Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 11:50 AM EST

PDB ID	:	1AFC
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 (i) 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 (i)) were used in the production of this report:

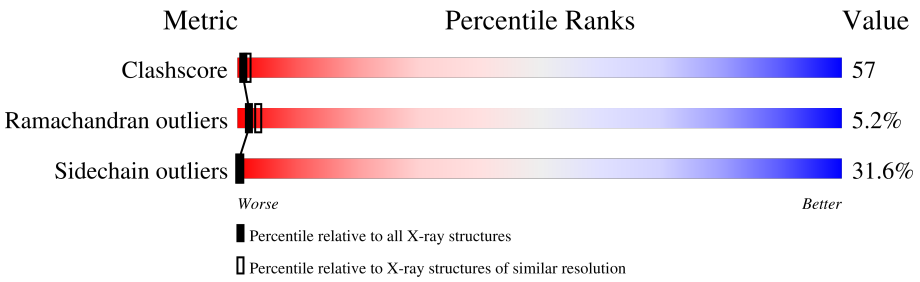
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	140	10% 39% 29% 13% 9%
1	B	140	11% 39% 31% 10% 9%
1	C	140	13% 34% 33% 11% 9%
1	D	140	16% 33% 30% 11% 9%
1	E	140	16% 29% 34% 12% 9%
1	F	140	13% 34% 30% 14% 9%
1	G	140	13% 36% 31% 11% 9%
1	H	140	11% 33% 28% 19% 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 (i)

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.

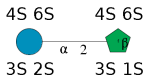
- Molecule 1 is a protein called ACIDIC FIBROBLAST GROWTH FACTOR.

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

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
			Total	C	O	S			
2	I	2	55	12	35	8	0	0	0
2	J	2	55	12	35	8	0	0	0
2	K	2	55	12	35	8	0	0	0
2	L	2	55	12	35	8	0	0	0
2	M	2	55	12	35	8	0	0	0
2	N	2	55	12	35	8	0	0	0
2	O	2	55	12	35	8	0	0	0
2	P	2	55	12	35	8	0	0	0

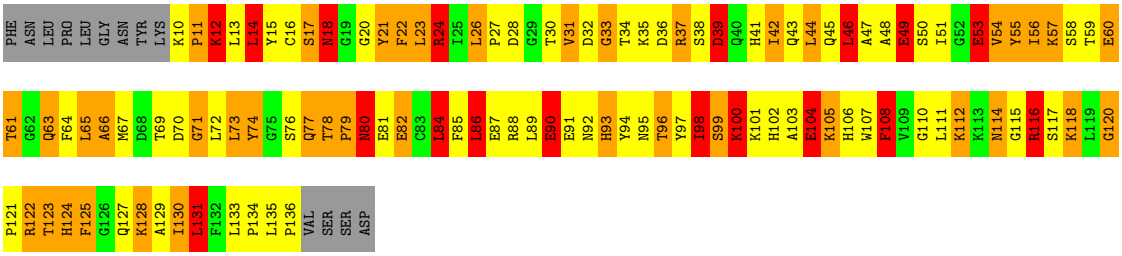
3 Residue-property plots (i)

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.

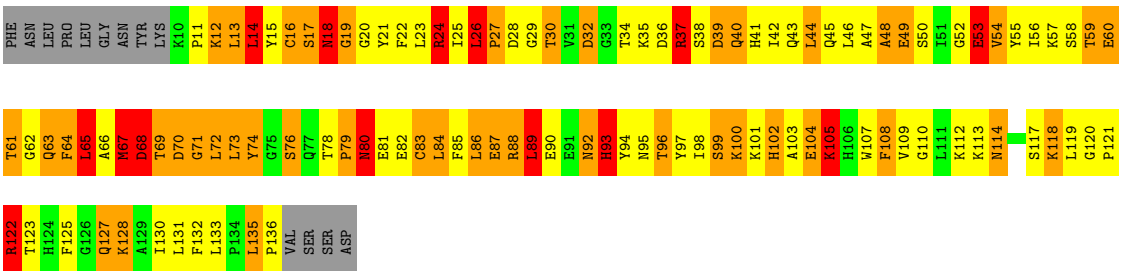
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 10% 39% 29% 13% 9%



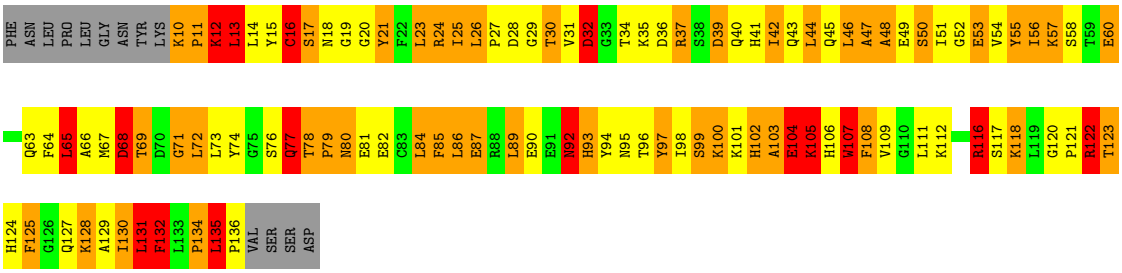
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain B: 11% 39% 31% 10% 9%



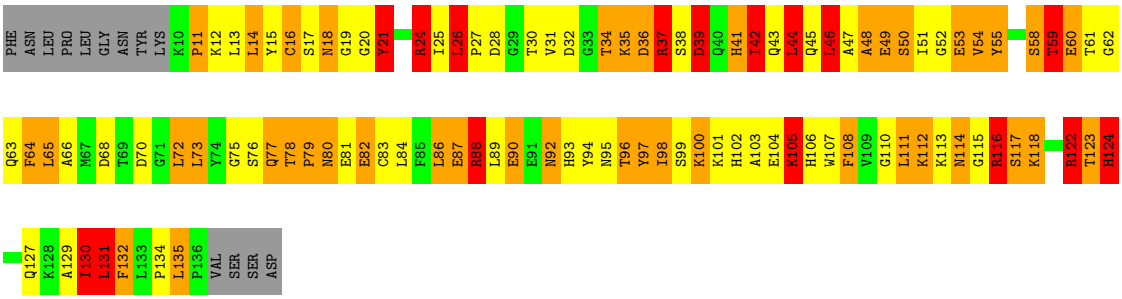
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain C: 13% 34% 33% 11% 9%



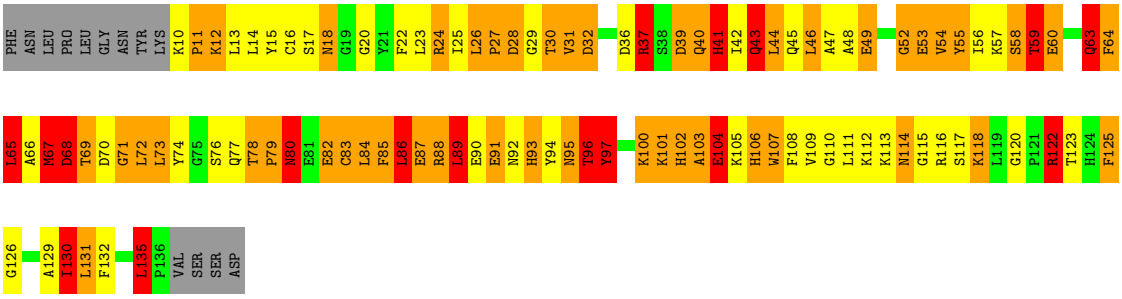
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain D: 16% 33% 30% 11% 9%



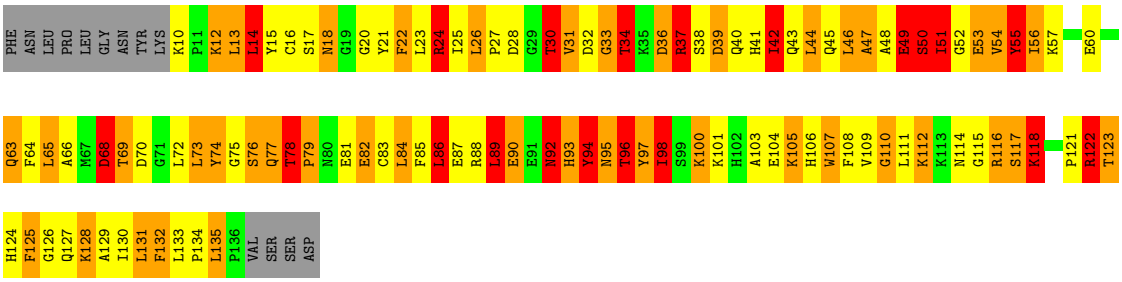
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain E: 16% 29% 34% 12% 9%



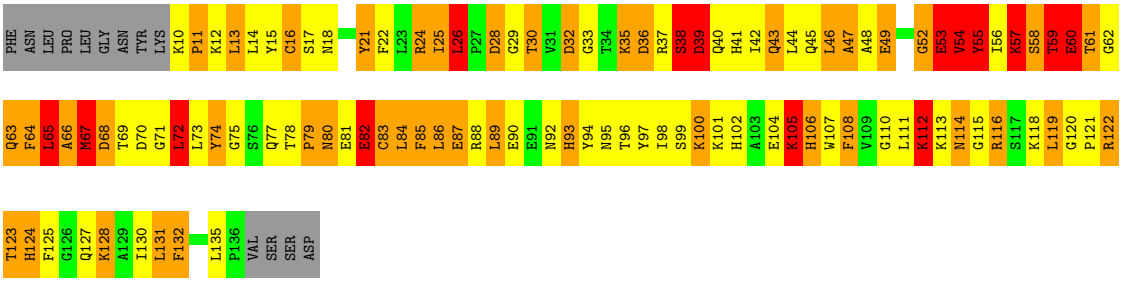
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain F: 13% 34% 30% 14% 9%



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain G: 13% 36% 31% 11% 9%



• 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:

• 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:

• 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:

• 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:

• 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:

• 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%

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 O: 100%

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 P: 100%

GU41
YYJ2

4 Data and refinement statistics (i)

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	0.87	0/1007	1.54	8/1363 (0.6%)
1	B	0.91	0/1007	1.48	8/1363 (0.6%)
1	C	0.89	0/1007	1.50	10/1363 (0.7%)
1	D	0.89	0/1007	1.49	11/1363 (0.8%)
1	E	0.91	0/1007	1.49	9/1363 (0.7%)
1	F	0.90	0/1007	1.52	8/1363 (0.6%)
1	G	0.89	0/1007	1.46	4/1363 (0.3%)
1	H	0.90	0/1007	1.51	8/1363 (0.6%)
All	All	0.89	0/8056	1.50	66/10904 (0.6%)

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

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	107	TRP	CD1-CG-CD2	11.01	115.11	106.30
1	A	24	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	D	37	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	E	24	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	D	24	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	107	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	C	107	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	F	24	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	H	122	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	E	107	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	F	107	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	D	107	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	B	107	TRP	CD1-CG-CD2	7.89	112.62	106.30
1	F	122	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	E	24	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	107	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	H	107	TRP	CD1-CG-CD2	7.47	112.27	106.30
1	B	122	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	107	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	21	TYR	O-C-N	-7.37	110.91	122.70
1	G	107	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	G	55	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	F	107	TRP	CG-CD1-NE1	-7.04	103.06	110.10
1	D	39	ASP	CB-CG-OD2	6.91	124.52	118.30
1	B	107	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	E	107	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	D	116	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	107	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	E	37	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	18	ASN	C-N-CA	-6.42	108.81	122.30
1	H	107	TRP	CE2-CD2-CG	-6.42	102.16	107.30
1	C	32	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	125	PHE	CB-CG-CD1	-6.21	116.46	120.80
1	G	107	TRP	CE2-CD2-CG	-6.17	102.37	107.30
1	D	122	ARG	CD-NE-CZ	-6.15	114.99	123.60
1	C	24	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	68	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	24	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	107	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	H	48	ALA	CB-CA-C	-5.85	101.32	110.10
1	E	78	THR	N-CA-CB	-5.75	99.38	110.30
1	D	21	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	C	122	ARG	NE-CZ-NH1	-5.51	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	107	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	D	116	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	H	55	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	H	27	PRO	O-C-N	-5.46	113.96	122.70
1	D	122	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	107	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	C	107	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	24	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	55	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	C	132	PHE	O-C-N	-5.41	114.05	122.70
1	G	107	TRP	NE1-CE2-CZ2	-5.30	124.57	130.40
1	E	68	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	E	107	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	C	116	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	H	37	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	F	42	ILE	O-C-N	-5.19	114.39	122.70
1	F	97	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	C	107	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	D	11	PRO	CA-N-CD	-5.08	104.39	111.50
1	E	122	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	H	68	ASP	CB-CA-C	-5.05	100.31	110.40
1	B	107	TRP	CB-CG-CD1	-5.04	120.45	127.00

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

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Mol	Chain	Res	Type	Group
1	A	123	THR	Mainchain
1	A	124	HIS	Mainchain
1	A	125	PHE	Mainchain,Sidechain
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
1	A	20	GLY	Mainchain
1	A	21	TYR	Mainchain
1	A	22	PHE	Mainchain
1	A	24	ARG	Mainchain,Sidechain
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	Mainchain,Sidechain
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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	Mainchain,Sidechain
1	A	76	SER	Mainchain
1	A	77	GLN	Mainchain
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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	Mainchain,Sidechain
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
1	B	34	THR	Mainchain
1	B	36	ASP	Mainchain
1	B	37	ARG	Mainchain
1	B	38	SER	Mainchain
1	B	39	ASP	Mainchain,Sidechain
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	Mainchain,Sidechain
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	Mainchain,Sidechain
1	B	69	THR	Mainchain
1	B	70	ASP	Sidechain
1	B	71	GLY	Mainchain
1	B	74	TYR	Mainchain,Sidechain
1	B	76	SER	Mainchain
1	B	79	PRO	Mainchain

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Mol	Chain	Res	Type	Group
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	Mainchain,Sidechain
1	B	88	ARG	Mainchain
1	B	89	LEU	Mainchain
1	B	92	ASN	Mainchain
1	B	93	HIS	Mainchain,Sidechain
1	B	95	ASN	Mainchain
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	Mainchain,Sidechain
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	Mainchain,Sidechain
1	C	16	CYS	Mainchain
1	C	20	GLY	Mainchain
1	C	21	TYR	Mainchain,Sidechain
1	C	23	LEU	Mainchain
1	C	25	ILE	Mainchain
1	C	27	PRO	Mainchain
1	C	29	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	C	30	THR	Mainchain
1	C	32	ASP	Mainchain,Sidechain
1	C	35	LYS	Mainchain
1	C	36	ASP	Mainchain,Sidechain
1	C	37	ARG	Mainchain
1	C	39	ASP	Mainchain,Sidechain
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
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	Mainchain,Sidechain
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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	Mainchain,Sidechain
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	Mainchain,Sidechain
1	D	37	ARG	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
1	D	52	GLY	Mainchain
1	D	53	GLU	Mainchain,Sidechain
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	Mainchain,Sidechain
1	D	65	LEU	Mainchain
1	D	70	ASP	Sidechain
1	D	72	LEU	Mainchain
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	Mainchain,Sidechain
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	Mainchain,Sidechain
1	D	99	SER	Mainchain
1	E	10	LYS	Mainchain
1	E	102	HIS	Mainchain
1	E	103	ALA	Mainchain
1	E	104	GLU	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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
1	E	28	ASP	Mainchain
1	E	31	VAL	Mainchain
1	E	32	ASP	Sidechain
1	E	36	ASP	Mainchain
1	E	37	ARG	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
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
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	Mainchain,Sidechain
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
1	F	97	TYR	Mainchain,Sidechain
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
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	Mainchain,Sidechain
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	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
1	G	60	GLU	Mainchain
1	G	64	PHE	Mainchain,Sidechain
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
1	G	82	GLU	Mainchain
1	G	83	CYS	Mainchain
1	G	85	PHE	Mainchain
1	G	86	LEU	Mainchain
1	G	87	GLU	Mainchain,Sidechain
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	Mainchain,Sidechain
1	H	125	PHE	Mainchain,Sidechain
1	H	129	ALA	Mainchain
1	H	13	LEU	Mainchain
1	H	130	ILE	Mainchain

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Mol	Chain	Res	Type	Group
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	Mainchain,Sidechain
1	H	27	PRO	Mainchain
1	H	28	ASP	Sidechain
1	H	30	THR	Mainchain
1	H	32	ASP	Mainchain
1	H	35	LYS	Mainchain
1	H	37	ARG	Mainchain
1	H	38	SER	Mainchain
1	H	39	ASP	Mainchain,Sidechain
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	Mainchain,Sidechain
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	Mainchain,Sidechain
1	H	76	SER	Mainchain
1	H	77	GLN	Mainchain
1	H	79	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	H	80	ASN	Mainchain
1	H	81	GLU	Mainchain
1	H	84	LEU	Mainchain
1	H	85	PHE	Mainchain,Sidechain
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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	983	0	944	109	0
1	B	983	0	944	95	0
1	C	983	0	944	112	0
1	D	983	0	944	96	0
1	E	983	0	944	86	0
1	F	983	0	944	84	0
1	G	983	0	944	122	0
1	H	983	0	944	121	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	27	0
2	P	55	0	6	18	0
All	All	8304	0	7600	899	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 57.

All (899) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:124:HIS:C	1:G:124:HIS:CD2	2.49	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:124:HIS:C	1:F:130:ILE:HD11	2.03	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:CD2	1:G:124:HIS:O	2.39	0.76
1:G:124:HIS:CD2	1:G:125:PHE:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:108:PHE:CD1	1:C:130:ILE:HD11	2.25	0.71
1:G:124:HIS:C	1:G:124:HIS:HD2	1.90	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:C:104:GLU:CD	1:C:104:GLU:H	1.95	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
1:H:79:PRO:O	1:H:80:ASN:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:47:ALA:O	1:F:55:TYR:HD2	1.76	0.67
1:G:47:ALA:C	1:G:54:VAL:HG12	2.14	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:G:124:HIS:HD2	1:G:125:PHE:C	1.97	0.67
1:F:26:LEU:CD1	1:F:26:LEU:N	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:134:PRO:C	1:C:135:LEU:HD23	2.15	0.66
1:D:87:GLU:O	1:D:88:ARG:CB	2.43	0.66
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
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:F:36:ASP:C	1:F:38:SER:H	1.98	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: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: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:H:24:ARG:NE	1:H:26:LEU:HD11	2.13	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:B:68:ASP:HB3	1:B:72:LEU:H	1.62	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
1:F:37:ARG:HH21	1:F:135:LEU:HD13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:PHE:HE1	1:D:78:THR:HA	1.62	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: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:F:89:LEU:C	1:F:90:GLU:HG2	2.20	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H:89:LEU:C	1:H:90:GLU:HG2	2.21	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:E:39:ASP:OD1	1:E:39:ASP:C	2.38	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: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: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:E:94:TYR:C	1:E:95:ASN:HD22	2.05	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
1:B:89:LEU:HD12	1:B:89:LEU:C	2.22	0.59
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:A:11:PRO:C	1:A:12:LYS:HD3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ALA:C	1:C:105:LYS:H	2.06	0.59
1:F:28:ASP:OD1	1:F:28:ASP:C	2.41	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:G:89:LEU:C	1:G:90:GLU:HG2	2.23	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: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
1:D:92:ASN:CG	1:D:92:ASN:O	2.39	0.58
1:C:103:ALA:C	1:C:105:LYS:N	2.57	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
2:P:2:YYJ:O3S3	2:P:2:YYJ:O1	2.22	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
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:C:131:LEU:HD23	1:C:131:LEU:C	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:ILE:HD11	1:D:106:HIS:C	2.24	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: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: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: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:H:85:PHE:CE2	1:H:109:VAL:CG2	2.89	0.55
1:H:85:PHE:CD2	1:H:109:VAL:HG21	2.42	0.55
1:C:19:GLY:HA3	1:C:21:TYR:CD2	2.41	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:D:58:SER:O	1:D:59:THR:C	2.42	0.55
1:H:13:LEU:N	1:H:13:LEU:HD13	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:60:GLU:N	1:C:60:GLU:CD	2.59	0.55
1:C:124:HIS:C	1:C:124:HIS:HD1	2.10	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:B:22:PHE:O	1:B:23:LEU:C	2.42	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:C:104:GLU:CD	1:C:104:GLU:N	2.58	0.54
1:E:122:ARG:HD2	2:M:2:YYJ:O2S3	2.06	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:80:ASN:C	1:B:82:GLU:N	2.59	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
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:E:27:PRO:C	1:E:29:GLY:N	2.60	0.53
1:E:49:GLU:N	1:E:53:GLU:O	2.41	0.53
2:O:1:GU4:S6	2:O:2:YYJ:C6	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:45:GLN:C	1:C:46:LEU:HD23	2.30	0.52
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:H:24:ARG:CD	1:H:26:LEU:CD1	2.87	0.52
1:E:104:GLU:H	1:E:104:GLU:CD	2.13	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:G:21:TYR:CE1	1:G:35:LYS:HD3	2.44	0.52
1:H:80:ASN:HD22	1:H:80:ASN:C	2.13	0.52
1:A:112:LYS:HB3	2:I:1:GU4:O25	2.10	0.51
1:G:24:ARG:HD2	1:G:26:LEU:HD22	1.92	0.51
1:H:37:ARG:C	1:H:42:ILE:HD11	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:124:HIS:ND1	1:D:124:HIS:C	2.64	0.51
1:B:102:HIS:CB	1:B:105:LYS:HG3	2.38	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: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: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:D:92:ASN:C	1:D:93:HIS:CD2	2.85	0.50
1:G:57:LYS:O	1:G:57:LYS:CG	2.58	0.50
1:H:124:HIS:C	1:H:125:PHE:O	2.48	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:D:45:GLN:C	1:D:46:LEU:HD23	2.32	0.50
1:E:27:PRO:C	1:E:29:GLY:H	2.13	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
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:F:13:LEU:O	1:F:134:PRO:HA	2.11	0.50
1:C:131:LEU:C	1:C:131:LEU:CD2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:39:ASP:O	1:G:42:ILE:CG1	2.57	0.50
1:G:122:ARG:C	1:G:123:THR:O	2.47	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:E:24:ARG:HD3	1:E:26:LEU:HD13	1.93	0.50
1:F:49:GLU:O	1:F:50:SER:CB	2.59	0.49
1:H:29:GLY:O	1:H:30:THR:C	2.50	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: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: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: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
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:A:112:LYS:HB3	1:A:112:LYS:HZ3	1.77	0.48
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:C:89:LEU:HD13	1:C:89:LEU:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:36:ASP:C	1:F:38:SER:N	2.66	0.48
1:H:14:LEU:HD12	1:H:23:LEU:HD23	1.95	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:C:28:ASP:OD1	1:C:28:ASP:C	2.52	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:H:104:GLU:CD	1:H:104:GLU:N	2.67	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: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:G:57:LYS:HD2	1:G:58:SER:C	2.34	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: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:57:LYS:O	1:A:57:LYS:HG2	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:112:LYS:HB3	1:A:112:LYS:HZ2	1.78	0.47
1:D:89:LEU:C	1:D:90:GLU:HG2	2.35	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:B:71:GLY:HA3	1:B:121:PRO:HD3	1.96	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: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:H:112:LYS:HE2	1:H:112:LYS:HB3	1.61	0.46
1:C:124:HIS:C	1:C:124:HIS:ND1	2.67	0.46
1:E:48:ALA:HA	1:E:53:GLU:O	2.15	0.46
1:B:119:LEU:O	1:B:120:GLY:C	2.52	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
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:80:ASN:HD22	1:A:80:ASN:C	2.20	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: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:B:99:SER:O	1:B:100:LYS:C	2.54	0.46
1:C:112:LYS:HA	2:K:1:GU4:O25	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLN:O	1:E:59:THR:HB	2.15	0.46
1:B:98:ILE:HG13	1:B:108:PHE:CE2	2.51	0.45
1:D:78:THR:HG23	1:D:79:PRO:CD	2.46	0.45
1:G:123:THR:O	1:G:124:HIS:HB3	2.16	0.45
1:B:112:LYS:C	1:B:114:ASN:H	2.20	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: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:E:80:ASN:C	1:E:80:ASN:HD22	2.19	0.45
1:H:27:PRO:CB	1:H:61:THR:HG21	2.22	0.45
1:B:64:PHE:O	1:B:65:LEU:C	2.55	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
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: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:H:38:SER:O	1:H:39:ASP:C	2.52	0.45
2:I:2:YYJ:O1S3	2:I:2:YYJ:O1S4	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:127:GLN:C	1:D:129:ALA:N	2.71	0.45
1:F:118:LYS:HD2	2:N:1:GU4:O25	2.17	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:B:68:ASP:OD2	1:B:72:LEU:HB2	2.17	0.44
1:G:18:ASN:CG	1:G:18:ASN:O	2.54	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:A:89:LEU:C	1:A:90:GLU:OE1	2.56	0.44
1:E:91:GLU:C	1:E:93:HIS:H	2.20	0.44
1:G:124:HIS:O	1:G:130:ILE:HD13	2.17	0.44
1:A:17:SER:O	1:A:18:ASN:C	2.55	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:F:63:GLN:HE21	1:F:63:GLN:HB2	1.46	0.44
2:P:1:GU4:O2	2:P:2:YYJ:C1	2.65	0.44
1:C:128:LYS:HB2	1:C:128:LYS:HZ3	1.81	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
1:E:130:ILE:N	1:E:130:ILE:HD13	2.32	0.44
1:G:112:LYS:HZ3	2:O:2:YYJ:C4	2.30	0.44
1:C:135:LEU:HD23	1:C:135:LEU:N	2.31	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: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:F:95:ASN:O	1:F:131:LEU:HD12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:TYR:HE2	1:H:113:LYS:O	2.01	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: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: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:B:89:LEU:C	1:B:89:LEU:CD1	2.87	0.43
1:F:77:GLN:H	1:F:77:GLN:HG2	1.59	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
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: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:78:THR:C	1:F:79:PRO:O	2.53	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:C:89:LEU:C	1:C:90:GLU:HG2	2.40	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:F:50:SER:O	1:F:51:ILE:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:53:GLU:CD	1:E:100:LYS:HE3	2.39	0.42
1:H:24:ARG:CZ	1:H:26:LEU:HD11	2.48	0.42
1:H:80:ASN:C	1:H:82:GLU:N	2.73	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:80:ASN:C	1:B:82:GLU:H	2.22	0.42
1:B:90:GLU:OE2	1:B:125:PHE:CZ	2.72	0.42
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:B:18:ASN:O	1:B:20:GLY:N	2.53	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: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: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:18:ASN:O	1:D:19:GLY:C	2.57	0.42
1:D:97:TYR:CD1	1:D:97:TYR:N	2.87	0.42
1:A:63:GLN:HG2	1:A:63:GLN:H	1.53	0.42
1:B:98:ILE:O	1:B:99:SER:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:80:ASN:O	1:H:81:GLU:C	2.57	0.42
1:B:49:GLU:OE1	1:B:50:SER:N	2.52	0.41
1:G:38:SER:O	1:G:39:ASP:C	2.56	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:A:94:TYR:CE2	1:A:133:LEU:HB2	2.55	0.41
1:B:112:LYS:C	1:B:114:ASN:N	2.74	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
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:A:78:THR:C	1:A:79:PRO:O	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:112:LYS:HZ2	1:F:112:LYS:HB3	1.86	0.41
1:B:19:GLY:C	1:B:35:LYS:HE2	2.40	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:32:ASP:C	1:G:32:ASP:OD1	2.58	0.41
1:G:58:SER:O	1:G:62:GLY:HA2	2.20	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:H:104:GLU:CD	1:H:104:GLU:H	2.23	0.41
1:A:84:LEU:N	1:A:84:LEU:CD2	2.84	0.40
1:G:67:MET:C	1:G:68:ASP:O	2.56	0.40
1:B:71:GLY:C	1:B:120:GLY:H	2.23	0.40
1:C:98:ILE:CG2	1:C:103:ALA:HA	2.51	0.40
1:D:127:GLN:C	1:D:129:ALA:H	2.25	0.40
1:F:16:CYS:HB2	1:F:132:PHE:CE2	2.56	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:D:124:HIS:C	1:D:124:HIS:HD1	2.19	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:B:24:ARG:HH11	1:B:32:ASP:CG	2.24	0.40
1:D:89:LEU:O	1:D:90:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	4 9
1	B	125/140 (89%)	112 (90%)	9 (7%)	4 (3%)	4 9
1	C	125/140 (89%)	103 (82%)	18 (14%)	4 (3%)	4 9
1	D	125/140 (89%)	104 (83%)	16 (13%)	5 (4%)	3 6
1	E	125/140 (89%)	102 (82%)	16 (13%)	7 (6%)	2 3
1	F	125/140 (89%)	105 (84%)	11 (9%)	9 (7%)	1 1
1	G	125/140 (89%)	105 (84%)	15 (12%)	5 (4%)	3 6
1	H	125/140 (89%)	92 (74%)	19 (15%)	14 (11%)	0 0
All	All	1000/1120 (89%)	827 (83%)	121 (12%)	52 (5%)	2 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	C	51	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/122 (83%)	69 (68%)	32 (32%)	0	0
1	B	101/122 (83%)	68 (67%)	33 (33%)	0	0
1	C	101/122 (83%)	67 (66%)	34 (34%)	0	0
1	D	101/122 (83%)	74 (73%)	27 (27%)	0	1
1	E	101/122 (83%)	69 (68%)	32 (32%)	0	0
1	F	101/122 (83%)	71 (70%)	30 (30%)	0	1
1	G	101/122 (83%)	64 (63%)	37 (37%)	0	0
1	H	101/122 (83%)	71 (70%)	30 (30%)	0	1
All	All	808/976 (83%)	553 (68%)	255 (32%)	0	0

All (255) 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	26	LEU
1	A	34	THR
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

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Mol	Chain	Res	Type
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	108	PHE
1	A	112	LYS
1	A	116	ARG
1	A	118	LYS
1	A	130	ILE
1	A	131	LEU
1	B	12	LYS
1	B	14	LEU
1	B	26	LEU
1	B	30	THR
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	70	ASP
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

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Mol	Chain	Res	Type
1	B	101	LYS
1	B	104	GLU
1	B	105	LYS
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	16	CYS
1	C	17	SER
1	C	26	LEU
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	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	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

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Mol	Chain	Res	Type
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
1	D	65	LEU
1	D	68	ASP
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	14	LEU
1	E	17	SER
1	E	30	THR
1	E	37	ARG
1	E	43	GLN
1	E	44	LEU
1	E	46	LEU
1	E	57	LYS
1	E	59	THR
1	E	63	GLN
1	E	65	LEU
1	E	67	MET
1	E	68	ASP
1	E	69	THR

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Mol	Chain	Res	Type
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	95	ASN
1	E	96	THR
1	E	97	TYR
1	E	100	LYS
1	E	101	LYS
1	E	104	GLU
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	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	65	LEU
1	F	68	ASP
1	F	69	THR
1	F	76	SER
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	94	TYR
1	F	96	THR
1	F	98	ILE

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Mol	Chain	Res	Type
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	13	LEU
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	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

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Mol	Chain	Res	Type
1	G	131	LEU
1	H	12	LYS
1	H	13	LEU
1	H	24	ARG
1	H	26	LEU
1	H	30	THR
1	H	34	THR
1	H	43	GLN
1	H	44	LEU
1	H	53	GLU
1	H	54	VAL
1	H	55	TYR
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	100	LYS
1	H	104	GLU
1	H	125	PHE
1	H	128	LYS
1	H	131	LEU
1	H	136	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	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

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Mol	Chain	Res	Type
1	B	93	HIS
1	B	124	HIS
1	B	127	GLN
1	C	63	GLN
1	C	77	GLN
1	C	93	HIS
1	C	102	HIS
1	D	63	GLN
1	D	93	HIS
1	D	106	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	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	43	GLN
1	H	63	GLN
1	H	80	ASN
1	H	95	ASN
1	H	102	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1.49	4 (14%)	29,43,45	2.28	7 (24%)
2	YYJ	I	2	2	27,28,28	2.09	6 (22%)	28,46,46	1.59	3 (10%)
2	GU4	J	1	2	27,27,28	1.47	5 (18%)	29,43,45	2.07	7 (24%)
2	YYJ	J	2	2	27,28,28	1.78	5 (18%)	28,46,46	0.95	1 (3%)
2	GU4	K	1	2	27,27,28	1.51	4 (14%)	29,43,45	2.24	8 (27%)
2	YYJ	K	2	2	27,28,28	1.80	4 (14%)	28,46,46	1.53	5 (17%)
2	GU4	L	1	2	27,27,28	1.93	5 (18%)	29,43,45	1.55	2 (6%)
2	YYJ	L	2	2	27,28,28	1.45	4 (14%)	28,46,46	1.23	3 (10%)
2	GU4	M	1	2	27,27,28	1.66	5 (18%)	29,43,45	2.70	10 (34%)
2	YYJ	M	2	2	27,28,28	1.77	4 (14%)	28,46,46	0.99	1 (3%)
2	GU4	N	1	2	27,27,28	1.54	5 (18%)	29,43,45	1.47	3 (10%)
2	YYJ	N	2	2	27,28,28	1.54	4 (14%)	28,46,46	1.39	5 (17%)
2	GU4	O	1	2	27,27,28	1.47	4 (14%)	29,43,45	2.28	8 (27%)
2	YYJ	O	2	2	27,28,28	1.43	4 (14%)	28,46,46	1.34	2 (7%)
2	GU4	P	1	2	27,27,28	1.87	5 (18%)	29,43,45	1.56	4 (13%)
2	YYJ	P	2	2	27,28,28	1.74	5 (18%)	28,46,46	1.52	3 (10%)

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	-	9/21/38/41	0/1/1/1
2	YYJ	I	2	2	-	6/23/42/42	0/1/1/1
2	GU4	J	1	2	-	10/21/38/41	0/1/1/1
2	YYJ	J	2	2	-	14/23/42/42	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	13/21/38/41	0/1/1/1
2	YYJ	L	2	2	-	7/23/42/42	0/1/1/1
2	GU4	M	1	2	-	13/21/38/41	0/1/1/1
2	YYJ	M	2	2	-	15/23/42/42	0/1/1/1
2	GU4	N	1	2	-	9/21/38/41	0/1/1/1
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 (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	YYJ	O3-S3	-6.04	1.39	1.57
2	J	2	YYJ	O3-S3	-4.96	1.42	1.57
2	P	1	GU4	O4-S4	-4.92	1.42	1.57
2	L	1	GU4	O6-S6	-4.90	1.43	1.56
2	P	1	GU4	O2-S2	-4.77	1.43	1.57
2	P	2	YYJ	O3-S3	-4.70	1.43	1.57
2	L	1	GU4	O2-S2	-4.61	1.43	1.57
2	I	1	GU4	O4-S4	-4.60	1.43	1.57
2	N	2	YYJ	O3-S3	-4.50	1.44	1.57
2	K	2	YYJ	O6-S6	-4.49	1.44	1.56
2	M	1	GU4	O4-S4	-4.47	1.44	1.57
2	K	2	YYJ	O3-S3	-4.46	1.44	1.57
2	M	2	YYJ	O1-S1	-4.44	1.44	1.56
2	M	2	YYJ	O3-S3	-4.33	1.44	1.57
2	L	2	YYJ	O3-S3	-4.32	1.44	1.57
2	O	2	YYJ	O1-S1	-4.31	1.45	1.56
2	N	1	GU4	O6-S6	-4.30	1.45	1.56
2	J	2	YYJ	O1-S1	-4.28	1.45	1.56
2	K	2	YYJ	O1-S1	-4.27	1.45	1.56
2	P	2	YYJ	O1-S1	-4.22	1.45	1.56
2	O	1	GU4	O6-S6	-4.21	1.45	1.56
2	M	2	YYJ	O6-S6	-4.18	1.45	1.56
2	L	1	GU4	O4-S4	-4.14	1.45	1.57
2	N	1	GU4	O4-S4	-4.10	1.45	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	GU4	O3-S3	-4.09	1.45	1.57
2	I	2	YYJ	O4-S4	-4.06	1.45	1.57
2	J	2	YYJ	O6-S6	-4.06	1.45	1.56
2	P	1	GU4	O6-S6	-4.05	1.45	1.56
2	K	1	GU4	O4-S4	-4.01	1.45	1.57
2	M	1	GU4	O6-S6	-3.94	1.46	1.56
2	K	2	YYJ	O4-S4	-3.93	1.45	1.57
2	P	2	YYJ	O4-S4	-3.89	1.45	1.57
2	I	2	YYJ	O6-S6	-3.79	1.46	1.56
2	M	2	YYJ	O4-S4	-3.74	1.46	1.57
2	J	2	YYJ	O4-S4	-3.73	1.46	1.57
2	I	2	YYJ	O1-S1	-3.72	1.46	1.56
2	J	1	GU4	O4-S4	-3.68	1.46	1.57
2	J	1	GU4	O6-S6	-3.63	1.47	1.56
2	O	1	GU4	O4-S4	-3.59	1.46	1.57
2	I	1	GU4	O6-S6	-3.48	1.47	1.56
2	O	2	YYJ	O6-S6	-3.46	1.47	1.56
2	N	2	YYJ	O1-S1	-3.40	1.47	1.56
2	I	2	YYJ	O3-C3	-3.39	1.40	1.47
2	O	1	GU4	O2-S2	-3.34	1.47	1.57
2	M	1	GU4	O3-S3	-3.33	1.47	1.57
2	K	1	GU4	O2-S2	-3.30	1.47	1.57
2	J	1	GU4	O2-S2	-3.28	1.47	1.57
2	K	1	GU4	O6-S6	-3.27	1.48	1.56
2	L	2	YYJ	O1-S1	-3.24	1.48	1.56
2	P	1	GU4	O3-S3	-3.22	1.47	1.57
2	N	2	YYJ	O4-S4	-3.12	1.48	1.57
2	L	2	YYJ	O6-S6	-3.09	1.48	1.56
2	O	2	YYJ	O4-S4	-3.06	1.48	1.57
2	P	2	YYJ	O6-S6	-3.06	1.48	1.56
2	N	2	YYJ	O6-S6	-3.01	1.48	1.56
2	L	2	YYJ	O4-S4	-3.01	1.48	1.57
2	P	1	GU4	O2-C2	-3.01	1.42	1.47
2	M	1	GU4	C1-C2	2.95	1.56	1.51
2	O	1	GU4	O3-S3	-2.91	1.48	1.57
2	K	1	GU4	O3-S3	-2.89	1.48	1.57
2	O	2	YYJ	O3-S3	-2.87	1.48	1.57
2	J	1	GU4	O3-S3	-2.86	1.48	1.57
2	I	1	GU4	O3-S3	-2.80	1.49	1.57
2	N	1	GU4	O2-S2	-2.78	1.49	1.57
2	L	1	GU4	O2-C2	-2.76	1.43	1.47
2	I	1	GU4	O2-S2	-2.75	1.49	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	GU4	O3-S3	-2.62	1.49	1.57
2	P	2	YYJ	O2-C2	2.56	1.45	1.40
2	I	2	YYJ	O2-C2	2.51	1.45	1.40
2	M	1	GU4	O2-S2	-2.37	1.50	1.57
2	N	1	GU4	C3-C4	2.30	1.57	1.52
2	J	2	YYJ	O3-C3	-2.03	1.43	1.47
2	J	1	GU4	C3-C4	2.01	1.56	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1	GU4	C1-O5-C5	-8.06	101.27	112.19
2	M	1	GU4	C2-O2-S2	7.14	127.22	117.91
2	I	1	GU4	O2-C2-C3	6.87	114.26	106.65
2	J	1	GU4	C2-O2-S2	6.38	126.23	117.91
2	O	1	GU4	C4-O4-S4	6.30	131.05	118.88
2	M	1	GU4	C1-O5-C5	-5.77	104.38	112.19
2	O	1	GU4	C3-O3-S3	5.55	129.59	118.88
2	L	1	GU4	O4-C4-C3	-5.40	96.61	108.48
2	M	1	GU4	O6-C6-C5	5.31	117.53	107.62
2	J	1	GU4	C1-O5-C5	5.06	119.05	112.19
2	P	2	YYJ	C4-O4-S4	-4.93	109.35	118.88
2	O	1	GU4	C2-O2-S2	4.68	124.01	117.91
2	M	1	GU4	O5-C5-C4	-4.59	101.47	110.07
2	O	2	YYJ	O5-C5-C6	4.59	119.55	109.45
2	I	2	YYJ	C4-O4-S4	-4.47	110.23	118.88
2	I	1	GU4	C1-C2-C3	-4.43	102.78	109.40
2	I	1	GU4	C2-O2-S2	4.37	123.61	117.91
2	O	1	GU4	O2-C2-C3	4.33	111.45	106.65
2	J	1	GU4	C3-C4-C5	4.19	119.30	110.55
2	P	1	GU4	C1-O5-C5	-4.08	106.66	112.19
2	N	1	GU4	C3-C4-C5	3.99	118.89	110.55
2	I	2	YYJ	O3-C3-C4	-3.99	98.12	109.32
2	N	1	GU4	O2-C2-C3	3.94	111.01	106.65
2	O	2	YYJ	O2-C2-O5	3.88	117.00	109.50
2	I	1	GU4	O6-C6-C5	3.78	114.67	107.62
2	I	2	YYJ	O6-C6-C5	3.73	114.58	107.62
2	M	1	GU4	O5-C1-C2	3.70	116.90	109.41
2	K	1	GU4	C6-C5-C4	3.64	122.34	113.33
2	L	1	GU4	C1-O5-C5	-3.64	107.26	112.19
2	M	1	GU4	O5-C5-C6	3.63	115.64	107.61
2	N	2	YYJ	O4-C4-C3	3.61	116.75	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1	GU4	C1-C2-C3	3.57	114.73	109.40
2	P	1	GU4	O2-C2-C3	-3.55	102.72	106.65
2	K	1	GU4	O6-C6-C5	3.45	114.06	107.62
2	P	1	GU4	O4-C4-C3	-3.42	100.97	108.48
2	I	1	GU4	C6-C5-C4	3.41	121.78	113.33
2	P	2	YYJ	O3-C3-C4	-3.40	99.77	109.32
2	I	1	GU4	O4-C4-C3	-3.33	101.17	108.48
2	L	2	YYJ	C4-O4-S4	3.31	125.28	118.88
2	K	2	YYJ	C6-C5-C4	-3.27	103.57	114.40
2	K	2	YYJ	O5-C5-C4	3.23	108.88	103.49
2	K	1	GU4	C4-O4-S4	3.10	124.86	118.88
2	K	1	GU4	C2-O2-S2	3.09	121.94	117.91
2	K	2	YYJ	O4-C4-C3	3.03	115.50	108.91
2	K	1	GU4	C1-C2-C3	2.92	113.77	109.40
2	M	1	GU4	C6-C5-C4	2.86	120.39	113.33
2	K	2	YYJ	C4-O4-S4	-2.84	113.38	118.88
2	M	1	GU4	C4-O4-S4	2.82	124.33	118.88
2	O	1	GU4	C1-O5-C5	2.82	116.01	112.19
2	N	2	YYJ	O5-C5-C4	2.79	108.15	103.49
2	M	1	GU4	O4-C4-C3	2.75	114.53	108.48
2	J	2	YYJ	O3-C3-C4	-2.72	101.68	109.32
2	J	1	GU4	O6-C6-C5	2.72	112.69	107.62
2	M	1	GU4	C1-C2-C3	2.71	113.45	109.40
2	J	1	GU4	O5-C5-C4	2.67	115.08	110.07
2	N	1	GU4	C3-O3-S3	2.65	124.00	118.88
2	M	2	YYJ	C4-O4-S4	2.61	123.92	118.88
2	L	2	YYJ	O1-S1-O3S1	2.59	114.71	106.88
2	I	1	GU4	C3-O3-S3	2.57	123.83	118.88
2	J	1	GU4	O5-C1-C2	2.41	114.29	109.41
2	O	1	GU4	C3-C4-C5	-2.36	105.63	110.55
2	O	1	GU4	O6-C6-C5	2.33	111.97	107.62
2	J	1	GU4	C4-O4-S4	2.32	123.35	118.88
2	K	1	GU4	O5-C5-C4	-2.31	105.74	110.07
2	K	1	GU4	O5-C5-C6	2.28	112.67	107.61
2	O	1	GU4	O5-C1-C2	2.21	113.88	109.41
2	N	2	YYJ	O3-C3-C4	-2.19	103.16	109.32
2	L	2	YYJ	O5-C5-C4	2.17	107.11	103.49
2	N	2	YYJ	C6-C5-C4	-2.16	107.23	114.40
2	K	2	YYJ	O6-C6-C5	2.09	111.52	107.62
2	N	2	YYJ	O5-C5-C6	2.04	113.94	109.45
2	P	2	YYJ	C5-C4-C3	2.01	108.66	103.36

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	GU4	C4-C5-C6-O6
2	I	1	GU4	C3-O3-S3-O29
2	I	1	GU4	C2-O2-S2-O10
2	I	2	YYJ	C2-C1-O1-S1
2	I	2	YYJ	C6-O6-S6-O1S6
2	J	1	GU4	C4-O4-S4-O25
2	J	1	GU4	C4-O4-S4-O24
2	J	1	GU4	C2-O2-S2-O11
2	J	1	GU4	C2-O2-S2-O12
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-O1S4
2	J	2	YYJ	C4-O4-S4-O3S4
2	J	2	YYJ	C6-O6-S6-O1S6
2	J	2	YYJ	C6-O6-S6-O3S6
2	K	1	GU4	C6-O6-S6-O21
2	K	1	GU4	C4-O4-S4-O24
2	K	1	GU4	C3-O3-S3-O29
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	C4-O4-S4-O24
2	L	1	GU4	C2-C3-O3-S3
2	L	1	GU4	C2-O2-S2-O10
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	C4-O4-S4-O25

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Mol	Chain	Res	Type	Atoms
2	M	1	GU4	C4-O4-S4-O26
2	M	1	GU4	C4-O4-S4-O24
2	M	1	GU4	C3-O3-S3-O28
2	M	1	GU4	C3-O3-S3-O29
2	M	1	GU4	C3-O3-S3-O27
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
2	M	2	YYJ	C4-C5-C6-O6
2	M	2	YYJ	C3-O3-S3-O1S3
2	M	2	YYJ	C6-O6-S6-O1S6
2	M	2	YYJ	C6-O6-S6-O2S6
2	N	1	GU4	C3-O3-S3-O29
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	C4-O4-S4-O1S4
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	O	2	YYJ	C4-O4-S4-O3S4
2	P	2	YYJ	C2-C3-O3-S3
2	P	2	YYJ	C4-C5-C6-O6
2	P	2	YYJ	C1-O1-S1-O1S1
2	P	2	YYJ	C1-O1-S1-O2S1
2	P	2	YYJ	C1-O1-S1-O3S1
2	I	2	YYJ	C6-O6-S6-O3S6
2	K	1	GU4	C6-O6-S6-O23
2	L	1	GU4	C6-O6-S6-O23

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Mol	Chain	Res	Type	Atoms
2	M	2	YYJ	C6-O6-S6-O3S6
2	N	2	YYJ	C6-O6-S6-O3S6
2	O	1	GU4	C6-O6-S6-O23
2	O	2	YYJ	C1-O1-S1-O2S1
2	O	2	YYJ	C1-O1-S1-O3S1
2	O	2	YYJ	C6-O6-S6-O3S6
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	M	1	GU4	C6-O6-S6-O22
2	M	1	GU4	C6-O6-S6-O23
2	O	1	GU4	C6-O6-S6-O22
2	P	1	GU4	C6-O6-S6-O22
2	P	1	GU4	C6-O6-S6-O23
2	P	2	YYJ	O5-C5-C6-O6
2	J	1	GU4	C6-O6-S6-O21
2	O	2	YYJ	C6-O6-S6-O1S6
2	P	1	GU4	C6-O6-S6-O21
2	I	1	GU4	C4-O4-S4-O25
2	I	1	GU4	C4-O4-S4-O26
2	J	1	GU4	C4-O4-S4-O26
2	J	2	YYJ	C3-O3-S3-O2S3
2	J	2	YYJ	C4-O4-S4-O2S4
2	K	1	GU4	C3-O3-S3-O27
2	K	1	GU4	C2-O2-S2-O11
2	K	1	GU4	C2-O2-S2-O12
2	L	1	GU4	C4-O4-S4-O25
2	L	1	GU4	C2-O2-S2-O11
2	M	2	YYJ	C4-O4-S4-O2S4
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	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-O22
2	J	1	GU4	C6-O6-S6-O23

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Mol	Chain	Res	Type	Atoms
2	L	2	YYJ	C1-O1-S1-O3S1
2	N	2	YYJ	C6-O6-S6-O2S6
2	I	2	YYJ	C3-C4-O4-S4
2	K	1	GU4	C6-O6-S6-O22
2	N	1	GU4	C6-O6-S6-O22
2	N	1	GU4	C6-O6-S6-O23
2	N	2	YYJ	C1-O1-S1-O2S1
2	N	2	YYJ	C1-O1-S1-O3S1
2	O	2	YYJ	C6-O6-S6-O2S6
2	I	1	GU4	O5-C5-C6-O6
2	N	2	YYJ	O5-C5-C6-O6
2	I	2	YYJ	C5-C6-O6-S6
2	M	2	YYJ	C5-C6-O6-S6
2	L	2	YYJ	C1-O1-S1-O1S1
2	M	1	GU4	C6-O6-S6-O21
2	N	1	GU4	C6-O6-S6-O21
2	I	1	GU4	C4-O4-S4-O24
2	J	2	YYJ	C3-O3-S3-O1S3
2	K	1	GU4	C2-O2-S2-O10
2	M	2	YYJ	C4-O4-S4-O1S4
2	N	1	GU4	C2-O2-S2-O10
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	C4-C5-C6-O6
2	L	2	YYJ	C1-O1-S1-O2S1
2	P	2	YYJ	C4-C3-O3-S3
2	N	2	YYJ	C1-O1-S1-O1S1
2	O	2	YYJ	O5-C5-C6-O6
2	I	1	GU4	C2-O2-S2-O11
2	I	1	GU4	C2-O2-S2-O12
2	K	1	GU4	C3-O3-S3-O28
2	L	1	GU4	C4-O4-S4-O26
2	L	1	GU4	C2-O2-S2-O12
2	M	2	YYJ	C3-O3-S3-O3S3
2	P	2	YYJ	C3-O3-S3-O1S3
2	L	1	GU4	C5-C6-O6-S6
2	M	2	YYJ	C1-O1-S1-O3S1
2	J	1	GU4	O5-C5-C6-O6
2	L	2	YYJ	C3-C4-O4-S4

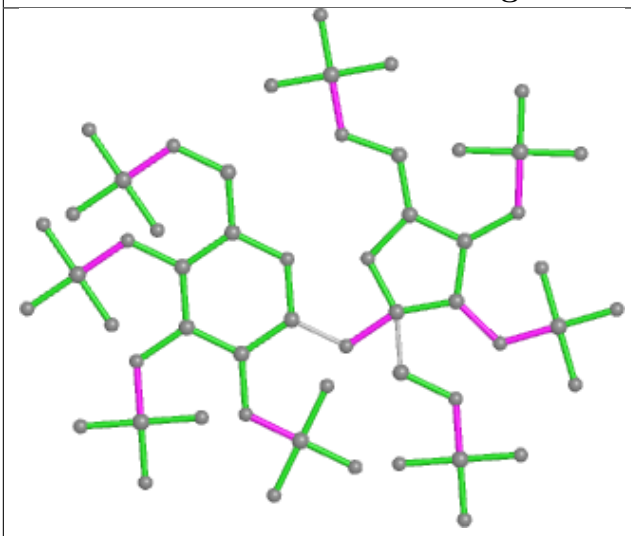
There are no ring outliers.

16 monomers are involved in 143 short contacts:

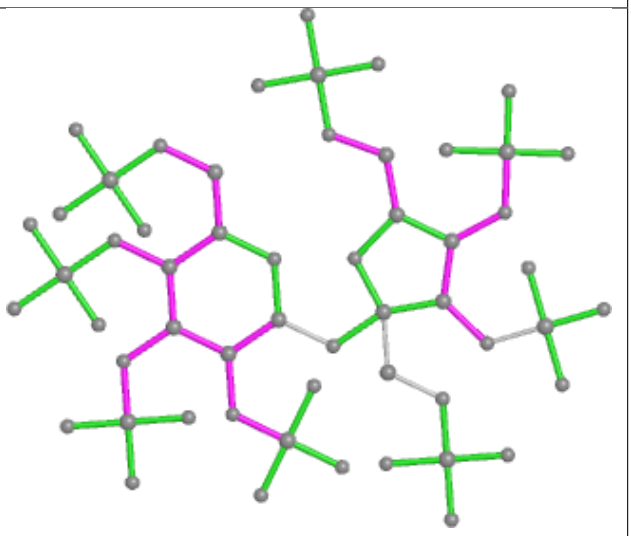
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	GU4	8	0
2	I	1	GU4	15	0
2	K	2	YYJ	9	0
2	P	1	GU4	13	0
2	O	2	YYJ	22	0
2	K	1	GU4	9	0
2	N	1	GU4	4	0
2	O	1	GU4	13	0
2	P	2	YYJ	11	0
2	N	2	YYJ	13	0
2	J	1	GU4	2	0
2	M	2	YYJ	14	0
2	L	2	YYJ	15	0
2	J	2	YYJ	6	0
2	I	2	YYJ	21	0
2	M	1	GU4	9	0

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

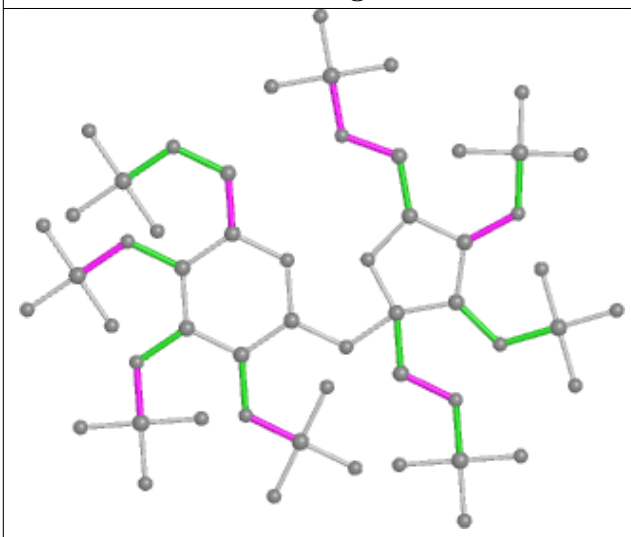
Oligosaccharide Chain I



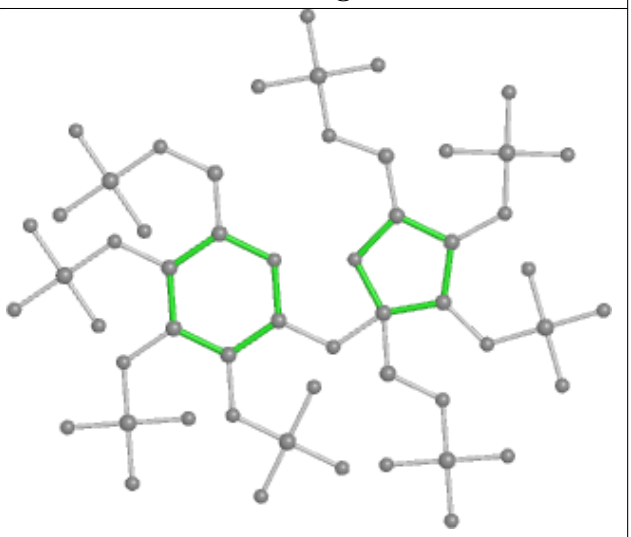
Bond lengths



Bond angles

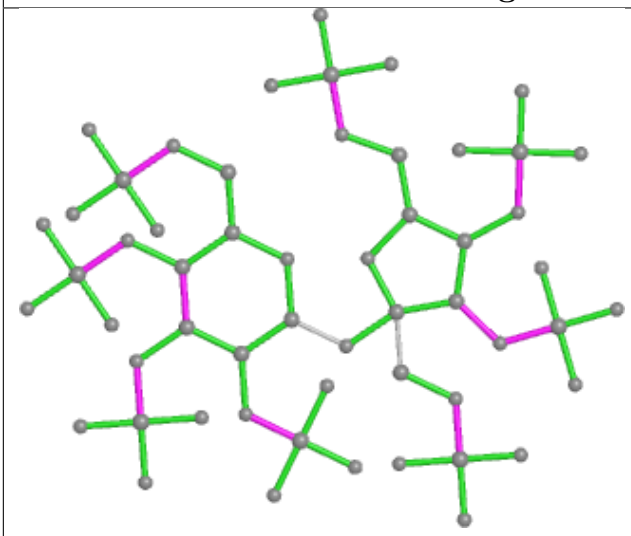


Torsions

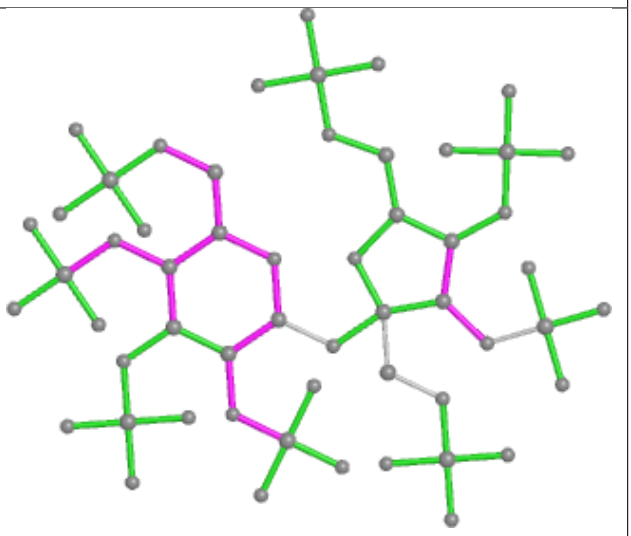


Rings

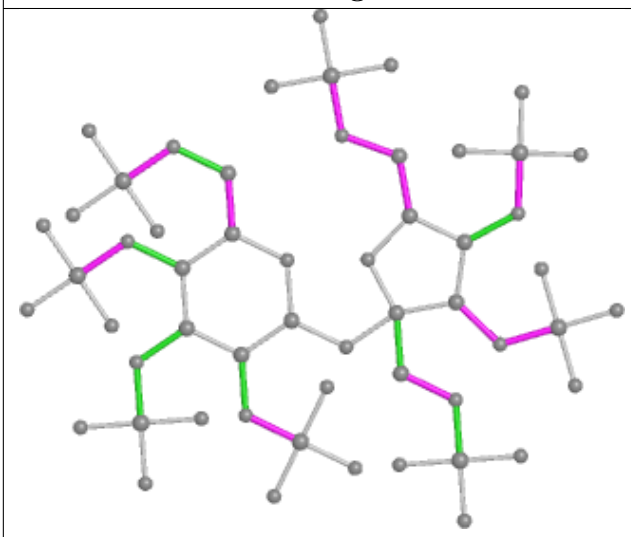
Oligosaccharide Chain J



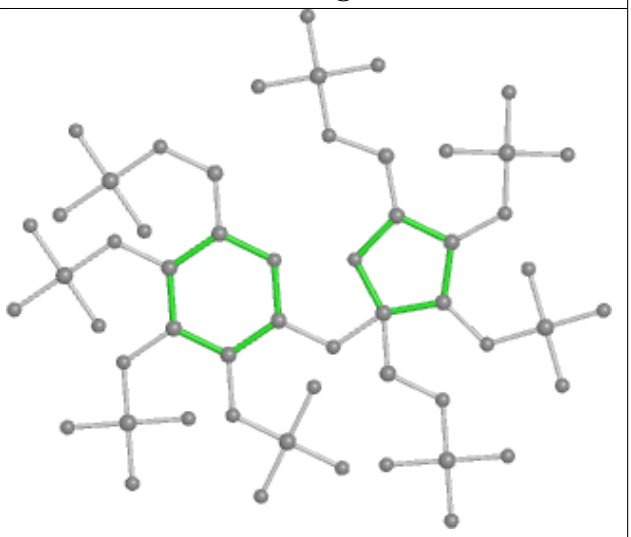
Bond lengths



Bond angles

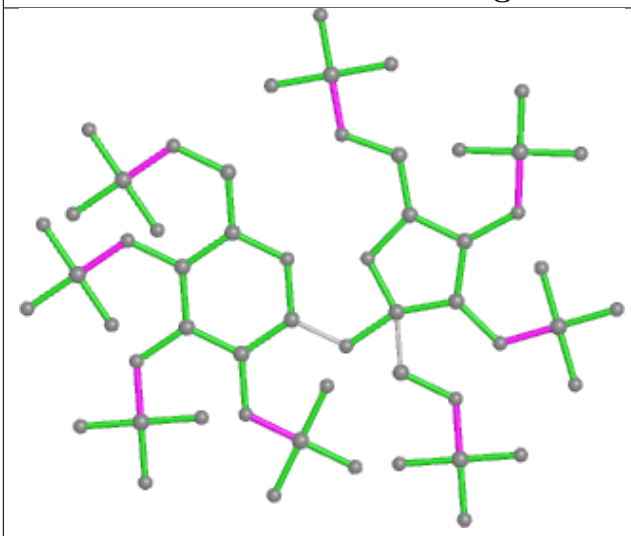


Torsions

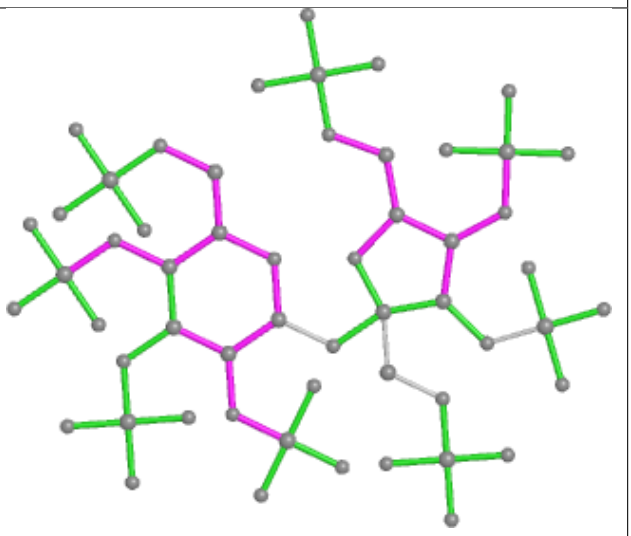


Rings

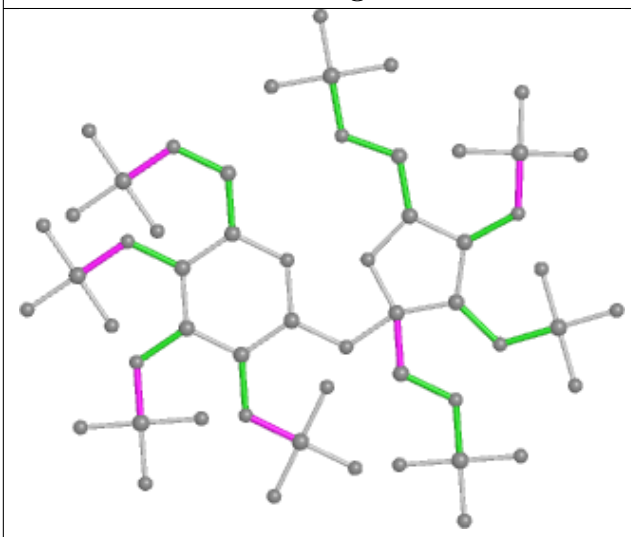
Oligosaccharide Chain K



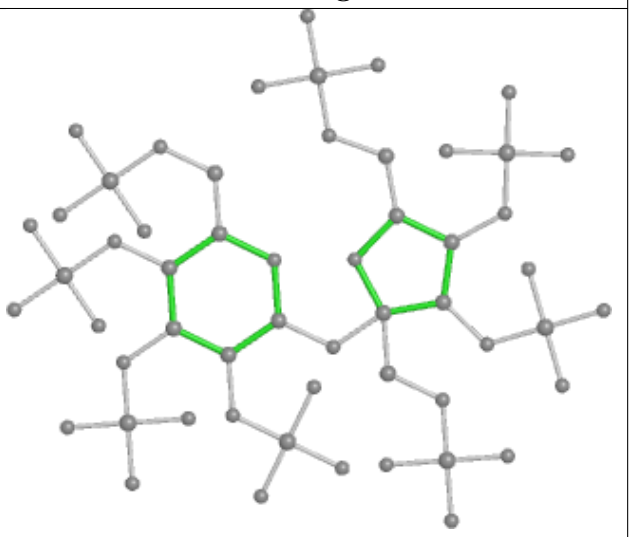
Bond lengths



Bond angles

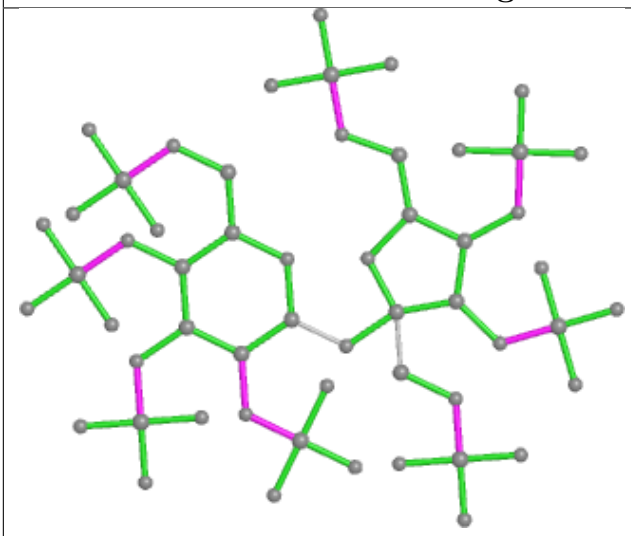


Torsions

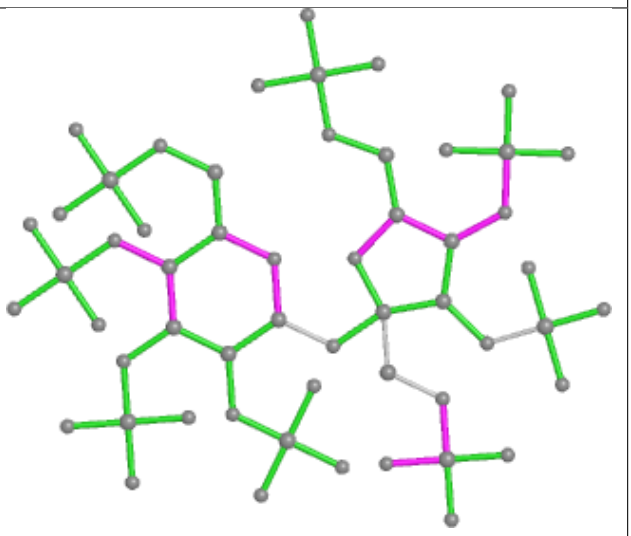


Rings

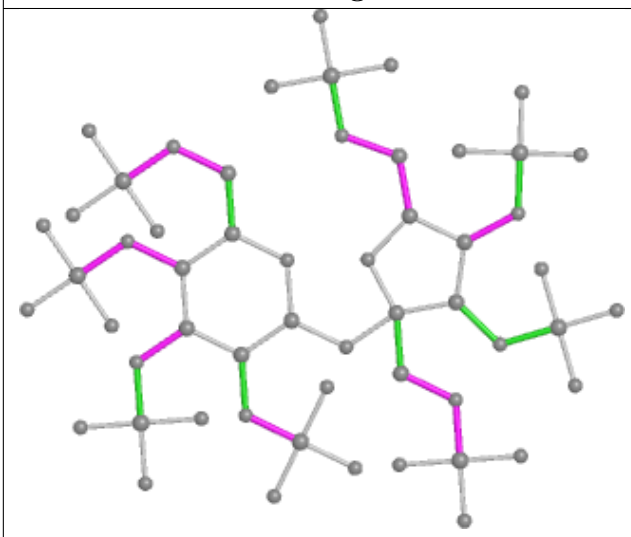
Oligosaccharide Chain L



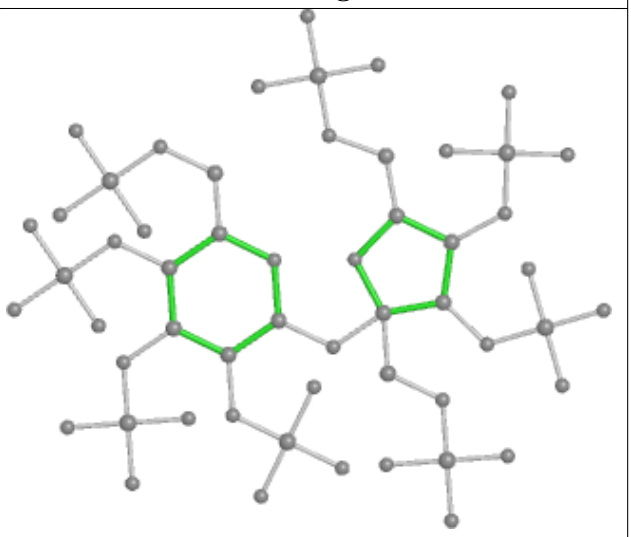
Bond lengths



Bond angles

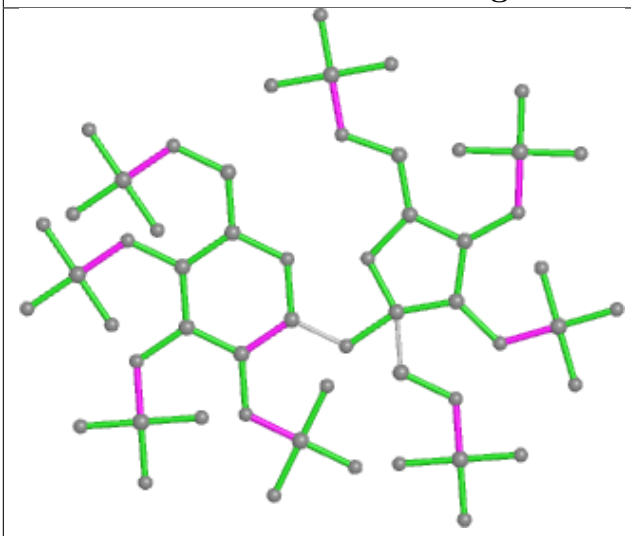


Torsions

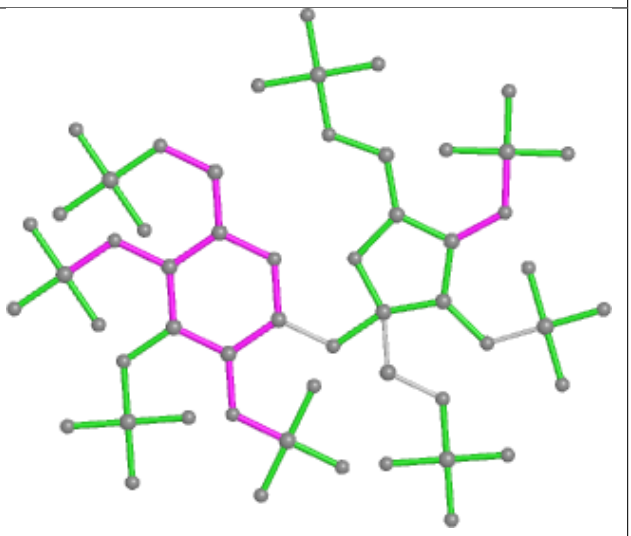


Rings

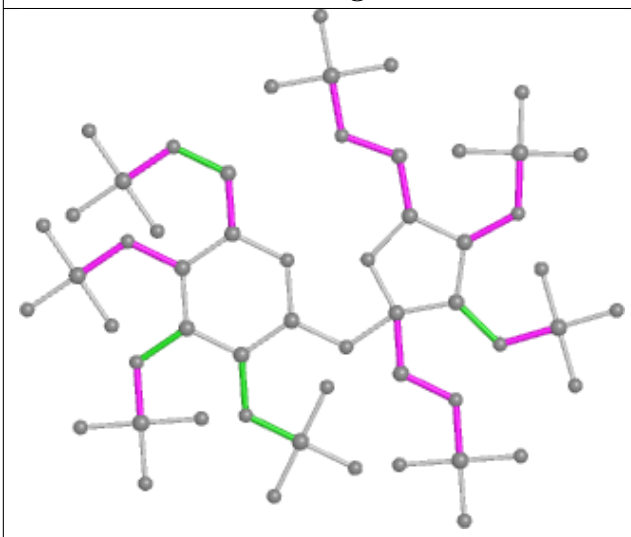
Oligosaccharide Chain M



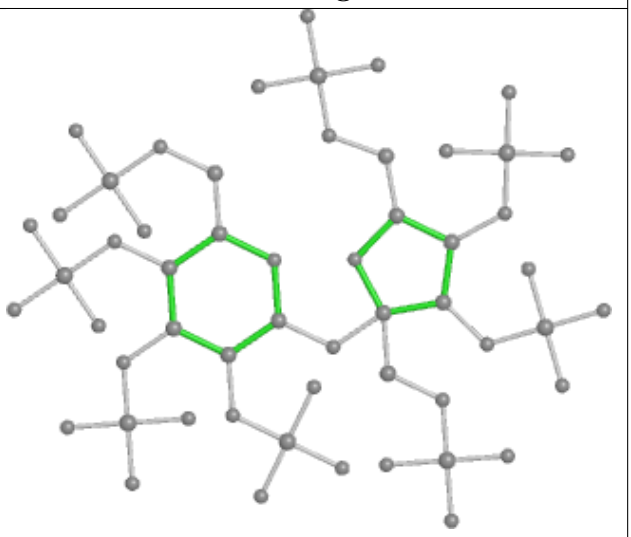
Bond lengths



Bond angles

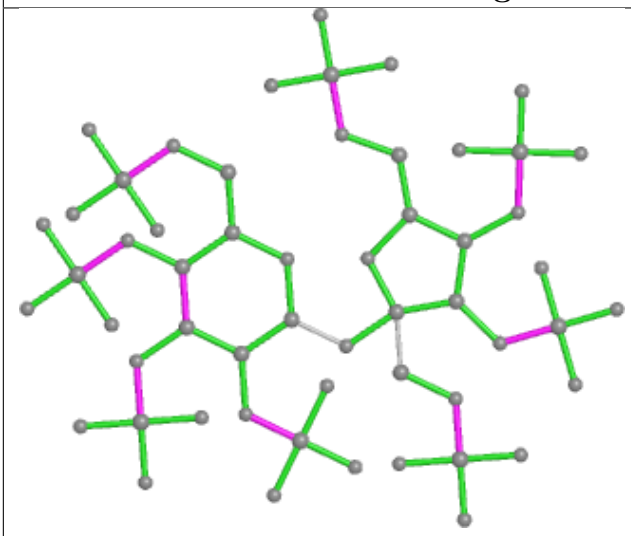


Torsions

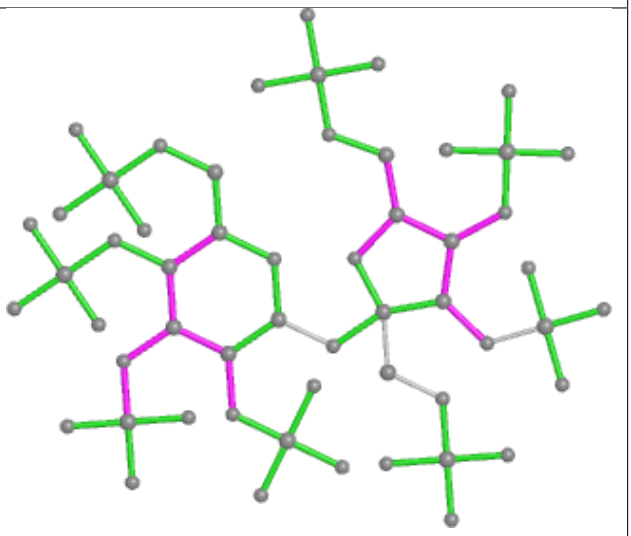


Rings

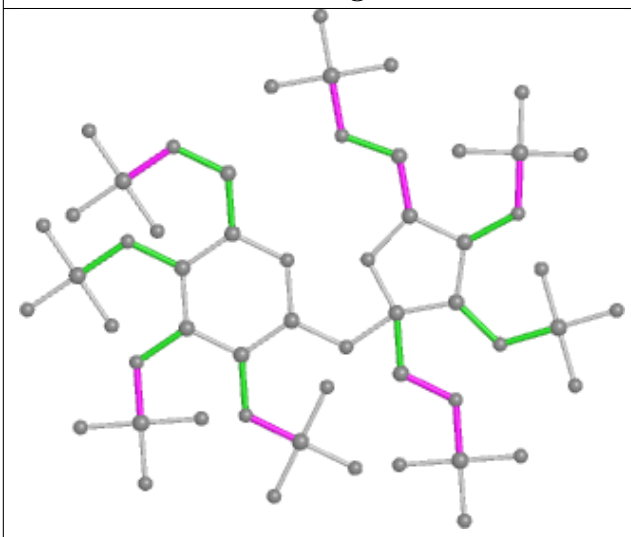
Oligosaccharide Chain N



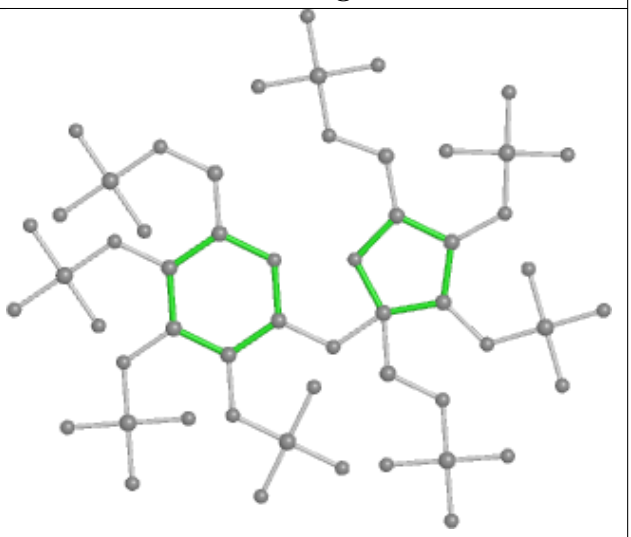
Bond lengths



Bond angles

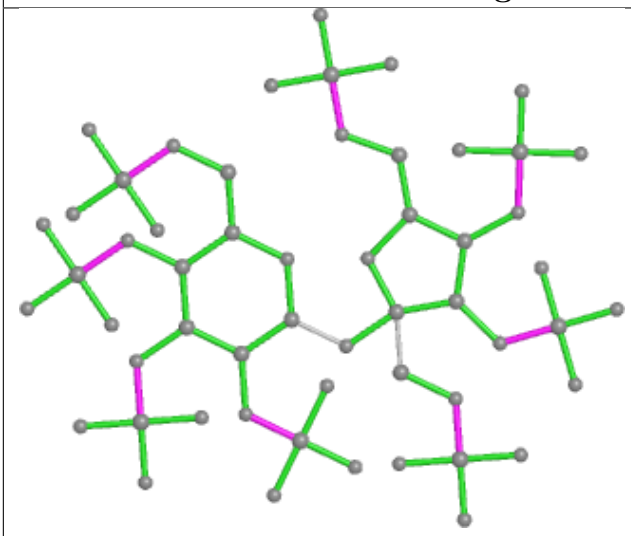


Torsions

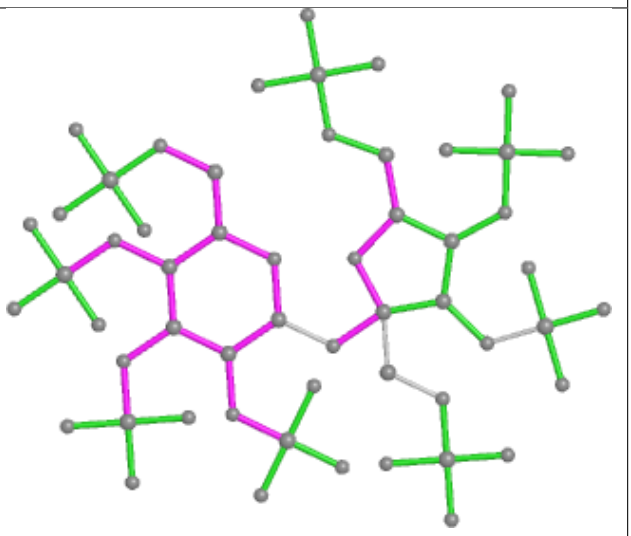


Rings

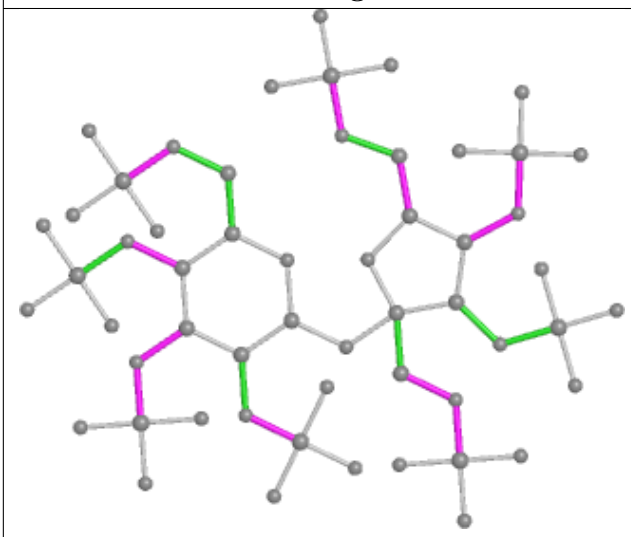
Oligosaccharide Chain O



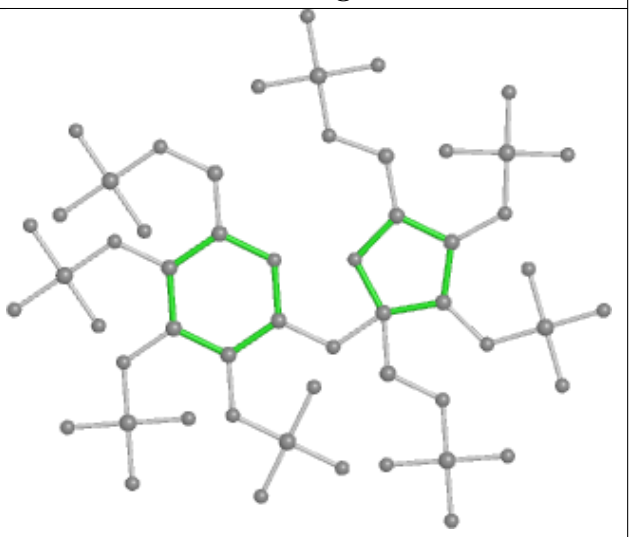
Bond lengths



Bond angles

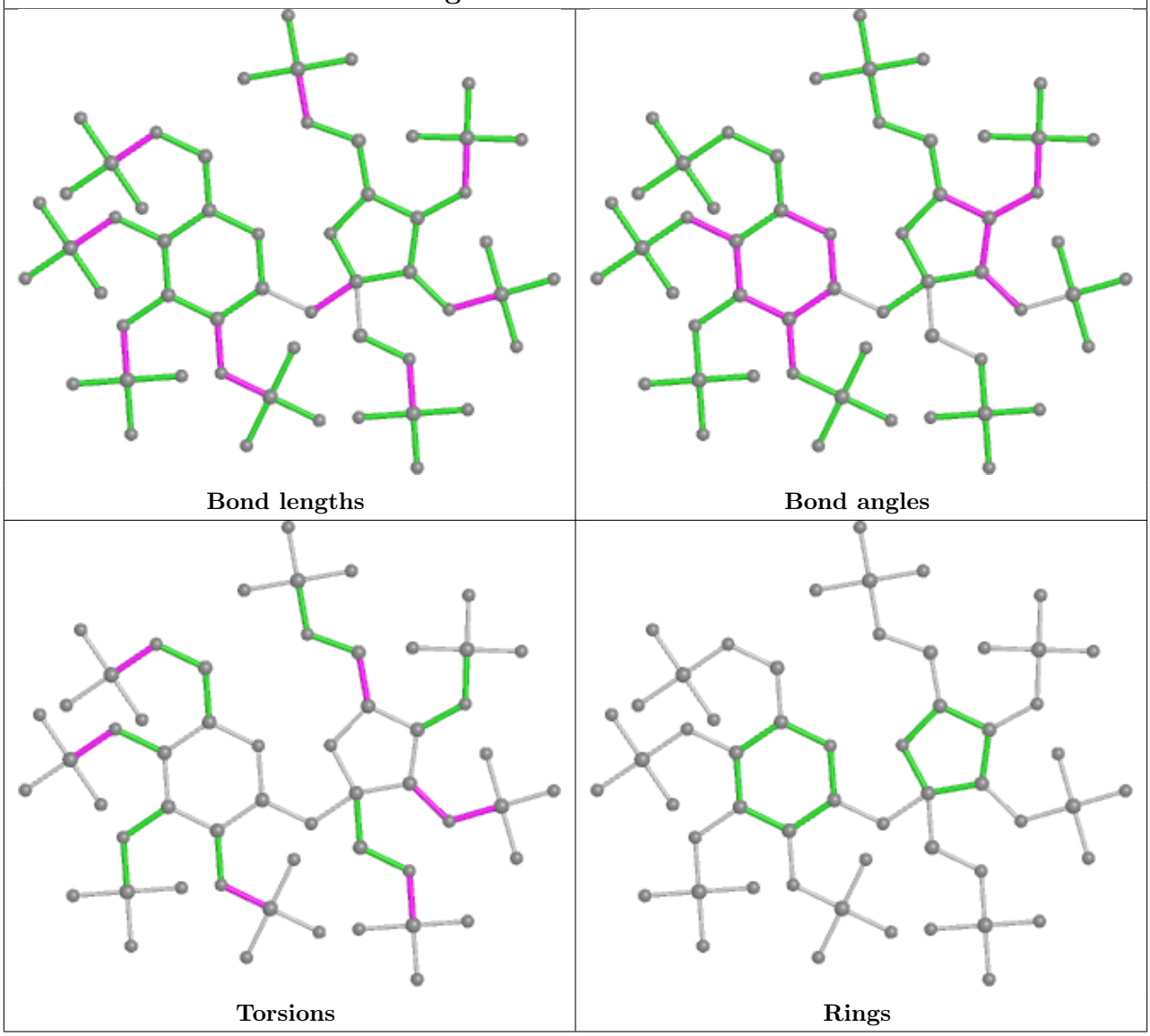


Torsions



Rings

Oligosaccharide Chain P



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.