



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:11 PM EDT

PDB ID : 1F6A
Title : Structure of the human ige-fc bound to its high affinity receptor fc(epsilon)ri(alpha)
Authors : Garman, S.C.; Wurzburg, B.A.; Tarchevskaya, S.S.; Kinet, J.P.; Jardetzky, T.S.
Deposited on : 2000-06-20
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.23.2

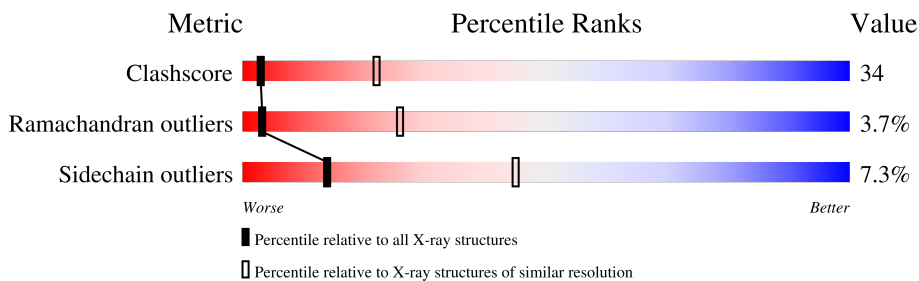
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	176	57% (Green), 38% (Yellow), ... (Red, Orange, Grey)
2	B	222	49% (Green), 40% (Yellow), 8% (Orange), ... (Red, Grey)
2	D	222	49% (Green), 40% (Yellow), 9% (Orange), ... (Red, Grey)
3	C	4	75% (Green), 25% (Yellow)
4	E	5	20% (Green), 40% (Yellow), 40% (Orange)
5	F	3	67% (Green), 33% (Yellow)
6	G	6	17% (Green), 67% (Yellow), 17% (Orange)
7	H	3	67% (Green), 33% (Yellow)

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
3	MAN	C	3	X	-	-	-
4	MAN	E	3	X	-	-	-
6	MAN	G	3	X	-	X	-
6	MAN	G	4	-	-	X	-
7	MAN	H	3	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5251 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1406	902	229	270	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	engineered mutation	UNP P12319
A	135	ALA	ASN	engineered mutation	UNP P12319
A	142	ALA	THR	engineered mutation	UNP P12319
A	143	ALA	VAL	cloning artifact	UNP P12319

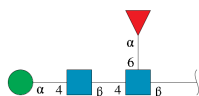
- Molecule 2 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	217	1711	1067	317	320	7	0	0	0
2	D	216	1704	1062	316	319	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

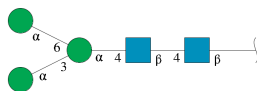
Chain	Residue	Modelled	Actual	Comment	Reference
B	326	ALA	-	cloning artifact	UNP P01854
B	327	ASP	-	cloning artifact	UNP P01854
B	328	PRO	-	cloning artifact	UNP P01854
B	329	CYS	-	cloning artifact	UNP P01854
D	326	ALA	-	cloning artifact	UNP P01854
D	327	ASP	-	cloning artifact	UNP P01854
D	328	PRO	-	cloning artifact	UNP P01854
D	329	CYS	-	cloning artifact	UNP P01854

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



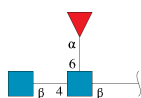
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	49	28	2	19	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



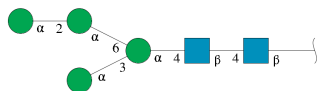
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	5	61	34	2	25	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



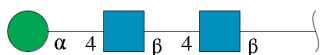
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	3	38	22	2	14	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



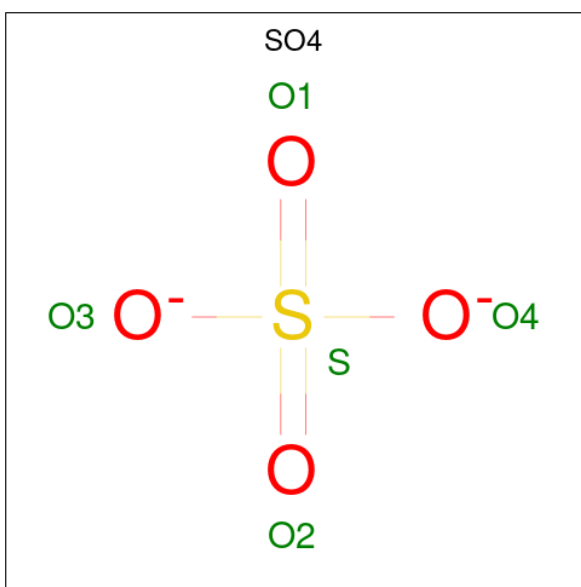
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	G	6	72	40	2	30	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



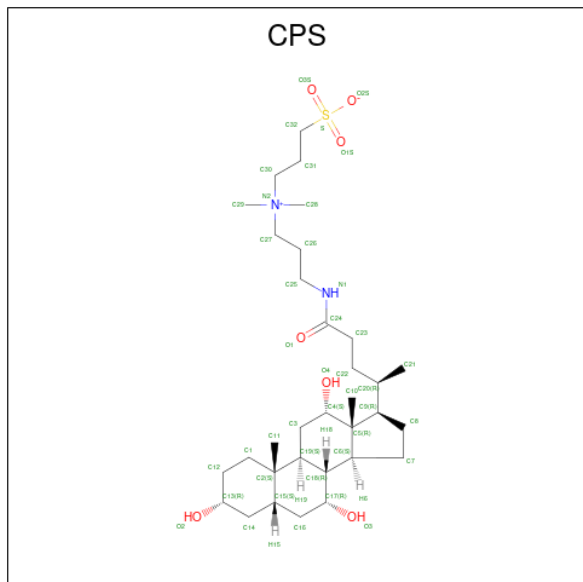
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	H	3	39	22	2	15	0	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
8	A	1	5	4	1	0	0
8	B	1	5	4	1	0	0
8	B	1	5	4	1	0	0
8	B	1	5	4	1	0	0
8	D	1	5	4	1	0	0

- Molecule 9 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	O				
9	A	1	Total	C	O	0	0		
			26	23	3				
9	A	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
9	D	1	Total	C	O	0	0		
			26	23	3				
9	D	1	Total	C	O	0	0		
			26	23	3				
9	D	1	Total	C	O	0	0		
			26	23	3				

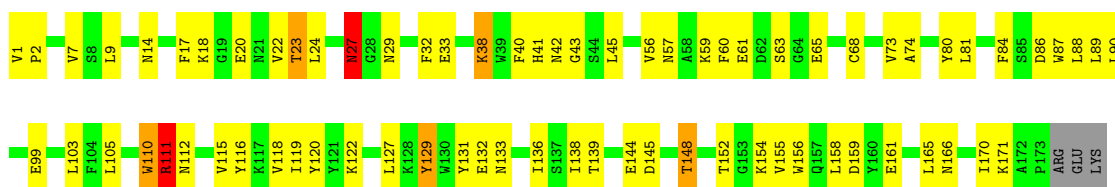
3 Residue-property plots

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

Note EDS was not executed.

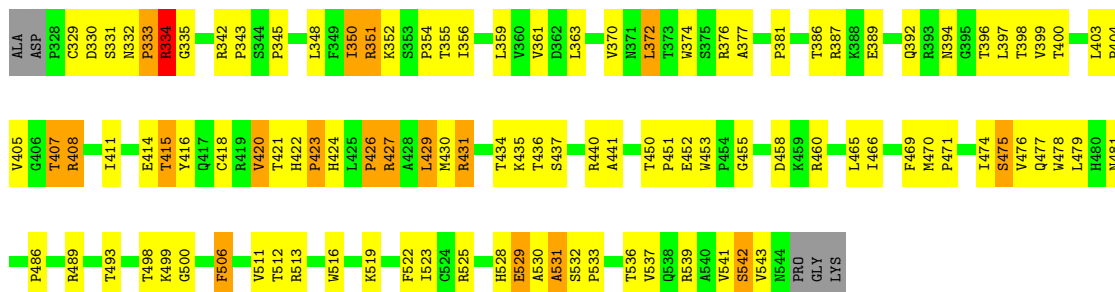
- Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT

Chain A: 



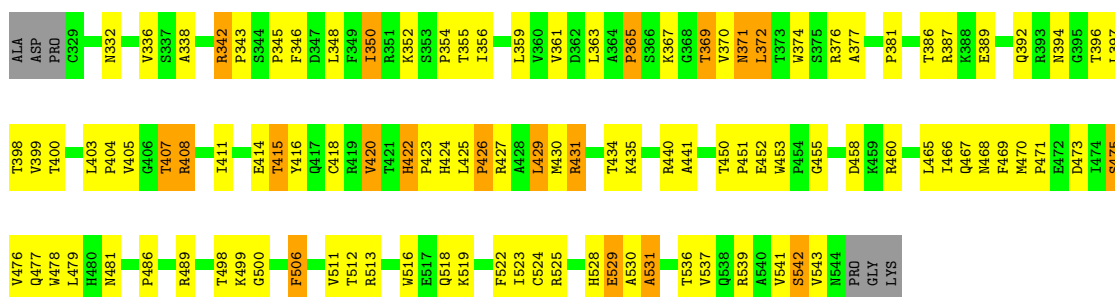
- Molecule 2: IG EPSILON CHAIN C REGION

Chain B: 



- Molecule 2: IG EPSILON CHAIN C REGION

Chain D: 




- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  75% 25%

 MAG1
MAG2
MAN3
FUC4

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  20% 40% 40%

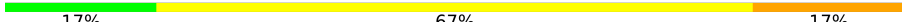
 MAG1
MAG2
MAN3
MAN4
MAN5


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

 MAG1
MAG2
FUC3

- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  17% 67% 17%

 MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

 MAG3
MAG2
MAN3

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.80Å 192.80Å 302.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.87 – 3.50	Depositor
% Data completeness (in resolution range)	99.6 (36.87-3.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	89.0	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: FUC, MAN, NAG, SO4, CPS

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	0.50	0/1448	0.73	1/1974 (0.1%)
2	B	0.49	2/1755 (0.1%)	0.77	2/2389 (0.1%)
2	D	0.48	2/1747 (0.1%)	0.76	2/2378 (0.1%)
All	All	0.49	4/4950 (0.1%)	0.76	5/6741 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	529	GLU	CD-OE1	-8.78	1.16	1.25
2	B	529	GLU	CD-OE1	-8.01	1.16	1.25
2	B	529	GLU	CD-OE2	-7.74	1.17	1.25
2	D	529	GLU	CD-OE2	-7.45	1.17	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	529	GLU	OE1-CD-OE2	-16.97	102.93	123.30
2	D	529	GLU	OE1-CD-OE2	-16.73	103.23	123.30
2	D	529	GLU	CG-CD-OE2	5.70	129.70	118.30
2	B	529	GLU	CG-CD-OE2	5.29	128.87	118.30
1	A	27	ASN	N-CA-C	5.24	125.15	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1406	0	1322	76	0
2	B	1711	0	1687	131	1
2	D	1704	0	1679	126	1
3	C	49	0	43	0	0
4	E	61	0	52	4	0
5	F	38	0	34	0	0
6	G	72	0	61	9	0
7	H	39	0	34	0	0
8	A	5	0	0	1	0
8	B	15	0	0	2	0
8	D	5	0	0	0	0
9	A	68	0	91	13	0
9	D	78	0	105	12	0
All	All	5251	0	5108	356	2

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 34.

All (356) 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)
9:A:371:CPS:C5	9:A:371:CPS:C10	1.75	1.65
9:D:105:CPS:C5	9:D:105:CPS:C10	1.75	1.58
9:A:371:CPS:N1	9:A:371:CPS:C25	1.67	1.50
6:G:3:MAN:H61	6:G:4:MAN:H3	1.41	1.00
1:A:115:VAL:HG22	1:A:155:VAL:HG22	1.49	0.92
2:B:333:PRO:HD2	2:B:429:LEU:HG	1.53	0.90
2:B:422:HIS:CD2	2:B:423:PRO:HD2	2.06	0.89
2:D:377:ALA:HB3	2:D:415:THR:HG23	1.54	0.88
2:B:415:THR:HB	2:B:434:THR:HG21	1.56	0.87
2:B:345:PRO:HB2	2:B:475:SER:HB2	1.55	0.87
2:B:377:ALA:HB3	2:B:415:THR:HG23	1.55	0.87
1:A:170:ILE:HG22	1:A:171:LYS:H	1.39	0.86
2:D:465:LEU:HB2	2:D:506:PHE:HE2	1.41	0.86
2:D:422:HIS:ND1	2:D:423:PRO:HD2	1.90	0.85
6:G:3:MAN:H61	6:G:4:MAN:C3	2.01	0.85
9:A:371:CPS:C10	9:A:371:CPS:C6	2.55	0.85
9:D:105:CPS:C10	9:D:105:CPS:C6	2.55	0.84
9:D:105:CPS:C10	9:D:105:CPS:C9	2.55	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG21	1:A:133:ASN:HA	1.60	0.84
1:A:105:LEU:HB2	1:A:136:ILE:HB	1.59	0.84
2:D:415:THR:HB	2:D:434:THR:HG21	1.59	0.84
2:B:389:GLU:HG2	2:B:399:VAL:HG22	1.61	0.83
9:A:371:CPS:C10	9:A:371:CPS:C9	2.56	0.82
2:B:465:LEU:HB2	2:B:506:PHE:HE2	1.42	0.82
1:A:110:TRP:NE1	1:A:111:ARG:HG3	1.93	0.82
2:B:331:SER:HB2	2:B:431:ARG:HH22	1.45	0.82
9:A:371:CPS:C10	9:A:371:CPS:C4	2.60	0.80
2:B:415:THR:HB	2:B:434:THR:CG2	2.12	0.80
2:D:389:GLU:HG2	2:D:399:VAL:HG22	1.64	0.79
9:D:105:CPS:C10	9:D:105:CPS:C4	2.60	0.79
2:D:541:VAL:HG22	2:D:542:SER:H	1.48	0.79
2:B:541:VAL:HG22	2:B:542:SER:H	1.46	0.79
2:B:426:PRO:HG2	2:B:427:ARG:H	1.47	0.78
1:A:40:PHE:CE2	1:A:45:LEU:HD12	2.18	0.78
1:A:99:GLU:HB2	1:A:170:ILE:O	1.84	0.77
2:D:415:THR:HB	2:D:434:THR:CG2	2.14	0.77
1:A:111:ARG:HH11	1:A:111:ARG:HB3	1.50	0.76
1:A:115:VAL:HG22	1:A:155:VAL:CG2	2.16	0.76
2:D:465:LEU:HB2	2:D:506:PHE:CE2	2.21	0.75
2:B:541:VAL:HG22	2:B:542:SER:N	2.03	0.74
1:A:116:TYR:CE2	9:A:371:CPS:H29	2.23	0.74
2:D:369:THR:HG22	2:D:370:VAL:H	1.54	0.73
2:D:452:GLU:HB3	2:D:460:ARG:HH21	1.53	0.73
1:A:115:VAL:HG12	1:A:118:VAL:HG22	1.71	0.73
2:B:435:LYS:HE2	2:B:529:GLU:OE1	1.89	0.72
2:D:345:PRO:HB2	2:D:475:SER:HB2	1.71	0.72
2:D:541:VAL:HG22	2:D:542:SER:N	2.04	0.72
2:B:452:GLU:HB3	2:B:460:ARG:HH21	1.54	0.71
2:B:465:LEU:HB2	2:B:506:PHE:CE2	2.23	0.71
1:A:170:ILE:HG22	1:A:171:LYS:N	2.05	0.71
2:D:408:ARG:N	2:D:408:ARG:HD3	2.05	0.71
2:B:415:THR:HA	2:B:434:THR:HG22	1.74	0.70
1:A:59:LYS:HZ3	1:A:60:PHE:HD1	1.40	0.70
2:B:377:ALA:CB	2:B:415:THR:HG23	2.21	0.70
2:D:377:ALA:CB	2:D:415:THR:HG23	2.20	0.69
2:B:430:MET:O	2:B:431:ARG:HG2	1.92	0.69
2:B:513:ARG:HA	2:B:516:TRP:CZ3	2.27	0.69
1:A:1:VAL:H2	1:A:2:PRO:HD2	1.57	0.69
2:B:408:ARG:HD3	2:B:408:ARG:N	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:3:MAN:C6	6:G:4:MAN:H5	2.23	0.68
2:B:465:LEU:HD12	2:B:466:ILE:N	2.07	0.68
2:D:430:MET:O	2:D:431:ARG:HG2	1.93	0.68
2:D:513:ARG:HA	2:D:516:TRP:CZ3	2.29	0.68
1:A:1:VAL:N	1:A:2:PRO:HD2	2.09	0.67
2:B:421:THR:O	2:B:421:THR:HG22	1.94	0.67
2:B:458:ASP:OD1	2:B:513:ARG:HD2	1.94	0.67
2:D:415:THR:HA	2:D:434:THR:HG22	1.73	0.67
2:D:458:ASP:OD1	2:D:513:ARG:HD2	1.94	0.67
9:A:371:CPS:C25	9:A:371:CPS:C24	2.67	0.67
1:A:1:VAL:N	1:A:2:PRO:CD	2.58	0.67
2:B:355:THR:HG22	2:B:404:PRO:HA	1.77	0.66
2:D:465:LEU:HD12	2:D:466:ILE:N	2.11	0.65
2:B:334:ARG:O	2:B:334:ARG:HG3	1.96	0.64
2:B:333:PRO:O	2:B:335:GLY:N	2.31	0.64
1:A:103:LEU:HD23	1:A:138:ILE:HD12	1.78	0.64
2:D:460:ARG:HH11	2:D:543:VAL:HG11	1.61	0.64
2:D:359:LEU:HD13	2:D:400:THR:HG22	1.79	0.64
2:B:486:PRO:HD2	2:B:489:ARG:HG3	1.80	0.63
2:B:359:LEU:HD13	2:B:400:THR:HG22	1.80	0.63
2:D:486:PRO:HD2	2:D:489:ARG:HG3	1.81	0.63
4:E:1:NAG:H61	4:E:2:NAG:N2	2.12	0.63
2:B:460:ARG:HH11	2:B:543:VAL:HG11	1.64	0.62
2:D:355:THR:HG22	2:D:404:PRO:HA	1.81	0.62
2:D:408:ARG:HD3	2:D:408:ARG:H	1.63	0.62
2:B:408:ARG:HD3	2:B:408:ARG:H	1.63	0.61
2:B:348:LEU:HD12	2:B:407:THR:HG23	1.82	0.61
2:B:513:ARG:HA	2:B:516:TRP:CE3	2.35	0.61
2:B:536:THR:HG22	2:B:537:VAL:N	2.16	0.60
2:D:528:HIS:HD2	2:D:530:ALA:H	1.49	0.60
6:G:1:NAG:H62	6:G:2:NAG:H83	1.84	0.60
2:D:338:ALA:O	2:D:431:ARG:HD2	2.02	0.60
2:B:506:PHE:CD1	2:D:506:PHE:HB3	2.37	0.59
2:B:470:MET:HA	2:B:471:PRO:O	2.01	0.59
2:D:348:LEU:HD12	2:D:407:THR:HG23	1.84	0.59
1:A:41:HIS:C	1:A:43:GLY:H	2.05	0.59
2:B:536:THR:O	2:B:537:VAL:HG23	2.03	0.59
2:D:470:MET:HA	2:D:471:PRO:O	2.02	0.59
2:D:422:HIS:ND1	2:D:423:PRO:CD	2.64	0.58
2:B:370:VAL:HG22	2:B:387:ARG:NH2	2.18	0.58
2:D:513:ARG:HA	2:D:516:TRP:CE3	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:PRO:HD3	2:B:356:ILE:HG22	1.86	0.58
2:D:528:HIS:CD2	2:D:529:GLU:N	2.71	0.58
2:D:453:TRP:HD1	2:D:455:GLY:H	1.51	0.58
2:D:536:THR:HG22	2:D:537:VAL:N	2.18	0.58
2:B:528:HIS:CD2	2:B:529:GLU:N	2.72	0.58
2:B:437:SER:HA	2:B:440:ARG:NH2	2.18	0.57
1:A:118:VAL:CG2	1:A:133:ASN:HA	2.33	0.57
2:D:367:LYS:HE2	9:D:105:CPS:H21B	1.86	0.57
6:G:4:MAN:O3	6:G:5:MAN:H2	2.04	0.57
2:B:453:TRP:HD1	2:B:455:GLY:H	1.51	0.57
1:A:27:ASN:ND2	1:A:29:ASN:HB2	2.20	0.57
2:B:403:LEU:HD12	2:B:404:PRO:HD2	1.85	0.57
2:D:424:HIS:N	2:D:424:HIS:CD2	2.70	0.57
2:D:403:LEU:HD12	2:D:404:PRO:HD2	1.86	0.57
2:D:528:HIS:CD2	2:D:530:ALA:H	2.23	0.57
2:D:398:THR:HG22	2:D:399:VAL:N	2.19	0.56
2:D:424:HIS:NE2	9:D:105:CPS:H11B	2.19	0.56
2:B:398:THR:HG22	2:B:399:VAL:N	2.20	0.56
2:D:336:VAL:HG21	2:D:363:LEU:HD23	1.86	0.56
1:A:40:PHE:CE2	1:A:45:LEU:CD1	2.89	0.56
2:B:528:HIS:HD2	2:B:530:ALA:H	1.53	0.56
1:A:154:LYS:HA	1:A:158:LEU:O	2.05	0.56
2:B:506:PHE:HB3	2:D:506:PHE:CD1	2.40	0.56
2:B:516:TRP:HA	2:B:519:LYS:O	2.06	0.56
1:A:119:ILE:HG12	1:A:129:TYR:HB2	1.88	0.56
1:A:110:TRP:CD1	1:A:111:ARG:HG3	2.42	0.55
2:D:498:THR:C	2:D:500:GLY:H	2.09	0.55
2:B:331:SER:HB2	2:B:431:ARG:NH2	2.20	0.55
2:D:460:ARG:HH11	2:D:543:VAL:CG1	2.19	0.55
2:D:516:TRP:HA	2:D:519:LYS:O	2.06	0.55
1:A:154:LYS:HG2	1:A:159:ASP:OD1	2.06	0.55
2:D:435:LYS:HE2	2:D:529:GLU:OE2	2.05	0.55
2:B:522:PHE:O	2:B:541:VAL:HG12	2.07	0.55
1:A:22:VAL:HG22	1:A:23:THR:N	2.22	0.55
2:B:477:GLN:HE22	2:B:525:ARG:HH21	1.55	0.55
1:A:87:TRP:O	1:A:88:LEU:HD23	2.06	0.54
1:A:115:VAL:CG2	1:A:155:VAL:HG22	2.31	0.54
2:B:460:ARG:HH11	2:B:543:VAL:CG1	2.20	0.54
2:B:498:THR:C	2:B:500:GLY:H	2.10	0.54
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.73	0.54
2:D:394:ASN:OD1	2:D:396:THR:HG22	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:PRO:HG3	2:B:427:ARG:CG	2.37	0.54
1:A:73:VAL:HG13	1:A:74:ALA:N	2.23	0.54
9:A:371:CPS:C10	9:A:371:CPS:C7	2.86	0.54
2:B:528:HIS:CD2	2:B:530:ALA:H	2.26	0.54
2:B:376:ARG:HD2	2:B:414:GLU:OE2	2.07	0.54
6:G:3:MAN:C6	6:G:4:MAN:C5	2.85	0.54
9:A:371:CPS:C10	9:A:371:CPS:C8	2.86	0.54
2:B:414:GLU:HG3	2:B:415:THR:N	2.23	0.53
1:A:116:TYR:CE2	9:A:371:CPS:C29	2.90	0.53
2:B:394:ASN:OD1	2:B:396:THR:HG22	2.08	0.53
2:B:348:LEU:HA	2:B:354:PRO:HG3	1.91	0.53
2:D:541:VAL:CG2	2:D:542:SER:H	2.20	0.53
2:D:525:ARG:HD2	2:D:536:THR:HG21	1.90	0.53
6:G:3:MAN:H62	6:G:4:MAN:H5	1.89	0.53
1:A:122:LYS:NZ	1:A:145:ASP:HA	2.22	0.53
2:B:333:PRO:CD	2:B:429:LEU:HG	2.32	0.53
1:A:156:TRP:CZ2	9:D:103:CPS:H11A	2.44	0.52
2:D:477:GLN:HE22	2:D:525:ARG:HH21	1.56	0.52
2:D:531:ALA:HB1	2:D:537:VAL:HG23	1.90	0.52
1:A:116:TYR:CD2	9:A:371:CPS:H29	2.43	0.52
1:A:120:TYR:CD1	1:A:136:ILE:HD11	2.43	0.52
2:B:531:ALA:HB1	2:B:537:VAL:HG23	1.91	0.52
2:D:450:THR:HG22	2:D:451:PRO:O	2.10	0.52
2:B:329:CYS:C	2:B:331:SER:H	2.12	0.52
2:D:536:THR:O	2:D:537:VAL:HG23	2.08	0.52
1:A:9:LEU:HD23	1:A:24:LEU:CD2	2.40	0.52
1:A:170:ILE:CG2	1:A:171:LYS:H	2.18	0.52
1:A:152:THR:HG22	1:A:161:GLU:HG3	1.92	0.52
2:D:367:LYS:HG3	9:D:105:CPS:O4	2.09	0.52
2:D:398:THR:CG2	2:D:399:VAL:N	2.72	0.52
2:B:386:THR:CG2	2:B:387:ARG:N	2.73	0.52
2:B:450:THR:HG22	2:B:451:PRO:O	2.08	0.52
2:B:372:LEU:HD11	2:B:418:CYS:SG	2.50	0.52
2:B:398:THR:CG2	2:B:399:VAL:N	2.73	0.52
2:B:415:THR:CB	2:B:434:THR:CG2	2.87	0.52
2:B:420:VAL:HG22	2:B:429:LEU:CB	2.40	0.52
2:D:372:LEU:HD11	2:D:418:CYS:SG	2.50	0.51
2:D:376:ARG:HD3	2:D:416:TYR:CE2	2.46	0.51
2:B:541:VAL:CG2	2:B:542:SER:N	2.73	0.51
2:D:376:ARG:HD2	2:D:414:GLU:OE2	2.11	0.51
2:D:392:GLN:HB2	2:D:396:THR:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG22	1:A:166:ASN:OD1	2.09	0.51
1:A:155:VAL:O	1:A:156:TRP:HB2	2.11	0.51
2:B:541:VAL:CG2	2:B:542:SER:H	2.19	0.51
1:A:86:ASP:OD1	1:A:87:TRP:N	2.38	0.51
1:A:132:GLU:OE1	2:B:334:ARG:NH1	2.42	0.51
2:D:522:PHE:O	2:D:541:VAL:HG12	2.10	0.51
2:B:477:GLN:NE2	2:B:525:ARG:HE	2.09	0.51
1:A:40:PHE:HE2	1:A:45:LEU:CD1	2.24	0.51
2:B:408:ARG:H	2:B:408:ARG:CD	2.24	0.51
2:D:522:PHE:HB2	2:D:541:VAL:HG13	1.92	0.51
1:A:56:VAL:O	1:A:57:ASN:C	2.48	0.50
2:D:408:ARG:H	2:D:408:ARG:CD	2.24	0.50
2:D:476:VAL:HG12	2:D:477:GLN:N	2.26	0.50
2:B:392:GLN:HB2	2:B:396:THR:HG22	1.92	0.50
2:B:528:HIS:CD2	2:B:529:GLU:H	2.29	0.50
2:D:525:ARG:HD2	2:D:536:THR:CG2	2.41	0.50
2:B:506:PHE:CE1	2:D:506:PHE:HB3	2.47	0.50
2:B:415:THR:CA	2:B:434:THR:HG22	2.40	0.50
2:B:350:ILE:O	2:B:352:LYS:HG3	2.11	0.50
2:B:530:ALA:O	2:B:531:ALA:O	2.30	0.50
1:A:41:HIS:C	1:A:43:GLY:N	2.65	0.50
2:D:530:ALA:O	2:D:531:ALA:O	2.30	0.50
2:B:525:ARG:HD2	2:B:536:THR:HG21	1.93	0.49
2:B:522:PHE:HB2	2:B:541:VAL:HG13	1.93	0.49
2:B:470:MET:HA	2:B:471:PRO:C	2.33	0.49
2:B:476:VAL:HG12	2:B:477:GLN:N	2.28	0.49
9:D:105:CPS:C10	9:D:105:CPS:C7	2.90	0.49
1:A:88:LEU:HD21	1:A:115:VAL:HG21	1.93	0.49
1:A:115:VAL:CG1	1:A:118:VAL:HG22	2.42	0.49
2:B:333:PRO:HG3	2:B:427:ARG:HG3	1.93	0.49
2:D:386:THR:CG2	2:D:387:ARG:N	2.75	0.49
1:A:1:VAL:HG12	1:A:1:VAL:O	2.13	0.49
2:B:407:THR:O	2:B:411:ILE:HG13	2.13	0.49
2:B:525:ARG:HD2	2:B:536:THR:CG2	2.43	0.49
2:D:414:GLU:HG3	2:D:415:THR:N	2.26	0.48
9:A:371:CPS:C8	9:A:371:CPS:H10	2.43	0.48
2:D:528:HIS:CD2	2:D:529:GLU:H	2.30	0.48
9:D:105:CPS:C10	9:D:105:CPS:C8	2.91	0.48
2:B:331:SER:O	2:B:429:LEU:HD21	2.13	0.48
2:B:415:THR:CB	2:B:434:THR:HG22	2.43	0.48
2:B:420:VAL:HG22	2:B:429:LEU:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:348:LEU:HA	2:D:354:PRO:HG3	1.96	0.48
2:D:407:THR:O	2:D:411:ILE:HG13	2.13	0.48
1:A:1:VAL:H3	1:A:2:PRO:CD	2.26	0.48
2:B:541:VAL:O	2:B:542:SER:HB3	2.14	0.48
2:D:408:ARG:N	2:D:408:ARG:CD	2.76	0.48
2:D:363:LEU:HB2	2:D:397:LEU:O	2.14	0.48
1:A:73:VAL:CG1	1:A:74:ALA:N	2.77	0.48
2:B:376:ARG:HD3	2:B:416:TYR:CE2	2.48	0.48
2:B:466:ILE:HD12	2:B:476:VAL:HG22	1.96	0.48
2:B:536:THR:CG2	2:B:537:VAL:N	2.76	0.48
2:D:350:ILE:O	2:D:352:LYS:HG3	2.12	0.48
2:D:477:GLN:NE2	2:D:525:ARG:HE	2.12	0.47
1:A:18:LYS:HD2	1:A:60:PHE:CE1	2.50	0.47
2:D:343:PRO:HD3	2:D:356:ILE:HG22	1.96	0.47
2:D:415:THR:CB	2:D:434:THR:HG22	2.44	0.47
2:B:511:VAL:HG12	2:B:512:THR:N	2.29	0.47
2:D:466:ILE:HD12	2:D:476:VAL:HG22	1.95	0.47
2:D:470:MET:HA	2:D:471:PRO:C	2.35	0.47
4:E:1:NAG:H62	4:E:2:NAG:H82	1.97	0.47
1:A:59:LYS:HG3	1:A:60:PHE:N	2.30	0.47
1:A:110:TRP:C	1:A:112:ASN:N	2.68	0.47
1:A:111:ARG:HB3	1:A:111:ARG:NH1	2.25	0.47
2:B:333:PRO:C	2:B:335:GLY:N	2.68	0.47
2:B:465:LEU:HD12	2:B:465:LEU:C	2.35	0.47
2:B:479:LEU:HB2	2:B:523:ILE:HB	1.97	0.47
2:D:415:THR:CA	2:D:434:THR:HG22	2.40	0.47
2:D:441:ALA:HB3	2:D:470:MET:HG2	1.97	0.47
2:D:541:VAL:O	2:D:542:SER:HB3	2.14	0.47
2:B:414:GLU:CG	2:B:415:THR:N	2.78	0.47
2:B:493:THR:HB	8:B:204:SO4:O3	2.14	0.47
2:D:411:ILE:O	2:D:435:LYS:HE3	2.15	0.47
2:D:336:VAL:CG2	2:D:363:LEU:HD23	2.44	0.47
1:A:17:PHE:CE2	1:A:89:LEU:HB2	2.51	0.46
1:A:110:TRP:CD1	2:D:426:PRO:HG3	2.50	0.46
2:B:426:PRO:HG2	2:B:427:ARG:N	2.23	0.46
2:B:477:GLN:HE21	2:B:525:ARG:HE	1.63	0.46
1:A:40:PHE:HE2	1:A:45:LEU:HD12	1.74	0.46
2:B:511:VAL:CG1	2:B:512:THR:N	2.79	0.46
2:D:415:THR:CB	2:D:434:THR:CG2	2.89	0.46
1:A:17:PHE:CE1	1:A:110:TRP:HA	2.50	0.46
2:D:536:THR:CG2	2:D:537:VAL:N	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:PRO:CG	2:B:427:ARG:H	2.23	0.46
2:D:405:VAL:HG22	2:D:416:TYR:CZ	2.51	0.45
1:A:32:PHE:O	1:A:33:GLU:HB2	2.16	0.45
2:D:511:VAL:HG12	2:D:512:THR:N	2.31	0.45
2:D:541:VAL:CG2	2:D:542:SER:N	2.74	0.45
2:D:345:PRO:HD2	2:D:475:SER:OG	2.17	0.45
6:G:3:MAN:H61	6:G:4:MAN:C5	2.46	0.45
9:A:370:CPS:H11A	9:A:371:CPS:H11A	1.98	0.45
2:D:528:HIS:HD2	2:D:529:GLU:N	2.14	0.45
2:B:333:PRO:C	2:B:335:GLY:H	2.19	0.45
2:B:441:ALA:HB3	2:B:470:MET:HG2	1.99	0.45
2:D:423:PRO:HB2	2:D:424:HIS:CD2	2.52	0.45
1:A:41:HIS:O	1:A:43:GLY:N	2.50	0.45
2:D:420:VAL:HG22	2:D:429:LEU:CB	2.47	0.45
2:D:478:TRP:CZ3	2:D:524:CYS:HB2	2.52	0.45
2:D:479:LEU:HB2	2:D:523:ILE:HB	1.99	0.45
2:D:522:PHE:HB2	2:D:541:VAL:CG1	2.47	0.45
2:B:345:PRO:HG2	2:B:474:ILE:C	2.37	0.44
1:A:103:LEU:HB3	1:A:138:ILE:HB	1.98	0.44
2:B:528:HIS:HD2	2:B:529:GLU:N	2.13	0.44
2:D:414:GLU:CG	2:D:415:THR:N	2.80	0.44
2:B:424:HIS:NE2	8:B:202:SO4:O1	2.36	0.44
2:D:369:THR:HG22	2:D:370:VAL:N	2.27	0.44
2:B:332:ASN:N	2:B:333:PRO:HD3	2.32	0.44
2:B:374:TRP:CD2	2:B:403:LEU:HD22	2.52	0.44
2:B:411:ILE:O	2:B:435:LYS:HE3	2.16	0.44
2:B:396:THR:HG23	2:B:397:LEU:N	2.32	0.44
2:B:403:LEU:HD12	2:B:404:PRO:CD	2.48	0.44
2:D:486:PRO:O	2:D:489:ARG:HB2	2.18	0.44
2:B:405:VAL:HG22	2:B:416:TYR:CZ	2.52	0.44
1:A:63:SER:HA	1:A:81:LEU:O	2.18	0.44
9:D:105:CPS:C8	9:D:105:CPS:H10	2.48	0.44
6:G:3:MAN:H61	6:G:4:MAN:H5	1.98	0.44
2:B:450:THR:HA	2:B:451:PRO:HD3	1.75	0.43
2:D:332:ASN:OD1	2:D:332:ASN:O	2.35	0.43
2:D:396:THR:HG23	2:D:397:LEU:N	2.33	0.43
2:D:465:LEU:HD12	2:D:465:LEU:C	2.39	0.43
1:A:99:GLU:OE2	1:A:171:LYS:HG2	2.18	0.43
2:D:511:VAL:CG1	2:D:512:THR:N	2.81	0.43
2:B:469:PHE:HD1	2:B:528:HIS:CE1	2.37	0.43
2:D:460:ARG:NH1	2:D:543:VAL:HG11	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:3:MAN:O2	4:E:4:MAN:H5	2.18	0.43
1:A:110:TRP:CG	2:D:426:PRO:HG3	2.54	0.43
2:B:437:SER:HA	2:B:440:ARG:HH22	1.83	0.43
2:B:522:PHE:HB2	2:B:541:VAL:CG1	2.48	0.43
2:D:476:VAL:CG1	2:D:477:GLN:N	2.82	0.43
1:A:65:GLU:HB2	1:A:80:TYR:CE2	2.54	0.42
2:D:450:THR:HA	2:D:451:PRO:HD3	1.78	0.42
2:D:478:TRP:O	2:D:479:LEU:HD23	2.19	0.42
1:A:65:GLU:HB2	1:A:80:TYR:HE2	1.83	0.42
2:B:440:ARG:HD3	2:B:471:PRO:HD3	2.02	0.42
2:D:374:TRP:CD2	2:D:403:LEU:HD22	2.53	0.42
2:B:486:PRO:O	2:B:489:ARG:HB2	2.19	0.42
1:A:144:GLU:HG3	1:A:145:ASP:N	2.34	0.42
2:D:403:LEU:HD12	2:D:404:PRO:CD	2.50	0.42
2:D:422:HIS:HB3	2:D:425:LEU:HD12	2.02	0.42
2:D:477:GLN:HE21	2:D:525:ARG:HE	1.67	0.42
2:B:332:ASN:O	2:B:333:PRO:C	2.56	0.42
2:D:469:PHE:HD1	2:D:528:HIS:CE1	2.38	0.42
1:A:90:LEU:HD23	1:A:165:LEU:HB3	2.01	0.42
2:B:450:THR:HG22	2:B:451:PRO:N	2.35	0.42
2:D:450:THR:HG22	2:D:451:PRO:N	2.35	0.42
2:B:532:SER:HB3	2:B:533:PRO:HA	2.02	0.41
2:D:338:ALA:C	2:D:431:ARG:HD2	2.40	0.41
2:D:440:ARG:HD3	2:D:471:PRO:HD3	2.02	0.41
2:D:467:GLN:NE2	2:D:468:ASN:HD21	2.18	0.41
9:D:105:CPS:H14	9:D:105:CPS:H19	2.00	0.41
1:A:41:HIS:HE1	1:A:63:SER:O	2.03	0.41
1:A:131:TYR:CG	2:B:334:ARG:HG2	2.55	0.41
1:A:17:PHE:O	1:A:20:GLU:HG3	2.21	0.41
1:A:139:THR:OG1	8:A:203:SO4:O4	2.36	0.41
2:B:478:TRP:O	2:B:479:LEU:HD23	2.20	0.41
2:B:330:ASP:OD1	2:B:330:ASP:O	2.39	0.41
2:B:348:LEU:HD13	2:B:354:PRO:CG	2.50	0.41
1:A:84:PHE:CD1	1:A:84:PHE:N	2.88	0.41
2:D:420:VAL:HG22	2:D:429:LEU:HB3	2.02	0.41
1:A:59:LYS:HG2	1:A:61:GLU:OE1	2.21	0.41
1:A:129:TYR:CD2	1:A:129:TYR:C	2.94	0.41
2:B:460:ARG:NH1	2:B:543:VAL:HG11	2.34	0.41
2:D:348:LEU:HD13	2:D:354:PRO:CG	2.51	0.41
2:B:506:PHE:HB3	2:D:506:PHE:CE1	2.55	0.41
2:D:342:ARG:HD2	2:D:473:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:ARG:CD	2:D:473:ASP:OD1	2.68	0.40
2:B:498:THR:C	2:B:500:GLY:N	2.75	0.40
2:D:370:VAL:O	2:D:371:ASN:C	2.60	0.40
1:A:14:ASN:O	1:A:81:LEU:HA	2.21	0.40
2:D:346:PHE:C	2:D:348:LEU:H	2.25	0.40
1:A:38:LYS:O	1:A:68:CYS:HA	2.22	0.40
2:B:363:LEU:HB2	2:B:397:LEU:O	2.22	0.40
2:D:425:LEU:HA	2:D:426:PRO:HD3	1.87	0.40
2:B:420:VAL:HG22	2:B:429:LEU:HB2	2.03	0.40
2:B:436:THR:O	2:B:440:ARG:NH1	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:GLN:OE1	2:D:518:GLN:OE1[11_566]	1.79	0.41
2:B:351:ARG:NH2	2:B:351:ARG:NH2[4_556]	2.12	0.08

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	171/176 (97%)	147 (86%)	20 (12%)	4 (2%)	6	36
2	B	215/222 (97%)	177 (82%)	29 (14%)	9 (4%)	3	23
2	D	214/222 (96%)	175 (82%)	30 (14%)	9 (4%)	3	23
All	All	600/620 (97%)	499 (83%)	79 (13%)	22 (4%)	3	26

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	334	ARG
2	B	531	ALA
2	D	426	PRO
2	D	531	ALA
2	B	426	PRO
2	D	371	ASN
2	B	350	ILE
2	D	350	ILE
2	D	369	THR
1	A	111	ARG
2	B	499	LYS
2	B	542	SER
2	D	365	PRO
2	D	499	LYS
2	D	542	SER
1	A	42	ASN
1	A	110	TRP
2	B	351	ARG
2	B	381	PRO
2	D	381	PRO
2	B	333	PRO

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	154/157 (98%)	147 (96%)	7 (4%)	27	61
2	B	192/195 (98%)	176 (92%)	16 (8%)	11	40
2	D	191/195 (98%)	175 (92%)	16 (8%)	11	40
All	All	537/547 (98%)	498 (93%)	39 (7%)	14	45

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	23	THR
1	A	38	LYS
1	A	111	ARG
1	A	127	LEU
1	A	129	TYR
1	A	148	THR
2	B	334	ARG
2	B	342	ARG
2	B	361	VAL
2	B	372	LEU
2	B	407	THR
2	B	408	ARG
2	B	415	THR
2	B	420	VAL
2	B	423	PRO
2	B	427	ARG
2	B	429	LEU
2	B	431	ARG
2	B	475	SER
2	B	481	ASN
2	B	506	PHE
2	B	539	ARG
2	D	342	ARG
2	D	361	VAL
2	D	365	PRO
2	D	372	LEU
2	D	407	THR
2	D	408	ARG
2	D	415	THR
2	D	420	VAL
2	D	422	HIS
2	D	427	ARG
2	D	429	LEU
2	D	431	ARG
2	D	475	SER
2	D	481	ASN
2	D	506	PHE
2	D	539	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	54	ASN
1	A	157	GLN
2	B	383	ASN
2	B	468	ASN
2	B	477	GLN
2	B	481	ASN
2	B	518	GLN
2	B	528	HIS
2	B	538	GLN
2	D	332	ASN
2	D	383	ASN
2	D	468	ASN
2	D	477	GLN
2	D	481	ASN
2	D	518	GLN
2	D	528	HIS
2	D	538	GLN

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](#)

21 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.50	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.52	0	17,19,21	0.76	0
3	MAN	C	3	3	11,11,12	0.47	0	15,15,17	0.23	0
3	FUC	C	4	3	10,10,11	0.52	0	14,14,16	0.45	0
4	NAG	E	1	1,4	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	0.85	1 (5%)
4	MAN	E	3	4	11,11,12	0.71	0	15,15,17	0.42	0
4	MAN	E	4	4	11,11,12	0.67	0	15,15,17	0.65	0
4	MAN	E	5	4	11,11,12	0.52	0	15,15,17	0.61	0
5	NAG	F	1	5,1	14,14,15	0.62	0	17,19,21	0.81	1 (5%)
5	NAG	F	2	5	14,14,15	0.48	0	17,19,21	0.64	0
5	FUC	F	3	5	10,10,11	0.48	0	14,14,16	0.44	0
6	NAG	G	1	2,6	14,14,15	0.39	0	17,19,21	0.77	0
6	NAG	G	2	6	14,14,15	0.71	0	17,19,21	0.69	0
6	MAN	G	3	6	11,11,12	0.64	0	15,15,17	0.91	0
6	MAN	G	4	6	11,11,12	0.75	0	15,15,17	1.18	0
6	MAN	G	5	6	11,11,12	1.07	1 (9%)	15,15,17	0.85	1 (6%)
6	MAN	G	6	6	11,11,12	0.60	0	15,15,17	0.56	0
7	NAG	H	1	2,7	14,14,15	0.65	0	17,19,21	0.68	0
7	NAG	H	2	7	14,14,15	0.72	0	17,19,21	0.77	1 (5%)
7	MAN	H	3	7	11,11,12	0.56	0	15,15,17	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
6	MAN	G	3	6	1/1/4/5	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
6	MAN	G	6	6	-	2/2/19/22	0/1/1/1
7	NAG	H	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	MAN	H	3	7	1/1/4/5	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5	MAN	O5-C5	2.11	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C2-N2-C7	-2.67	119.10	122.90
6	G	5	MAN	C1-O5-C5	2.61	115.73	112.19
4	E	1	NAG	C2-N2-C7	-2.55	119.27	122.90
5	F	1	NAG	C2-N2-C7	-2.38	119.51	122.90
4	E	2	NAG	C2-N2-C7	-2.37	119.53	122.90
7	H	2	NAG	C2-N2-C7	-2.08	119.94	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	MAN	C1
4	E	3	MAN	C1
6	G	3	MAN	C1
7	H	3	MAN	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	H	2	NAG	C8-C7-N2-C2
7	H	2	NAG	O7-C7-N2-C2
6	G	6	MAN	O5-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
6	G	3	MAN	O5-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
6	G	3	MAN	C4-C5-C6-O6
6	G	6	MAN	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
5	F	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C1-C2-N2-C7
5	F	2	NAG	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
7	H	3	MAN	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
7	H	3	MAN	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	G	5	MAN	C4-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 13 short contacts:

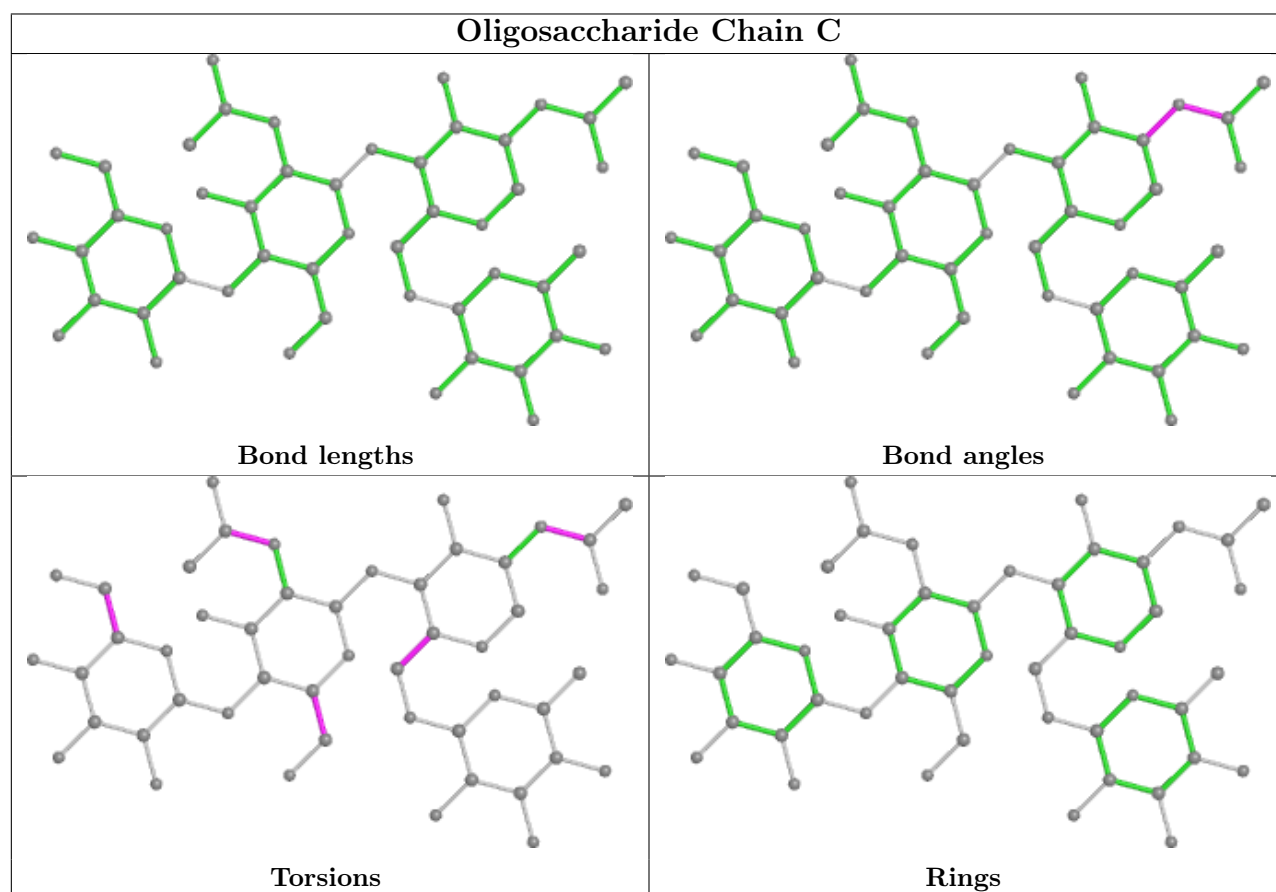
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	1	0
4	E	2	NAG	3	0

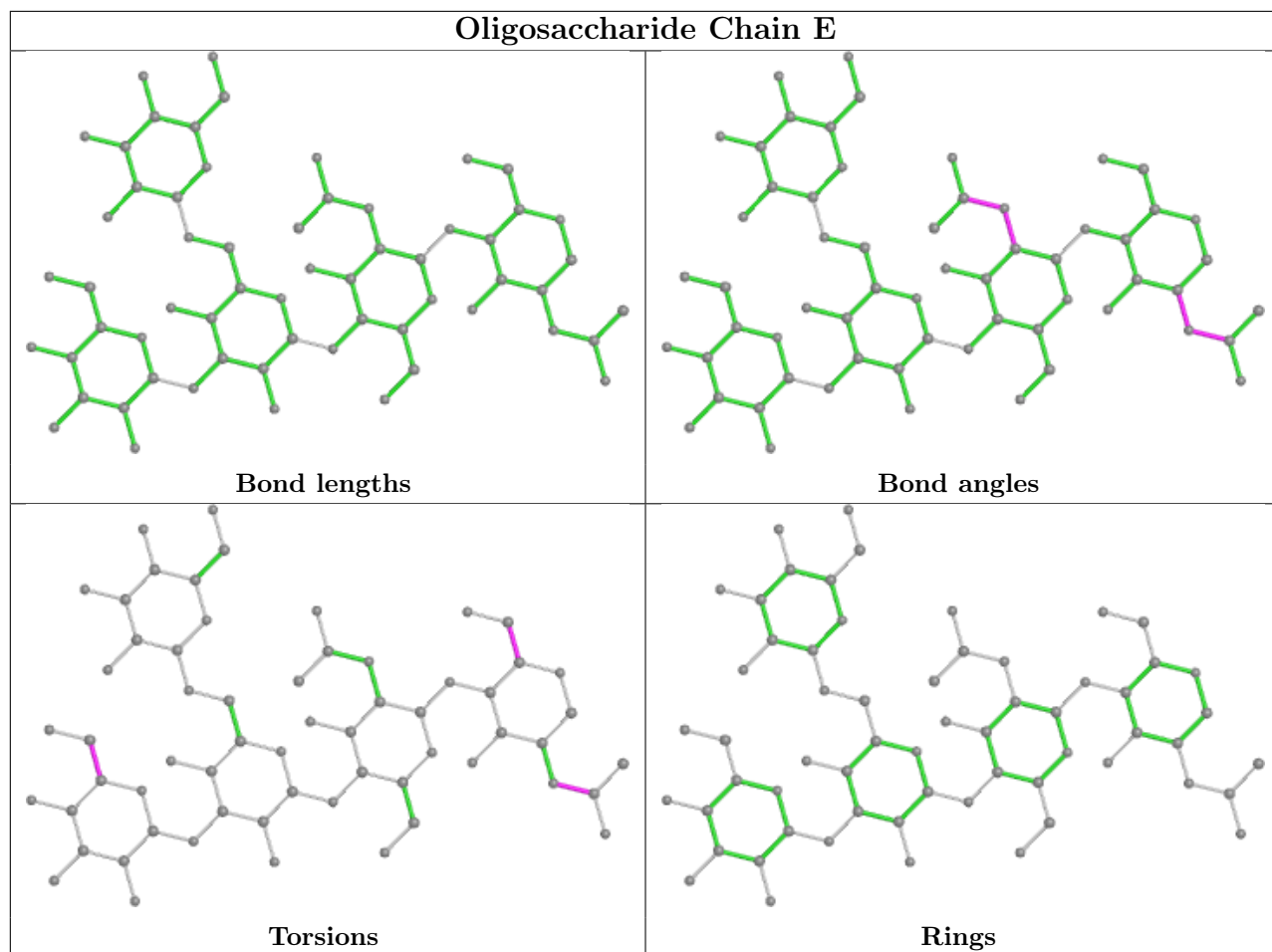
Continued on next page...

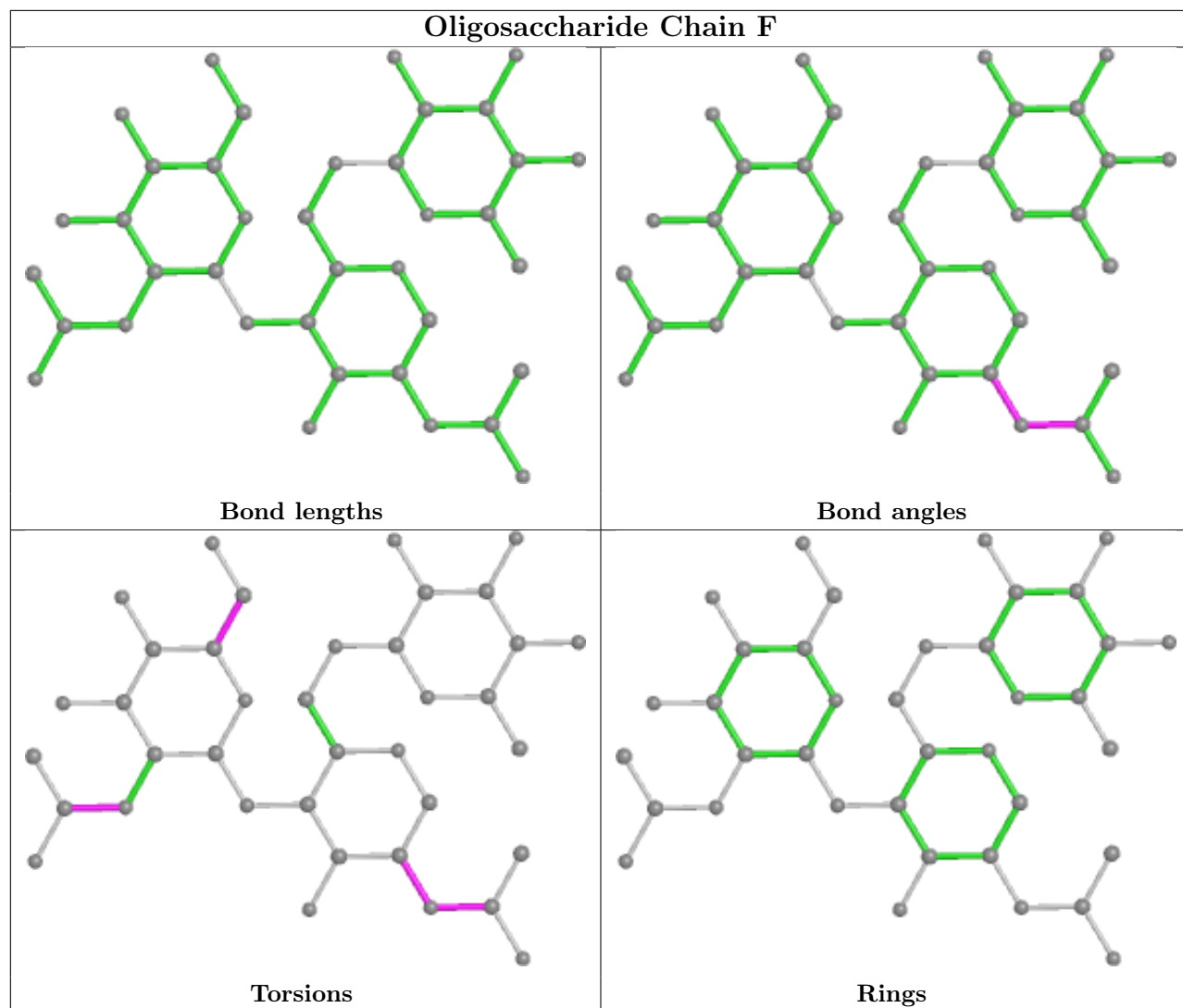
Continued from previous page...

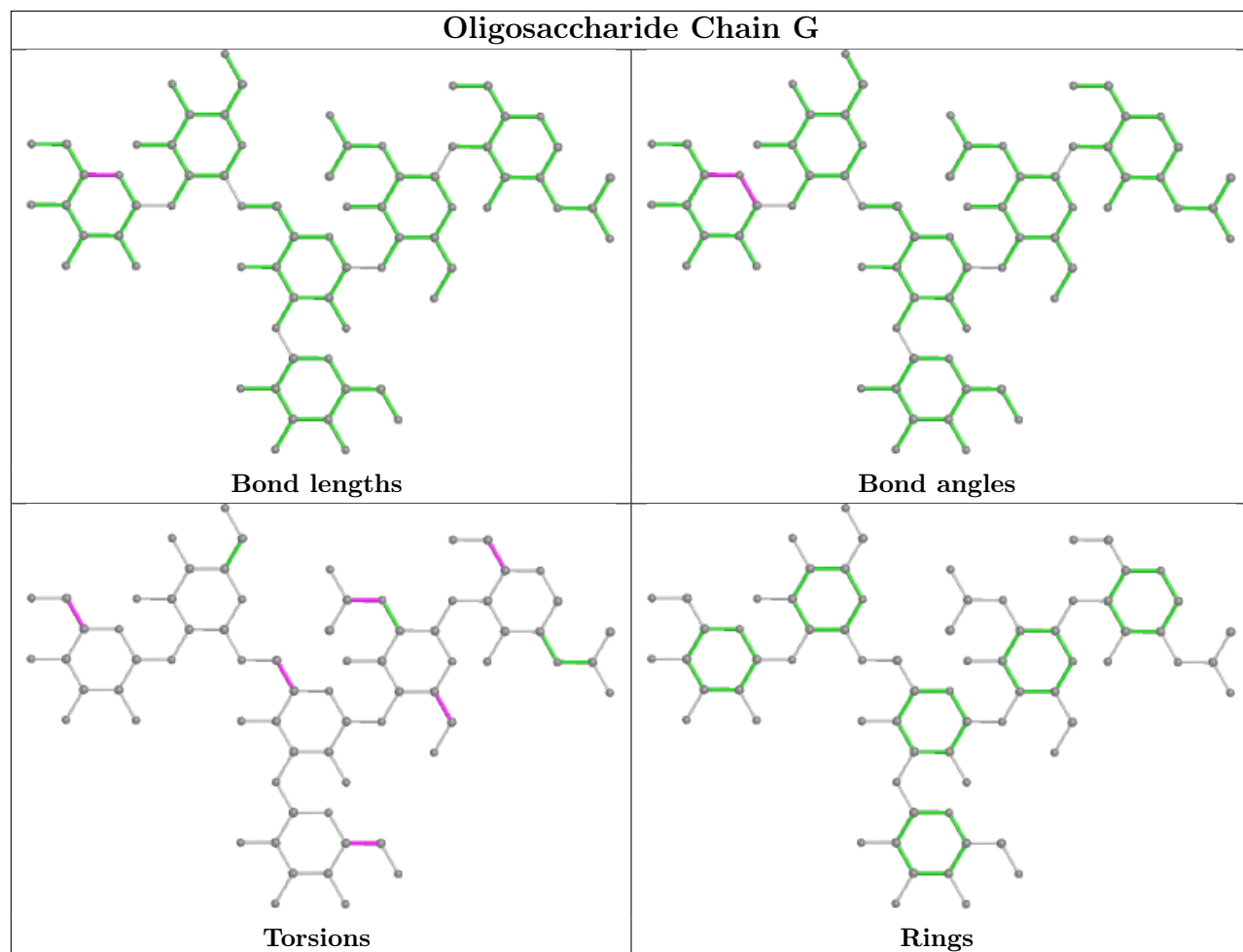
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2	NAG	1	0
4	E	1	NAG	3	0
6	G	4	MAN	8	0
6	G	3	MAN	7	0
6	G	5	MAN	1	0
6	G	1	NAG	1	0
4	E	3	MAN	1	0

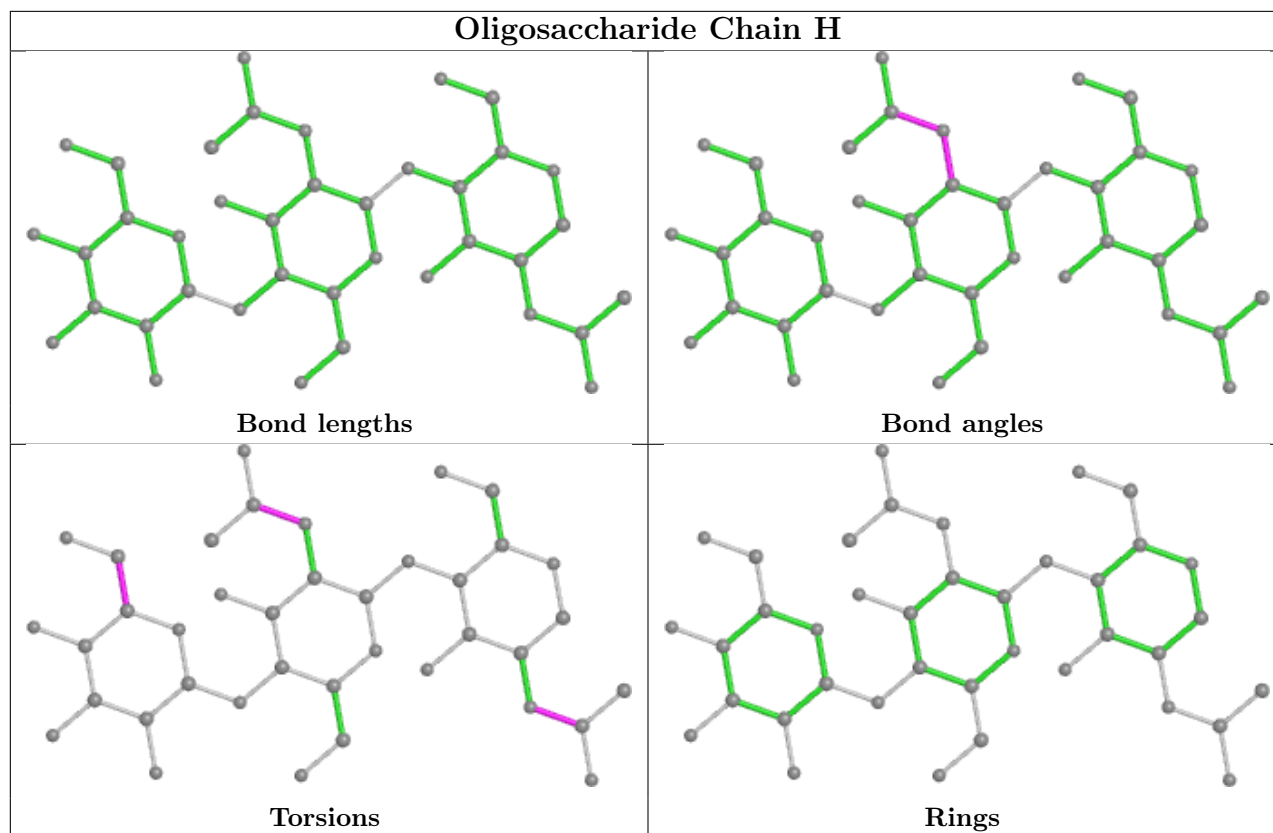
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	SO4	D	205	-	4,4,4	0.50	0	6,6,6	0.27	0
8	SO4	A	203	-	4,4,4	0.51	0	6,6,6	0.25	0
9	CPS	A	370	-	29,29,45	4.70	17 (58%)	47,47,70	4.09	28 (59%)
9	CPS	A	371	-	45,45,45	4.98	23 (51%)	69,70,70	3.38	33 (47%)
8	SO4	B	201	-	4,4,4	0.42	0	6,6,6	0.12	0
8	SO4	B	204	-	4,4,4	0.55	0	6,6,6	0.43	0
9	CPS	D	103	-	29,29,45	4.86	18 (62%)	47,47,70	3.94	28 (59%)
9	CPS	D	105	-	29,29,45	5.07	17 (58%)	47,47,70	3.86	28 (59%)
8	SO4	B	202	-	4,4,4	0.26	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CPS	D	104	-	29,29,45	4.89	17 (58%)	47,47,70	3.94	28 (59%)

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
9	CPS	A	370	-	-	0/6/71/90	0/4/4/4
9	CPS	A	371	-	-	7/25/90/90	0/4/4/4
9	CPS	D	103	-	-	0/6/71/90	0/4/4/4
9	CPS	D	105	-	-	0/6/71/90	0/4/4/4
9	CPS	D	104	-	-	0/6/71/90	0/4/4/4

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	371	CPS	C32-S	-16.17	1.54	1.77
9	D	103	CPS	O4-C4	-13.58	1.21	1.43
9	A	370	CPS	O4-C4	-13.39	1.21	1.43
9	D	104	CPS	O4-C4	-13.25	1.21	1.43
9	D	105	CPS	O4-C4	-13.14	1.21	1.43
9	A	371	CPS	C10-C5	12.81	1.75	1.54
9	A	371	CPS	O4-C4	-12.77	1.22	1.43
9	D	105	CPS	C10-C5	12.76	1.75	1.54
9	D	104	CPS	C10-C5	12.02	1.74	1.54
9	D	103	CPS	C10-C5	11.96	1.74	1.54
9	A	370	CPS	C10-C5	10.65	1.71	1.54
9	A	371	CPS	C25-N1	9.37	1.67	1.46
9	D	105	CPS	C18-C19	9.09	1.71	1.53
9	A	371	CPS	C5-C9	-8.49	1.41	1.55
9	A	371	CPS	C18-C19	8.22	1.69	1.53
9	D	105	CPS	C5-C9	-8.17	1.41	1.55
9	D	103	CPS	C5-C9	-7.81	1.42	1.55
9	D	104	CPS	C18-C19	7.78	1.69	1.53
9	D	103	CPS	C18-C19	7.44	1.68	1.53
9	D	104	CPS	C5-C9	-7.24	1.43	1.55
9	D	105	CPS	C18-C17	7.20	1.65	1.53
9	D	104	CPS	C18-C17	7.01	1.65	1.53
9	A	370	CPS	C3-C4	6.95	1.65	1.53
9	A	370	CPS	C18-C19	6.88	1.67	1.53
9	A	370	CPS	C5-C9	-6.80	1.43	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	370	CPS	C18-C17	6.63	1.64	1.53
9	A	371	CPS	C3-C4	6.58	1.64	1.53
9	A	371	CPS	C18-C17	6.53	1.64	1.53
9	D	103	CPS	O3-C17	-6.42	1.29	1.43
9	D	104	CPS	C3-C4	6.28	1.63	1.53
9	D	103	CPS	C18-C17	6.00	1.63	1.53
9	A	371	CPS	C23-C24	-5.76	1.40	1.51
9	D	105	CPS	C3-C4	5.67	1.62	1.53
9	D	104	CPS	O3-C17	-5.62	1.31	1.43
9	A	370	CPS	O3-C17	-5.54	1.31	1.43
9	D	103	CPS	C3-C4	5.51	1.62	1.53
9	D	105	CPS	O3-C17	-5.51	1.31	1.43
9	D	104	CPS	C8-C9	5.05	1.64	1.54
9	D	105	CPS	C8-C9	4.89	1.64	1.54
9	A	371	CPS	O3-C17	-4.81	1.33	1.43
9	D	103	CPS	C8-C9	4.71	1.64	1.54
9	D	103	CPS	C16-C15	-4.64	1.46	1.53
9	A	371	CPS	C8-C7	4.47	1.66	1.54
9	D	105	CPS	C14-C15	4.35	1.60	1.53
9	D	104	CPS	C16-C15	-4.25	1.47	1.53
9	A	370	CPS	C16-C15	-4.23	1.47	1.53
9	A	370	CPS	C5-C4	-4.09	1.48	1.54
9	A	370	CPS	C8-C9	4.07	1.62	1.54
9	A	371	CPS	O2S-S	-4.04	1.33	1.47
9	A	371	CPS	C16-C15	-4.01	1.47	1.53
9	D	105	CPS	C8-C7	3.96	1.64	1.54
9	A	371	CPS	C8-C9	3.91	1.62	1.54
9	D	104	CPS	O2-C13	3.91	1.55	1.43
9	D	105	CPS	O2-C13	3.84	1.54	1.43
9	A	370	CPS	O2-C13	3.81	1.54	1.43
9	D	105	CPS	C20-C9	3.77	1.61	1.54
9	A	371	CPS	O2-C13	3.76	1.54	1.43
9	A	371	CPS	C14-C15	3.67	1.59	1.53
9	D	105	CPS	C5-C4	-3.63	1.48	1.54
9	D	104	CPS	C14-C15	3.63	1.59	1.53
9	D	105	CPS	C14-C13	3.60	1.58	1.51
9	D	104	CPS	C8-C7	3.59	1.63	1.54
9	D	103	CPS	C8-C7	3.55	1.63	1.54
9	A	370	CPS	C8-C7	3.32	1.63	1.54
9	D	104	CPS	C5-C4	-3.31	1.49	1.54
9	D	104	CPS	C20-C9	3.30	1.60	1.54
9	D	103	CPS	O2-C13	3.30	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	103	CPS	C14-C15	3.26	1.59	1.53
9	A	370	CPS	C14-C15	3.22	1.59	1.53
9	D	103	CPS	C20-C9	3.14	1.59	1.54
9	D	104	CPS	C14-C13	3.09	1.57	1.51
9	A	371	CPS	C5-C6	-3.08	1.50	1.55
9	A	370	CPS	C14-C13	3.04	1.57	1.51
9	A	370	CPS	C7-C6	-3.02	1.48	1.54
9	D	105	CPS	C16-C15	-2.88	1.49	1.53
9	A	370	CPS	C11-C2	2.81	1.59	1.54
9	D	103	CPS	C5-C4	-2.81	1.50	1.54
9	A	371	CPS	C20-C9	2.73	1.59	1.54
9	D	103	CPS	C11-C2	2.68	1.59	1.54
9	A	371	CPS	C14-C13	2.67	1.56	1.51
9	D	105	CPS	C11-C2	2.58	1.58	1.54
9	D	103	CPS	C14-C13	2.58	1.56	1.51
9	D	103	CPS	C7-C6	-2.54	1.49	1.54
9	A	371	CPS	C5-C4	-2.46	1.50	1.54
9	A	371	CPS	C11-C2	2.32	1.58	1.54
9	D	104	CPS	C11-C2	2.28	1.58	1.54
9	A	371	CPS	C22-C23	-2.23	1.45	1.52
9	D	103	CPS	C5-C6	-2.19	1.51	1.55
9	A	371	CPS	C3-C19	-2.17	1.50	1.53
9	D	104	CPS	C7-C6	-2.13	1.50	1.54
9	D	105	CPS	C7-C6	-2.12	1.50	1.54
9	A	370	CPS	C22-C20	2.03	1.60	1.53

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	CPS	C6-C18-C17	11.16	126.61	111.81
9	A	370	CPS	C6-C18-C17	10.52	125.76	111.81
9	D	104	CPS	C6-C18-C17	10.45	125.66	111.81
9	D	103	CPS	C6-C18-C17	9.53	124.45	111.81
9	A	370	CPS	C19-C18-C17	-9.30	100.75	111.88
9	D	104	CPS	C19-C18-C17	-8.90	101.23	111.88
9	D	103	CPS	C19-C3-C4	8.60	125.66	114.30
9	A	371	CPS	C6-C18-C17	8.53	123.12	111.81
9	D	105	CPS	C19-C3-C4	8.50	125.53	114.30
9	D	104	CPS	C19-C3-C4	8.42	125.42	114.30
9	D	105	CPS	C19-C18-C17	-8.38	101.85	111.88
9	A	370	CPS	C19-C3-C4	8.32	125.29	114.30
9	D	103	CPS	C19-C18-C17	-8.22	102.04	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	371	CPS	C19-C18-C17	-8.13	102.15	111.88
9	A	371	CPS	C27-C26-C25	8.10	126.66	111.04
9	A	371	CPS	C19-C3-C4	7.73	124.51	114.30
9	A	370	CPS	C9-C5-C4	7.63	124.63	117.67
9	A	371	CPS	C26-C27-N2	7.29	130.82	115.38
9	D	105	CPS	C2-C19-C18	7.06	119.40	111.82
9	D	103	CPS	C2-C19-C18	6.88	119.21	111.82
9	D	104	CPS	C2-C19-C18	6.88	119.20	111.82
9	A	370	CPS	C5-C6-C18	6.75	123.36	114.74
9	A	370	CPS	C7-C6-C18	-6.68	109.00	118.33
9	A	371	CPS	C2-C19-C18	6.59	118.89	111.82
9	D	104	CPS	C9-C5-C4	6.38	123.49	117.67
9	D	103	CPS	C10-C5-C6	-6.38	101.22	111.21
9	A	371	CPS	C3-C19-C18	-6.17	101.84	110.88
9	D	103	CPS	C3-C19-C18	-6.10	101.95	110.88
9	D	103	CPS	C7-C6-C18	-6.03	109.90	118.33
9	A	370	CPS	C3-C19-C18	-6.02	102.07	110.88
9	D	103	CPS	C9-C5-C4	5.99	123.13	117.67
9	D	104	CPS	C7-C6-C18	-5.93	110.04	118.33
9	D	104	CPS	C3-C19-C18	-5.92	102.21	110.88
9	D	105	CPS	C3-C19-C18	-5.89	102.25	110.88
9	D	105	CPS	C10-C5-C6	-5.82	102.10	111.21
9	D	103	CPS	C15-C16-C17	5.80	120.86	114.46
9	D	104	CPS	C5-C6-C18	5.64	121.94	114.74
9	D	104	CPS	C10-C5-C6	-5.63	102.40	111.21
9	A	370	CPS	C5-C9-C20	5.59	126.17	119.50
9	A	370	CPS	C2-C19-C18	5.57	117.80	111.82
9	D	105	CPS	C9-C5-C6	5.56	105.69	100.09
9	D	103	CPS	C5-C6-C18	5.54	121.81	114.74
9	D	105	CPS	C15-C16-C17	5.44	120.46	114.46
9	D	105	CPS	C7-C6-C18	-5.36	110.84	118.33
9	D	105	CPS	C5-C6-C18	5.33	121.55	114.74
9	A	370	CPS	C10-C5-C6	-5.32	102.88	111.21
9	A	371	CPS	C10-C5-C6	-5.23	103.03	111.21
9	A	371	CPS	C31-C30-N2	5.20	126.39	115.38
9	A	371	CPS	C6-C5-C4	5.12	112.17	107.40
9	D	105	CPS	C9-C5-C4	4.96	122.20	117.67
9	A	371	CPS	C15-C16-C17	4.95	119.93	114.46
9	D	103	CPS	C7-C6-C5	4.92	108.38	103.55
9	D	104	CPS	C7-C6-C5	4.86	108.32	103.55
9	A	370	CPS	C10-C5-C4	-4.79	104.19	109.07
9	D	103	CPS	C5-C9-C20	4.77	125.19	119.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	371	CPS	C9-C5-C4	4.72	121.98	117.67
9	D	104	CPS	C9-C5-C6	4.57	104.70	100.09
9	A	370	CPS	C8-C9-C20	-4.48	105.21	112.15
9	D	104	CPS	C10-C5-C4	-4.38	104.60	109.07
9	A	370	CPS	C7-C6-C5	4.36	107.83	103.55
9	A	371	CPS	C5-C6-C18	4.32	120.26	114.74
9	D	104	CPS	C15-C16-C17	4.27	119.17	114.46
9	A	371	CPS	C7-C6-C18	-4.25	112.39	118.33
9	A	370	CPS	C15-C16-C17	4.24	119.14	114.46
9	D	103	CPS	C21-C20-C9	4.20	119.35	112.92
9	D	105	CPS	C21-C20-C9	4.20	119.35	112.92
9	A	371	CPS	O1S-S-C32	-4.17	101.90	106.92
9	D	103	CPS	C6-C5-C4	4.16	111.28	107.40
9	D	104	CPS	C5-C9-C20	4.10	124.39	119.50
9	A	371	CPS	C9-C5-C6	4.08	104.20	100.09
9	A	371	CPS	O4-C4-C5	-3.97	104.32	111.03
9	D	105	CPS	C16-C17-C18	3.96	115.71	111.48
9	A	370	CPS	C11-C2-C1	3.96	114.64	108.26
9	D	103	CPS	C9-C5-C6	3.90	104.02	100.09
9	A	370	CPS	C11-C2-C19	-3.86	105.86	111.18
9	D	104	CPS	C6-C5-C4	3.84	110.98	107.40
9	D	105	CPS	O4-C4-C5	-3.84	104.53	111.03
9	A	370	CPS	O4-C4-C5	-3.83	104.56	111.03
9	D	105	CPS	C6-C5-C4	3.83	110.96	107.40
9	D	103	CPS	C16-C17-C18	3.79	115.53	111.48
9	D	104	CPS	C21-C20-C9	3.78	118.71	112.92
9	A	371	CPS	C16-C17-C18	3.73	115.46	111.48
9	A	370	CPS	C6-C5-C4	3.68	110.83	107.40
9	D	103	CPS	C10-C5-C4	-3.67	105.33	109.07
9	D	104	CPS	C16-C17-C18	3.63	115.36	111.48
9	D	104	CPS	O4-C4-C5	-3.53	105.06	111.03
9	D	105	CPS	C7-C6-C5	3.48	106.97	103.55
9	A	370	CPS	C16-C17-C18	3.47	115.19	111.48
9	A	370	CPS	C21-C20-C9	3.35	118.05	112.92
9	D	104	CPS	C8-C9-C20	-3.33	106.99	112.15
9	A	370	CPS	C9-C5-C6	3.30	103.42	100.09
9	D	103	CPS	C15-C14-C13	-3.29	107.93	112.76
9	D	104	CPS	C1-C12-C13	3.28	114.68	110.47
9	D	103	CPS	O4-C4-C3	-3.27	102.46	109.12
9	D	103	CPS	O4-C4-C5	-3.25	105.54	111.03
9	D	105	CPS	C5-C9-C20	3.22	123.34	119.50
9	A	371	CPS	C10-C5-C4	-3.21	105.80	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	371	CPS	O4-C4-C3	-3.19	102.62	109.12
9	A	371	CPS	C11-C2-C19	-3.17	106.81	111.18
9	A	371	CPS	C5-C9-C20	3.08	123.17	119.50
9	A	371	CPS	C26-C25-N1	3.07	121.00	112.21
9	A	370	CPS	C1-C12-C13	3.06	114.39	110.47
9	D	105	CPS	C19-C2-C15	-3.05	104.29	108.58
9	D	103	CPS	C8-C9-C20	-3.01	107.49	112.15
9	D	103	CPS	C1-C12-C13	3.01	114.33	110.47
9	D	105	CPS	C1-C12-C13	2.99	114.31	110.47
9	A	370	CPS	C15-C14-C13	-2.99	108.37	112.76
9	A	370	CPS	O3-C17-C18	-2.98	102.77	109.43
9	D	105	CPS	C11-C2-C1	2.95	113.01	108.26
9	D	103	CPS	C11-C2-C1	2.93	112.99	108.26
9	D	104	CPS	C15-C14-C13	-2.89	108.52	112.76
9	D	104	CPS	C16-C15-C14	-2.86	107.89	111.19
9	A	371	CPS	O3-C17-C18	-2.84	103.07	109.43
9	A	371	CPS	O2S-S-C32	2.81	110.31	105.77
9	D	104	CPS	C11-C2-C1	2.80	112.78	108.26
9	D	104	CPS	O3-C17-C18	-2.74	103.30	109.43
9	D	103	CPS	C16-C15-C14	-2.73	108.04	111.19
9	A	371	CPS	C16-C15-C14	-2.73	108.05	111.19
9	A	371	CPS	C15-C14-C13	-2.73	108.75	112.76
9	A	370	CPS	C14-C15-C2	2.68	115.50	112.66
9	D	103	CPS	C19-C2-C15	-2.67	104.83	108.58
9	D	105	CPS	O3-C17-C18	-2.66	103.48	109.43
9	D	105	CPS	C10-C5-C9	-2.65	107.06	111.21
9	A	371	CPS	C21-C20-C9	2.65	116.98	112.92
9	D	105	CPS	O4-C4-C3	-2.64	103.74	109.12
9	D	104	CPS	O4-C4-C3	-2.64	103.75	109.12
9	D	103	CPS	O3-C17-C18	-2.61	103.60	109.43
9	D	104	CPS	C11-C2-C19	-2.60	107.60	111.18
9	D	105	CPS	C15-C14-C13	-2.60	108.94	112.76
9	D	103	CPS	C11-C2-C19	-2.55	107.67	111.18
9	A	371	CPS	O1-C24-C23	2.54	126.67	122.02
9	D	103	CPS	C14-C15-C2	2.49	115.31	112.66
9	A	370	CPS	O4-C4-C3	-2.43	104.17	109.12
9	A	371	CPS	C7-C8-C9	-2.33	100.51	105.13
9	D	104	CPS	C19-C2-C15	-2.25	105.42	108.58
9	D	105	CPS	C16-C15-C14	-2.19	108.67	111.19
9	A	370	CPS	C3-C4-C5	-2.19	109.00	111.24
9	D	104	CPS	C14-C15-C2	2.18	114.97	112.66
9	D	105	CPS	C8-C9-C20	-2.14	108.83	112.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	371	CPS	C19-C2-C15	-2.07	105.67	108.58
9	D	105	CPS	C10-C5-C4	-2.04	106.99	109.07
9	A	371	CPS	O2-C13-C12	2.04	115.35	110.16
9	D	105	CPS	C11-C2-C19	-2.02	108.41	111.18
9	A	371	CPS	C1-C12-C13	2.01	113.05	110.47
9	A	370	CPS	C12-C1-C2	2.00	116.22	112.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	371	CPS	C20-C22-C23-C24
9	A	371	CPS	C25-C26-C27-N2
9	A	371	CPS	C30-C31-C32-S
9	A	371	CPS	C26-C25-N1-C24
9	A	371	CPS	C26-C27-N2-C28
9	A	371	CPS	C26-C27-N2-C30
9	A	371	CPS	C26-C27-N2-C29

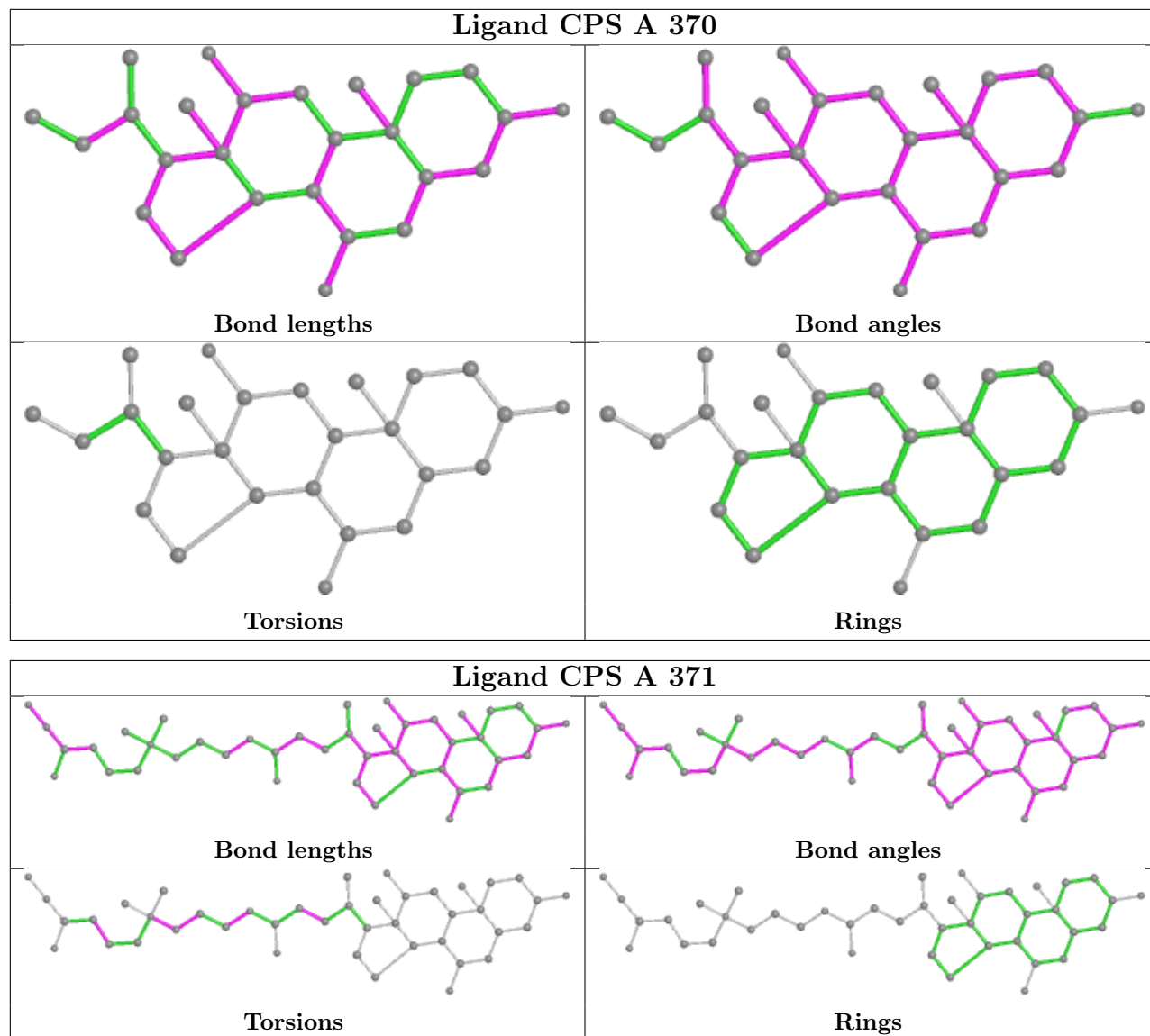
There are no ring outliers.

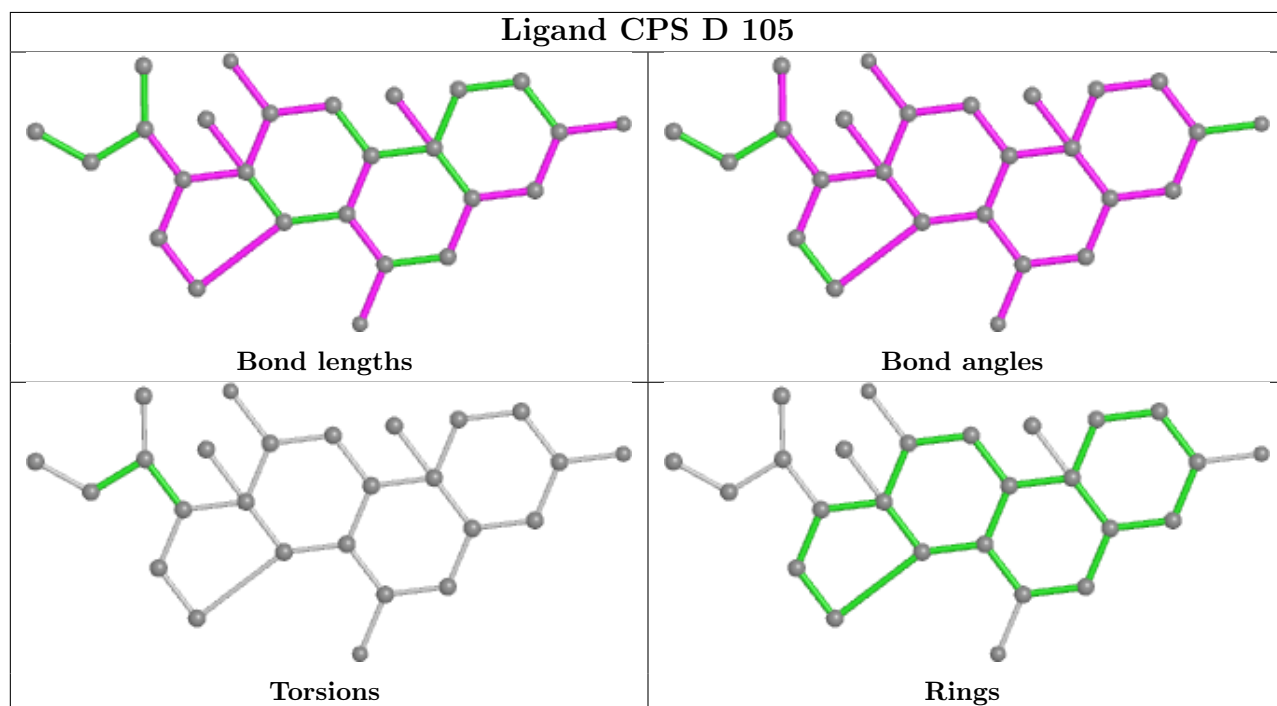
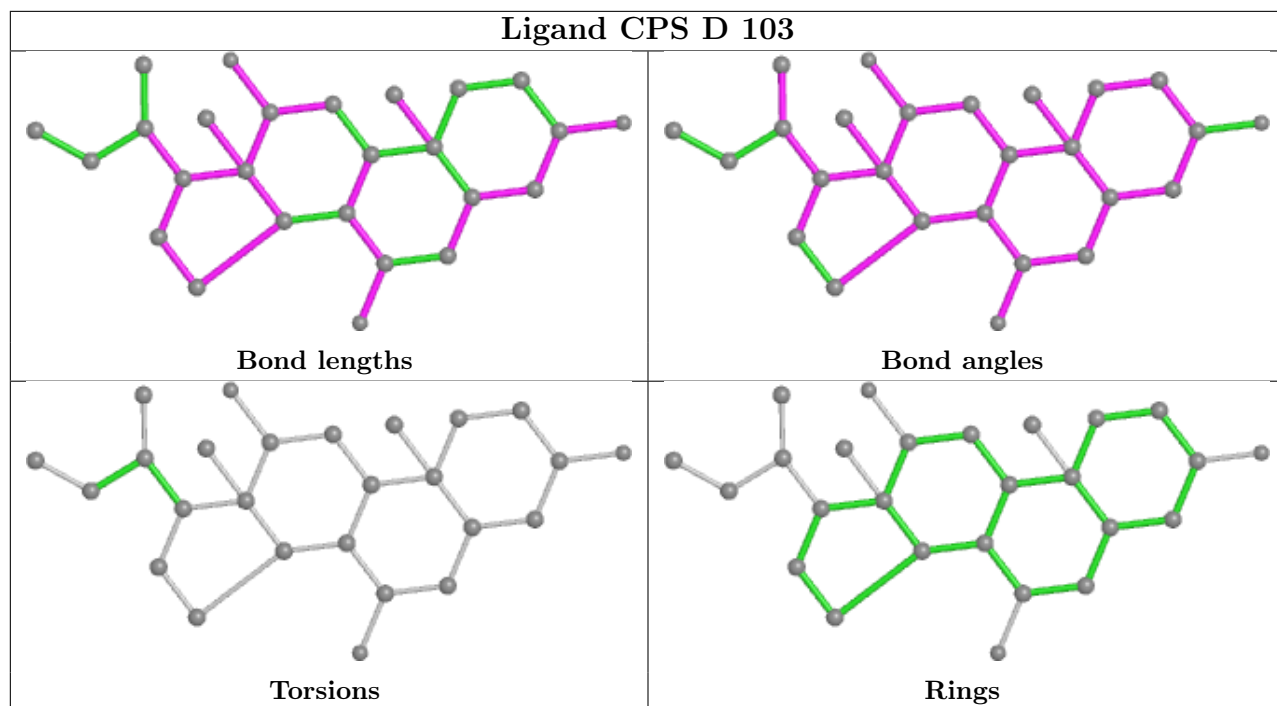
7 monomers are involved in 28 short contacts:

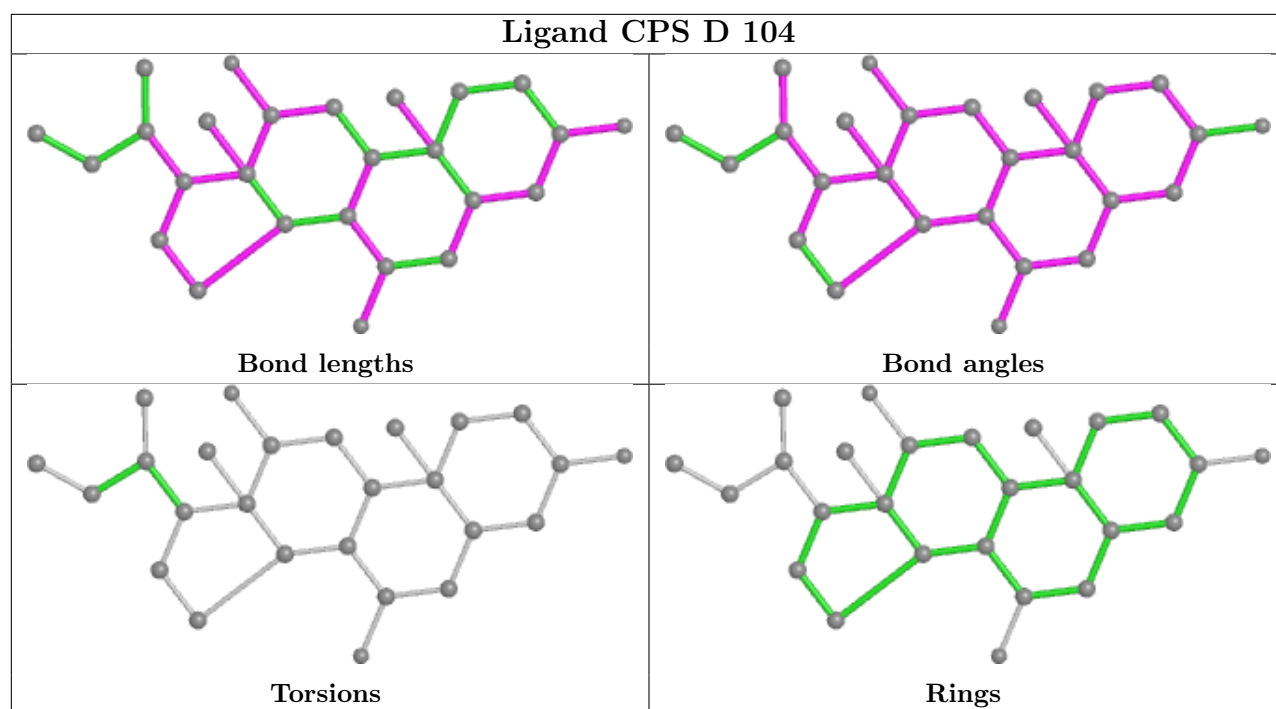
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	203	SO4	1	0
9	A	370	CPS	1	0
9	A	371	CPS	13	0
8	B	204	SO4	1	0
9	D	103	CPS	1	0
9	D	105	CPS	11	0
8	B	202	SO4	1	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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.