	YYJ	C6-O6-S6-O3S6
2	O	2	YYJ	C1-O1-S1-O2S1
2	O	2	YYJ	C6-O6-S6-O3S6
2	P	1	GU4	C6-O6-S6-O23
2	I	1	GU4	C4-O4-S4-O25
2	I	1	GU4	C4-O4-S4-O26
2	J	1	GU4	C4-O4-S4-O25
2	J	1	GU4	C2-O2-S2-O11
2	J	1	GU4	C2-O2-S2-O12
2	J	2	YYJ	C3-O3-S3-O2S3
2	J	2	YYJ	C4-O4-S4-O2S4

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Mol	Chain	Res	Type	Atoms
2	K	1	GU4	C2-O2-S2-O11
2	K	1	GU4	C2-O2-S2-O12
2	M	1	GU4	C4-O4-S4-O25
2	M	1	GU4	C3-O3-S3-O28
2	M	1	GU4	C3-O3-S3-O27
2	N	1	GU4	C3-O3-S3-O28
2	N	1	GU4	C2-O2-S2-O11
2	N	1	GU4	C2-O2-S2-O12
2	N	2	YYJ	C4-O4-S4-O2S4
2	O	1	GU4	C3-O3-S3-O28
2	O	1	GU4	C3-O3-S3-O27
2	O	1	GU4	C2-O2-S2-O11
2	O	2	YYJ	C4-O4-S4-O3S4
2	P	1	GU4	C4-O4-S4-O25
2	P	1	GU4	C4-O4-S4-O26
2	P	1	GU4	C2-O2-S2-O11
2	P	1	GU4	C2-O2-S2-O12
2	J	1	GU4	C6-O6-S6-O21
2	J	2	YYJ	C6-O6-S6-O1S6
2	K	1	GU4	C6-O6-S6-O21
2	M	2	YYJ	C6-O6-S6-O1S6
2	P	2	YYJ	C1-O1-S1-O1S1
2	I	2	YYJ	C6-O6-S6-O2S6
2	J	2	YYJ	C6-O6-S6-O2S6
2	L	1	GU4	C6-O6-S6-O22
2	L	1	GU4	C6-O6-S6-O23
2	M	1	GU4	C6-O6-S6-O22
2	N	2	YYJ	C6-O6-S6-O2S6
2	O	1	GU4	C6-O6-S6-O22
2	O	1	GU4	C6-O6-S6-O23
2	P	1	GU4	C6-O6-S6-O22
2	I	2	YYJ	C3-C4-O4-S4
2	I	1	GU4	C4-O4-S4-O24
2	J	1	GU4	C4-O4-S4-O24
2	J	2	YYJ	C3-O3-S3-O1S3
2	J	2	YYJ	C4-O4-S4-O1S4
2	K	1	GU4	C3-O3-S3-O29
2	K	1	GU4	C2-O2-S2-O10
2	M	1	GU4	C4-O4-S4-O26
2	M	1	GU4	C4-O4-S4-O24
2	N	1	GU4	C3-O3-S3-O29
2	N	1	GU4	C2-O2-S2-O10

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Mol	Chain	Res	Type	Atoms
2	N	2	YYJ	C4-O4-S4-O1S4
2	O	1	GU4	C2-O2-S2-O10
2	P	1	GU4	C4-O4-S4-O24
2	P	1	GU4	C2-O2-S2-O10
2	L	2	YYJ	C1-O1-S1-O1S1
2	O	2	YYJ	C6-O6-S6-O1S6
2	P	1	GU4	C6-O6-S6-O21
2	I	2	YYJ	C5-C6-O6-S6
2	M	2	YYJ	C5-C6-O6-S6
2	J	1	GU4	C6-O6-S6-O22
2	J	1	GU4	C6-O6-S6-O23
2	L	2	YYJ	C1-O1-S1-O3S1
2	N	1	GU4	C6-O6-S6-O23
2	N	2	YYJ	C1-O1-S1-O3S1
2	K	1	GU4	C6-O6-S6-O22
2	N	1	GU4	C6-O6-S6-O22
2	N	2	YYJ	C1-O1-S1-O2S1
2	O	2	YYJ	C6-O6-S6-O2S6
2	J	1	GU4	C4-O4-S4-O26
2	M	1	GU4	C6-O6-S6-O21
2	N	1	GU4	C6-O6-S6-O21
2	L	2	YYJ	C4-C5-C6-O6
2	L	2	YYJ	C1-O1-S1-O2S1
2	J	1	GU4	O5-C5-C6-O6
2	J	1	GU4	C4-C5-C6-O6
2	I	1	GU4	C3-O3-S3-O29
2	I	1	GU4	C2-O2-S2-O10
2	K	1	GU4	C4-O4-S4-O24
2	L	1	GU4	C4-O4-S4-O25
2	L	1	GU4	C4-O4-S4-O24
2	L	1	GU4	C2-O2-S2-O10
2	M	2	YYJ	C3-O3-S3-O1S3
2	P	2	YYJ	C4-C3-O3-S3
2	N	2	YYJ	C1-O1-S1-O1S1
2	K	1	GU4	C3-O3-S3-O27
2	L	1	GU4	C2-O2-S2-O11
2	L	1	GU4	C5-C6-O6-S6
2	M	2	YYJ	C4-O4-S4-O1S4
2	M	2	YYJ	C4-O4-S4-O2S4
2	I	1	GU4	C3-C4-O4-S4
2	K	1	GU4	C3-C4-O4-S4
2	L	1	GU4	C4-C3-O3-S3

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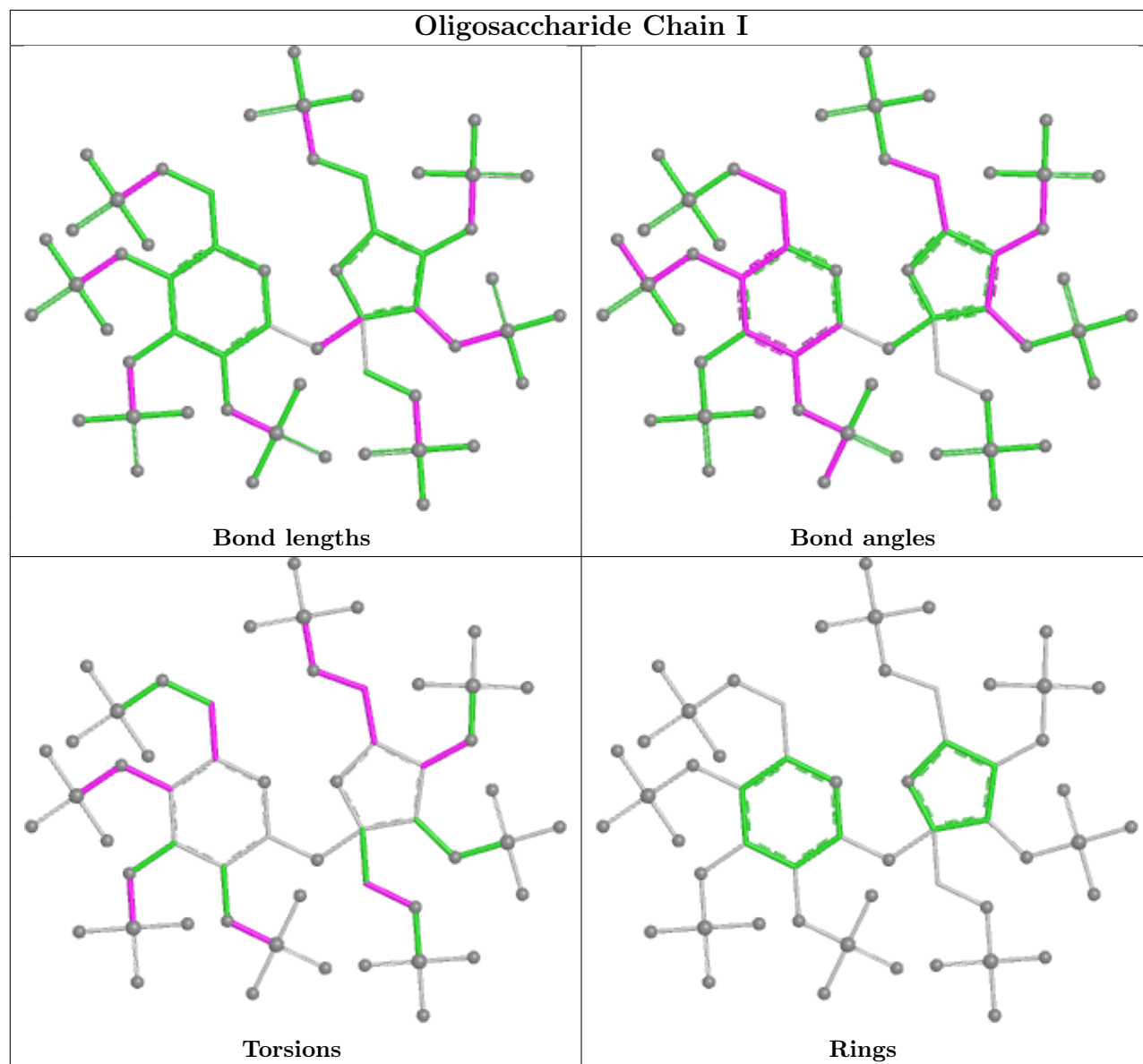
Mol	Chain	Res	Type	Atoms
2	J	1	GU4	C5-C6-O6-S6
2	N	1	GU4	C5-C6-O6-S6
2	P	2	YYJ	C5-C6-O6-S6
2	I	2	YYJ	O5-C5-C6-O6
2	J	2	YYJ	O1-C1-C2-O2
2	L	2	YYJ	C3-C4-O4-S4
2	L	2	YYJ	O5-C5-C6-O6
2	M	2	YYJ	O5-C5-C6-O6
2	O	2	YYJ	O5-C5-C6-O6
2	I	1	GU4	O5-C5-C6-O6

There are no ring outliers.

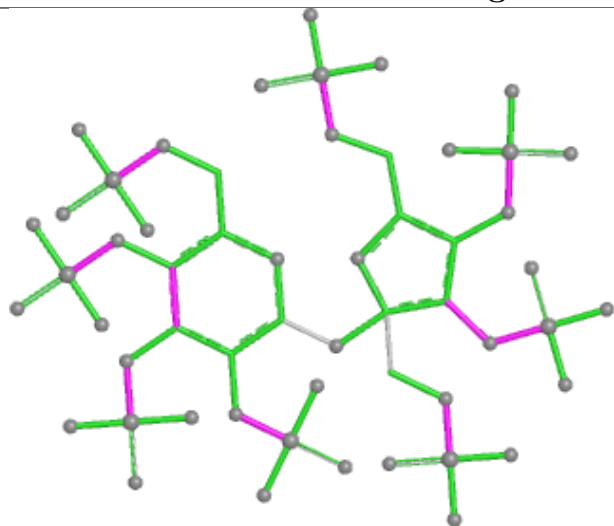
16 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	GU4	2	0
2	P	1	GU4	13	0
2	O	2	YYJ	21	0
2	K	2	YYJ	9	0
2	L	1	GU4	8	0
2	M	2	YYJ	14	0
2	I	1	GU4	15	0
2	L	2	YYJ	15	0
2	N	2	YYJ	13	0
2	O	1	GU4	13	0
2	M	1	GU4	9	0
2	P	2	YYJ	11	0
2	I	2	YYJ	21	0
2	K	1	GU4	9	0
2	N	1	GU4	4	0
2	J	2	YYJ	6	0

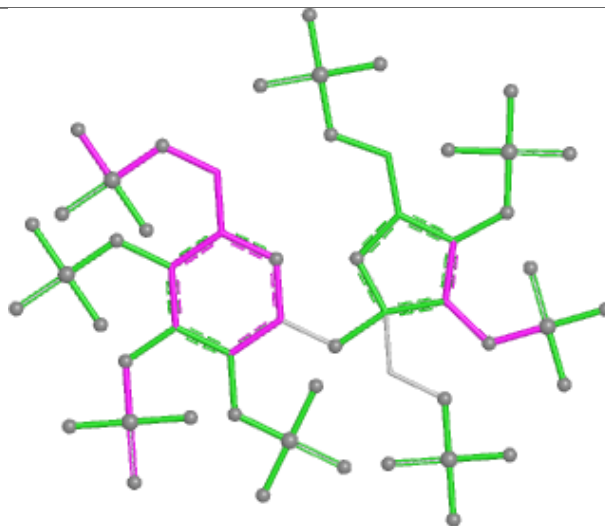
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



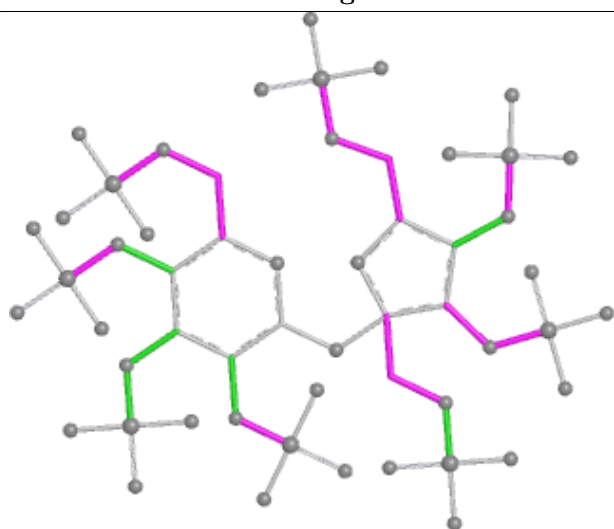
Oligosaccharide Chain J



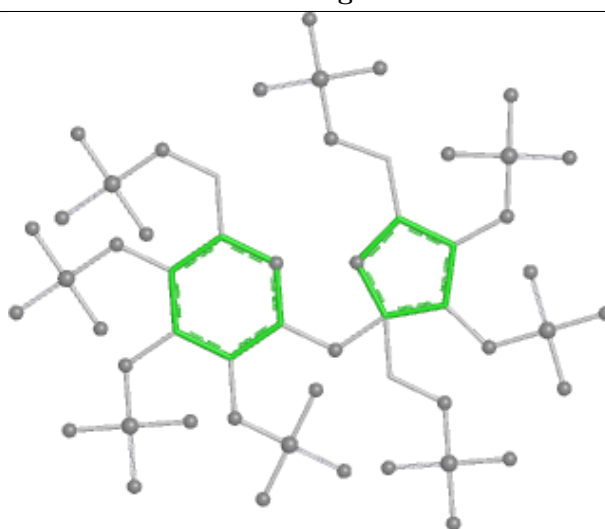
Bond lengths



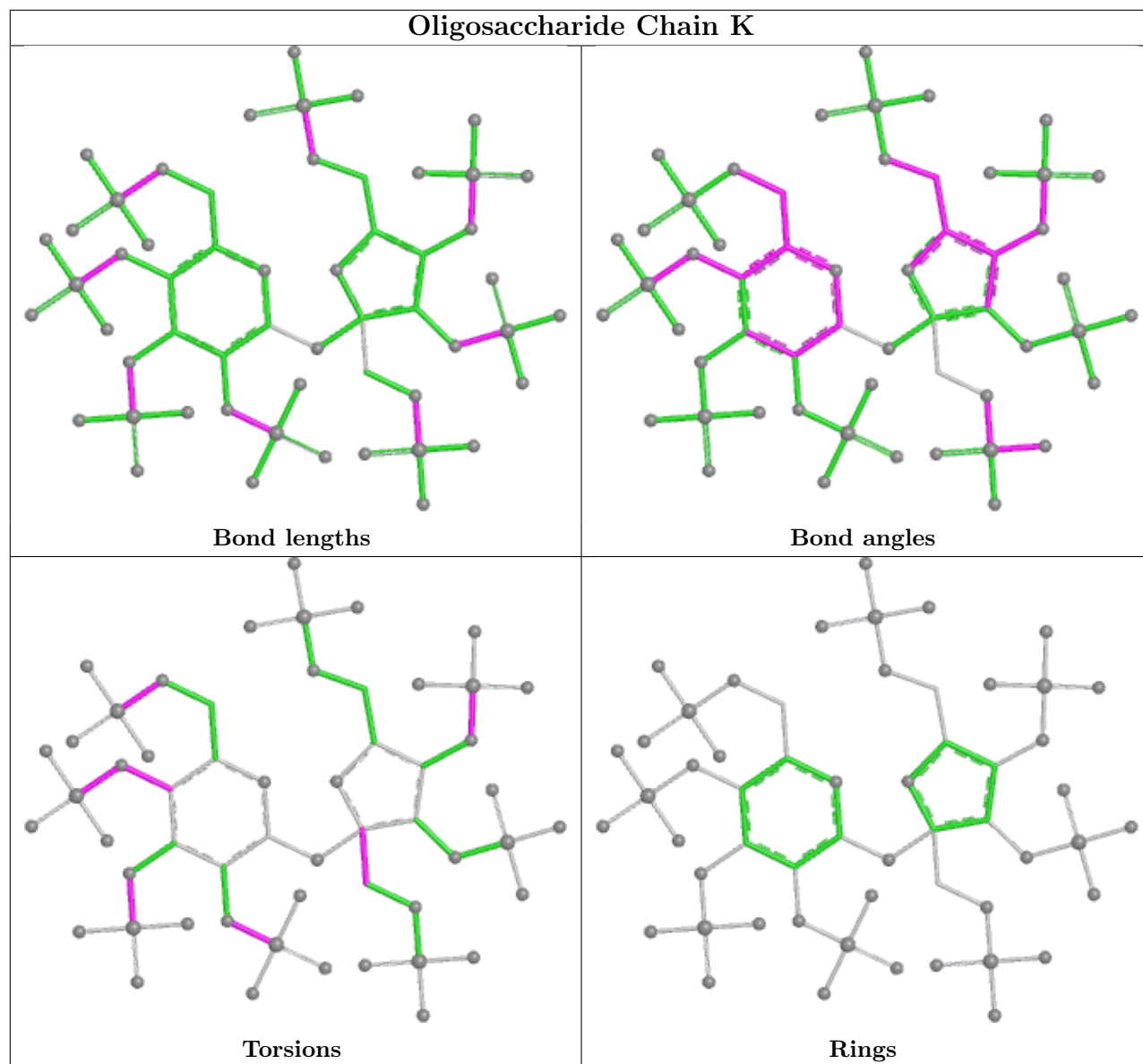
Bond angles

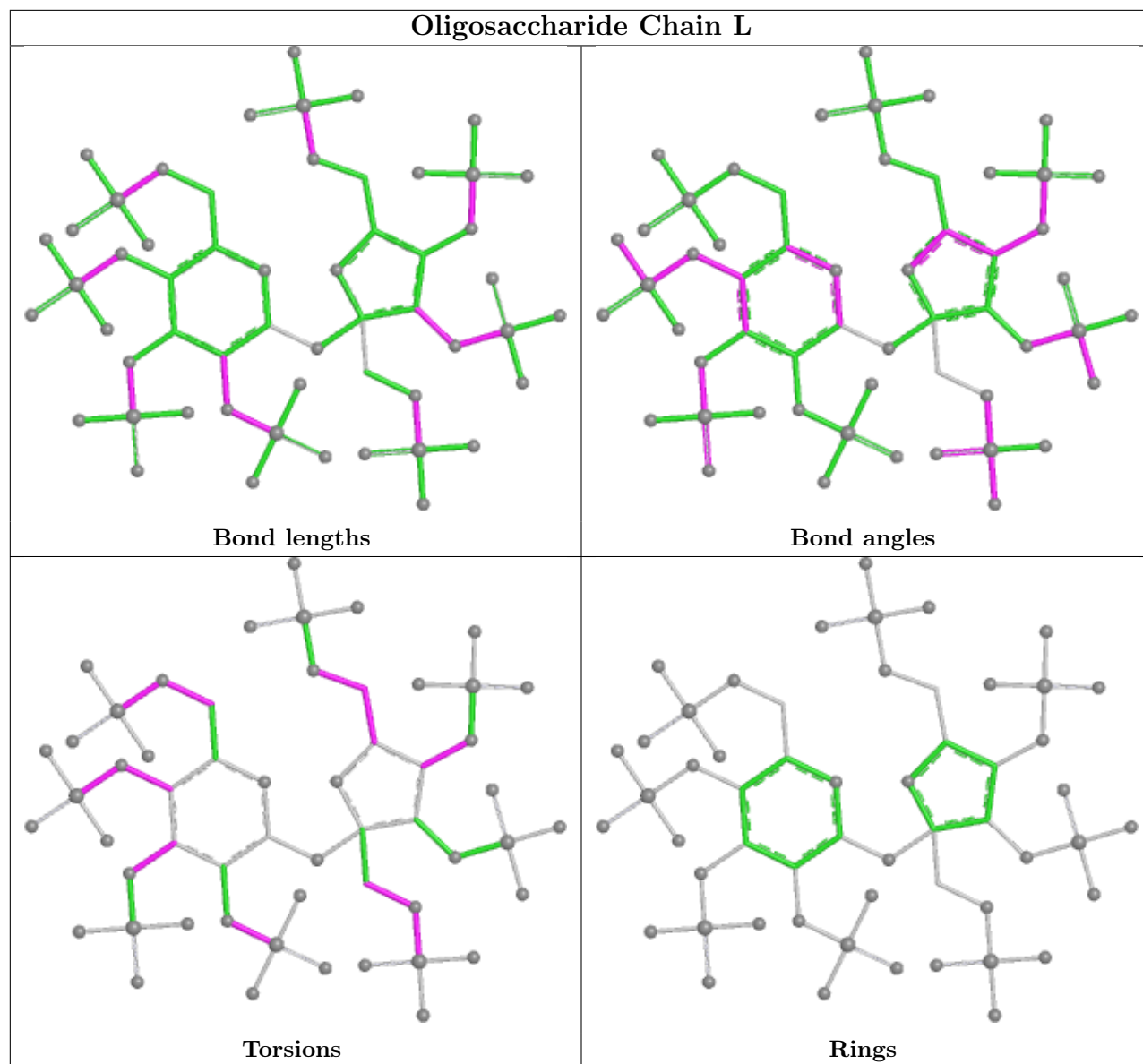


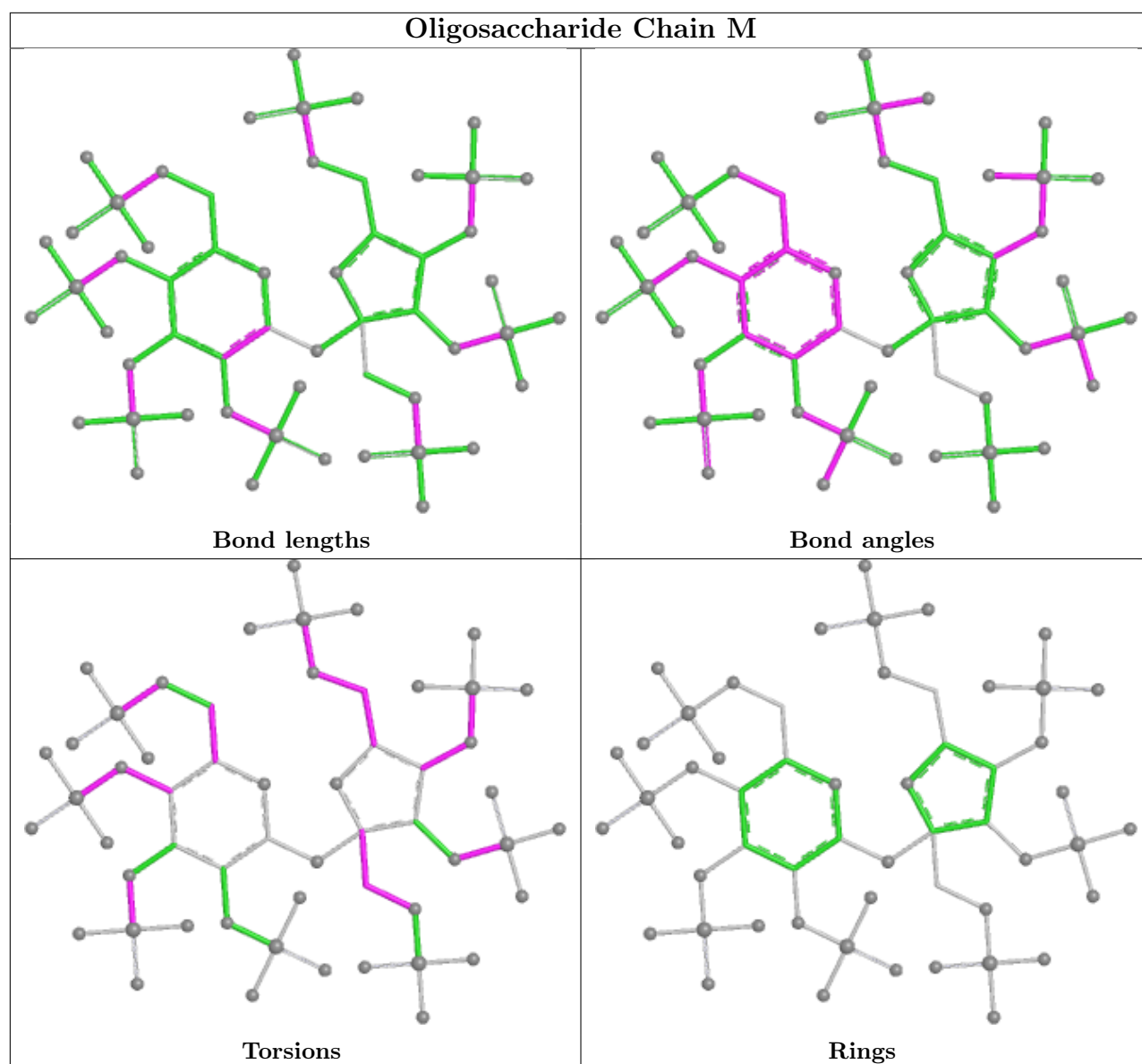
Torsions

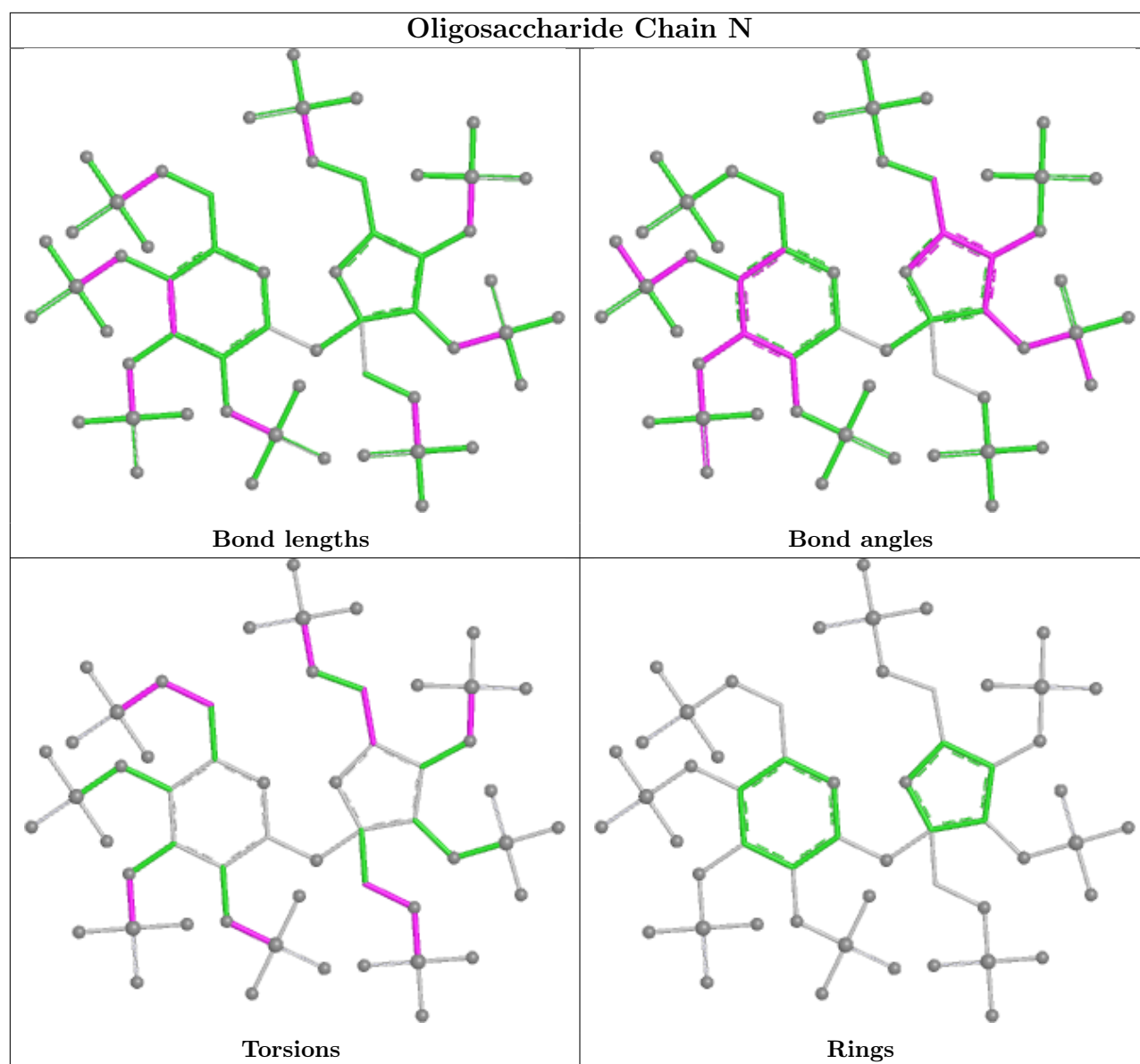


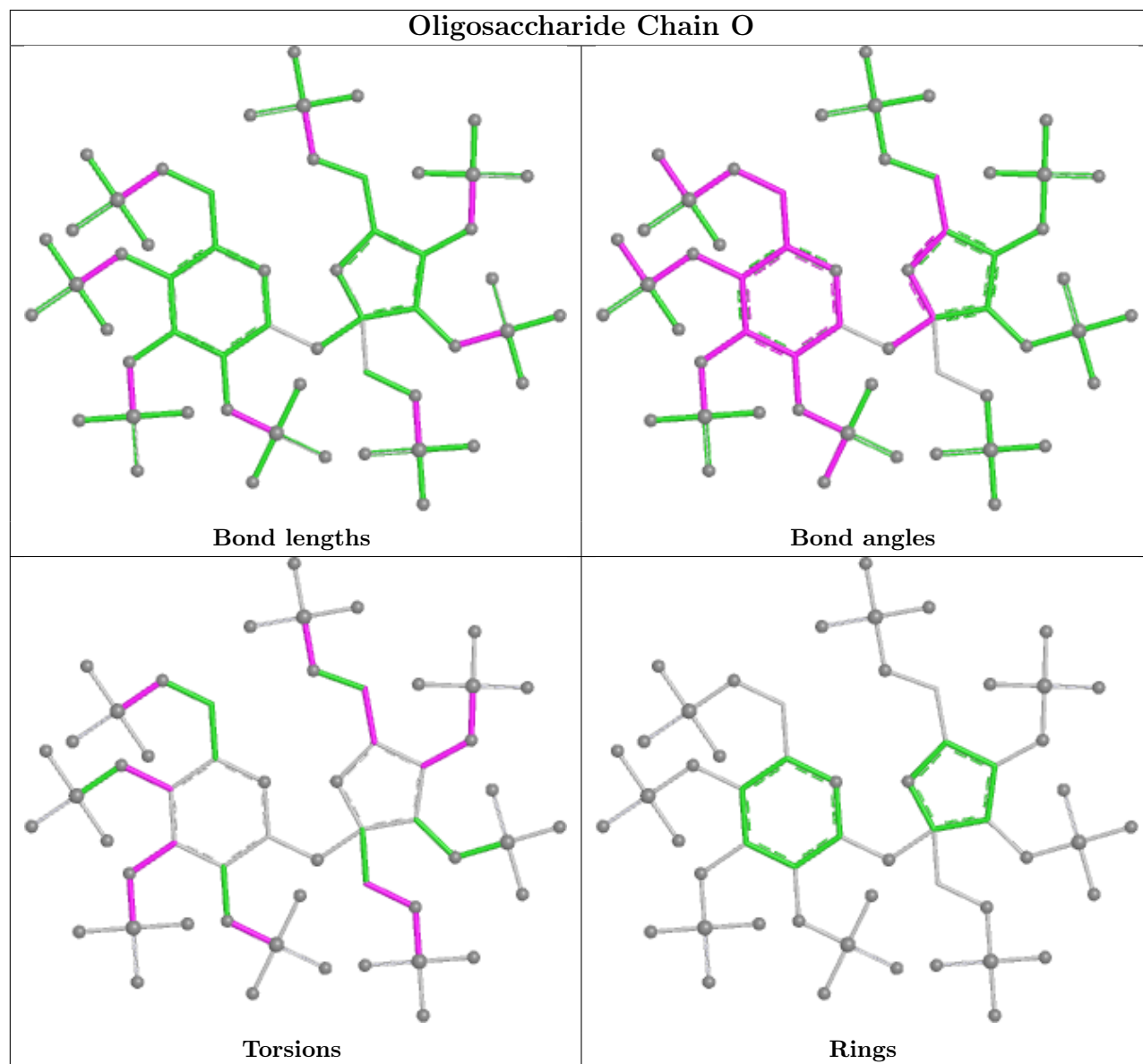
Rings

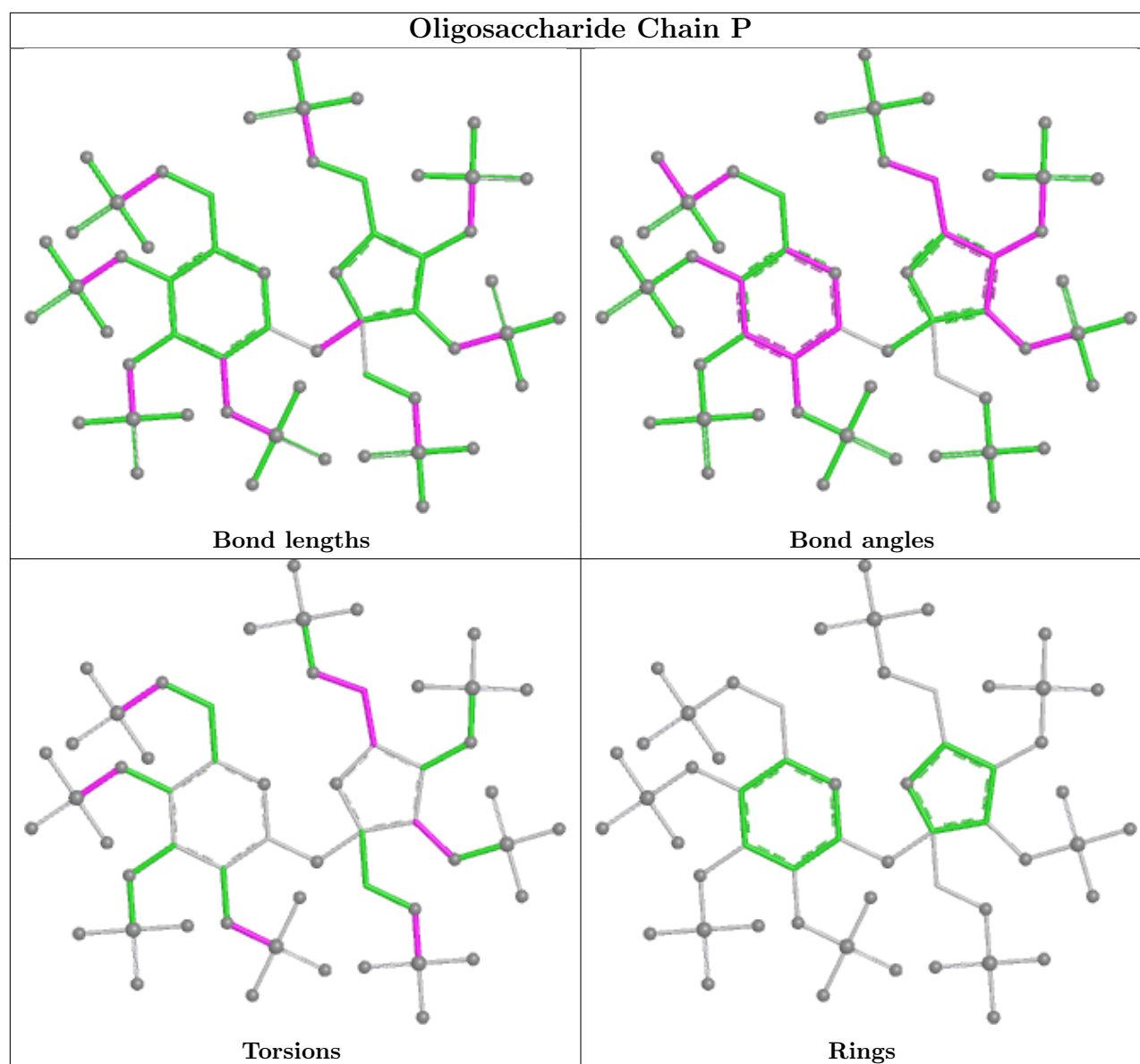












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.