



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:56 AM BST

PDB ID : 1MX1
Title : Crystal Structure of Human Liver Carboxylesterase in complex with tacrine
Authors : Bencharit, S.; Morton, C.L.; Hyatt, J.L.; Kuhn, P.; Danks, M.K.; Potter, P.M.;
Redinbo, M.R.
Deposited on : 2002-10-01
Resolution : 2.40 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) : 2.13.1

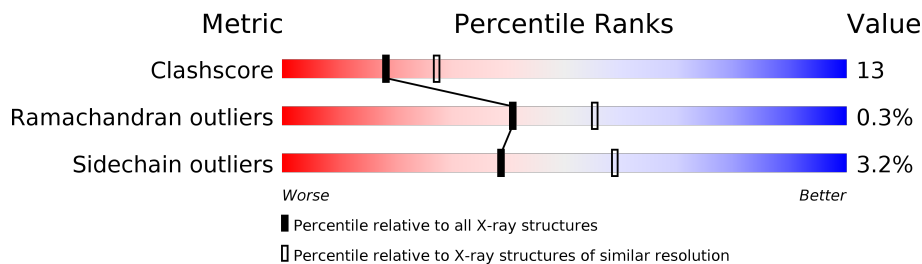
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
2	G	2	

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
4	SIA	A	182	-	-	X	-
4	SIA	B	282	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 27468 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.

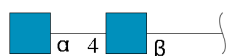
- Molecule 1 is a protein called liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4130	2662	685	763	20	0	0	0
1	B	531	4124	2659	684	761	20	0	0	0
1	C	531	4124	2659	684	761	20	0	0	0
1	D	531	4124	2659	684	761	20	0	0	0
1	E	531	4124	2659	684	761	20	0	0	0
1	F	531	4124	2659	684	761	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

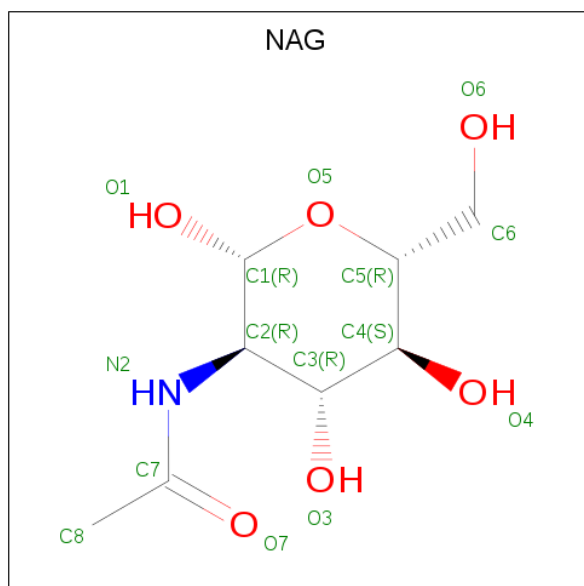
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141
F	?	-	GLN	deletion	UNP P23141

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



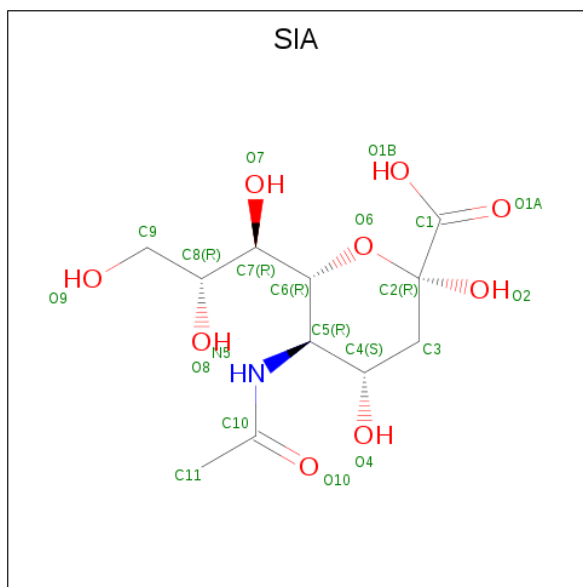
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



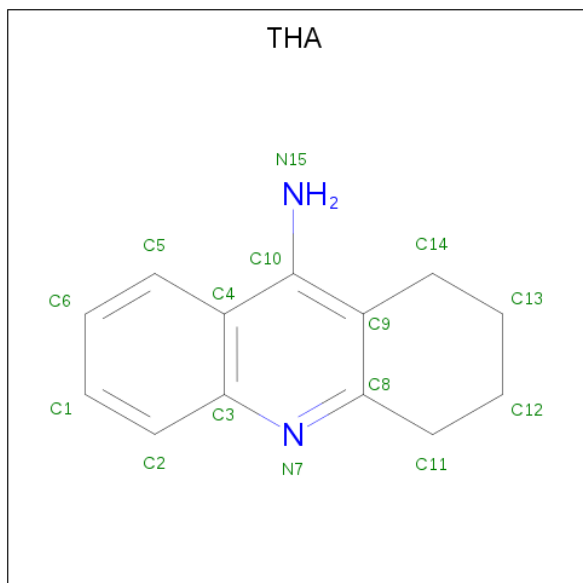
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0
3	F	1	14	8	1	5	0	0
3	F	1	14	8	1	5	0	0

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	21	11	1	9	0	0
4	B	1	21	11	1	9	0	0
4	D	1	21	11	1	9	1	0
4	E	1	21	11	1	9	1	0

- Molecule 5 is TACRINE (three-letter code: THA) (formula: $C_{13}H_{14}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	1
			60	52	8		
5	B	1	Total	C	N	0	1
			60	52	8		
5	C	1	Total	C	N	0	1
			75	65	10		
5	D	1	Total	C	N	0	1
			75	65	10		
5	E	1	Total	C	N	0	1
			75	65	10		
5	F	1	Total	C	N	0	1
			60	52	8		

- Molecule 6 is water.

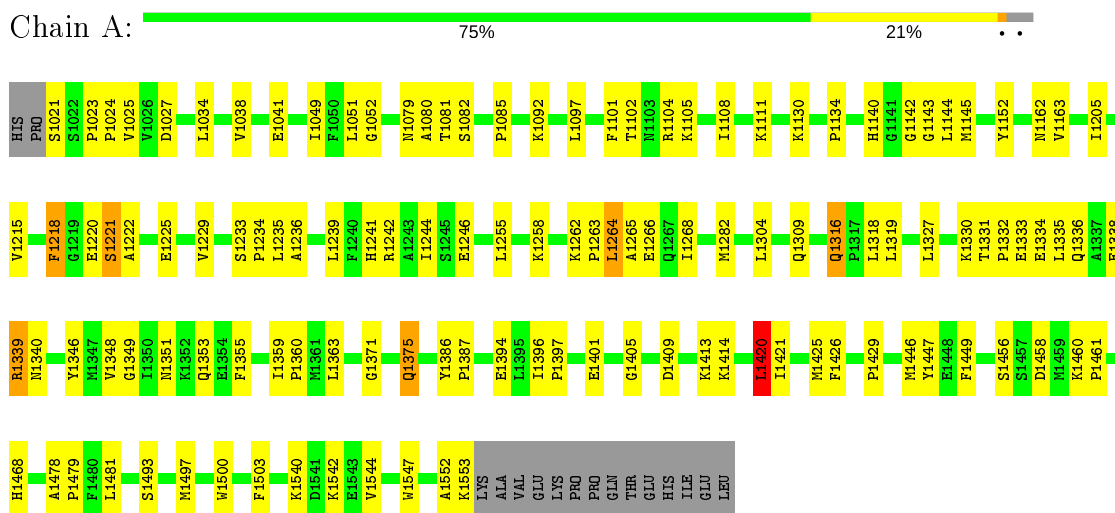
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	364	Total	O	0	0
			364	364		
6	B	360	Total	O	0	0
			360	360		
6	C	371	Total	O	0	0
			371	371		
6	D	306	Total	O	0	0
			306	306		
6	E	353	Total	O	0	0
			353	353		
6	F	363	Total	O	0	0
			363	363		

3 Residue-property plots [i](#)

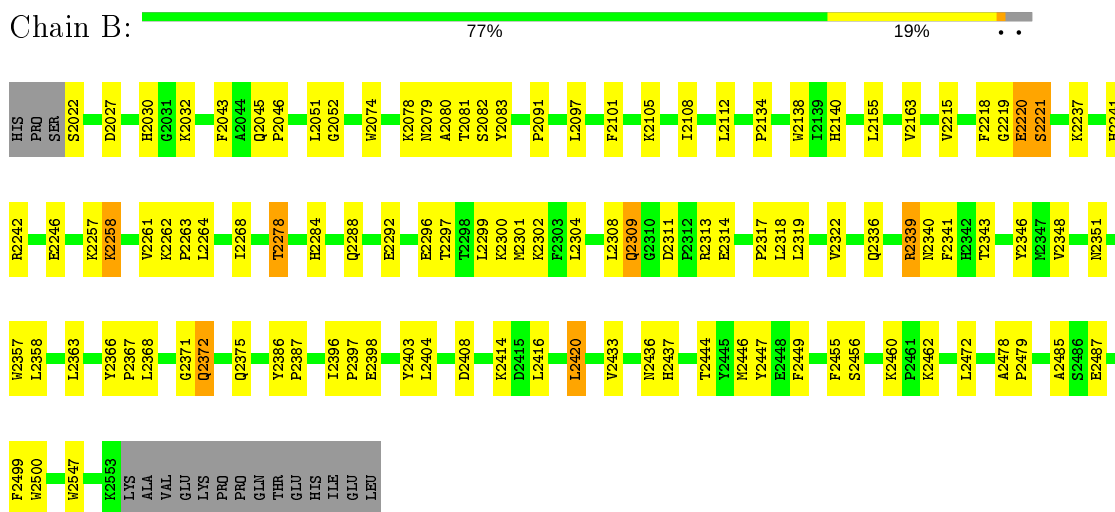
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

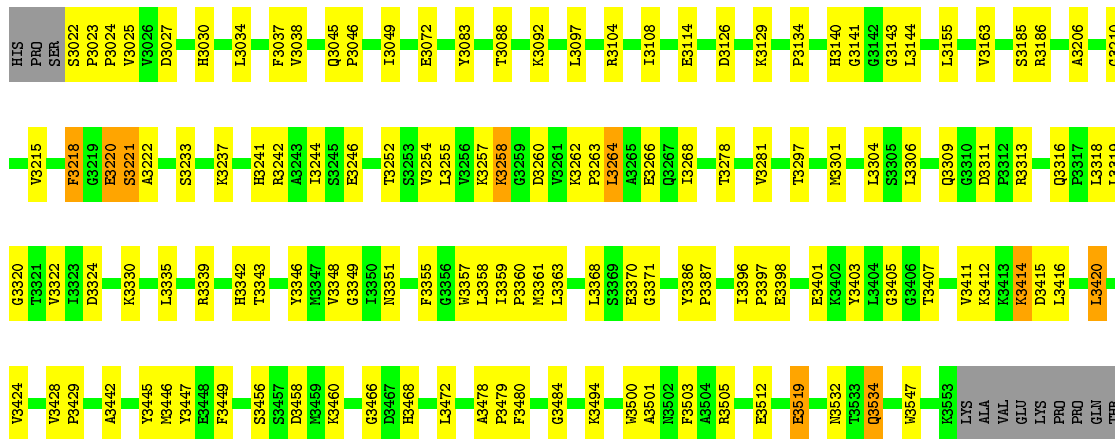


- Molecule 1: liver Carboxylesterase I



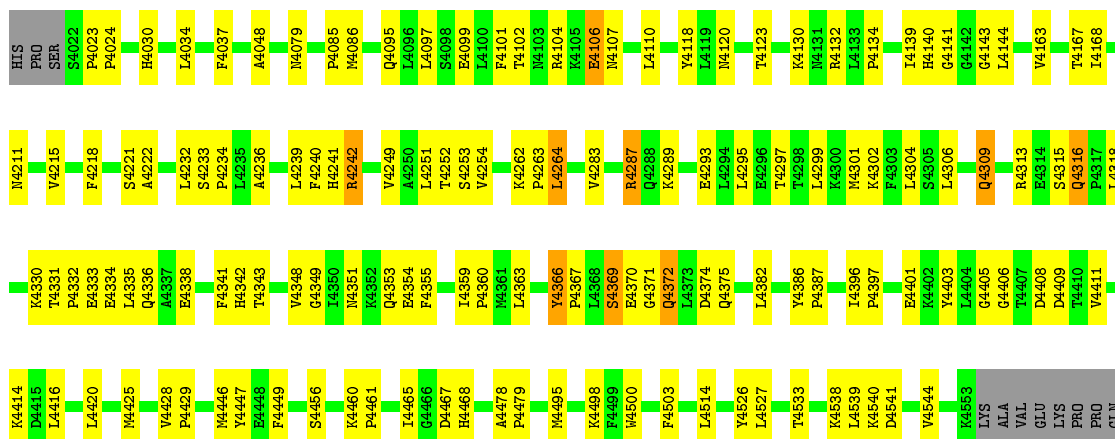
- Molecule 1: liver Carboxylesterase I





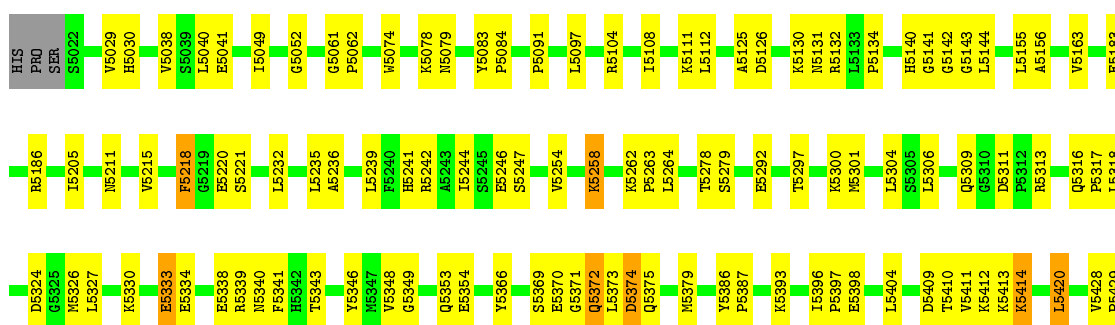
GLU
HIS
ILE
GLU
LEU

• Molecule 1: liver Carboxylesterase I



THR
GLU
HIS
ILE
GLU
LEU

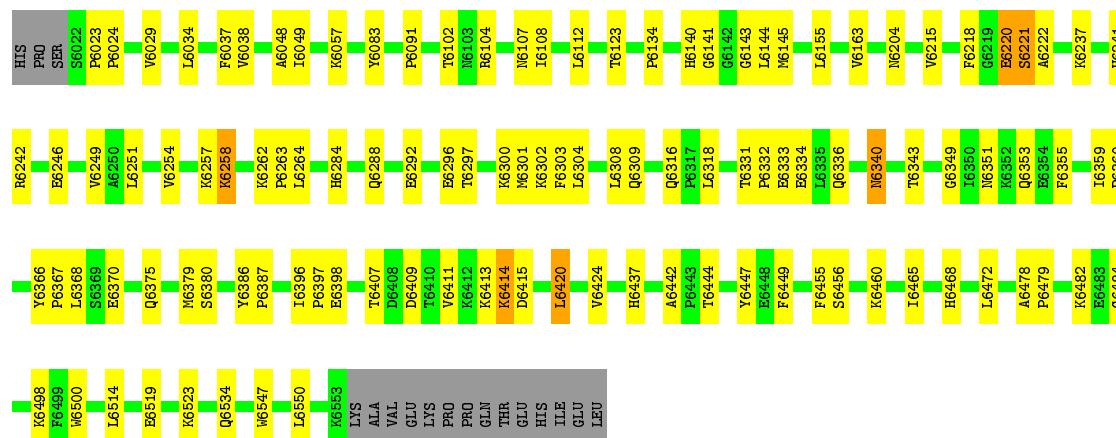
• Molecule 1: liver Carboxylesterase I





- Molecule 1: liver Carboxylesterase I

Chain F: 76% 20%



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

Chain G: 50% 50%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.02Å 117.03Å 176.01Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40	Depositor
% Data completeness (in resolution range)	99.4 (19.98-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.162 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	27468	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: SIA, THA, NAG, NDG

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	0.33	0/4236	0.58	1/5754 (0.0%)
1	B	0.33	0/4230	0.58	0/5746
1	C	0.34	0/4230	0.59	0/5746
1	D	0.32	0/4230	0.56	0/5746
1	E	0.33	0/4230	0.58	0/5746
1	F	0.34	0/4230	0.57	0/5746
All	All	0.33	0/25386	0.58	1/34484 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1420	LEU	CA-CB-CG	5.36	127.63	115.30

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	4130	0	4131	117	0
1	B	4124	0	4126	107	0
1	C	4124	0	4126	126	0
1	D	4124	0	4126	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4124	0	4125	112	0
1	F	4124	0	4126	97	0
2	G	28	0	24	2	0
3	A	14	0	13	0	0
3	B	14	0	13	3	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
3	F	28	0	26	1	0
4	A	21	0	18	30	0
4	B	21	0	18	16	0
4	D	21	0	18	7	0
4	E	21	0	18	7	0
5	A	60	0	56	13	0
5	B	60	0	56	9	0
5	C	75	0	70	12	0
5	D	75	0	70	10	0
5	E	75	0	70	14	0
5	F	60	0	56	7	0
6	A	364	0	0	25	0
6	B	360	0	0	16	0
6	C	371	0	0	17	0
6	D	306	0	0	9	0
6	E	353	0	0	22	0
6	F	363	0	0	12	0
All	All	27468	0	25312	671	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 13.

All (671) 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:1052:GLY:HA3	4:A:182:SIA:H32	1.24	1.19
4:B:282:SIA:H111	6:C:7197:HOH:O	1.42	1.18
4:B:282:SIA:H113	1:C:3278:THR:HB	1.29	1.14
4:A:182:SIA:H111	1:B:2278:THR:HB	1.31	1.12
1:C:3258:LYS:HE2	1:C:3258:LYS:H	1.09	1.12
4:A:182:SIA:C11	1:B:2278:THR:HB	1.82	1.08
1:C:3363:LEU:HD13	5:C:3[E]:THA:H131	1.35	1.04
1:A:1242:ARG:HG2	1:A:1242:ARG:HH11	1.26	1.00
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.07	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.10	0.98
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.09	0.97
1:E:5371:GLY:HA2	1:E:5414:LYS:HD3	1.45	0.97
1:F:6215:VAL:H	1:F:6241:HIS:HD2	1.09	0.96
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.27	0.96
1:A:1085:PRO:HD3	6:A:8501:HOH:O	1.66	0.94
1:A:1080:ALA:HA	4:A:182:SIA:C1	1.99	0.93
1:E:5215:VAL:H	1:E:5241:HIS:HD2	1.07	0.93
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.06	0.93
1:B:2078:LYS:HG3	4:B:282:SIA:H91	1.51	0.92
4:B:282:SIA:C11	1:C:3278:THR:HB	1.99	0.92
1:A:1080:ALA:HA	4:A:182:SIA:O1B	1.70	0.91
1:B:2398:GLU:HG3	6:B:7028:HOH:O	1.71	0.91
1:E:5398:GLU:HG3	6:E:7131:HOH:O	1.70	0.91
1:C:3242:ARG:HH11	1:C:3242:ARG:HG2	1.40	0.86
1:C:3258:LYS:HE2	1:C:3258:LYS:N	1.91	0.85
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.59	0.85
1:F:6134:PRO:HG2	1:F:6163:VAL:HG12	1.59	0.85
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.58	0.84
1:E:5091:PRO:HG3	1:E:5112:LEU:HD11	1.58	0.84
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.58	0.84
1:A:1363:LEU:HD13	5:A:1[C]:THA:H6	1.60	0.84
4:A:182:SIA:C11	1:B:2278:THR:CB	2.56	0.84
1:B:2339:ARG:HH22	1:B:2436:ASN:HD22	1.23	0.83
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.60	0.82
1:B:2340:ASN:HB2	6:B:8374:HOH:O	1.77	0.82
1:D:4264:LEU:HG	1:D:4316:GLN:HG2	1.62	0.81
1:A:1082:SER:HB2	6:A:7946:HOH:O	1.80	0.81
4:E:582:SIA:H111	6:E:8910:HOH:O	1.79	0.81
4:B:282:SIA:H112	6:C:7272:HOH:O	1.80	0.80
1:B:2363:LEU:HD13	5:B:2[B]:THA:H131	1.64	0.80
1:B:2080:ALA:HA	4:B:282:SIA:O1B	1.81	0.80
1:C:3258:LYS:CE	1:C:3258:LYS:H	1.94	0.79
1:F:6258:LYS:H	1:F:6258:LYS:CE	1.96	0.79
1:C:3407:THR:HB	6:C:7546:HOH:O	1.83	0.78
1:F:6304:LEU:HD22	5:F:6[D]:THA:H122	1.66	0.78
1:E:5029:VAL:HB	6:E:8655:HOH:O	1.82	0.77
1:E:5215:VAL:H	1:E:5241:HIS:CD2	1.98	0.77
1:E:5304:LEU:HD22	5:E:5[D]:THA:H112	1.64	0.77
1:F:6215:VAL:H	1:F:6241:HIS:CD2	2.00	0.77
4:A:182:SIA:H111	1:B:2278:THR:CB	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:182:SIA:H112	1:B:2278:THR:HB	1.68	0.75
1:B:2215:VAL:H	1:B:2241:HIS:CD2	1.99	0.75
1:F:6258:LYS:N	1:F:6258:LYS:HE2	2.02	0.74
1:F:6251:LEU:HD11	1:F:6336:GLN:HE22	1.51	0.74
1:F:6340:ASN:HB3	6:F:7188:HOH:O	1.85	0.74
1:B:2220:GLU:HG2	1:B:2472:LEU:HD21	1.69	0.74
1:F:6318:LEU:HD11	5:F:6[C]:THA:H141	1.68	0.74
1:F:6023:PRO:HB2	1:F:6034:LEU:HD21	1.69	0.74
1:F:6257:LYS:HE2	1:F:6316:GLN:HE21	1.54	0.73
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.01	0.73
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.71	0.73
1:C:3104:ARG:HD2	6:C:7871:HOH:O	1.88	0.73
1:A:1052:GLY:HA3	4:A:182:SIA:C3	2.13	0.72
1:A:1024:PRO:HA	6:A:7684:HOH:O	1.90	0.72
1:C:3458:ASP:HB2	6:D:7637:HOH:O	1.88	0.71
1:D:4079:ASN:O	4:D:482:SIA:H31	1.91	0.71
1:B:2082:SER:O	4:B:282:SIA:O1A	2.09	0.71
1:A:1130:LYS:HB3	6:A:8340:HOH:O	1.90	0.71
1:B:2221:SER:OG	5:B:2[B]:THA:H5	1.91	0.71
4:A:182:SIA:H112	1:B:2278:THR:CB	2.19	0.70
1:A:1041:GLU:CD	1:A:1041:GLU:H	1.92	0.70
1:D:4134:PRO:HG2	1:D:4163:VAL:HG12	1.74	0.70
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.73	0.70
1:A:1242:ARG:HH11	1:A:1242:ARG:CG	2.04	0.69
1:A:1052:GLY:CA	4:A:182:SIA:H32	2.14	0.69
1:C:3215:VAL:H	1:C:3241:HIS:CD2	2.00	0.69
1:F:6242:ARG:HH11	1:F:6242:ARG:HG2	1.58	0.69
1:B:2052:GLY:HA3	4:B:282:SIA:H32	1.75	0.69
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.03	0.69
1:B:2371:GLY:HA3	1:E:5371:GLY:HA3	1.75	0.69
4:B:282:SIA:H113	1:C:3278:THR:CB	2.16	0.68
1:F:6257:LYS:HE2	1:F:6316:GLN:NE2	2.08	0.68
1:F:6353:GLN:NE2	1:F:6465:ILE:H	1.92	0.68
1:E:5409:ASP:HB2	1:E:5412:LYS:HB2	1.76	0.68
1:C:3221:SER:HB3	6:C:7018:HOH:O	1.93	0.68
1:B:2339:ARG:HB3	1:B:2339:ARG:NH1	2.09	0.68
4:A:182:SIA:C11	1:B:2278:THR:CG2	2.73	0.67
1:B:2314:GLU:HB3	6:B:8159:HOH:O	1.93	0.67
1:B:2339:ARG:HH22	1:B:2436:ASN:ND2	1.91	0.67
1:A:1221:SER:HB3	6:A:7019:HOH:O	1.95	0.67
1:B:2051:LEU:O	4:B:282:SIA:O1A	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6221:SER:OG	5:F:6[D]:THA:H5	1.95	0.67
1:D:4332:PRO:O	1:D:4336:GLN:HG2	1.95	0.66
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.30	0.66
1:A:1333:GLU:H	1:A:1333:GLU:CD	1.98	0.66
1:B:2304:LEU:HD23	1:B:2318:LEU:CD2	2.26	0.65
1:C:3252:THR:HG21	5:C:3[D]:THA:H132	1.77	0.65
2:G:1:NAG:O3	2:G:2:NDG:H8C2	1.95	0.65
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.78	0.65
1:C:3414:LYS:HE2	1:C:3415:ASP:OD2	1.96	0.65
1:E:5420:LEU:HD13	1:E:5547:TRP:HZ2	1.62	0.65
4:E:582:SIA:H113	6:E:8318:HOH:O	1.96	0.65
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.32	0.65
1:F:6398:GLU:HG3	6:F:7017:HOH:O	1.97	0.65
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	1.78	0.65
1:C:3268:ILE:HD11	1:C:3319:LEU:HD21	1.79	0.65
1:A:1332:PRO:O	1:A:1336:GLN:HG2	1.98	0.64
1:D:4355:PHE:CD2	1:D:4425:MET:HE1	2.32	0.64
1:D:4353:GLN:NE2	1:D:4465:ILE:H	1.96	0.64
1:E:5292:GLU:HG2	6:E:8311:HOH:O	1.97	0.64
1:E:5220:GLU:HG2	1:E:5472:LEU:HD21	1.79	0.64
1:E:5254:VAL:HG11	5:E:5[E]:THA:H1	1.80	0.64
6:B:7243:HOH:O	1:E:5462:LYS:HB3	1.98	0.64
1:C:3304:LEU:HD23	1:C:3318:LEU:HD21	1.80	0.63
1:F:6254:VAL:HG11	5:F:6[B]:THA:H6	1.81	0.63
1:F:6220:GLU:OE2	1:F:6221:SER:HB2	1.99	0.63
1:B:2339:ARG:HH11	1:B:2339:ARG:HB3	1.64	0.63
1:B:2052:GLY:O	4:B:282:SIA:O2	2.17	0.63
1:D:4236:ALA:HA	1:D:4239:LEU:HD12	1.79	0.63
1:E:5079:ASN:O	4:E:582:SIA:O10	2.16	0.63
1:D:4304:LEU:HG	5:D:4[A]:THA:H2	1.81	0.63
1:F:6102:THR:OG1	1:F:6104:ARG:HG2	1.99	0.62
1:F:6292:GLU:HG3	6:F:7630:HOH:O	1.99	0.62
1:E:5414:LYS:HB3	1:E:5414:LYS:NZ	2.14	0.62
1:A:1339:ARG:HH11	1:A:1339:ARG:HG3	1.64	0.62
1:D:4406:GLY:HA3	6:D:7429:HOH:O	2.00	0.62
1:E:5374:ASP:HB2	6:E:7207:HOH:O	1.98	0.62
1:C:3114:GLU:HB3	6:C:8433:HOH:O	1.99	0.62
1:B:2339:ARG:HA	1:B:2341:PHE:CE2	2.34	0.62
1:D:4024:PRO:HG3	1:D:4037:PHE:CZ	2.35	0.62
1:C:3220:GLU:HG2	1:C:3472:LEU:HD11	1.82	0.62
1:F:6024:PRO:HG3	1:F:6037:PHE:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.82	0.61
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.35	0.61
1:E:5304:LEU:HD23	1:E:5318:LEU:HD21	1.82	0.61
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.35	0.61
4:A:182:SIA:H113	6:A:8501:HOH:O	2.00	0.61
1:B:2097:LEU:HD13	5:B:2[D]:THA:H6	1.82	0.61
1:A:1355:PHE:CD1	1:A:1360:PRO:HG3	2.36	0.61
1:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.81	0.61
1:A:1371:GLY:O	1:A:1414:LYS:HD3	2.00	0.61
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.82	0.61
1:D:4382:LEU:HD23	1:D:4396:ILE:HG23	1.83	0.61
1:D:4023:PRO:HB2	1:D:4034:LEU:HD11	1.83	0.60
1:D:4085:PRO:HD3	4:D:482:SIA:H112	1.81	0.60
1:A:1264:LEU:HG	1:A:1316:GLN:HG2	1.83	0.60
1:B:2246:GLU:HG2	1:B:2447:TYR:OH	2.01	0.60
6:A:7397:HOH:O	1:F:6309:GLN:HB3	2.01	0.60
1:C:3398:GLU:HG3	6:C:7168:HOH:O	2.02	0.60
1:F:6023:PRO:CB	1:F:6034:LEU:HD21	2.32	0.60
1:C:3242:ARG:HH11	1:C:3242:ARG:CG	2.14	0.59
1:A:1552:ALA:O	1:A:1553:LYS:HB2	2.02	0.59
1:A:1097:LEU:HD13	5:A:1[A]:THA:H132	1.83	0.59
1:C:3309:GLN:HB3	6:D:7906:HOH:O	2.01	0.59
1:D:4097:LEU:HD13	5:D:4[C]:THA:H6	1.82	0.59
1:E:5097:LEU:HD13	5:E:5[E]:THA:H132	1.85	0.59
6:B:8017:HOH:O	1:E:5300:LYS:HE2	2.01	0.59
1:E:5456:SER:HB3	1:E:5460:LYS:HD3	1.83	0.59
1:E:5343:THR:HB	1:E:5442:ALA:HB2	1.84	0.59
1:D:4095:GLN:O	1:D:4099:GLU:HG3	2.03	0.59
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.86	0.59
1:A:1338:GLU:O	1:A:1340:ASN:N	2.34	0.59
1:A:1038:VAL:HG21	1:A:1049:ILE:HD12	1.83	0.58
1:A:1097:LEU:HD13	5:A:1[D]:THA:H6	1.85	0.58
1:E:5304:LEU:HD23	1:E:5318:LEU:CD2	2.33	0.58
1:E:5428:VAL:HB	1:E:5429:PRO:HD3	1.85	0.58
1:C:3257:LYS:HE2	1:C:3316:GLN:NE2	2.18	0.58
1:F:6420:LEU:HD13	1:F:6547:TRP:HZ2	1.68	0.58
1:A:1355:PHE:CD2	1:A:1425:MET:HE1	2.38	0.58
1:D:4232:LEU:HD23	1:D:4341:PHE:CB	2.33	0.58
1:E:5083:TYR:CE2	1:E:5108:ILE:HD13	2.39	0.58
1:B:2371:GLY:HA2	1:B:2414:LYS:HD3	1.86	0.58
1:D:4355:PHE:CE1	1:D:4360:PRO:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4097:LEU:HD13	5:D:4[E]:THA:H132	1.84	0.58
1:B:2336:GLN:HE22	1:B:2433:VAL:HA	1.68	0.58
1:B:2078:LYS:CG	4:B:282:SIA:H91	2.31	0.58
1:C:3097:LEU:HD13	5:C:3[C]:THA:H6	1.84	0.58
1:C:3221:SER:OG	1:C:3468:HIS:NE2	2.36	0.57
1:E:5396:ILE:HB	1:E:5397:PRO:HD3	1.85	0.57
1:E:5318:LEU:HD11	5:E:5[C]:THA:H141	1.86	0.57
1:D:4330:LYS:HG3	1:D:4335:LEU:HG	1.87	0.57
1:D:4264:LEU:CG	1:D:4316:GLN:HG2	2.32	0.57
1:F:6241:HIS:O	1:F:6242:ARG:HG2	2.04	0.57
1:C:3371:GLY:O	1:C:3411:VAL:HA	2.04	0.57
1:B:2051:LEU:C	4:B:282:SIA:O1A	2.43	0.57
1:C:3255:LEU:HD11	5:C:3[D]:THA:H122	1.85	0.57
1:D:4221:SER:OG	1:D:4468:HIS:NE2	2.38	0.57
4:A:182:SIA:C1	6:A:7946:HOH:O	2.51	0.57
1:F:6221:SER:HB3	6:F:7002:HOH:O	2.05	0.57
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.68	0.57
4:D:482:SIA:H4	6:D:7646:HOH:O	2.04	0.57
1:E:5333:GLU:CD	1:E:5333:GLU:H	2.08	0.57
1:B:2221:SER:OG	5:B:2[A]:THA:H142	2.04	0.56
1:A:1242:ARG:HG2	1:A:1242:ARG:NH1	2.06	0.56
1:D:4363:LEU:HD13	5:D:4[A]:THA:H6	1.88	0.56
1:D:4236:ALA:HB1	1:D:4240:PHE:HE1	1.69	0.56
1:D:4304:LEU:HG	5:D:4[B]:THA:H112	1.88	0.56
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.40	0.56
1:A:1262:LYS:HG3	1:A:1266:GLU:OE2	2.05	0.56
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.87	0.56
1:D:4343:THR:HG21	6:D:7992:HOH:O	2.05	0.56
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.87	0.56
1:A:1266:GLU:HA	1:A:1282:MET:HE3	1.88	0.56
1:A:1420:LEU:C	1:A:1420:LEU:HD12	2.27	0.56
1:A:1097:LEU:CD1	5:A:1[D]:THA:H6	2.36	0.56
1:B:2420:LEU:HD13	1:B:2547:TRP:CZ2	2.41	0.56
4:A:182:SIA:C4	6:A:8501:HOH:O	2.53	0.56
1:D:4498:LYS:HB3	1:D:4514:LEU:HD11	1.87	0.55
1:E:5254:VAL:HG11	5:E:5[B]:THA:H6	1.87	0.55
1:E:5373:LEU:H	1:E:5410:THR:HB	1.72	0.55
4:A:182:SIA:C2	6:A:7946:HOH:O	2.54	0.55
1:D:4456:SER:HB3	1:D:4460:LYS:HD3	1.88	0.55
1:E:5334:GLU:O	1:E:5338:GLU:HG3	2.07	0.55
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4252:THR:HG22	1:D:4254:VAL:HG12	1.89	0.55
1:E:5487:GLU:O	1:E:5491:ARG:HG3	2.07	0.55
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.88	0.55
1:E:5386:TYR:N	1:E:5387:PRO:HD2	2.22	0.55
1:A:1461:PRO:HG3	1:F:6370:GLU:HG3	1.89	0.55
1:A:1353:GLN:HA	6:A:8437:HOH:O	2.06	0.55
1:B:2308:LEU:HD11	1:B:2367:PRO:HG3	1.87	0.55
1:B:2296:GLU:HG2	6:B:8017:HOH:O	2.07	0.55
1:D:4106:GLU:CD	1:D:4106:GLU:H	2.11	0.55
1:E:5420:LEU:HD13	1:E:5547:TRP:CZ2	2.40	0.55
1:F:6420:LEU:HD13	1:F:6547:TRP:CZ2	2.42	0.55
1:B:2079:ASN:ND2	3:B:279:NAG:H82	2.22	0.55
1:B:2262:LYS:HB3	1:B:2263:PRO:HD3	1.89	0.54
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.41	0.54
1:C:3092:LYS:HD2	1:D:4302:LYS:HD2	1.89	0.54
3:F:679:NAG:O4	3:F:680:NAG:C1	2.55	0.54
1:B:2079:ASN:OD1	1:B:2081:THR:HG23	2.08	0.54
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.90	0.54
1:B:2097:LEU:HD13	5:B:2[C]:THA:H132	1.90	0.54
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.90	0.54
1:C:3420:LEU:HD13	1:C:3547:TRP:CZ2	2.42	0.54
1:F:6375:GLN:HG3	1:F:6413:LYS:NZ	2.23	0.54
1:B:2264:LEU:HD21	1:B:2319:LEU:HD23	1.90	0.54
1:A:1079:ASN:O	4:A:182:SIA:O1B	2.26	0.54
1:A:1080:ALA:CA	4:A:182:SIA:O1B	2.49	0.54
1:C:3420:LEU:HD12	1:C:3420:LEU:C	2.27	0.54
1:B:2051:LEU:O	4:B:282:SIA:C1	2.56	0.53
1:E:5393:LYS:HA	1:E:5396:ILE:HG12	1.88	0.53
4:A:182:SIA:C10	6:A:8501:HOH:O	2.56	0.53
1:C:3330:LYS:HG3	1:C:3335:LEU:CD2	2.38	0.53
1:E:5330:LYS:HB3	1:E:5334:GLU:OE2	2.07	0.53
1:B:2081:THR:OG1	3:B:279:NAG:H82	2.08	0.53
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.23	0.53
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.90	0.53
1:F:6107:ASN:HB3	6:F:8982:HOH:O	2.08	0.53
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.23	0.53
1:D:4313:ARG:HG2	1:D:4386:TYR:CE2	2.43	0.53
1:B:2311:ASP:OD1	1:B:2313:ARG:HB2	2.09	0.53
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.91	0.53
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	1.89	0.53
1:A:1304:LEU:HG	5:A:1[B]:THA:H142	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3512:GLU:CD	1:C:3512:GLU:H	2.12	0.53
1:B:2420:LEU:C	1:B:2420:LEU:HD12	2.29	0.53
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.91	0.53
1:C:3304:LEU:HD23	1:C:3318:LEU:CD2	2.39	0.53
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.91	0.53
1:F:6038:VAL:HG21	1:F:6049:ILE:HD12	1.90	0.53
1:F:6420:LEU:O	1:F:6420:LEU:HD12	2.09	0.52
1:B:2292:GLU:O	1:B:2296:GLU:HG3	2.09	0.52
1:C:3339:ARG:NE	6:C:7471:HOH:O	2.42	0.52
1:E:5420:LEU:HD12	1:E:5420:LEU:O	2.08	0.52
1:F:6296:GLU:O	1:F:6300:LYS:HG3	2.08	0.52
1:C:3420:LEU:HD12	1:C:3420:LEU:O	2.09	0.52
1:B:2339:ARG:HH11	1:B:2339:ARG:CB	2.23	0.52
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.09	0.52
6:A:7567:HOH:O	1:F:6302:LYS:HE2	2.10	0.52
1:B:2027:ASP:OD2	1:B:2032:LYS:HG2	2.10	0.52
1:E:5084:PRO:HB3	4:E:582:SIA:O1A	2.09	0.52
1:F:6498:LYS:HB3	1:F:6514:LEU:HD11	1.92	0.52
1:C:3260:ASP:OD2	1:C:3263:PRO:HD3	2.10	0.52
1:D:4331:THR:OG1	1:D:4334:GLU:HG3	2.10	0.52
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.91	0.52
1:A:1082:SER:CB	6:A:7946:HOH:O	2.49	0.51
1:C:3242:ARG:NH1	1:C:3242:ARG:HG2	2.17	0.51
1:B:2351:ASN:ND2	1:B:2449:PHE:HB3	2.25	0.51
1:C:3263:PRO:HD2	6:C:8024:HOH:O	2.11	0.51
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.91	0.51
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.73	0.51
1:C:3401:GLU:HB2	6:C:8182:HOH:O	2.09	0.51
1:E:5398:GLU:HB3	6:E:8267:HOH:O	2.09	0.51
1:A:1304:LEU:HG	5:A:1[C]:THA:H2	1.91	0.51
1:C:3480:PHE:HZ	1:C:3494:LYS:HG3	1.74	0.51
1:C:3264:LEU:HD11	1:C:3316:GLN:HG2	1.93	0.51
1:F:6420:LEU:C	1:F:6420:LEU:HD12	2.30	0.51
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.91	0.51
1:F:6221:SER:OG	1:F:6468:HIS:NE2	2.38	0.51
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.73	0.51
1:D:4540:LYS:O	1:D:4544:VAL:HG23	2.10	0.51
1:F:6455:PHE:CD2	1:F:6482:LYS:HD3	2.46	0.51
1:E:5084:PRO:HA	4:E:582:SIA:O1B	2.11	0.51
4:A:182:SIA:H112	1:B:2278:THR:CG2	2.39	0.51
1:E:5132:ARG:HD2	6:E:7329:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3255:LEU:CD1	5:C:3[D]:THA:H122	2.41	0.51
1:A:1080:ALA:HA	4:A:182:SIA:O1A	2.10	0.50
1:D:4295:LEU:O	1:D:4299:LEU:HG	2.11	0.50
1:E:5420:LEU:HD12	1:E:5420:LEU:C	2.32	0.50
1:E:5254:VAL:HG11	5:E:5[C]:THA:H132	1.93	0.50
1:A:1221:SER:OG	5:A:1[C]:THA:H142	2.12	0.50
1:D:4241:HIS:O	1:D:4242:ARG:HG3	2.11	0.50
1:D:4315:SER:HB3	6:D:8975:HOH:O	2.12	0.50
1:C:3186:ARG:HB3	1:C:3324:ASP:HB2	1.94	0.50
1:F:6038:VAL:CG2	1:F:6049:ILE:HD12	2.41	0.50
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.47	0.50
1:D:4428:VAL:HB	1:D:4429:PRO:HD3	1.94	0.50
1:D:4264:LEU:HG	1:D:4316:GLN:CG	2.40	0.50
1:D:4468:HIS:NE2	5:D:4[E]:THA:H112	2.26	0.50
1:C:3348:VAL:O	1:C:3446:MET:HA	2.12	0.50
1:D:4221:SER:HB3	6:D:7004:HOH:O	2.11	0.50
1:F:6375:GLN:HG3	1:F:6413:LYS:HZ2	1.75	0.50
1:B:2414:LYS:HD2	6:E:7998:HOH:O	2.11	0.50
1:C:3252:THR:CG2	5:C:3[D]:THA:H132	2.42	0.50
1:A:1104:ARG:HD2	1:A:1108:ILE:HG12	1.93	0.49
4:A:182:SIA:H112	1:B:2278:THR:HG22	1.94	0.49
1:B:2487:GLU:HG2	6:B:8088:HOH:O	2.11	0.49
1:D:4262:LYS:HB3	1:D:4263:PRO:HD3	1.93	0.49
1:D:4396:ILE:HB	1:D:4397:PRO:HD3	1.94	0.49
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.75	0.49
1:E:5375:GLN:O	1:E:5379:MET:HG3	2.11	0.49
1:E:5404:LEU:HD13	1:E:5413:LYS:HB3	1.93	0.49
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.27	0.49
1:F:6411:VAL:HG13	6:F:9011:HOH:O	2.11	0.49
1:D:4538:LYS:HG2	6:D:7570:HOH:O	2.11	0.49
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.26	0.49
1:C:3445:TYR:CE1	1:C:3519:GLU:HA	2.48	0.49
1:B:2317:PRO:O	1:B:2318:LEU:HD23	2.13	0.49
1:D:4024:PRO:HG3	1:D:4037:PHE:CE2	2.48	0.49
1:E:5349:GLY:HA3	1:E:5447:TYR:CE1	2.47	0.49
1:A:1266:GLU:HA	1:A:1282:MET:CE	2.42	0.49
1:A:1420:LEU:HD13	1:A:1547:TRP:CZ2	2.47	0.49
1:D:4348:VAL:O	1:D:4446:MET:HA	2.12	0.49
1:E:5125:ALA:HB1	1:E:5131:ASN:HD22	1.77	0.49
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.28	0.49
1:F:6254:VAL:HG11	5:F:6[C]:THA:H132	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:HIS:HE1	6:A:7162:HOH:O	1.94	0.49
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.47	0.49
1:D:4030:HIS:HD2	6:D:7529:HOH:O	1.96	0.49
1:A:1092:LYS:HD2	1:F:6302:LYS:HD2	1.95	0.49
1:A:1225:GLU:O	1:A:1229:VAL:HG23	2.13	0.49
1:C:3206:ALA:HA	1:C:3210:GLY:O	2.12	0.48
1:E:5371:GLY:O	1:E:5411:VAL:HA	2.13	0.48
1:A:1335:LEU:O	1:A:1338:GLU:O	2.30	0.48
1:E:5104:ARG:HD2	6:E:8627:HOH:O	2.13	0.48
1:F:6242:ARG:HG2	1:F:6242:ARG:NH1	2.27	0.48
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.75	0.48
1:C:3030:HIS:HD2	6:C:7837:HOH:O	1.95	0.48
1:C:3257:LYS:HZ2	1:C:3320:GLY:H	1.60	0.48
1:D:4079:ASN:HB3	4:D:482:SIA:C1	2.42	0.48
1:D:4538:LYS:HB3	1:D:4541:ASP:HB2	1.94	0.48
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	1.95	0.48
1:D:4526:TYR:CD2	1:D:4539:LEU:HB2	2.47	0.48
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.49	0.48
1:F:6284:HIS:O	1:F:6288:GLN:HG2	2.12	0.48
4:A:182:SIA:C11	1:B:2278:THR:HG22	2.43	0.48
1:C:3363:LEU:HD13	5:C:3[E]:THA:C13	2.25	0.48
1:F:6343:THR:HB	1:F:6442:ALA:HB2	1.94	0.48
1:A:1264:LEU:HG	1:A:1316:GLN:CD	2.34	0.48
1:C:3022:SER:HB2	1:C:3023:PRO:HD2	1.96	0.48
1:C:3038:VAL:HG21	1:C:3049:ILE:HD12	1.96	0.48
1:E:5262:LYS:HB3	1:E:5263:PRO:HD3	1.94	0.48
1:A:1409:ASP:O	1:A:1413:LYS:HG3	2.13	0.48
4:A:182:SIA:N5	6:A:8501:HOH:O	2.35	0.48
1:B:2304:LEU:HD22	5:B:2[A]:THA:C2	2.44	0.48
1:B:2437:HIS:HD2	1:B:2444:THR:OG1	1.95	0.48
1:D:4401:GLU:OE2	1:D:4405:GLY:HA3	2.14	0.48
1:E:5126:ASP:H	1:E:5131:ASN:ND2	2.12	0.48
1:F:6024:PRO:HG3	1:F:6037:PHE:CE1	2.49	0.48
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	2.14	0.48
1:B:2341:PHE:CE1	1:B:2343:THR:HG22	2.49	0.48
1:C:3241:HIS:C	1:C:3242:ARG:HG3	2.34	0.48
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.49	0.48
1:C:3420:LEU:O	1:C:3424:VAL:HG23	2.14	0.48
1:C:3351:ASN:HB3	1:C:3466:GLY:O	2.14	0.48
1:D:4289:LYS:HA	1:D:4293:GLU:OE2	2.14	0.48
1:E:5232:LEU:HD23	1:E:5341:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6220:GLU:HA	1:F:6246:GLU:O	2.13	0.48
1:A:1258:LYS:HB2	6:A:7269:HOH:O	2.14	0.47
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.14	0.47
1:C:3140:HIS:HE1	6:C:7022:HOH:O	1.97	0.47
1:E:5040:LEU:HD22	1:E:5156:ALA:HA	1.96	0.47
1:E:5218:PHE:CB	1:E:5244:ILE:HB	2.44	0.47
1:E:5220:GLU:HA	1:E:5246:GLU:O	2.15	0.47
1:E:5140:HIS:HE1	6:E:7160:HOH:O	1.97	0.47
1:F:6355:PHE:CD1	1:F:6360:PRO:HG3	2.49	0.47
1:A:1142:GLY:HA2	5:A:1[A]:THA:H131	1.95	0.47
1:B:2363:LEU:HD13	5:B:2[B]:THA:C13	2.40	0.47
1:D:4242:ARG:HD3	1:D:4503:PHE:O	2.15	0.47
1:F:6333:GLU:OE1	1:F:6333:GLU:N	2.46	0.47
1:B:2462:LYS:HE2	1:E:5374:ASP:HB3	1.96	0.47
1:E:5030:HIS:HD2	6:E:7857:HOH:O	1.96	0.47
1:E:5186:ARG:HB3	1:E:5324:ASP:HB2	1.96	0.47
1:F:6359:ILE:HB	1:F:6360:PRO:HD3	1.96	0.47
1:F:6258:LYS:CD	1:F:6258:LYS:H	2.27	0.47
1:B:2304:LEU:HD13	5:B:2[B]:THA:H122	1.97	0.47
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.74	0.47
1:E:5221:SER:HA	1:E:5247:SER:O	2.15	0.47
1:A:1330:LYS:HG3	1:A:1335:LEU:HG	1.97	0.47
1:A:1142:GLY:HA2	5:A:1[B]:THA:H111	1.97	0.47
1:C:3512:GLU:CD	1:C:3512:GLU:N	2.68	0.47
1:F:6145:MET:HB2	1:F:6304:LEU:HD21	1.96	0.47
1:C:3257:LYS:HD2	6:C:8696:HOH:O	2.13	0.47
1:C:3368:LEU:O	1:D:4369:SER:HA	2.15	0.47
1:D:4102:THR:OG1	1:D:4104:ARG:HG2	2.14	0.47
1:D:4354:GLU:O	1:D:4468:HIS:HB2	2.14	0.47
1:E:5236:ALA:HA	1:E:5239:LEU:HD12	1.96	0.47
1:E:5097:LEU:CD1	5:E:5[E]:THA:H132	2.45	0.47
1:F:6303:PHE:O	1:F:6304:LEU:HB2	2.15	0.47
1:A:1101:PHE:CE2	5:A:1[D]:THA:H1	2.49	0.47
1:C:3257:LYS:HZ1	1:C:3319:LEU:HA	1.80	0.46
1:F:6375:GLN:O	1:F:6379:MET:HG3	2.15	0.46
4:A:182:SIA:H31	6:A:7946:HOH:O	2.15	0.46
1:D:4249:VAL:HG23	1:D:4251:LEU:H	1.80	0.46
1:E:5074:TRP:CD2	1:E:5078:LYS:HE2	2.51	0.46
1:A:1339:ARG:NH1	1:A:1339:ARG:HG3	2.30	0.46
1:B:2052:GLY:HA3	4:B:282:SIA:C3	2.45	0.46
1:E:5264:LEU:HD22	1:E:5316:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5414:LYS:HZ2	1:E:5414:LYS:HB3	1.80	0.46
1:A:1221:SER:HB3	1:A:1222:ALA:H	1.44	0.46
1:A:1540:LYS:O	1:A:1544:VAL:HG23	2.15	0.46
1:B:2079:ASN:O	4:B:282:SIA:H8	2.15	0.46
1:D:4318:LEU:HD12	1:D:4318:LEU:C	2.36	0.46
1:E:5183:GLU:OE2	1:E:5183:GLU:N	2.43	0.46
1:A:1021:SER:N	6:A:7616:HOH:O	2.48	0.46
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.97	0.46
1:F:6386:TYR:N	1:F:6387:PRO:HD2	2.31	0.46
1:A:1421:ILE:HG22	1:A:1425:MET:HE1	1.97	0.46
1:C:3262:LYS:HG3	1:C:3266:GLU:OE2	2.15	0.46
1:E:5078:LYS:HD3	4:E:582:SIA:O4	2.16	0.46
1:F:6420:LEU:O	1:F:6424:VAL:HG23	2.16	0.46
1:B:2261:VAL:HB	6:B:8950:HOH:O	2.15	0.46
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.16	0.46
3:B:279:NAG:H83	6:B:7733:HOH:O	2.15	0.46
1:F:6221:SER:HB3	1:F:6222:ALA:H	1.54	0.46
1:A:1145:MET:HG3	1:A:1304:LEU:HD13	1.97	0.46
1:B:2304:LEU:HD23	1:B:2318:LEU:HD21	1.98	0.46
1:D:4403:TYR:O	1:D:4416:LEU:HD13	2.16	0.46
1:D:4349:GLY:HA3	1:D:4447:TYR:CZ	2.51	0.46
1:D:4304:LEU:HG	5:D:4[A]:THA:C2	2.44	0.46
1:A:1331:THR:OG1	1:A:1334:GLU:HG3	2.16	0.45
1:B:2022:SER:HA	6:B:8573:HOH:O	2.16	0.45
1:B:2051:LEU:O	1:B:2080:ALA:HB1	2.16	0.45
1:F:6249:VAL:HG23	1:F:6251:LEU:H	1.81	0.45
1:A:1264:LEU:HG	1:A:1316:GLN:CG	2.44	0.45
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.16	0.45
1:D:4309:GLN:C	1:D:4309:GLN:NE2	2.70	0.45
1:D:4334:GLU:O	1:D:4338:GLU:HG2	2.16	0.45
1:D:4363:LEU:HD13	5:D:4[B]:THA:C13	2.47	0.45
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.92	0.45
1:D:4363:LEU:HD13	5:D:4[B]:THA:H131	1.98	0.45
1:E:5311:ASP:OD1	1:E:5313:ARG:HB2	2.17	0.45
1:E:5318:LEU:HD11	5:E:5[A]:THA:H111	1.98	0.45
1:E:5491:ARG:HH11	1:E:5491:ARG:HG2	1.81	0.45
1:B:2372:GLN:HG2	1:B:2372:GLN:H	1.53	0.45
1:B:2420:LEU:HD13	1:B:2547:TRP:HZ2	1.81	0.45
1:E:5348:VAL:O	1:E:5446:MET:HA	2.17	0.45
1:F:6437:HIS:HD2	1:F:6444:THR:OG1	1.99	0.45
1:B:2348:VAL:O	1:B:2446:MET:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4283:VAL:O	1:D:4287:ARG:HB2	2.17	0.45
1:E:5538:LYS:HE2	6:E:7328:HOH:O	2.16	0.45
1:C:3257:LYS:HB2	1:C:3322:VAL:HG12	1.98	0.45
1:D:4371:GLY:O	1:D:4414:LYS:HD3	2.16	0.45
1:E:5052:GLY:O	4:E:582:SIA:H32	2.15	0.45
1:E:5078:LYS:NZ	6:E:8318:HOH:O	2.49	0.45
1:F:6332:PRO:O	1:F:6336:GLN:HG3	2.16	0.45
1:A:1242:ARG:NH1	1:A:1242:ARG:CG	2.68	0.45
1:C:3532:ASN:HB3	1:C:3534:GLN:NE2	2.32	0.45
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.16	0.45
1:C:3221:SER:HB3	1:C:3222:ALA:H	1.47	0.45
1:C:3412:LYS:O	1:C:3416:LEU:HG	2.17	0.45
1:C:3403:TYR:O	1:C:3416:LEU:HD13	2.17	0.45
1:E:5297:THR:O	1:E:5301:MET:HG2	2.16	0.45
1:E:5340:ASN:HA	6:E:8083:HOH:O	2.16	0.45
1:A:1461:PRO:CG	1:F:6370:GLU:HG3	2.46	0.45
1:A:1143:GLY:O	1:A:1144:LEU:HB2	2.17	0.45
1:A:1394:GLU:H	1:A:1394:GLU:CD	2.20	0.45
1:C:3254:VAL:HG11	5:C:3[A]:THA:H5	1.99	0.45
1:D:4233:SER:HA	1:D:4234:PRO:HD3	1.82	0.45
1:E:5468:HIS:NE2	5:E:5[E]:THA:H112	2.32	0.45
1:A:1349:GLY:HA3	1:A:1447:TYR:CZ	2.52	0.45
1:C:3401:GLU:OE2	1:C:3405:GLY:HA3	2.16	0.45
1:E:5097:LEU:HD13	5:E:5[B]:THA:H132	1.99	0.45
1:E:5547:TRP:CZ3	1:E:5550:LEU:HD23	2.52	0.45
1:F:6251:LEU:CD1	1:F:6336:GLN:HE22	2.27	0.45
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.52	0.44
1:B:2257:LYS:HD3	6:B:8330:HOH:O	2.17	0.44
1:C:3045:GLN:HA	1:C:3046:PRO:HD3	1.88	0.44
1:D:4079:ASN:HB3	4:D:482:SIA:O1B	2.17	0.44
1:F:6262:LYS:HB3	1:F:6263:PRO:HD3	1.98	0.44
1:F:6297:THR:O	1:F:6301:MET:HG2	2.18	0.44
1:B:2284:HIS:NE2	1:B:2288:GLN:OE1	2.50	0.44
1:B:2304:LEU:HD22	5:B:2[B]:THA:H122	1.98	0.44
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.51	0.44
1:D:4099:GLU:HG2	1:D:4107:ASN:OD1	2.17	0.44
1:D:4526:TYR:CE2	1:D:4539:LEU:HB2	2.52	0.44
1:E:5235:LEU:HD12	1:E:5327:LEU:HA	1.97	0.44
1:F:6143:GLY:O	1:F:6144:LEU:HB2	2.17	0.44
1:A:1375:GLN:HB3	1:A:1375:GLN:HE21	1.54	0.44
1:A:1051:LEU:C	4:A:182:SIA:O1A	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2258:LYS:HD2	1:B:2258:LYS:H	1.82	0.44
1:C:3023:PRO:HA	1:C:3024:PRO:HD3	1.78	0.44
1:C:3297:THR:O	1:C:3301:MET:HG2	2.17	0.44
1:D:4023:PRO:HA	1:D:4024:PRO:HD3	1.87	0.44
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.99	0.44
1:E:5306:LEU:HD22	1:E:5366:TYR:CD1	2.52	0.44
1:F:6057:LYS:HD2	6:F:7839:HOH:O	2.17	0.44
1:F:6351:ASN:ND2	1:F:6449:PHE:HB3	2.32	0.44
1:C:3330:LYS:HG3	1:C:3335:LEU:HD21	1.99	0.44
1:F:6409:ASP:OD1	1:F:6411:VAL:HB	2.17	0.44
1:F:6437:HIS:HE1	6:F:7001:HOH:O	1.99	0.44
1:B:2257:LYS:HB2	1:B:2322:VAL:HG12	2.00	0.44
1:C:3246:GLU:HG2	1:C:3447:TYR:OH	2.17	0.44
1:F:6304:LEU:HD23	1:F:6318:LEU:CD2	2.46	0.44
1:A:1038:VAL:CG2	1:A:1049:ILE:HD12	2.47	0.44
1:A:1233:SER:HA	1:A:1234:PRO:HD3	1.78	0.44
1:C:3281:VAL:HG13	6:C:9007:HOH:O	2.17	0.44
1:D:4527:LEU:HD11	1:D:4533:THR:HG22	1.99	0.44
1:E:5317:PRO:O	1:E:5318:LEU:HD23	2.17	0.44
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.16	0.44
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.80	0.44
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.53	0.44
1:C:3371:GLY:H	1:D:4414:LYS:HZ3	1.65	0.44
1:D:4086:MET:CE	1:D:4110:LEU:HB2	2.48	0.44
1:D:4232:LEU:HA	1:D:4341:PHE:HB2	1.98	0.44
1:F:6547:TRP:CZ3	1:F:6550:LEU:HD23	2.53	0.44
1:D:4101:PHE:CE2	5:D:4[C]:THA:H1	2.53	0.44
1:A:1426:PHE:C	1:A:1429:PRO:HD2	2.38	0.44
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.17	0.44
1:C:3371:GLY:HA2	1:D:4371:GLY:HA3	1.99	0.44
1:F:6029:VAL:HG23	1:F:6204:ASN:OD1	2.17	0.44
1:A:1105:LYS:HG3	1:A:1481:LEU:O	2.17	0.43
1:B:2215:VAL:N	1:B:2241:HIS:HD2	1.91	0.43
1:D:4120:ASN:HB2	1:D:4167:THR:OG1	2.18	0.43
3:E:579:NAG:H83	3:E:579:NAG:O3	2.17	0.43
1:D:4130:LYS:HE3	1:D:4132:ARG:HH21	1.82	0.43
1:E:5262:LYS:NZ	1:E:5279:SER:OG	2.51	0.43
1:A:1458:ASP:HB3	1:F:6380:SER:OG	2.19	0.43
1:F:6407:THR:HB	6:F:7621:HOH:O	2.18	0.43
1:A:1152:TYR:CD1	1:A:1152:TYR:N	2.86	0.43
1:B:2030:HIS:HD2	6:B:7686:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3257:LYS:NZ	1:C:3319:LEU:HA	2.34	0.43
1:D:4048:ALA:HB3	1:D:4123:THR:HG23	2.00	0.43
1:E:5104:ARG:HD3	6:E:8519:HOH:O	2.19	0.43
1:E:5326:MET:HE2	6:E:8489:HOH:O	2.18	0.43
1:A:1221:SER:HG	1:A:1468:HIS:CE1	2.34	0.43
1:A:1318:LEU:HD12	1:A:1318:LEU:C	2.39	0.43
1:B:2302:LYS:NZ	6:B:8096:HOH:O	2.51	0.43
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.33	0.43
1:E:5142:GLY:HA2	5:E:5[D]:THA:H141	2.01	0.43
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.53	0.43
1:F:6308:LEU:HD11	1:F:6367:PRO:HG3	1.99	0.43
1:C:3023:PRO:CB	1:C:3034:LEU:HD21	2.48	0.43
1:D:4139:ILE:HG12	1:D:4168:ILE:HD11	1.99	0.43
1:A:1348:VAL:O	1:A:1446:MET:HA	2.18	0.43
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.99	0.43
1:B:2097:LEU:HD11	1:B:2101:PHE:CE2	2.54	0.43
1:C:3221:SER:OG	5:C:3[E]:THA:H5	2.18	0.43
1:F:6091:PRO:HB3	1:F:6112:LEU:HD11	2.00	0.43
1:F:6254:VAL:CG1	5:F:6[B]:THA:H6	2.49	0.43
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	2.00	0.43
1:D:4409:ASP:OD1	1:D:4411:VAL:HB	2.19	0.43
4:D:482:SIA:H111	1:E:5278:THR:HG21	2.01	0.43
1:E:5097:LEU:HD13	5:E:5[A]:THA:H6	2.01	0.43
1:F:6366:TYR:HA	1:F:6367:PRO:HD3	1.80	0.43
1:A:1255:LEU:HD11	5:A:1[C]:THA:H131	2.01	0.43
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.34	0.43
1:E:5218:PHE:HB2	1:E:5244:ILE:HB	2.01	0.43
1:E:5353:GLN:NE2	1:E:5465:ILE:H	2.16	0.43
1:C:3532:ASN:HB3	1:C:3534:GLN:HE21	1.84	0.42
1:E:5221:SER:OG	5:E:5[D]:THA:N15	2.49	0.42
1:F:6048:ALA:HB3	1:F:6123:THR:HG23	2.01	0.42
2:G:1:NAG:H61	2:G:2:NDG:C5	2.49	0.42
1:C:3233:SER:O	1:C:3342:HIS:HE1	2.02	0.42
1:F:6523:LYS:HB2	6:F:7657:HOH:O	2.19	0.42
1:C:3237:LYS:HG3	1:C:3237:LYS:O	2.18	0.42
1:E:5528:GLN:O	1:E:5533:THR:HA	2.20	0.42
1:C:3218:PHE:HB2	1:C:3244:ILE:HB	2.00	0.42
1:C:3370:GLU:HG3	1:D:4461:PRO:HG3	2.01	0.42
1:E:5132:ARG:HB3	1:E:5211:ASN:HB2	2.01	0.42
1:F:6237:LYS:HD3	6:F:7710:HOH:O	2.19	0.42
1:A:1265:ALA:C	1:A:1282:MET:HE1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:SER:OG	5:A:1[B]:THA:H2	2.19	0.42
1:B:2140:HIS:HE1	6:B:7057:HOH:O	2.01	0.42
4:A:182:SIA:C11	6:A:8501:HOH:O	2.65	0.42
1:C:3252:THR:HG21	5:C:3[A]:THA:H6	2.00	0.42
1:D:4130:LYS:HE3	1:D:4132:ARG:NH2	2.35	0.42
1:E:5130:LYS:HA	6:E:7877:HOH:O	2.19	0.42
1:A:1542:LYS:HG3	6:A:7508:HOH:O	2.20	0.42
4:A:182:SIA:H4	6:A:8501:HOH:O	2.19	0.42
1:C:3311:ASP:OD1	1:C:3313:ARG:HB2	2.19	0.42
1:C:3358:LEU:HG	1:C:3363:LEU:HD12	2.02	0.42
1:E:5258:LYS:HD2	6:E:7098:HOH:O	2.19	0.42
1:C:3221:SER:OG	5:C:3[A]:THA:H2	2.19	0.42
1:C:3398:GLU:HB3	6:C:7228:HOH:O	2.19	0.42
1:F:6331:THR:OG1	1:F:6334:GLU:HG3	2.20	0.42
1:A:1401:GLU:OE2	1:A:1405:GLY:HA3	2.20	0.42
1:B:2296:GLU:O	1:B:2300:LYS:HG3	2.20	0.42
1:E:5143:GLY:O	1:E:5144:LEU:HB2	2.20	0.42
1:E:5262:LYS:HE3	6:E:7678:HOH:O	2.19	0.42
1:F:6368:LEU:HD23	6:F:8373:HOH:O	2.19	0.42
1:A:1264:LEU:CG	1:A:1316:GLN:HG2	2.48	0.41
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.50	0.41
1:C:3306:LEU:HD12	6:C:8873:HOH:O	2.19	0.41
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.88	0.41
1:A:1235:LEU:HD12	1:A:1327:LEU:HA	2.02	0.41
1:E:5038:VAL:HG21	1:E:5049:ILE:HD12	2.02	0.41
1:A:1081:THR:N	4:A:182:SIA:O1B	2.52	0.41
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.50	0.41
1:A:1493:SER:O	1:A:1497:MET:HG3	2.20	0.41
1:C:3022:SER:N	6:C:7425:HOH:O	2.53	0.41
1:C:3358:LEU:O	1:C:3363:LEU:HD12	2.21	0.41
1:C:3361:MET:CE	1:C:3363:LEU:HG	2.50	0.41
1:A:1111:LYS:HG3	6:A:7685:HOH:O	2.19	0.41
1:C:3143:GLY:O	1:C:3144:LEU:HB2	2.20	0.41
1:A:1420:LEU:O	1:A:1420:LEU:HD12	2.21	0.41
1:B:2043:PHE:HA	6:B:9057:HOH:O	2.20	0.41
1:B:2366:TYR:HA	1:B:2367:PRO:HD3	1.83	0.41
1:B:2455:PHE:HZ	1:B:2485:ALA:HB2	1.85	0.41
1:D:4232:LEU:HD23	1:D:4341:PHE:HB3	2.02	0.41
1:E:5461:PRO:HG2	1:E:5464:VAL:HG23	2.02	0.41
1:B:2309:GLN:C	1:B:2309:GLN:NE2	2.74	0.41
1:F:6368:LEU:HD23	1:F:6368:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1331:THR:HB	1:A:1333:GLU:OE1	2.20	0.41
1:A:1221:SER:OG	1:A:1468:HIS:NE2	2.45	0.41
1:B:2045:GLN:HA	1:B:2046:PRO:HD3	1.90	0.41
1:D:4143:GLY:O	1:D:4144:LEU:HB2	2.20	0.41
1:D:4221:SER:HB3	1:D:4222:ALA:H	1.56	0.41
1:D:4353:GLN:O	1:D:4467:ASP:HA	2.21	0.41
1:D:4495:MET:HE3	1:D:4533:THR:HG21	2.02	0.41
1:A:1097:LEU:CD1	5:A:1[A]:THA:H132	2.50	0.41
1:B:2220:GLU:OE2	1:B:2221:SER:HB2	2.20	0.41
1:D:4132:ARG:HB3	1:D:4211:ASN:HB2	2.01	0.41
1:E:5097:LEU:HD13	5:E:5[C]:THA:H6	2.02	0.41
1:A:1268:ILE:HD11	1:A:1319:LEU:HD21	2.03	0.41
1:B:2420:LEU:HD12	1:B:2420:LEU:O	2.20	0.41
1:C:3242:ARG:HD3	1:C:3503:PHE:O	2.21	0.41
1:C:3351:ASN:HD22	1:C:3449:PHE:HB3	1.84	0.41
1:D:4297:THR:O	1:D:4301:MET:HG2	2.20	0.41
1:E:5205:ILE:HD12	1:E:5205:ILE:HA	1.92	0.41
1:F:6254:VAL:CG1	5:F:6[C]:THA:H132	2.51	0.41
1:A:1426:PHE:O	1:A:1429:PRO:HD2	2.21	0.41
1:A:1140:HIS:CE1	6:A:7162:HOH:O	2.73	0.40
1:B:2237:LYS:HD3	1:B:2237:LYS:HA	1.90	0.40
1:C:3022:SER:HB2	1:C:3023:PRO:CD	2.52	0.40
1:C:3363:LEU:HD13	5:C:3[B]:THA:C6	2.50	0.40
1:E:5258:LYS:HE2	6:E:7910:HOH:O	2.20	0.40
1:E:5339:ARG:HG2	6:E:7869:HOH:O	2.20	0.40
1:A:1051:LEU:O	1:A:1080:ALA:HB1	2.20	0.40
4:A:182:SIA:O6	6:A:7946:HOH:O	2.22	0.40
1:C:3126:ASP:OD2	1:C:3129:LYS:HG3	2.20	0.40
1:D:4118:TYR:CZ	4:D:482:SIA:H113	2.57	0.40
1:E:5540:LYS:O	1:E:5544:VAL:HG23	2.21	0.40
1:B:2297:THR:O	1:B:2301:MET:HG2	2.22	0.40
1:B:2372:GLN:HB3	1:B:2372:GLN:HE21	1.52	0.40
1:C:3024:PRO:HG3	1:C:3037:PHE:CE2	2.56	0.40
1:D:4331:THR:HB	1:D:4333:GLU:OE1	2.21	0.40
1:F:6304:LEU:HD23	1:F:6318:LEU:HD21	2.02	0.40
1:B:2105:LYS:HD2	6:B:7487:HOH:O	2.22	0.40
1:B:2138:TRP:CZ3	1:B:2219:GLY:HA2	2.57	0.40
1:C:3532:ASN:C	1:C:3534:GLN:NE2	2.75	0.40
1:D:4370:GLU:O	1:D:4372:GLN:HG2	2.21	0.40
1:E:5061:GLY:HA3	1:E:5062:PRO:HD3	1.91	0.40
1:B:2368:LEU:O	1:E:5369:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5370:GLU:C	1:E:5372:GLN:H	2.24	0.40
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.95	0.40
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	2.03	0.40
1:A:1242:ARG:HD3	1:A:1503:PHE:O	2.20	0.40
1:D:4306:LEU:HD22	1:D:4366:TYR:CE1	2.57	0.40
1:F:6414:LYS:HE2	1:F:6415:ASP:OD2	2.21	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	530/548 (97%)	509 (96%)	20 (4%)	1 (0%)	47	62
1	B	529/548 (96%)	508 (96%)	20 (4%)	1 (0%)	47	62
1	C	529/548 (96%)	509 (96%)	17 (3%)	3 (1%)	25	36
1	D	529/548 (96%)	499 (94%)	28 (5%)	2 (0%)	34	48
1	E	529/548 (96%)	505 (96%)	24 (4%)	0	100	100
1	F	529/548 (96%)	505 (96%)	22 (4%)	2 (0%)	34	48
All	All	3175/3288 (97%)	3035 (96%)	131 (4%)	9 (0%)	41	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1339	ARG
1	D	4253	SER
1	C	3185	SER
1	F	6340	ASN
1	B	2357	TRP
1	C	3357	TRP

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Mol	Chain	Res	Type
1	F	6484	GLY
1	D	4369	SER
1	C	3484	GLY

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	448/463 (97%)	437 (98%)	11 (2%)	47 67
1	B	447/463 (96%)	428 (96%)	19 (4%)	29 46
1	C	447/463 (96%)	432 (97%)	15 (3%)	37 56
1	D	447/463 (96%)	432 (97%)	15 (3%)	37 56
1	E	447/463 (96%)	433 (97%)	14 (3%)	40 60
1	F	447/463 (96%)	436 (98%)	11 (2%)	47 67
All	All	2683/2778 (97%)	2598 (97%)	85 (3%)	39 59

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1027	ASP
1	A	1162	ASN
1	A	1218	PHE
1	A	1221	SER
1	A	1264	LEU
1	A	1309	GLN
1	A	1316	GLN
1	A	1346	TYR
1	A	1375	GLN
1	A	1420	LEU
1	A	1500	TRP
1	B	2155	LEU
1	B	2218	PHE
1	B	2220	GLU
1	B	2221	SER

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Mol	Chain	Res	Type
1	B	2242	ARG
1	B	2258	LYS
1	B	2278	THR
1	B	2299	LEU
1	B	2309	GLN
1	B	2339	ARG
1	B	2346	TYR
1	B	2358	LEU
1	B	2372	GLN
1	B	2375	GLN
1	B	2404	LEU
1	B	2408	ASP
1	B	2420	LEU
1	B	2499	PHE
1	B	2500	TRP
1	C	3027	ASP
1	C	3072	GLU
1	C	3088	THR
1	C	3155	LEU
1	C	3218	PHE
1	C	3220	GLU
1	C	3221	SER
1	C	3258	LYS
1	C	3264	LEU
1	C	3346	TYR
1	C	3414	LYS
1	C	3420	LEU
1	C	3500	TRP
1	C	3519	GLU
1	C	3534	GLN
1	D	4106	GLU
1	D	4218	PHE
1	D	4242	ARG
1	D	4264	LEU
1	D	4287	ARG
1	D	4309	GLN
1	D	4316	GLN
1	D	4342	HIS
1	D	4366	TYR
1	D	4372	GLN
1	D	4374	ASP
1	D	4375	GLN

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Mol	Chain	Res	Type
1	D	4408	ASP
1	D	4420	LEU
1	D	4500	TRP
1	E	5041	GLU
1	E	5111	LYS
1	E	5155	LEU
1	E	5218	PHE
1	E	5242	ARG
1	E	5258	LYS
1	E	5309	GLN
1	E	5333	GLU
1	E	5346	TYR
1	E	5372	GLN
1	E	5374	ASP
1	E	5414	LYS
1	E	5420	LEU
1	E	5500	TRP
1	F	6155	LEU
1	F	6218	PHE
1	F	6220	GLU
1	F	6221	SER
1	F	6258	LYS
1	F	6264	LEU
1	F	6414	LYS
1	F	6420	LEU
1	F	6500	TRP
1	F	6519	GLU
1	F	6534	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1045	GLN
1	A	1140	HIS
1	A	1162	ASN
1	A	1238	ASN
1	A	1241	HIS
1	A	1309	GLN
1	A	1316	GLN
1	A	1351	ASN
1	A	1353	GLN

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Mol	Chain	Res	Type
1	A	1372	GLN
1	A	1450	GLN
1	A	1537	GLN
1	B	2030	HIS
1	B	2045	GLN
1	B	2131	ASN
1	B	2140	HIS
1	B	2241	HIS
1	B	2309	GLN
1	B	2336	GLN
1	B	2340	ASN
1	B	2351	ASN
1	B	2372	GLN
1	B	2436	ASN
1	B	2437	HIS
1	B	2450	GLN
1	B	2532	ASN
1	B	2537	GLN
1	C	3030	HIS
1	C	3140	HIS
1	C	3241	HIS
1	C	3351	ASN
1	C	3436	ASN
1	C	3534	GLN
1	C	3537	GLN
1	D	4030	HIS
1	D	4140	HIS
1	D	4241	HIS
1	D	4309	GLN
1	D	4316	GLN
1	D	4340	ASN
1	D	4342	HIS
1	D	4351	ASN
1	D	4353	GLN
1	D	4372	GLN
1	D	4375	GLN
1	D	4450	GLN
1	D	4537	GLN
1	E	5045	GLN
1	E	5131	ASN
1	E	5140	HIS
1	E	5162	ASN

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Mol	Chain	Res	Type
1	E	5241	HIS
1	E	5309	GLN
1	E	5340	ASN
1	E	5351	ASN
1	E	5353	GLN
1	E	5372	GLN
1	E	5436	ASN
1	E	5537	GLN
1	F	6045	GLN
1	F	6140	HIS
1	F	6162	ASN
1	F	6241	HIS
1	F	6316	GLN
1	F	6351	ASN
1	F	6353	GLN
1	F	6437	HIS
1	F	6532	ASN
1	F	6534	GLN
1	F	6537	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](#)

2 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	NAG	G	1	1,2	14,14,15	0.78	0	17,19,21	0.66	0
2	NDG	G	2	2	14,14,15	1.09	1 (7%)	17,19,21	1.51	4 (23%)

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	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NDG	G	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NDG	O5-C5	2.90	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NDG	C6-C5-C4	-3.23	105.43	113.00
2	G	2	NDG	C3-C4-C5	2.74	115.12	110.24
2	G	2	NDG	O5-C1-C2	-2.21	107.80	111.29
2	G	2	NDG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NDG	C1-C2-N2-C7
2	G	2	NDG	C8-C7-N2-C2
2	G	2	NDG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

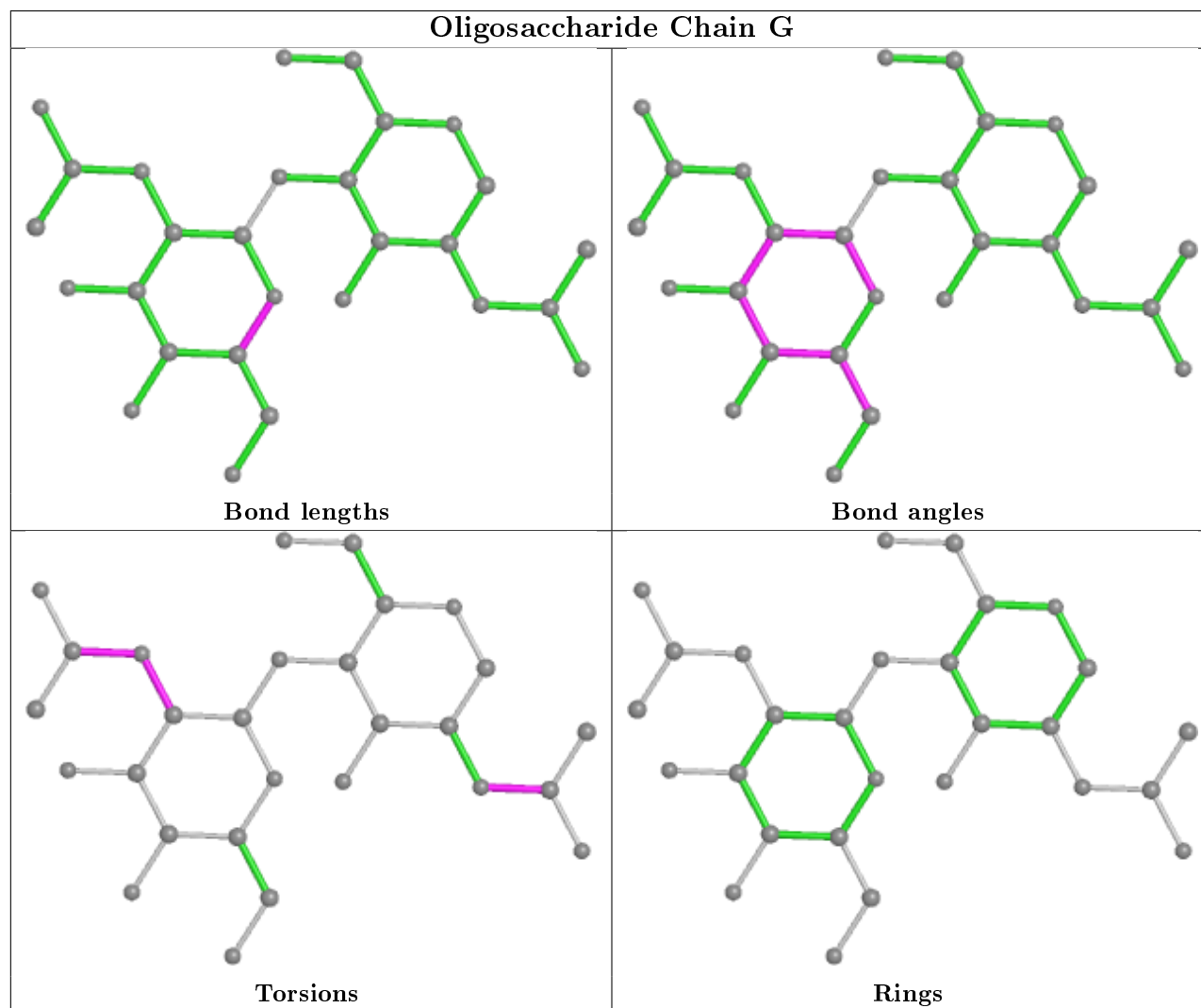
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NDG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	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](#)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	THA	F	6[C]	-	17,17,17	2.27	7 (41%)	21,24,24	1.58	3 (14%)
5	THA	F	6[B]	-	17,17,17	2.29	7 (41%)	21,24,24	1.53	3 (14%)
3	NAG	B	279	1	14,14,15	0.56	0	17,19,21	0.82	1 (5%)
5	THA	A	1[D]	-	17,17,17	2.31	6 (35%)	21,24,24	1.53	3 (14%)
5	THA	B	2[D]	-	17,17,17	2.32	7 (41%)	21,24,24	1.53	3 (14%)
5	THA	A	1[A]	-	17,17,17	2.32	7 (41%)	21,24,24	1.58	3 (14%)
4	SIA	B	282	-	18,21,21	0.99	0	21,31,31	0.99	1 (4%)
3	NAG	F	680	-	14,14,15	0.49	0	17,19,21	0.64	0
5	THA	A	1[C]	-	17,17,17	2.28	7 (41%)	21,24,24	1.59	3 (14%)
5	THA	B	2[A]	-	17,17,17	2.32	7 (41%)	21,24,24	1.63	3 (14%)
5	THA	A	1[B]	-	17,17,17	2.35	7 (41%)	21,24,24	1.57	3 (14%)
5	THA	D	4[E]	-	17,17,17	2.29	7 (41%)	21,24,24	1.52	3 (14%)
5	THA	B	2[C]	-	17,17,17	2.30	7 (41%)	21,24,24	1.56	3 (14%)
5	THA	D	4[D]	-	17,17,17	2.35	7 (41%)	21,24,24	1.57	3 (14%)
5	THA	B	2[B]	-	17,17,17	2.36	7 (41%)	21,24,24	1.56	3 (14%)
5	THA	D	4[A]	-	17,17,17	2.34	7 (41%)	21,24,24	1.59	3 (14%)
5	THA	D	4[C]	-	17,17,17	2.33	7 (41%)	21,24,24	1.55	3 (14%)
5	THA	D	4[B]	-	17,17,17	2.34	7 (41%)	21,24,24	1.54	3 (14%)
3	NAG	F	679	1	14,14,15	0.50	0	17,19,21	0.87	1 (5%)
4	SIA	A	182	1	18,21,21	1.00	1 (5%)	21,31,31	1.25	2 (9%)
5	THA	C	3[E]	-	17,17,17	2.37	7 (41%)	21,24,24	1.54	4 (19%)
5	THA	C	3[D]	-	17,17,17	2.24	7 (41%)	21,24,24	1.58	3 (14%)
3	NAG	E	579	1	14,14,15	0.56	0	17,19,21	0.68	1 (5%)
5	THA	C	3[A]	-	17,17,17	2.34	7 (41%)	21,24,24	1.54	3 (14%)
5	THA	E	5[E]	-	17,17,17	2.31	7 (41%)	21,24,24	1.56	3 (14%)
5	THA	C	3[C]	-	17,17,17	2.34	7 (41%)	21,24,24	1.53	3 (14%)
5	THA	E	5[D]	-	17,17,17	2.34	7 (41%)	21,24,24	1.54	3 (14%)
5	THA	C	3[B]	-	17,17,17	2.37	7 (41%)	21,24,24	1.61	3 (14%)
3	NAG	A	179	1	14,14,15	0.63	0	17,19,21	0.62	0
5	THA	F	6[D]	-	17,17,17	2.31	7 (41%)	21,24,24	1.56	3 (14%)
5	THA	E	5[A]	-	17,17,17	2.36	7 (41%)	21,24,24	1.54	3 (14%)
4	SIA	E	582	-	18,21,21	1.05	1 (5%)	21,31,31	1.23	2 (9%)
5	THA	E	5[C]	-	17,17,17	2.33	7 (41%)	21,24,24	1.57	3 (14%)
5	THA	F	6[A]	-	17,17,17	2.31	7 (41%)	21,24,24	1.63	3 (14%)
5	THA	E	5[B]	-	17,17,17	2.32	7 (41%)	21,24,24	1.56	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	479	1	14,14,15	0.50	0	17,19,21	0.65	0
4	SIA	D	482	-	18,21,21	1.21	2 (11%)	21,31,31	0.93	2 (9%)

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
5	THA	F	6[C]	-	-	-	0/3/3/3
5	THA	D	4[A]	-	-	-	0/3/3/3
5	THA	F	6[B]	-	-	-	0/3/3/3
5	THA	C	3[E]	-	-	-	0/3/3/3
5	THA	A	1[D]	-	-	-	0/3/3/3
5	THA	B	2[D]	-	-	-	0/3/3/3
5	THA	A	1[A]	-	-	-	0/3/3/3
4	SIA	B	282	-	-	0/14/38/38	0/1/1/1
3	NAG	F	680	-	-	2/6/23/26	0/1/1/1
5	THA	A	1[C]	-	-	-	0/3/3/3
5	THA	B	2[A]	-	-	-	0/3/3/3
5	THA	A	1[B]	-	-	-	0/3/3/3
5	THA	D	4[E]	-	-	-	0/3/3/3
5	THA	B	2[C]	-	-	-	0/3/3/3
5	THA	D	4[D]	-	-	-	0/3/3/3
5	THA	B	2[B]	-	-	-	0/3/3/3
3	NAG	A	179	1	-	2/6/23/26	0/1/1/1
5	THA	D	4[C]	-	-	-	0/3/3/3
5	THA	D	4[B]	-	-	-	0/3/3/3
3	NAG	F	679	1	-	2/6/23/26	0/1/1/1
4	SIA	A	182	1	-	2/14/38/38	0/1/1/1
3	NAG	B	279	1	-	4/6/23/26	0/1/1/1
5	THA	C	3[D]	-	-	-	0/3/3/3
3	NAG	E	579	1	-	4/6/23/26	0/1/1/1
5	THA	C	3[A]	-	-	-	0/3/3/3
5	THA	E	5[E]	-	-	-	0/3/3/3
5	THA	C	3[C]	-	-	-	0/3/3/3
5	THA	E	5[D]	-	-	-	0/3/3/3
5	THA	C	3[B]	-	-	-	0/3/3/3
5	THA	F	6[D]	-	-	-	0/3/3/3
5	THA	E	5[A]	-	-	-	0/3/3/3
4	SIA	E	582	-	-	0/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	THA	E	5[C]	-	-	-	0/3/3/3
5	THA	F	6[A]	-	-	-	0/3/3/3
5	THA	E	5[B]	-	-	-	0/3/3/3
3	NAG	D	479	1	-	2/6/23/26	0/1/1/1
4	SIA	D	482	-	-	0/14/38/38	0/1/1/1

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3[E]	THA	C14-C9	5.08	1.59	1.51
5	B	2[B]	THA	C14-C9	5.01	1.59	1.51
5	D	4[B]	THA	C14-C9	4.92	1.59	1.51
5	E	5[D]	THA	C14-C9	4.91	1.59	1.51
5	C	3[A]	THA	C14-C9	4.91	1.59	1.51
5	D	4[C]	THA	C14-C9	4.89	1.59	1.51
5	A	1[D]	THA	C14-C9	4.84	1.59	1.51
5	D	4[D]	THA	C14-C9	4.84	1.59	1.51
5	B	2[D]	THA	C14-C9	4.84	1.59	1.51
5	C	3[C]	THA	C14-C9	4.83	1.59	1.51
5	A	1[B]	THA	C14-C9	4.82	1.59	1.51
5	E	5[A]	THA	C14-C9	4.79	1.59	1.51
5	D	4[E]	THA	C14-C9	4.79	1.59	1.51
5	C	3[B]	THA	C14-C9	4.75	1.59	1.51
5	D	4[A]	THA	C14-C9	4.73	1.59	1.51
5	E	5[C]	THA	C14-C9	4.73	1.59	1.51
5	F	6[D]	THA	C14-C9	4.70	1.59	1.51
5	E	5[B]	THA	C14-C9	4.69	1.59	1.51
5	F	6[B]	THA	C14-C9	4.59	1.58	1.51
5	B	2[C]	THA	C14-C9	4.53	1.58	1.51
5	F	6[A]	THA	C14-C9	4.53	1.58	1.51
5	B	2[A]	THA	C14-C9	4.52	1.58	1.51
5	F	6[C]	THA	C14-C9	4.52	1.58	1.51
5	E	5[E]	THA	C14-C9	4.51	1.58	1.51
5	A	1[C]	THA	C14-C9	4.46	1.58	1.51
5	A	1[A]	THA	C14-C9	4.42	1.58	1.51
5	C	3[D]	THA	C14-C9	4.08	1.58	1.51
5	E	5[E]	THA	C4-C3	4.02	1.49	1.42
5	A	1[A]	THA	C4-C3	4.02	1.49	1.42
5	E	5[C]	THA	C4-C3	4.00	1.49	1.42
5	C	3[D]	THA	C4-C3	3.99	1.49	1.42
5	C	3[B]	THA	C11-C8	3.99	1.57	1.50
5	D	4[E]	THA	C4-C3	3.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	6[B]	THA	C4-C3	3.97	1.49	1.42
5	A	1[C]	THA	C4-C3	3.97	1.49	1.42
5	B	2[C]	THA	C4-C3	3.97	1.49	1.42
5	E	5[D]	THA	C4-C3	3.97	1.49	1.42
5	B	2[D]	THA	C4-C3	3.94	1.49	1.42
5	E	5[A]	THA	C4-C3	3.94	1.49	1.42
5	E	5[B]	THA	C4-C3	3.94	1.49	1.42
5	C	3[C]	THA	C4-C3	3.93	1.49	1.42
5	C	3[B]	THA	C4-C3	3.93	1.49	1.42
5	F	6[A]	THA	C11-C8	3.91	1.57	1.50
5	D	4[B]	THA	C4-C3	3.90	1.48	1.42
5	B	2[A]	THA	C11-C8	3.89	1.57	1.50
5	F	6[A]	THA	C4-C3	3.89	1.48	1.42
5	D	4[A]	THA	C4-C3	3.88	1.48	1.42
5	B	2[A]	THA	C4-C3	3.88	1.48	1.42
5	D	4[D]	THA	C4-C3	3.88	1.48	1.42
5	C	3[D]	THA	C11-C8	3.86	1.57	1.50
5	B	2[B]	THA	C4-C3	3.85	1.48	1.42
5	F	6[C]	THA	C4-C3	3.85	1.48	1.42
5	C	3[E]	THA	C4-C3	3.84	1.48	1.42
5	A	1[A]	THA	C11-C8	3.84	1.57	1.50
5	A	1[B]	THA	C4-C3	3.83	1.48	1.42
5	C	3[C]	THA	C11-C8	3.83	1.57	1.50
5	E	5[A]	THA	C11-C8	3.82	1.57	1.50
5	A	1[B]	THA	C11-C8	3.81	1.57	1.50
5	A	1[D]	THA	C4-C3	3.81	1.48	1.42
5	C	3[A]	THA	C4-C3	3.80	1.48	1.42
5	D	4[C]	THA	C4-C3	3.79	1.48	1.42
5	C	3[A]	THA	C9-C8	3.77	1.46	1.40
5	F	6[D]	THA	C4-C3	3.77	1.48	1.42
5	D	4[A]	THA	C11-C8	3.77	1.56	1.50
5	A	1[C]	THA	C11-C8	3.77	1.56	1.50
5	E	5[E]	THA	C11-C8	3.76	1.56	1.50
5	D	4[C]	THA	C11-C8	3.76	1.56	1.50
5	D	4[A]	THA	C9-C8	3.75	1.46	1.40
5	A	1[D]	THA	C11-C8	3.75	1.56	1.50
5	E	5[C]	THA	C9-C8	3.74	1.46	1.40
5	A	1[D]	THA	C9-C8	3.74	1.46	1.40
5	B	2[D]	THA	C9-C8	3.74	1.46	1.40
5	E	5[A]	THA	C9-C8	3.73	1.46	1.40
5	F	6[B]	THA	C9-C8	3.73	1.46	1.40
5	D	4[D]	THA	C11-C8	3.71	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	6[D]	THA	C11-C8	3.71	1.56	1.50
5	F	6[D]	THA	C9-C8	3.70	1.46	1.40
5	B	2[B]	THA	C9-C8	3.70	1.46	1.40
5	A	1[B]	THA	C9-C8	3.70	1.46	1.40
5	D	4[D]	THA	C9-C8	3.70	1.46	1.40
5	E	5[C]	THA	C11-C8	3.69	1.56	1.50
5	F	6[C]	THA	C11-C8	3.69	1.56	1.50
5	D	4[C]	THA	C9-C8	3.69	1.46	1.40
5	C	3[C]	THA	C9-C8	3.69	1.46	1.40
5	E	5[B]	THA	C11-C8	3.69	1.56	1.50
5	A	1[A]	THA	C9-C8	3.69	1.46	1.40
5	B	2[C]	THA	C9-C8	3.69	1.46	1.40
5	E	5[E]	THA	C9-C8	3.68	1.46	1.40
5	E	5[B]	THA	C9-C8	3.68	1.46	1.40
5	B	2[C]	THA	C11-C8	3.68	1.56	1.50
5	F	6[C]	THA	C9-C8	3.67	1.46	1.40
5	C	3[A]	THA	C11-C8	3.66	1.56	1.50
5	E	5[D]	THA	C9-C8	3.66	1.46	1.40
5	D	4[B]	THA	C9-C8	3.65	1.46	1.40
5	B	2[B]	THA	C11-C8	3.64	1.56	1.50
5	C	3[E]	THA	C9-C8	3.64	1.46	1.40
5	C	3[B]	THA	C9-C8	3.62	1.45	1.40
5	C	3[E]	THA	C11-C8	3.61	1.56	1.50
5	A	1[C]	THA	C9-C8	3.61	1.45	1.40
5	B	2[A]	THA	C9-C8	3.61	1.45	1.40
5	F	6[B]	THA	C11-C8	3.59	1.56	1.50
5	B	2[D]	THA	C11-C8	3.55	1.56	1.50
5	E	5[D]	THA	C11-C8	3.54	1.56	1.50
5	F	6[A]	THA	C9-C8	3.52	1.45	1.40
5	C	3[D]	THA	C9-C8	3.50	1.45	1.40
5	D	4[B]	THA	C11-C8	3.49	1.56	1.50
5	D	4[E]	THA	C9-C8	3.48	1.45	1.40
5	D	4[E]	THA	C11-C8	3.40	1.56	1.50
4	A	182	SIA	C3-C2	2.81	1.55	1.51
5	F	6[C]	THA	C3-N7	-2.45	1.33	1.37
5	A	1[B]	THA	C6-C5	2.40	1.42	1.36
5	B	2[A]	THA	C6-C5	2.40	1.42	1.36
5	B	2[B]	THA	C1-C2	2.40	1.42	1.36
5	C	3[E]	THA	C6-C5	2.39	1.42	1.36
5	D	4[D]	THA	C6-C5	2.38	1.42	1.36
5	D	4[B]	THA	C1-C2	2.37	1.42	1.36
5	E	5[B]	THA	C3-N7	-2.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3[E]	THA	C1-C2	2.36	1.42	1.36
5	E	5[D]	THA	C1-C2	2.35	1.42	1.36
5	F	6[B]	THA	C3-N7	-2.35	1.33	1.37
5	A	1[A]	THA	C1-C2	2.34	1.42	1.36
5	C	3[B]	THA	C6-C5	2.34	1.42	1.36
5	F	6[A]	THA	C6-C5	2.34	1.42	1.36
5	A	1[A]	THA	C6-C5	2.33	1.42	1.36
5	D	4[A]	THA	C6-C5	2.33	1.42	1.36
5	F	6[D]	THA	C1-C2	2.33	1.42	1.36
5	E	5[A]	THA	C1-C2	2.33	1.42	1.36
5	D	4[E]	THA	C6-C5	2.33	1.42	1.36
5	D	4[E]	THA	C1-C2	2.32	1.42	1.36
5	E	5[C]	THA	C3-N7	-2.32	1.33	1.37
5	B	2[A]	THA	C1-C2	2.32	1.42	1.36
5	A	1[C]	THA	C3-N7	-2.32	1.33	1.37
5	E	5[D]	THA	C6-C5	2.32	1.42	1.36
5	D	4[A]	THA	C1-C2	2.31	1.42	1.36
5	C	3[B]	THA	C1-C2	2.31	1.42	1.36
5	E	5[E]	THA	C3-N7	-2.31	1.33	1.37
5	C	3[D]	THA	C1-C2	2.30	1.41	1.36
5	E	5[A]	THA	C6-C5	2.30	1.41	1.36
5	B	2[D]	THA	C3-N7	-2.28	1.33	1.37
5	C	3[D]	THA	C6-C5	2.28	1.41	1.36
5	B	2[C]	THA	C3-N7	-2.28	1.33	1.37
5	C	3[A]	THA	C6-C5	2.28	1.41	1.36
5	B	2[C]	THA	C1-C2	2.28	1.41	1.36
5	E	5[E]	THA	C1-C2	2.28	1.41	1.36
5	D	4[D]	THA	C3-N7	-2.27	1.33	1.37
5	F	6[A]	THA	C1-C2	2.27	1.41	1.36
5	D	4[B]	THA	C3-N7	-2.27	1.33	1.37
5	E	5[E]	THA	C6-C5	2.27	1.41	1.36
5	F	6[D]	THA	C3-N7	-2.26	1.33	1.37
5	D	4[B]	THA	C6-C5	2.26	1.41	1.36
5	B	2[B]	THA	C6-C5	2.26	1.41	1.36
5	B	2[C]	THA	C6-C5	2.25	1.41	1.36
5	D	4[A]	THA	C3-N7	-2.25	1.33	1.37
5	B	2[D]	THA	C6-C5	2.25	1.41	1.36
5	C	3[C]	THA	C3-N7	-2.25	1.33	1.37
5	E	5[A]	THA	C3-N7	-2.24	1.33	1.37
5	E	5[C]	THA	C6-C5	2.24	1.41	1.36
5	D	4[D]	THA	C1-C2	2.24	1.41	1.36
5	C	3[A]	THA	C3-N7	-2.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5[B]	THA	C6-C5	2.23	1.41	1.36
5	E	5[C]	THA	C1-C2	2.23	1.41	1.36
5	F	6[C]	THA	C6-C5	2.22	1.41	1.36
5	A	1[C]	THA	C6-C5	2.21	1.41	1.36
5	E	5[B]	THA	C1-C2	2.21	1.41	1.36
5	C	3[B]	THA	C3-N7	-2.21	1.34	1.37
5	B	2[D]	THA	C1-C2	2.21	1.41	1.36
5	B	2[B]	THA	C3-N7	-2.20	1.34	1.37
5	A	1[C]	THA	C1-C2	2.20	1.41	1.36
5	F	6[B]	THA	C1-C2	2.20	1.41	1.36
5	D	4[C]	THA	C3-N7	-2.19	1.34	1.37
5	A	1[B]	THA	C1-C2	2.19	1.41	1.36
5	A	1[D]	THA	C3-N7	-2.19	1.34	1.37
5	D	4[E]	THA	C3-N7	-2.19	1.34	1.37
5	F	6[D]	THA	C6-C5	2.19	1.41	1.36
5	B	2[A]	THA	C3-N7	-2.19	1.34	1.37
5	C	3[C]	THA	C1-C2	2.19	1.41	1.36
5	C	3[A]	THA	C1-C2	2.18	1.41	1.36
4	D	482	SIA	C3-C2	2.18	1.54	1.51
5	D	4[C]	THA	C6-C5	2.17	1.41	1.36
5	F	6[B]	THA	C6-C5	2.16	1.41	1.36
5	F	6[A]	THA	C3-N7	-2.16	1.34	1.37
5	C	3[D]	THA	C3-N7	-2.16	1.34	1.37
4	E	582	SIA	O6-C2	2.15	1.45	1.43
5	A	1[B]	THA	C3-N7	-2.15	1.34	1.37
5	C	3[C]	THA	C6-C5	2.14	1.41	1.36
5	A	1[A]	THA	C3-N7	-2.12	1.34	1.37
5	C	3[E]	THA	C3-N7	-2.10	1.34	1.37
5	D	4[C]	THA	C1-C2	2.09	1.41	1.36
5	A	1[D]	THA	C6-C5	2.07	1.41	1.36
5	E	5[D]	THA	C3-N7	-2.07	1.34	1.37
5	F	6[C]	THA	C1-C2	2.07	1.41	1.36
4	D	482	SIA	C4-C5	2.03	1.54	1.53

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6[C]	THA	C8-N7-C3	4.59	123.33	117.67
5	D	4[D]	THA	C8-N7-C3	4.58	123.32	117.67
5	B	2[A]	THA	C8-N7-C3	4.58	123.31	117.67
5	B	2[B]	THA	C8-N7-C3	4.56	123.29	117.67
5	E	5[B]	THA	C8-N7-C3	4.55	123.29	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6[A]	THA	C8-N7-C3	4.53	123.26	117.67
5	C	3[B]	THA	C8-N7-C3	4.52	123.25	117.67
5	D	4[A]	THA	C8-N7-C3	4.52	123.24	117.67
5	E	5[C]	THA	C8-N7-C3	4.52	123.24	117.67
5	A	1[B]	THA	C8-N7-C3	4.51	123.23	117.67
5	C	3[E]	THA	C8-N7-C3	4.50	123.23	117.67
5	A	1[C]	THA	C8-N7-C3	4.50	123.22	117.67
5	F	6[D]	THA	C8-N7-C3	4.49	123.21	117.67
5	E	5[A]	THA	C8-N7-C3	4.47	123.19	117.67
5	C	3[A]	THA	C8-N7-C3	4.47	123.18	117.67
5	D	4[B]	THA	C8-N7-C3	4.46	123.18	117.67
5	E	5[E]	THA	C8-N7-C3	4.45	123.16	117.67
5	A	1[A]	THA	C8-N7-C3	4.45	123.16	117.67
5	C	3[D]	THA	C8-N7-C3	4.44	123.15	117.67
5	F	6[B]	THA	C8-N7-C3	4.44	123.14	117.67
5	B	2[C]	THA	C8-N7-C3	4.43	123.14	117.67
5	E	5[D]	THA	C8-N7-C3	4.43	123.13	117.67
5	C	3[C]	THA	C8-N7-C3	4.42	123.12	117.67
5	D	4[C]	THA	C8-N7-C3	4.41	123.11	117.67
5	A	1[D]	THA	C8-N7-C3	4.41	123.11	117.67
5	B	2[D]	THA	C8-N7-C3	4.41	123.11	117.67
5	D	4[E]	THA	C8-N7-C3	4.39	123.08	117.67
4	A	182	SIA	O6-C6-C5	3.72	113.41	109.78
5	F	6[A]	THA	C14-C9-C8	-3.36	117.94	121.08
5	B	2[A]	THA	C14-C9-C8	-3.33	117.97	121.08
5	A	1[C]	THA	C14-C9-C8	-3.24	118.05	121.08
5	C	3[B]	THA	C14-C9-C8	-3.22	118.07	121.08
5	D	4[A]	THA	C14-C9-C8	-3.12	118.16	121.08
4	E	582	SIA	O6-C6-C5	3.12	112.82	109.78
5	C	3[D]	THA	C14-C9-C8	-3.08	118.20	121.08
5	A	1[A]	THA	C14-C9-C8	-3.06	118.22	121.08
5	E	5[C]	THA	C14-C9-C8	-2.99	118.28	121.08
5	E	5[E]	THA	C14-C9-C8	-2.99	118.28	121.08
5	F	6[C]	THA	C14-C9-C8	-2.95	118.32	121.08
5	A	1[B]	THA	C14-C9-C8	-2.95	118.32	121.08
5	D	4[C]	THA	C14-C9-C8	-2.95	118.33	121.08
5	D	4[D]	THA	C14-C9-C8	-2.94	118.33	121.08
5	B	2[C]	THA	C14-C9-C8	-2.93	118.34	121.08
5	E	5[B]	THA	C14-C9-C8	-2.91	118.36	121.08
5	E	5[A]	THA	C14-C9-C8	-2.89	118.38	121.08
5	A	1[D]	THA	C14-C9-C8	-2.87	118.40	121.08
5	F	6[D]	THA	C14-C9-C8	-2.87	118.40	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3[C]	THA	C14-C9-C8	-2.86	118.40	121.08
5	C	3[A]	THA	C14-C9-C8	-2.85	118.41	121.08
5	B	2[D]	THA	C14-C9-C8	-2.85	118.41	121.08
5	F	6[B]	THA	C14-C9-C8	-2.85	118.42	121.08
5	D	4[E]	THA	C14-C9-C8	-2.79	118.47	121.08
4	E	582	SIA	O6-C6-C7	2.77	111.56	107.29
5	B	2[B]	THA	C14-C9-C8	-2.76	118.50	121.08
5	D	4[B]	THA	C14-C9-C8	-2.71	118.55	121.08
5	E	5[D]	THA	C14-C9-C8	-2.68	118.57	121.08
5	C	3[D]	THA	C9-C8-N7	-2.68	121.39	123.68
5	D	4[A]	THA	C9-C8-N7	-2.67	121.40	123.68
5	B	2[A]	THA	C9-C8-N7	-2.65	121.42	123.68
5	F	6[A]	THA	C9-C8-N7	-2.65	121.42	123.68
5	C	3[B]	THA	C9-C8-N7	-2.65	121.42	123.68
5	A	1[A]	THA	C9-C8-N7	-2.63	121.44	123.68
5	F	6[C]	THA	C9-C8-N7	-2.62	121.44	123.68
5	A	1[B]	THA	C9-C8-N7	-2.62	121.45	123.68
5	B	2[C]	THA	C9-C8-N7	-2.60	121.46	123.68
5	D	4[C]	THA	C9-C8-N7	-2.60	121.46	123.68
5	A	1[D]	THA	C9-C8-N7	-2.59	121.47	123.68
5	E	5[C]	THA	C9-C8-N7	-2.59	121.47	123.68
5	A	1[C]	THA	C9-C8-N7	-2.57	121.48	123.68
5	E	5[B]	THA	C9-C8-N7	-2.57	121.49	123.68
5	C	3[A]	THA	C9-C8-N7	-2.55	121.50	123.68
5	E	5[E]	THA	C9-C8-N7	-2.54	121.51	123.68
5	C	3[E]	THA	C14-C9-C8	-2.54	118.71	121.08
5	D	4[D]	THA	C9-C8-N7	-2.54	121.51	123.68
5	E	5[D]	THA	C9-C8-N7	-2.53	121.52	123.68
5	E	5[A]	THA	C9-C8-N7	-2.53	121.52	123.68
5	B	2[B]	THA	C9-C8-N7	-2.52	121.53	123.68
5	C	3[C]	THA	C9-C8-N7	-2.51	121.53	123.68
5	F	6[D]	THA	C9-C8-N7	-2.51	121.53	123.68
5	C	3[E]	THA	C9-C8-N7	-2.50	121.54	123.68
5	D	4[B]	THA	C9-C8-N7	-2.48	121.56	123.68
5	B	2[D]	THA	C9-C8-N7	-2.48	121.57	123.68
5	F	6[B]	THA	C9-C8-N7	-2.46	121.58	123.68
5	D	4[E]	THA	C9-C8-N7	-2.38	121.65	123.68
4	A	182	SIA	C8-C7-C6	-2.31	108.66	113.03
3	B	279	NAG	C2-N2-C7	-2.26	119.69	122.90
4	D	482	SIA	O6-C6-C7	2.17	110.64	107.29
4	B	282	SIA	O6-C6-C7	2.11	110.55	107.29
3	F	679	NAG	C2-N2-C7	-2.09	119.93	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3[E]	THA	C13-C14-C9	2.08	117.12	112.84
4	D	482	SIA	O6-C6-C5	2.04	111.77	109.78
3	E	579	NAG	C2-N2-C7	-2.03	120.02	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	279	NAG	C8-C7-N2-C2
3	B	279	NAG	O7-C7-N2-C2
3	E	579	NAG	C8-C7-N2-C2
3	E	579	NAG	O7-C7-N2-C2
3	F	680	NAG	C8-C7-N2-C2
3	B	279	NAG	O5-C5-C6-O6
3	A	179	NAG	C8-C7-N2-C2
3	B	279	NAG	C4-C5-C6-O6
3	F	680	NAG	O7-C7-N2-C2
3	A	179	NAG	O7-C7-N2-C2
3	F	679	NAG	C8-C7-N2-C2
3	F	679	NAG	O7-C7-N2-C2
3	E	579	NAG	C4-C5-C6-O6
3	E	579	NAG	O5-C5-C6-O6
4	A	182	SIA	C11-C10-N5-C5
3	D	479	NAG	C8-C7-N2-C2
4	A	182	SIA	O10-C10-N5-C5
3	D	479	NAG	O7-C7-N2-C2

There are no ring outliers.

33 monomers are involved in 130 short contacts:

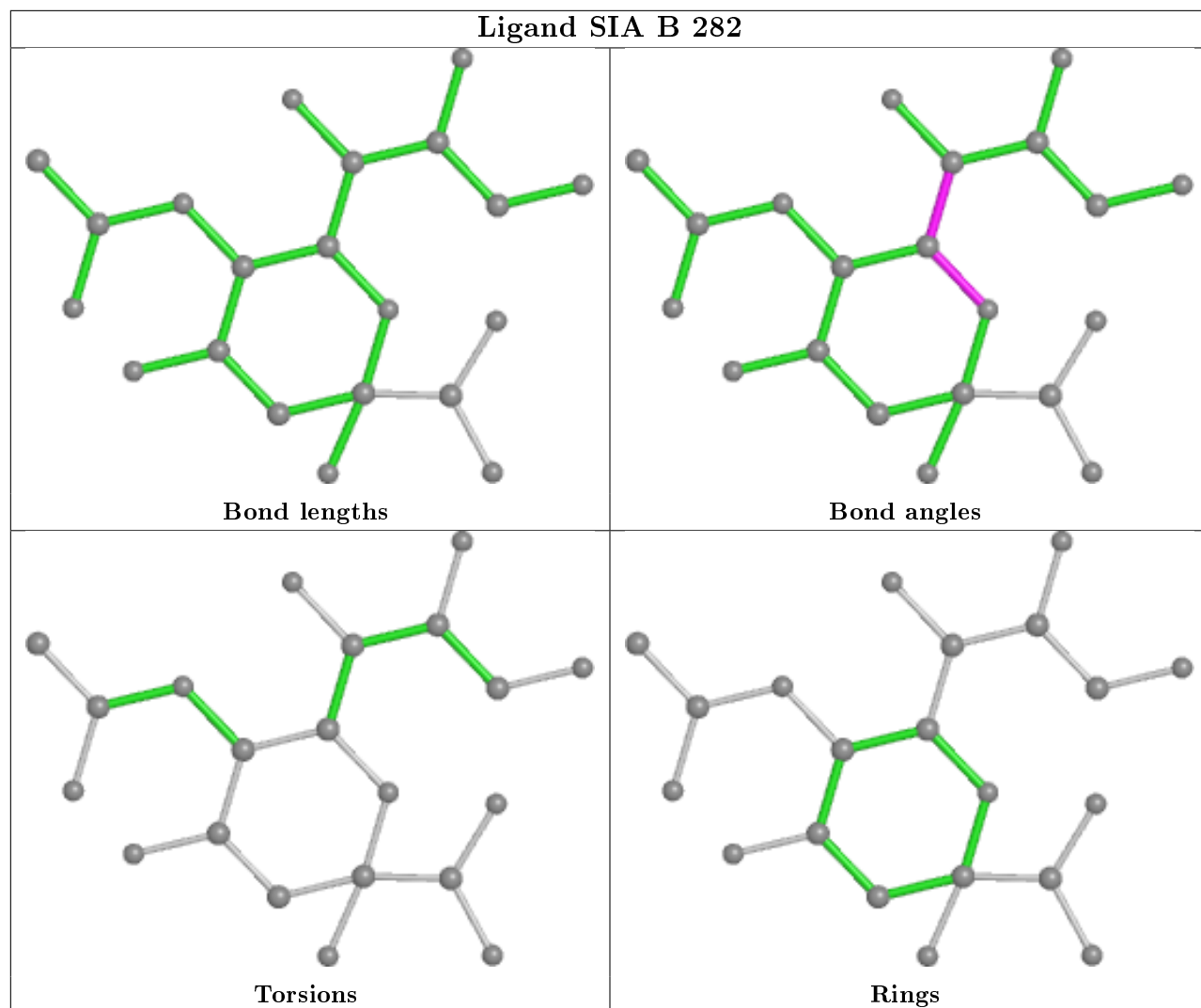
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	6[C]	THA	3	0
5	F	6[B]	THA	2	0
3	B	279	NAG	3	0
5	A	1[D]	THA	3	0
5	B	2[D]	THA	1	0
5	A	1[A]	THA	3	0
4	B	282	SIA	16	0
3	F	680	NAG	1	0
5	A	1[C]	THA	4	0
5	B	2[A]	THA	2	0

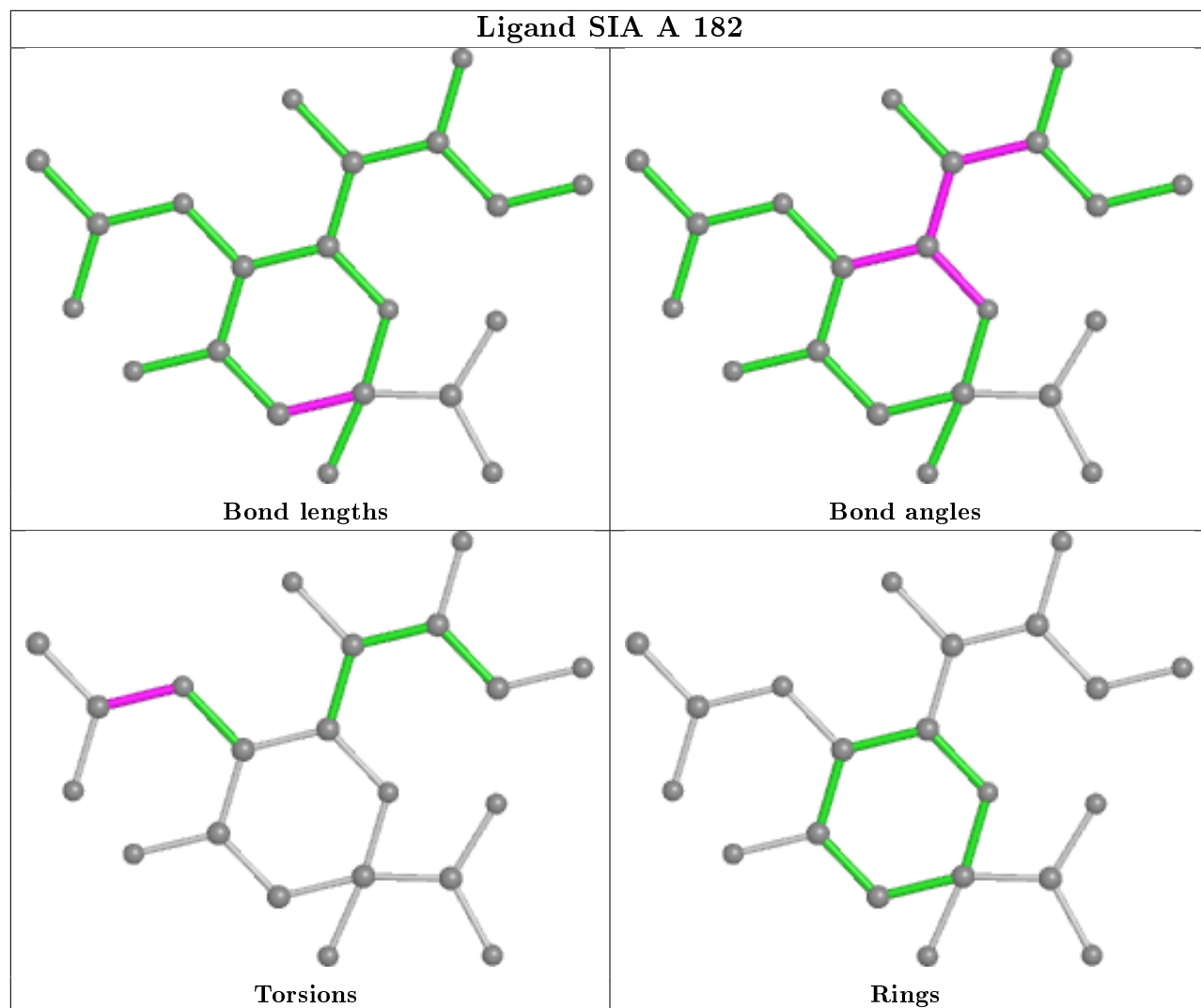
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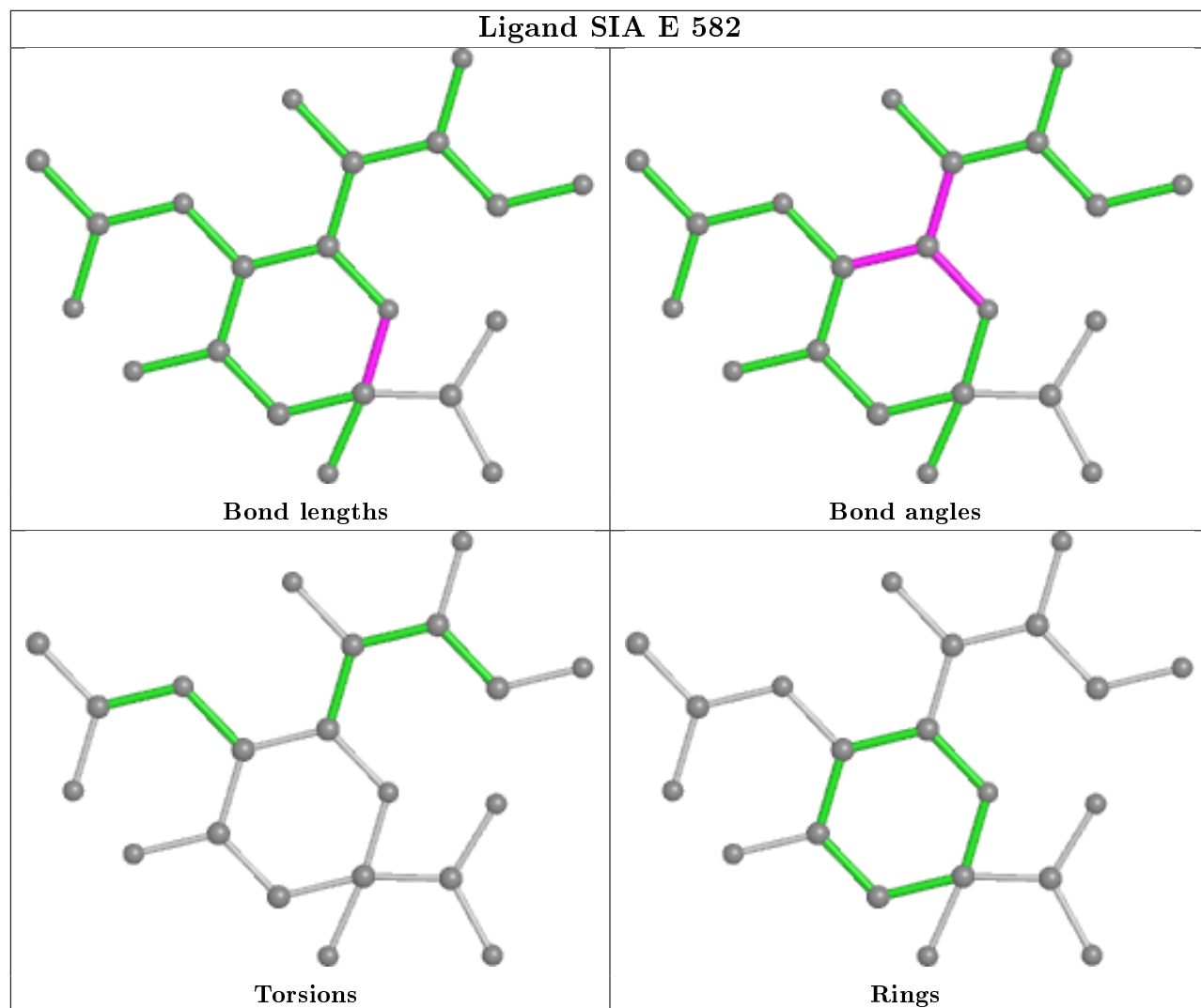
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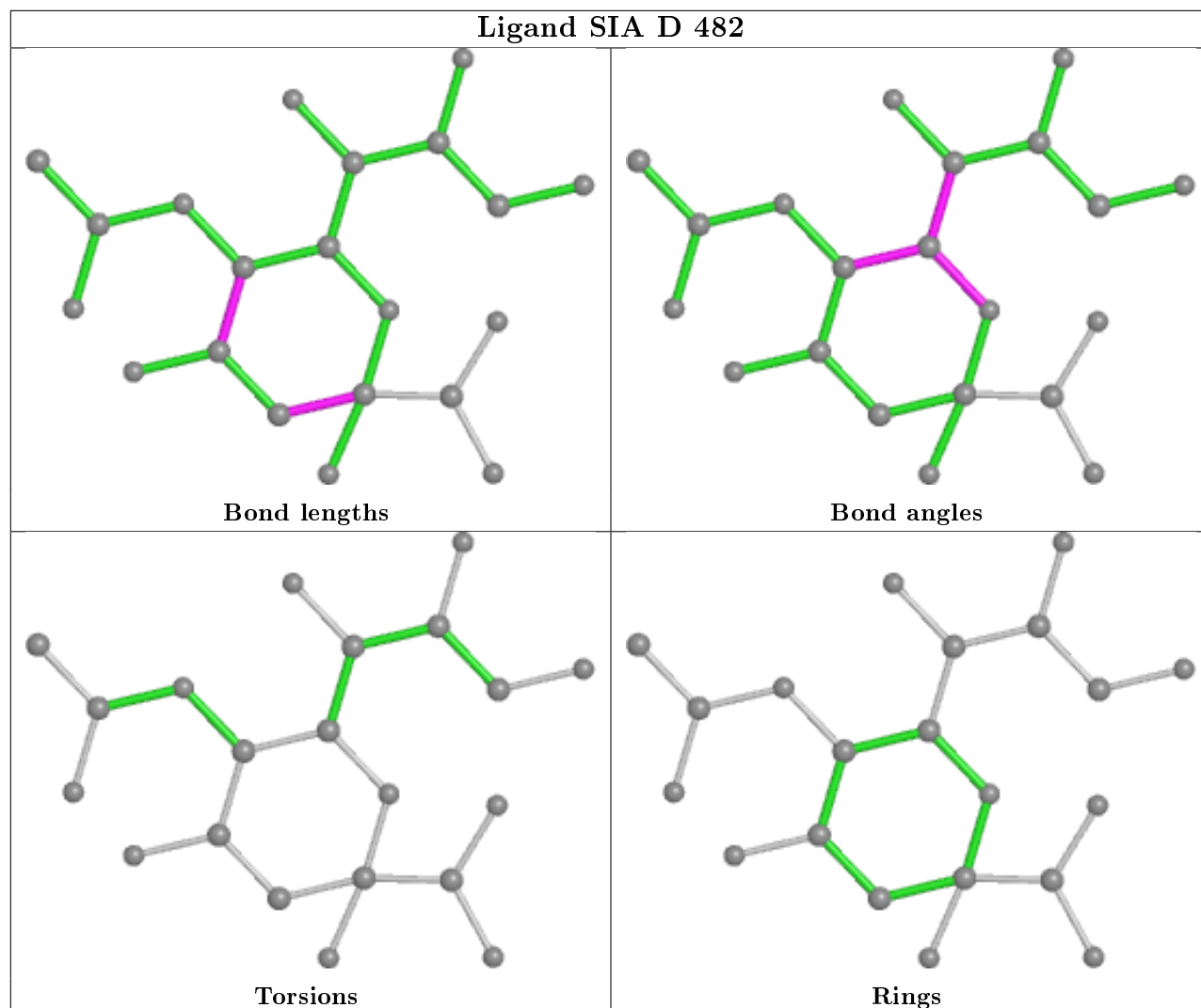
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1[B]	THA	3	0
5	D	4[E]	THA	2	0
5	B	2[C]	THA	1	0
5	B	2[B]	THA	5	0
5	D	4[A]	THA	3	0
5	D	4[C]	THA	2	0
5	D	4[B]	THA	3	0
3	F	679	NAG	1	0
4	A	182	SIA	30	0
5	C	3[E]	THA	3	0
5	C	3[D]	THA	4	0
3	E	579	NAG	1	0
5	C	3[A]	THA	3	0
5	E	5[E]	THA	4	0
5	C	3[C]	THA	1	0
5	E	5[D]	THA	3	0
5	C	3[B]	THA	1	0
5	F	6[D]	THA	2	0
5	E	5[A]	THA	2	0
4	E	582	SIA	7	0
5	E	5[C]	THA	3	0
5	E	5[B]	THA	2	0
4	D	482	SIA	7	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.