



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 PM UTC

PDB ID : 2HRR / pdb_00002hrr
Title : Crystal structure of Human Liver Carboxylesterase 1 (hCE1) in covalent complex with the nerve agent Tabun (GA)
Authors : Fleming, C.D.; Redinbo, M.R.
Deposited on : 2006-07-20
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

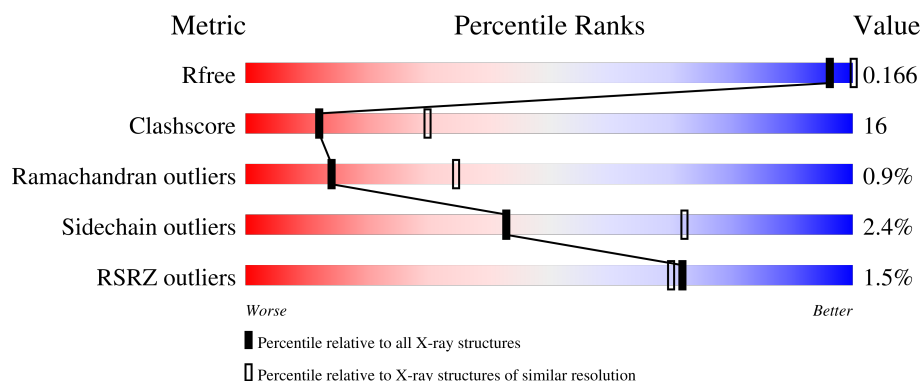
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	532	2% 67% 31% .
1	B	532	2% 69% 30% .
1	C	532	% 71% 27% .
2	D	2	50% 50%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	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
6	SO4	A	1604	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13429 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.

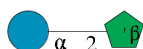
- Molecule 1 is a protein called Liver carboxylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	C	531	Total	C	N	O	S	0	0	0
			4125	2659	684	762	20			

There are 3 discrepancies between the modelled and reference sequences:

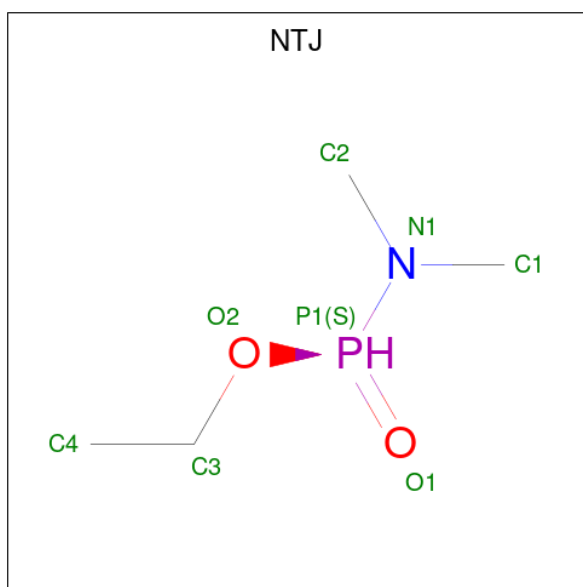
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q9UK77
B	?	-	GLN	deletion	UNP Q9UK77
C	?	-	GLN	deletion	UNP Q9UK77

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is R-ETHYL N,N-DIMETHYLPHOSPHONAMIDATE (CCD ID: NTJ) (formula: C₄H₁₂NO₂P).



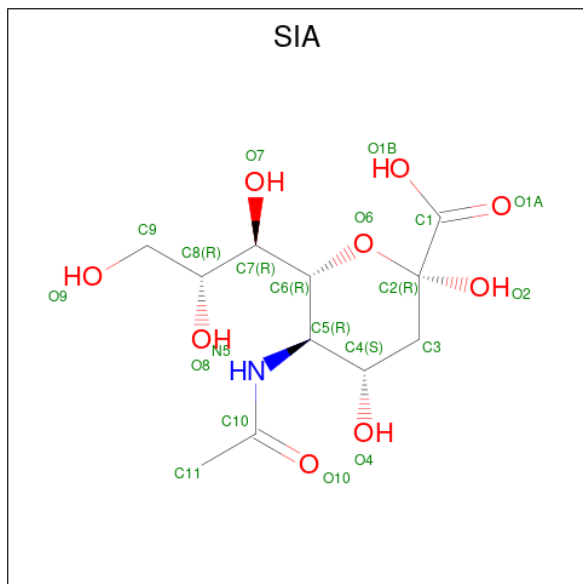
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
3	B	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
3	C	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

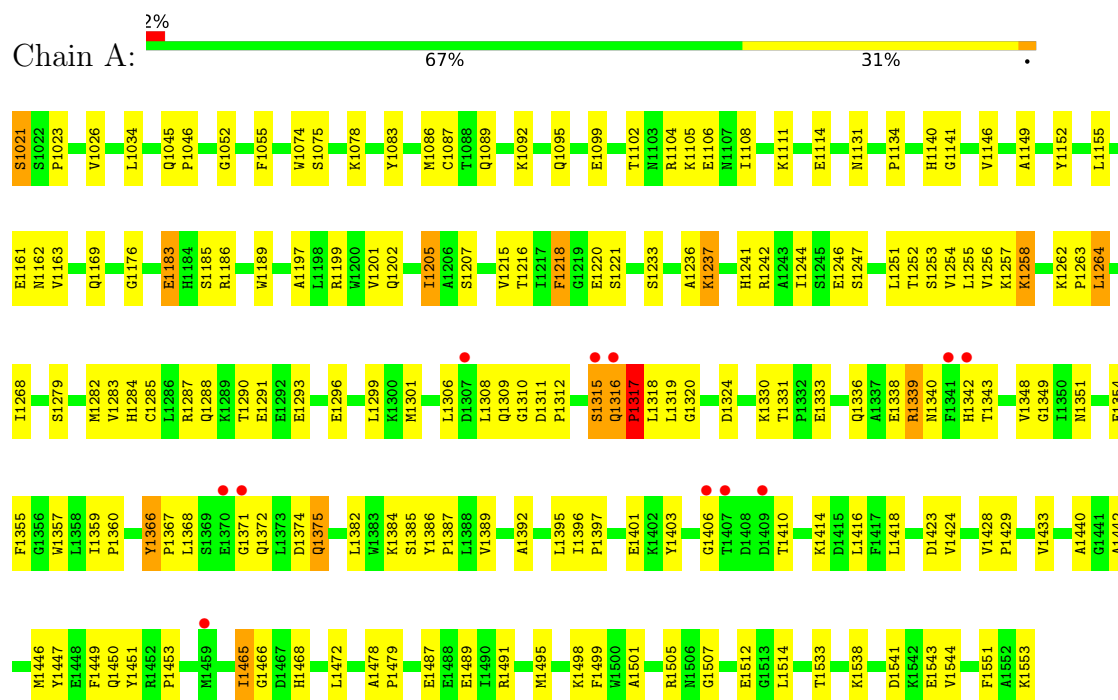
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	242	Total	O	0	0
			242	242		
7	C	326	Total	O	0	0
			326	326		

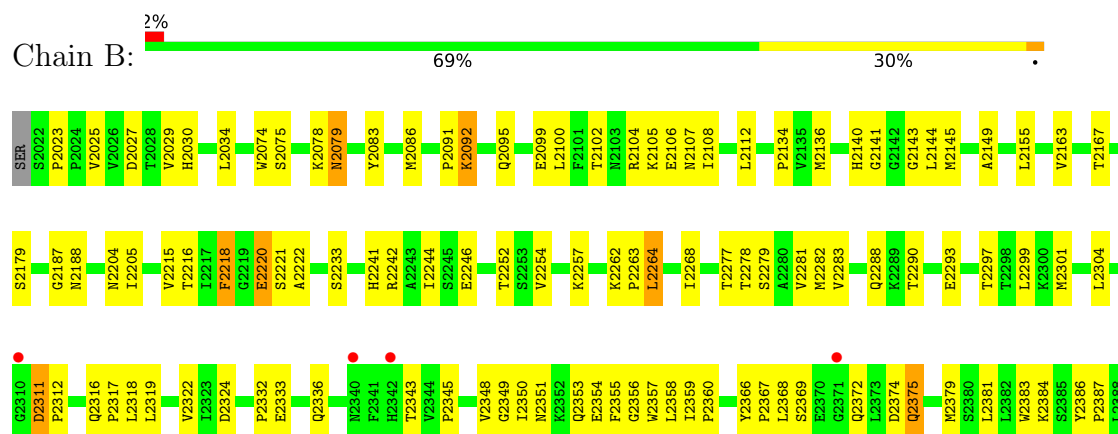
3 Residue-property plots [i](#)

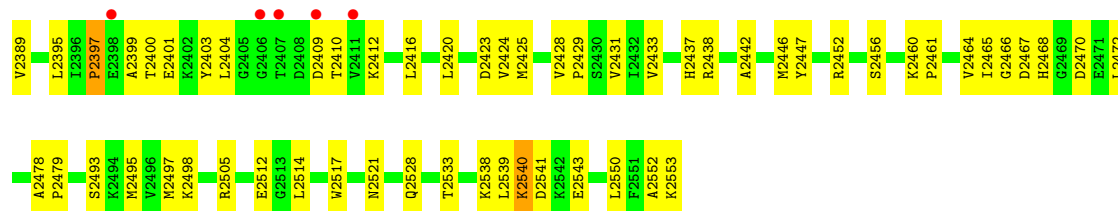
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Liver carboxylesterase 1

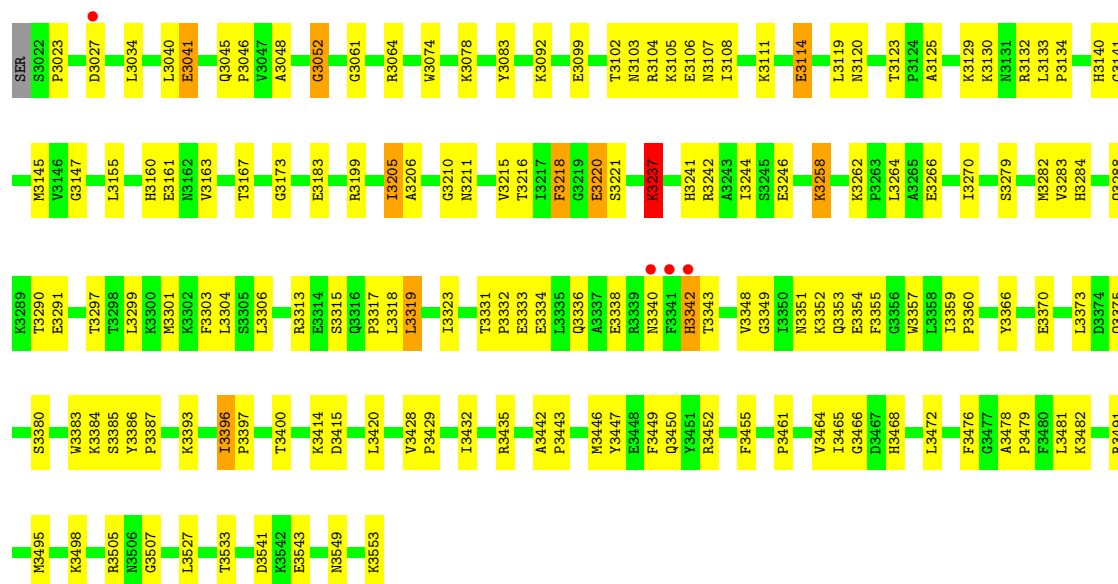


• Molecule 1: Liver carboxylesterase 1





• Molecule 1: Liver carboxylesterase 1



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.57Å 181.05Å 202.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.78 – 2.70 41.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (41.78-2.70) 91.9 (41.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.32 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.167 , 0.232 0.169 , 0.166	Depositor DCC
R_{free} test set	2701 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13429	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FRU, GLC, SIA, NTJ, SO4

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	0.44	1/4236 (0.0%)	0.94	11/5754 (0.2%)
1	B	0.40	1/4230 (0.0%)	0.88	7/5746 (0.1%)
1	C	0.43	1/4231 (0.0%)	0.91	9/5746 (0.2%)
All	All	0.42	3/12697 (0.0%)	0.91	27/17246 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2092	LYS	CE-NZ	-5.25	1.33	1.49
1	C	3092	LYS	CE-NZ	-5.19	1.33	1.49
1	A	1092	LYS	CE-NZ	-5.15	1.33	1.49

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1316	GLN	CA-C-N	-9.42	110.29	119.90
1	A	1316	GLN	C-N-CA	-9.42	110.29	119.90
1	A	1317	PRO	N-CA-C	-9.34	96.40	111.15
1	A	1075	SER	N-CA-C	9.27	121.47	111.36
1	B	2075	SER	N-CA-C	8.94	122.68	111.69
1	A	1316	GLN	N-CA-C	6.99	125.25	109.81
1	A	1311	ASP	CA-C-N	5.99	125.47	119.24
1	A	1311	ASP	C-N-CA	5.99	125.47	119.24
1	C	3160	HIS	N-CA-C	5.95	118.72	111.82
1	C	3114	GLU	N-CA-C	-5.90	105.58	112.89
1	C	3541	ASP	N-CA-C	5.69	117.16	111.07
1	A	1507	GLY	N-CA-C	-5.67	106.35	115.08
1	A	1183	GLU	N-CA-C	5.63	118.19	111.71
1	B	2233	SER	N-CA-C	5.45	116.69	109.93
1	A	1114	GLU	N-CA-C	-5.34	105.63	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3396	ILE	CB-CA-C	-5.31	108.65	113.70
1	C	3507	GLY	N-CA-C	-5.25	106.81	114.90
1	A	1233	SER	N-CA-C	5.25	117.23	109.62
1	C	3052	GLY	CA-C-N	-5.21	118.84	122.59
1	C	3052	GLY	C-N-CA	-5.21	118.84	122.59
1	C	3183	GLU	N-CA-C	5.14	118.65	112.38
1	C	3481	LEU	N-CA-C	-5.11	107.71	114.04
1	B	2356	GLY	N-CA-C	5.05	118.79	112.73
1	B	2366	TYR	CA-C-N	5.05	126.15	119.84
1	B	2366	TYR	C-N-CA	5.05	126.15	119.84
1	B	2311	ASP	CA-C-N	5.03	125.30	119.47
1	B	2311	ASP	C-N-CA	5.03	125.30	119.47

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	4129	141	0
1	B	4124	0	4125	125	0
1	C	4125	0	4124	117	0
2	D	23	0	21	1	0
2	E	23	0	21	1	0
2	F	23	0	21	1	0
3	A	8	0	11	1	0
3	B	8	0	11	0	0
3	C	8	0	11	0	0
4	A	14	0	12	0	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
5	A	21	0	18	3	0
5	B	21	0	18	6	0
5	C	21	0	18	7	0
6	A	10	0	0	3	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	10	0	0	1	0
7	A	259	0	0	15	0
7	B	242	0	0	8	0
7	C	326	0	0	20	0
All	All	13429	0	12566	393	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 16.

All (393) 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:C:3343:THR:HB	1:C:3442:ALA:HB2	1.31	1.11
1:B:2343:THR:HB	1:B:2442:ALA:HB2	1.46	0.98
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.12	0.95
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.17	0.92
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.07	0.90
1:C:3353:GLN:NE2	1:C:3465:ILE:H	1.71	0.88
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.56	0.87
1:C:3105:LYS:HG3	1:C:3106:GLU:H	1.37	0.87
1:A:1258:LYS:H	1:A:1258:LYS:HD2	1.40	0.86
1:A:1105:LYS:HG3	1:A:1106:GLU:H	1.39	0.86
1:A:1257:LYS:HE2	1:A:1318:LEU:O	1.77	0.85
1:A:1264:LEU:HG	1:A:1317:PRO:HB2	1.59	0.84
1:A:1268:ILE:HG12	1:A:1301:MET:HE2	1.57	0.84
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.57	0.82
1:B:2105:LYS:HG3	1:B:2106:GLU:H	1.45	0.81
1:A:1336:GLN:HE22	1:A:1433:VAL:HA	1.44	0.80
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.62	0.80
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	1.81	0.80
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	1.82	0.79
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.66	0.78
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.19	0.78
1:A:1290:THR:OG1	1:A:1293:GLU:HG3	1.84	0.77
1:A:1220:GLU:HG2	1:A:1472:LEU:HD21	1.66	0.77
1:B:2220:GLU:HG2	1:B:2472:LEU:HD21	1.66	0.76
1:C:3215:VAL:H	1:C:3241:HIS:CD2	1.99	0.74
1:A:1316:GLN:O	1:A:1317:PRO:C	2.29	0.74
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.04	0.74
1:A:1553:LYS:HG2	7:A:1819:HOH:O	1.88	0.73
1:C:3129:LYS:HG2	1:C:3130:LYS:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2602:NAG:H83	5:B:2603:SIA:H31	1.69	0.73
1:A:1105:LYS:HG3	1:A:1106:GLU:N	2.03	0.73
1:C:3216:THR:HG23	1:C:3242:ARG:HB2	1.70	0.73
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.71	0.73
1:B:2332:PRO:O	1:B:2336:GLN:HG3	1.89	0.72
1:A:1105:LYS:HG2	7:A:1820:HOH:O	1.90	0.72
1:A:1397:PRO:O	1:A:1401:GLU:HG3	1.92	0.70
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.27	0.69
5:C:3604:SIA:H7	7:C:3723:HOH:O	1.92	0.69
1:C:3129:LYS:HG2	1:C:3130:LYS:N	2.09	0.68
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.88	0.68
1:C:3353:GLN:HE22	1:C:3465:ILE:H	1.39	0.67
1:B:2091:PRO:HB3	1:B:2112:LEU:HD11	1.77	0.67
1:C:3105:LYS:HD3	7:C:3991:HOH:O	1.95	0.66
1:B:2372:GLN:HG2	1:B:2410:THR:HB	1.77	0.66
1:A:1306:LEU:HD11	1:A:1385:SER:HA	1.77	0.66
1:C:3303:PHE:CZ	1:C:3319:LEU:HD11	2.30	0.66
1:B:2268:ILE:HG12	1:B:2301:MET:HE2	1.79	0.65
1:B:2252:THR:HG22	1:B:2425:MET:O	1.96	0.65
1:C:3105:LYS:HG3	1:C:3106:GLU:N	2.09	0.64
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.80	0.64
1:C:3199:ARG:HG3	7:C:3990:HOH:O	1.98	0.63
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.78	0.63
1:B:2355:PHE:CD1	1:B:2360:PRO:HG3	2.33	0.63
1:B:2423:ASP:OD2	1:B:2543:GLU:HG2	1.98	0.63
1:A:1262:LYS:HE3	1:A:1279:SER:OG	1.99	0.63
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.14	0.63
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.34	0.63
1:C:3315:SER:HB2	7:C:3977:HOH:O	1.99	0.62
1:C:3262:LYS:O	1:C:3266:GLU:HG3	1.99	0.62
5:C:3604:SIA:H4	5:C:3604:SIA:H113	1.82	0.62
1:A:1338:GLU:C	1:A:1340:ASN:H	2.06	0.62
1:B:2086:MET:HE3	1:B:2112:LEU:HD21	1.79	0.62
1:A:1501:ALA:O	1:A:1505:ARG:HG2	2.00	0.62
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.35	0.61
1:C:3491:ARG:HD2	7:C:3929:HOH:O	1.99	0.61
1:B:2246:GLU:HG2	1:B:2447:TYR:OH	2.00	0.61
1:B:2278:THR:OG1	1:B:2281:VAL:HG23	2.00	0.61
5:C:3604:SIA:C7	7:C:3723:HOH:O	2.48	0.61
1:B:2423:ASP:O	1:B:2428:VAL:HG23	2.02	0.60
1:B:2355:PHE:CE1	1:B:2360:PRO:HG3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.16	0.60
1:A:1140:HIS:HD2	1:A:1141:GLY:O	1.85	0.60
1:C:3414:LYS:HD3	1:C:3415:ASP:N	2.17	0.60
1:A:1382:LEU:HD23	1:A:1396:ILE:HG23	1.84	0.59
1:A:1339:ARG:CD	1:A:1440:ALA:HA	2.33	0.59
1:A:1279:SER:O	1:A:1283:VAL:HG23	2.02	0.59
1:A:1512:GLU:HG3	7:A:1838:HOH:O	2.02	0.58
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.34	0.58
1:B:2369:SER:HA	2:E:2:FRU:H61	1.85	0.58
1:B:2452:ARG:HG2	1:B:2452:ARG:HH11	1.69	0.58
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.84	0.58
1:A:1257:LYS:HE3	1:A:1320:GLY:H	1.69	0.57
1:A:1551:PHE:C	1:A:1553:LYS:H	2.12	0.57
1:A:1372:GLN:HG3	1:A:1410:THR:OG1	2.03	0.57
1:A:1161:GLU:OE2	1:A:1498:LYS:HG2	2.05	0.57
1:A:1538:LYS:HB3	1:A:1541:ASP:HB2	1.86	0.57
1:B:2351:ASN:HB3	1:B:2466:GLY:O	2.04	0.57
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.04	0.57
1:B:2079:ASN:O	5:B:2603:SIA:O2	2.17	0.57
1:B:2107:ASN:HD22	1:B:2108:ILE:H	1.52	0.57
1:B:2428:VAL:HB	1:B:2429:PRO:HD3	1.87	0.57
1:A:1403:TYR:O	1:A:1416:LEU:HD13	2.06	0.56
5:A:1603:SIA:N5	5:A:1603:SIA:O7	2.38	0.56
1:B:2029:VAL:HG23	1:B:2204:ASN:OD1	2.05	0.56
1:C:3414:LYS:HE3	2:F:1:GLC:O2	2.05	0.56
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.20	0.56
1:B:2357:TRP:O	1:B:2360:PRO:HD2	2.05	0.56
5:B:2603:SIA:H6	5:B:2603:SIA:H113	1.87	0.56
1:B:2092:LYS:HE3	7:B:2812:HOH:O	2.05	0.56
1:A:1083:TYR:CE2	1:A:1108:ILE:HD13	2.39	0.56
1:A:1338:GLU:C	1:A:1340:ASN:N	2.62	0.56
1:C:3246:GLU:HG2	1:C:3447:TYR:OH	2.06	0.55
1:A:1026:VAL:HG13	1:A:1207:SER:HB3	1.87	0.55
1:A:1052:GLY:HA3	5:A:1603:SIA:C9	2.37	0.55
1:B:2215:VAL:H	1:B:2241:HIS:CD2	2.05	0.55
1:A:1308:LEU:HB2	1:A:1309:GLN:HE22	1.71	0.55
1:A:1339:ARG:HD3	1:A:1440:ALA:HA	1.88	0.55
1:A:1026:VAL:CG1	1:A:1207:SER:HB3	2.37	0.55
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.97	0.55
1:A:1264:LEU:HD22	1:A:1264:LEU:O	2.07	0.55
1:A:1308:LEU:HB2	1:A:1309:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.41	0.55
1:C:3319:LEU:N	1:C:3319:LEU:HD12	2.22	0.55
1:B:2353:GLN:NE2	1:B:2465:ILE:H	2.05	0.55
1:B:2102:THR:OG1	1:B:2104:ARG:HG2	2.06	0.54
1:A:1423:ASP:OD2	1:A:1543:GLU:HG2	2.07	0.54
1:B:2375:GLN:O	1:B:2379:MET:HG3	2.08	0.54
1:C:3111:LYS:HD2	7:C:3704:HOH:O	2.08	0.54
1:A:1262:LYS:HE2	1:A:1282:MET:HE1	1.89	0.54
1:A:1241:HIS:O	1:A:1242:ARG:HD3	2.07	0.54
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.08	0.54
1:B:2025:VAL:HG22	1:B:2034:LEU:HD23	1.90	0.54
1:A:1257:LYS:HE3	1:A:1320:GLY:N	2.23	0.54
1:A:1318:LEU:HB3	7:A:1763:HOH:O	2.07	0.54
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.90	0.54
1:B:2512:GLU:O	1:B:2512:GLU:HG3	2.07	0.54
1:B:2105:LYS:HG3	1:B:2106:GLU:N	2.19	0.54
5:B:2603:SIA:H7	7:B:2805:HOH:O	2.07	0.54
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.43	0.54
1:A:1316:GLN:O	1:A:1318:LEU:HG	2.07	0.53
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.90	0.53
1:B:2100:LEU:HD13	1:B:2358:LEU:HD13	1.89	0.53
1:C:3114:GLU:HG3	1:C:3291:GLU:OE1	2.09	0.53
1:B:2140:HIS:HD2	1:B:2141:GLY:O	1.90	0.53
1:C:3366:TYR:OH	1:C:3385:SER:HB3	2.08	0.53
1:A:1336:GLN:NE2	1:A:1433:VAL:HA	2.20	0.53
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.71	0.53
1:C:3074:TRP:CD2	1:C:3078:LYS:HE2	2.44	0.53
1:B:2437:HIS:HE1	7:B:2703:HOH:O	1.93	0.52
1:A:1236:ALA:O	1:A:1237:LYS:C	2.52	0.52
1:B:2395:LEU:HD13	1:B:2550:LEU:HG	1.91	0.52
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.89	0.52
1:C:3173:GLY:HA3	7:C:3767:HOH:O	2.10	0.52
1:A:1257:LYS:HD3	7:A:1947:HOH:O	2.09	0.52
1:A:1357:TRP:O	1:A:1360:PRO:HD2	2.10	0.52
1:B:2400:THR:CG2	1:B:2404:LEU:HD12	2.39	0.52
1:A:1342:HIS:HE1	7:A:1721:HOH:O	1.93	0.52
1:B:2447:TYR:HB3	1:B:2517:TRP:CZ2	2.44	0.52
1:A:1089:GLN:HB2	1:A:1146:VAL:HG12	1.92	0.52
1:C:3045:GLN:NE2	1:C:3046:PRO:HD2	2.25	0.52
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	1.90	0.51
1:C:3258:LYS:H	1:C:3258:LYS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:PHE:CD2	1:A:1514:LEU:HD13	2.45	0.51
1:B:2297:THR:O	1:B:2301:MET:HG2	2.09	0.51
1:A:1216:THR:HG23	1:A:1242:ARG:HB2	1.93	0.51
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.39	0.51
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.09	0.51
1:C:3129:LYS:HB2	7:C:3985:HOH:O	2.10	0.51
1:C:3297:THR:O	1:C:3301:MET:HG2	2.10	0.51
5:C:3604:SIA:H4	5:C:3604:SIA:C11	2.40	0.51
1:A:1087:CYS:HB3	7:A:1811:HOH:O	2.10	0.51
1:B:2288:GLN:HG3	7:B:2865:HOH:O	2.10	0.51
1:B:2493:SER:O	1:B:2497:MET:HG3	2.10	0.51
1:C:3352:LYS:HG2	1:C:3450:GLN:HE21	1.76	0.51
1:A:1258:LYS:HD2	1:A:1258:LYS:N	2.18	0.51
1:C:3279:SER:O	1:C:3283:VAL:HG23	2.09	0.51
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.92	0.51
1:C:3354:GLU:O	1:C:3468:HIS:HB2	2.10	0.51
1:A:1111:LYS:HD3	7:A:1936:HOH:O	2.10	0.51
1:A:1283:VAL:HG12	1:A:1287:ARG:NH1	2.26	0.50
1:A:1140:HIS:HE1	7:A:1766:HOH:O	1.94	0.50
1:A:1285:CYS:HB2	7:C:3963:HOH:O	2.10	0.50
7:A:1717:HOH:O	5:C:3604:SIA:H31	2.11	0.50
1:B:2467:ASP:N	1:B:2470:ASP:OD2	2.44	0.50
1:C:3343:THR:CB	1:C:3442:ALA:HB2	2.23	0.50
1:A:1348:VAL:O	1:A:1446:MET:HA	2.11	0.50
1:B:2106:GLU:HG2	7:B:2834:HOH:O	2.10	0.50
1:C:3040:LEU:O	1:C:3041:GLU:C	2.54	0.50
1:C:3319:LEU:HD12	1:C:3319:LEU:H	1.76	0.50
1:C:3241:HIS:O	1:C:3242:ARG:HD3	2.12	0.50
1:A:1045:GLN:NE2	1:A:1046:PRO:HD2	2.26	0.50
1:B:2539:LEU:C	1:B:2541:ASP:H	2.19	0.50
1:A:1338:GLU:O	1:A:1340:ASN:N	2.45	0.50
1:A:1551:PHE:C	1:A:1553:LYS:N	2.70	0.50
1:A:1201:VAL:O	1:A:1205:ILE:HB	2.12	0.50
1:B:2397:PRO:O	1:B:2401:GLU:HG3	2.11	0.50
1:C:3290:THR:HA	6:C:3602:SO4:O3	2.12	0.50
1:A:1023:PRO:CB	1:A:1034:LEU:HD21	2.42	0.49
1:B:2221:SER:OG	1:B:2222:ALA:N	2.42	0.49
1:B:2279:SER:HA	1:B:2282:MET:HE3	1.95	0.49
1:A:1333:GLU:H	1:A:1333:GLU:CD	2.21	0.49
1:B:2216:THR:HG23	1:B:2242:ARG:HB2	1.95	0.49
1:B:2333:GLU:H	1:B:2333:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2357:TRP:C	1:B:2360:PRO:HD2	2.37	0.49
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.94	0.49
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.27	0.49
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.42	0.49
1:A:1428:VAL:HG13	1:A:1544:VAL:HG22	1.95	0.49
1:C:3052:GLY:O	5:C:3604:SIA:H92	2.13	0.49
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.95	0.49
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.95	0.48
1:B:2543:GLU:OE2	1:B:2543:GLU:N	2.43	0.48
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.77	0.48
1:A:1354:GLU:O	1:A:1468:HIS:HB2	2.13	0.48
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.13	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:HG21	1.95	0.48
1:C:3048:ALA:HB3	1:C:3123:THR:HG23	1.96	0.48
1:B:2241:HIS:C	1:B:2242:ARG:HD3	2.39	0.48
1:C:3111:LYS:HE2	7:C:4008:HOH:O	2.14	0.48
1:A:1021:SER:O	1:A:1021:SER:OG	2.32	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.96	0.48
1:B:2336:GLN:HE22	1:B:2433:VAL:HG22	1.79	0.48
1:B:2100:LEU:HD13	1:B:2358:LEU:CD1	2.44	0.48
1:B:2107:ASN:ND2	1:B:2108:ILE:H	2.11	0.48
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.95	0.48
1:C:3348:VAL:O	1:C:3446:MET:HA	2.14	0.48
1:C:3495:MET:HE1	1:C:3533:THR:OG1	2.13	0.48
1:C:3543:GLU:OE2	1:C:3543:GLU:N	2.35	0.48
1:A:1149:ALA:HB2	1:A:1169:GLN:HG3	1.96	0.47
1:A:1284:HIS:HA	6:A:1604:SO4:O2	2.14	0.47
1:A:1342:HIS:CE1	7:A:1721:HOH:O	2.66	0.47
1:A:1355:PHE:CD1	1:A:1360:PRO:HG3	2.49	0.47
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.96	0.47
1:A:1074:TRP:CD2	1:A:1078:LYS:HE2	2.49	0.47
1:C:3111:LYS:HG2	7:C:4008:HOH:O	2.15	0.47
5:B:2603:SIA:H6	5:B:2603:SIA:C11	2.43	0.47
1:B:2420:LEU:C	1:B:2420:LEU:HD23	2.39	0.47
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.78	0.47
1:C:3323:ILE:HG12	7:C:3732:HOH:O	2.13	0.47
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.50	0.47
1:A:1360:PRO:HB2	2:D:1:GLC:H61	1.96	0.47
1:B:2030:HIS:HD2	7:B:2737:HOH:O	1.96	0.47
1:B:2107:ASN:ND2	1:B:2108:ILE:N	2.62	0.47
1:C:3370:GLU:HG3	7:C:3833:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2348:VAL:O	1:B:2446:MET:HA	2.15	0.46
1:B:2354:GLU:O	1:B:2468:HIS:HB2	2.15	0.46
1:C:3218:PHE:HB3	1:C:3244:ILE:HB	1.97	0.46
1:C:3428:VAL:O	1:C:3432:ILE:HG13	2.16	0.46
1:C:3288:GLN:NE2	7:C:3703:HOH:O	2.47	0.46
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.50	0.46
1:B:2215:VAL:N	1:B:2241:HIS:HD2	1.95	0.46
1:B:2409:ASP:HB3	1:B:2412:LYS:HB2	1.98	0.46
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.49	0.46
1:B:2179:SER:HB2	1:B:2187:GLY:HA3	1.98	0.46
1:B:2145:MET:HG3	1:B:2304:LEU:HD13	1.98	0.46
1:B:2498:LYS:HB3	1:B:2514:LEU:HD11	1.97	0.46
1:C:3351:ASN:HB3	1:C:3466:GLY:O	2.16	0.46
1:C:3083:TYR:CZ	1:C:3108:ILE:HD13	2.51	0.45
1:C:3161:GLU:OE2	1:C:3498:LYS:HG2	2.16	0.45
1:A:1371:GLY:HA2	1:A:1414:LYS:HE3	1.97	0.45
1:A:1389:VAL:HB	1:A:1424:VAL:HG11	1.99	0.45
5:A:1603:SIA:H112	1:B:2277:THR:O	2.16	0.45
1:C:3103:ASN:ND2	1:C:3476:PHE:HB3	2.30	0.45
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.98	0.45
1:B:2262:LYS:HB3	1:B:2263:PRO:HD3	1.98	0.45
1:A:1284:HIS:O	1:A:1288:GLN:HG3	2.17	0.45
1:A:1291:GLU:HB2	6:A:1605:SO4:O3	2.16	0.45
1:B:2367:PRO:C	1:B:2369:SER:H	2.23	0.45
1:A:1451:TYR:CE2	1:A:1489:GLU:HG3	2.51	0.45
1:A:1330:LYS:HB3	1:A:1330:LYS:HE2	1.81	0.45
1:B:2149:ALA:HB1	1:B:2167:THR:HB	1.97	0.45
1:B:2241:HIS:O	1:B:2345:PRO:HD2	2.17	0.45
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.16	0.45
1:A:1251:LEU:HB2	1:A:1429:PRO:HB3	1.99	0.45
1:B:2350:ILE:C	1:B:2351:ASN:HD22	2.25	0.45
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	1.99	0.45
1:A:1199:ARG:HG2	1:A:1199:ARG:HH11	1.82	0.45
1:A:1287:ARG:HD2	6:A:1604:SO4:O2	2.16	0.45
1:B:2188:ASN:HD22	1:B:2324:ASP:CG	2.25	0.45
1:B:2343:THR:CB	1:B:2442:ALA:HB2	2.32	0.45
1:B:2539:LEU:O	1:B:2541:ASP:N	2.50	0.45
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.99	0.44
1:C:3505:ARG:NH1	7:C:3714:HOH:O	2.50	0.44
1:C:3140:HIS:CD2	1:C:3147:GLY:HA3	2.53	0.44
1:C:3386:TYR:N	1:C:3387:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3455:PHE:CD2	1:C:3482:LYS:HD3	2.52	0.44
1:C:3317:PRO:HD3	1:C:3387:PRO:HB2	1.98	0.44
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.23	0.44
1:A:1199:ARG:HG2	1:A:1199:ARG:NH1	2.32	0.44
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.18	0.44
1:B:2452:ARG:HG2	1:B:2452:ARG:NH1	2.32	0.44
1:C:3205:ILE:HD12	1:C:3205:ILE:HA	1.84	0.44
1:A:1197:ALA:O	1:A:1201:VAL:HG23	2.17	0.44
1:A:1366:TYR:C	1:A:1368:LEU:H	2.26	0.44
1:B:2343:THR:HB	1:B:2442:ALA:CB	2.31	0.44
1:B:2438:ARG:HD2	1:B:2521:ASN:HA	2.00	0.44
1:C:3064:ARG:CZ	7:C:3843:HOH:O	2.65	0.44
1:C:3140:HIS:HD2	1:C:3141:GLY:O	2.01	0.44
1:C:3333:GLU:OE1	1:C:3333:GLU:N	2.42	0.44
1:C:3373:LEU:HB2	1:C:3414:LYS:HB2	1.98	0.44
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.18	0.44
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.18	0.44
1:B:2395:LEU:HB3	1:B:2550:LEU:HD11	1.98	0.44
1:A:1331:THR:HB	1:A:1333:GLU:OE1	2.18	0.44
1:A:1395:LEU:O	1:A:1396:ILE:C	2.60	0.44
1:A:1453:PRO:HA	1:A:1489:GLU:OE1	2.18	0.44
1:C:3338:GLU:C	1:C:3340:ASN:N	2.75	0.44
1:C:3125:ALA:HB2	1:C:3133:LEU:CD1	2.48	0.43
1:A:1149:ALA:CB	1:A:1169:GLN:HG3	2.48	0.43
1:A:1312:PRO:HA	1:A:1315:SER:HB2	2.00	0.43
1:C:3383:TRP:CD1	1:C:3393:LYS:HZ3	2.35	0.43
1:A:1131:ASN:HB2	7:A:1745:HOH:O	2.17	0.43
1:B:2539:LEU:C	1:B:2541:ASP:N	2.77	0.43
1:A:1366:TYR:HA	1:A:1367:PRO:HD3	1.82	0.43
1:A:1374:ASP:O	1:A:1375:GLN:C	2.62	0.43
1:B:2372:GLN:HG2	1:B:2410:THR:CB	2.45	0.43
1:B:2400:THR:HG23	1:B:2404:LEU:HD12	2.01	0.43
1:A:1392:ALA:HB3	1:A:1395:LEU:HG	2.01	0.43
1:B:2107:ASN:HD22	1:B:2108:ILE:N	2.14	0.43
1:C:3357:TRP:O	1:C:3360:PRO:HD2	2.18	0.43
1:C:3375:GLN:HE22	1:C:3400:THR:HG22	1.83	0.43
1:A:1306:LEU:HD11	1:A:1384:LYS:O	2.18	0.43
1:C:3099:GLU:HG2	1:C:3107:ASN:OD1	2.19	0.43
1:C:3145:MET:SD	1:C:3173:GLY:HA2	2.59	0.43
1:B:2257:LYS:HB2	1:B:2322:VAL:HG12	2.01	0.43
1:C:3241:HIS:C	1:C:3242:ARG:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3331:THR:OG1	1:C:3334:GLU:HG3	2.18	0.43
1:A:1252:THR:HG22	1:A:1254:VAL:HG12	2.00	0.43
1:B:2205:ILE:HD12	1:B:2205:ILE:HA	1.88	0.43
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.49	0.43
1:A:1495:MET:HE1	1:A:1533:THR:OG1	2.19	0.42
1:B:2552:ALA:C	1:B:2553:LYS:HG3	2.43	0.42
1:A:1414:LYS:O	1:A:1418:LEU:HG	2.20	0.42
1:C:3220:GLU:OE2	1:C:3221:SER:HB2	2.19	0.42
1:C:3306:LEU:HA	7:C:3949:HOH:O	2.18	0.42
1:B:2399:ALA:N	7:B:2709:HOH:O	2.52	0.42
1:B:2528:GLN:O	1:B:2533:THR:HA	2.19	0.42
1:B:2312:PRO:HG3	1:B:2384:LYS:HA	2.02	0.42
1:C:3102:THR:OG1	1:C:3104:ARG:HG2	2.20	0.42
1:A:1202:GLN:HG3	7:A:1940:HOH:O	2.20	0.42
1:C:3279:SER:HA	1:C:3282:MET:HE3	2.01	0.42
1:C:3284:HIS:O	1:C:3288:GLN:HG2	2.19	0.42
1:A:1152:TYR:CD1	1:A:1152:TYR:N	2.88	0.42
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	2.00	0.42
1:A:1257:LYS:NZ	1:A:1319:LEU:HA	2.34	0.42
1:C:3452:ARG:HD2	1:C:3464:VAL:O	2.20	0.42
1:C:3549:ASN:O	1:C:3553:LYS:HG3	2.20	0.42
1:B:2025:VAL:CG2	1:B:2034:LEU:HD23	2.50	0.42
1:C:3313:ARG:HD3	1:C:3383:TRP:HH2	1.85	0.42
1:B:2553:LYS:HD3	7:B:2768:HOH:O	2.18	0.42
1:A:1372:GLN:HG3	1:A:1410:THR:CB	2.49	0.41
1:B:2538:LYS:HB3	1:B:2541:ASP:HB2	2.02	0.41
5:B:2603:SIA:H111	1:C:3262:LYS:NZ	2.35	0.41
1:C:3027:ASP:O	1:C:3027:ASP:CG	2.64	0.41
1:A:1086:MET:HG2	1:A:1111:LYS:O	2.19	0.41
1:A:1256:VAL:O	1:A:1258:LYS:HE3	2.20	0.41
1:B:2279:SER:O	1:B:2283:VAL:HG23	2.20	0.41
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.34	0.41
1:B:2264:LEU:HD11	1:B:2319:LEU:HD23	2.03	0.41
1:B:2312:PRO:HG3	1:B:2384:LYS:HD3	2.01	0.41
1:A:1221:SER:HA	1:A:1247:SER:O	2.21	0.41
1:C:3380:SER:O	1:C:3384:LYS:HG2	2.20	0.41
1:C:3442:ALA:HA	1:C:3443:PRO:HD3	1.90	0.41
1:B:2311:ASP:HA	1:B:2312:PRO:HD3	1.92	0.41
1:C:3237:LYS:HD3	1:C:3342:HIS:HB3	2.02	0.41
1:A:1055:PHE:CD1	1:A:1055:PHE:C	2.99	0.41
1:A:1254:VAL:HG13	1:A:1255:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:LEU:HD12	7:A:1706:HOH:O	2.21	0.41
1:B:2431:VAL:HG21	1:B:2540:LYS:HB2	2.02	0.41
1:C:3125:ALA:HB2	1:C:3133:LEU:HD12	2.03	0.41
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	2.02	0.41
1:A:1386:TYR:N	1:A:1387:PRO:CD	2.83	0.41
1:B:2257:LYS:NZ	1:B:2318:LEU:O	2.52	0.41
1:B:2374:ASP:O	1:B:2375:GLN:C	2.64	0.41
1:A:1254:VAL:HG23	1:A:1387:PRO:O	2.21	0.41
1:B:2086:MET:HG3	1:B:2112:LEU:HD23	2.02	0.41
1:B:2136:MET:HB3	1:B:2218:PHE:CE1	2.56	0.41
1:B:2317:PRO:HD3	1:B:2387:PRO:HB2	2.03	0.41
1:B:2349:GLY:HA3	1:B:2447:TYR:CZ	2.55	0.41
1:C:3266:GLU:O	1:C:3270:ILE:HG13	2.21	0.41
1:C:3420:LEU:HD23	1:C:3420:LEU:C	2.46	0.41
1:C:3461:PRO:HG2	1:C:3464:VAL:HG23	2.03	0.41
1:A:1183:GLU:HG3	7:A:1737:HOH:O	2.21	0.40
1:A:1218:PHE:HA	1:A:1244:ILE:O	2.21	0.40
1:A:1296:GLU:OE1	1:A:1296:GLU:HA	2.21	0.40
1:B:2495:MET:HG3	1:B:2514:LEU:HD22	2.03	0.40
1:C:3061:GLY:HA2	7:C:3843:HOH:O	2.21	0.40
1:C:3119:LEU:C	1:C:3119:LEU:HD12	2.46	0.40
1:C:3120:ASN:HB2	1:C:3167:THR:OG1	2.21	0.40
1:C:3318:LEU:HD12	1:C:3318:LEU:C	2.46	0.40
1:B:2381:LEU:C	1:B:2383:TRP:N	2.76	0.40
1:C:3435:ARG:HD2	7:C:3738:HOH:O	2.21	0.40
1:A:1095:GLN:O	1:A:1099:GLU:HG3	2.21	0.40
1:A:1357:TRP:C	1:A:1360:PRO:HD2	2.47	0.40
1:A:1468:HIS:CD2	3:A:1601:NTJ:H1C2	2.55	0.40
1:B:2254:VAL:O	1:B:2254:VAL:HG22	2.21	0.40
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	2.03	0.40
1:C:3461:PRO:HG2	1:C:3464:VAL:CG2	2.52	0.40
1:A:1451:TYR:C	1:A:1465:ILE:HG13	2.47	0.40
1:C:3078:LYS:HG3	5:C:3604:SIA:O1A	2.21	0.40
1:A:1487:GLU:O	1:A:1491:ARG:HB2	2.21	0.40
1:C:3132:ARG:O	1:C:3211:ASN:HB2	2.22	0.40
1:C:3206:ALA:HA	1:C:3210:GLY:O	2.22	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	530/532 (100%)	493 (93%)	29 (6%)	8 (2%)	8	22
1	B	529/532 (99%)	491 (93%)	34 (6%)	4 (1%)	16	37
1	C	529/532 (99%)	505 (96%)	22 (4%)	2 (0%)	30	54
All	All	1588/1596 (100%)	1489 (94%)	85 (5%)	14 (1%)	14	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1237	LYS
1	A	1315	SER
1	B	2540	LYS
1	A	1310	GLY
1	A	1406	GLY
1	B	2368	LEU
1	B	2375	GLN
1	A	1185	SER
1	A	1253	SER
1	A	1339	ARG
1	C	3237	LYS
1	A	1375	GLN
1	C	3041	GLU
1	B	2397	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	448/448 (100%)	436 (97%)	12 (3%)	39	69
1	B	447/448 (100%)	438 (98%)	9 (2%)	48	76
1	C	447/448 (100%)	436 (98%)	11 (2%)	42	71
All	All	1342/1344 (100%)	1310 (98%)	32 (2%)	43	72

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	SER
1	A	1155	LEU
1	A	1162	ASN
1	A	1205	ILE
1	A	1218	PHE
1	A	1258	LYS
1	A	1264	LEU
1	A	1299	LEU
1	A	1317	PRO
1	A	1366	TYR
1	A	1450	GLN
1	A	1465	ILE
1	B	2027	ASP
1	B	2079	ASN
1	B	2155	LEU
1	B	2218	PHE
1	B	2220	GLU
1	B	2264	LEU
1	B	2299	LEU
1	B	2316	GLN
1	B	2505	ARG
1	C	3155	LEU
1	C	3205	ILE
1	C	3218	PHE
1	C	3220	GLU
1	C	3237	LYS
1	C	3258	LYS
1	C	3264	LEU
1	C	3299	LEU
1	C	3304	LEU
1	C	3319	LEU
1	C	3342	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1045	GLN
1	A	1069	GLN
1	A	1140	HIS
1	A	1162	ASN
1	A	1241	HIS
1	A	1309	GLN
1	A	1316	GLN
1	A	1336	GLN
1	A	1351	ASN
1	A	1353	GLN
1	A	1375	GLN
1	A	1436	ASN
1	A	1450	GLN
1	A	1532	ASN
1	A	1537	GLN
1	B	2030	HIS
1	B	2045	GLN
1	B	2069	GLN
1	B	2107	ASN
1	B	2140	HIS
1	B	2162	ASN
1	B	2202	GLN
1	B	2241	HIS
1	B	2351	ASN
1	B	2353	GLN
1	B	2372	GLN
1	B	2436	ASN
1	B	2450	GLN
1	B	2532	ASN
1	B	2537	GLN
1	C	3140	HIS
1	C	3160	HIS
1	C	3184	HIS
1	C	3241	HIS
1	C	3340	ASN
1	C	3353	GLN
1	C	3436	ASN
1	C	3450	GLN
1	C	3506	ASN
1	C	3516	HIS
1	C	3534	GLN

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Mol	Chain	Res	Type
1	C	3537	GLN
1	C	3549	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	GLC	D	1	2	11,11,12	1.48	3 (27%)	15,15,17	0.84	0
2	FRU	D	2	2	11,12,12	1.64	1 (9%)	10,18,18	1.11	0
2	GLC	E	1	2	11,11,12	1.59	3 (27%)	15,15,17	1.04	1 (6%)
2	FRU	E	2	2	11,12,12	1.68	1 (9%)	10,18,18	0.79	0
2	GLC	F	1	2	11,11,12	1.38	1 (9%)	15,15,17	0.87	1 (6%)
2	FRU	F	2	2	11,12,12	1.34	1 (9%)	10,18,18	0.95	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
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	3/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	FRU	E	2	2	-	3/5/24/24	0/1/1/1
2	GLC	F	1	2	-	2/2/19/22	0/1/1/1
2	FRU	F	2	2	-	0/5/24/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	FRU	O2-C2	5.28	1.49	1.40
2	D	2	FRU	O2-C2	5.17	1.49	1.40
2	F	2	FRU	O2-C2	4.14	1.47	1.40
2	E	1	GLC	O5-C1	3.69	1.49	1.43
2	F	1	GLC	O5-C1	3.38	1.49	1.43
2	D	1	GLC	O5-C1	3.05	1.48	1.43
2	E	1	GLC	C2-C3	2.26	1.55	1.52
2	D	1	GLC	C2-C3	2.20	1.55	1.52
2	D	1	GLC	O5-C5	2.09	1.47	1.43
2	E	1	GLC	O5-C5	2.07	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	C1-O5-C5	2.77	115.91	112.19
2	F	1	GLC	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

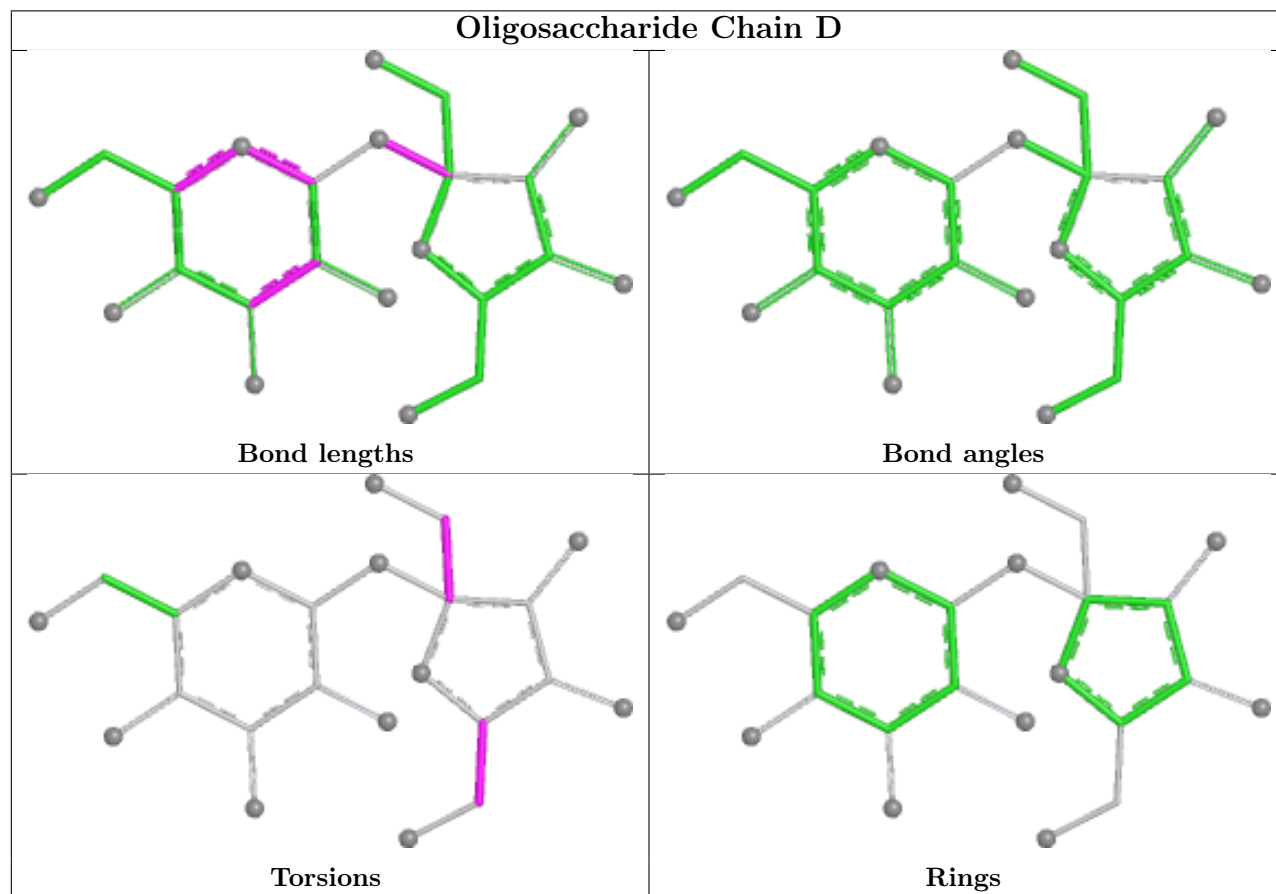
Mol	Chain	Res	Type	Atoms
2	E	2	FRU	O1-C1-C2-O2
2	E	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	D	2	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-C3
2	D	2	FRU	O5-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	D	2	FRU	O1-C1-C2-O2
2	E	2	FRU	O1-C1-C2-O5

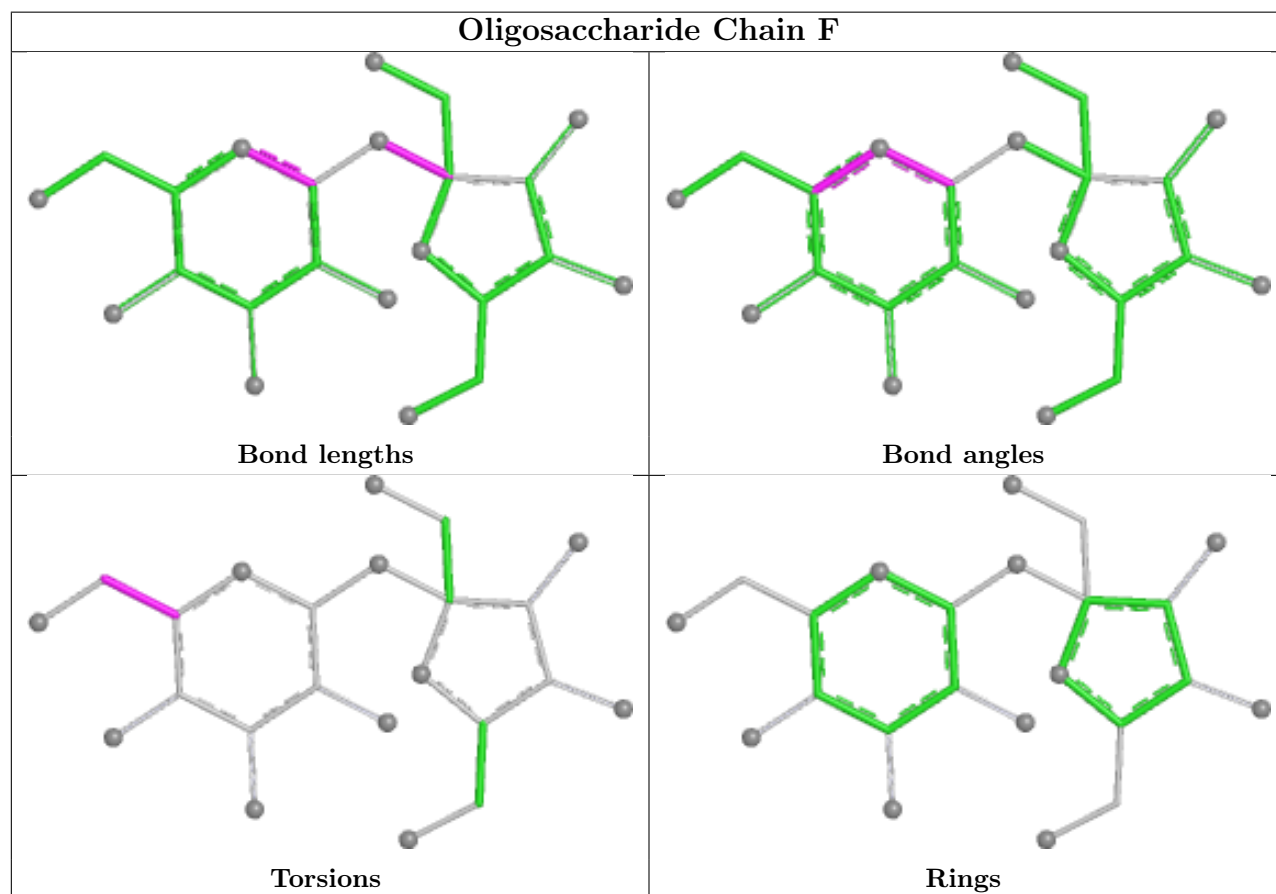
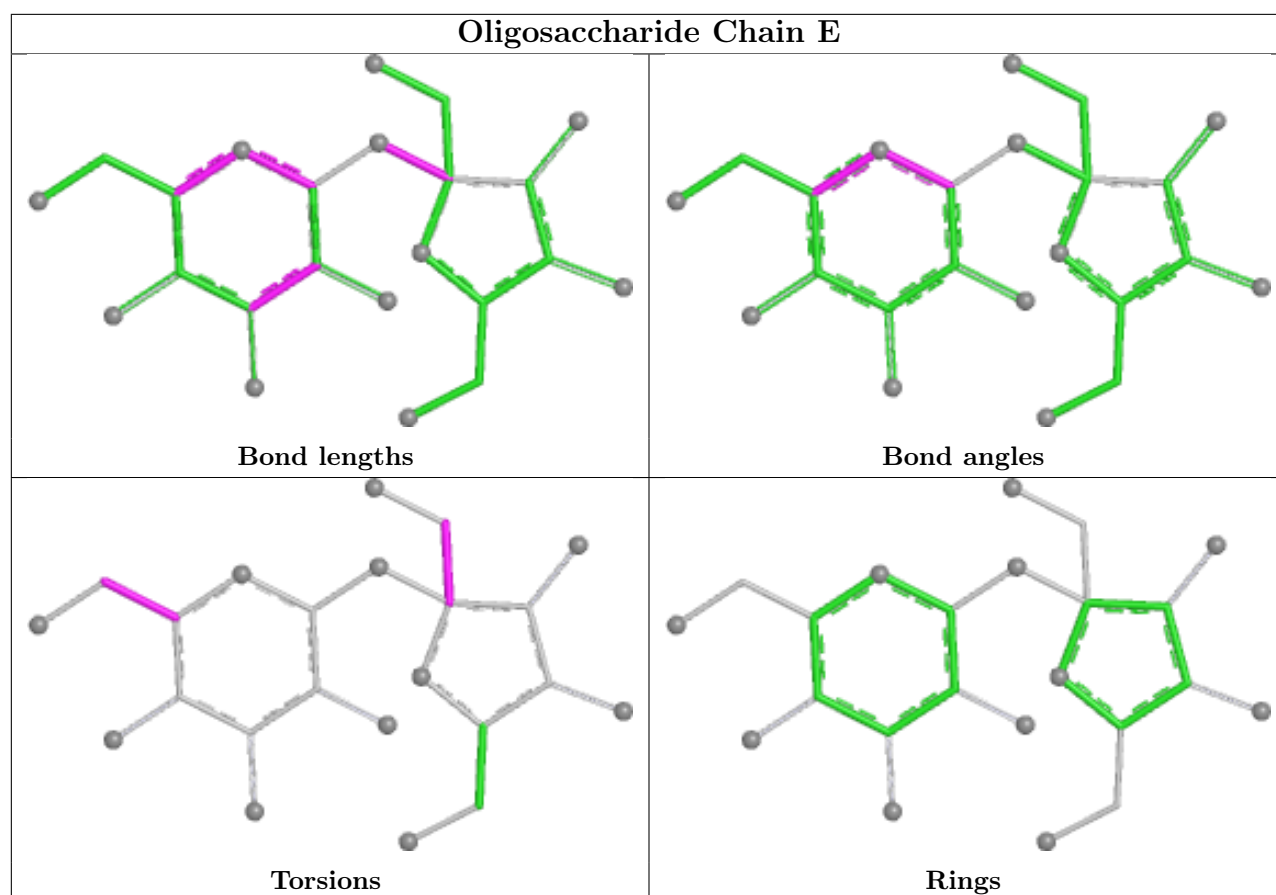
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	1	0
2	E	2	FRU	1	0
2	F	1	GLC	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

14 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
3	NTJ	C	3601	1	4,7,7	1.37	0	4,8,8	2.33	3 (75%)
4	NAG	B	2602	1	14,14,15	0.55	0	17,19,21	0.69	1 (5%)
3	NTJ	A	1601	1	4,7,7	1.31	0	4,8,8	2.34	3 (75%)
4	NAG	C	3603	1	14,14,15	0.71	0	17,19,21	0.73	0
5	SIA	A	1603	-	21,21,21	1.03	0	24,31,31	1.07	2 (8%)
6	SO4	B	2604	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	C	3605	-	4,4,4	0.36	0	6,6,6	0.07	0
3	NTJ	B	2601	1	4,7,7	1.24	0	4,8,8	2.39	3 (75%)
6	SO4	A	1605	-	4,4,4	0.36	0	6,6,6	0.10	0
6	SO4	C	3602	-	4,4,4	0.38	0	6,6,6	0.07	0
6	SO4	A	1604	-	4,4,4	0.36	0	6,6,6	0.08	0
5	SIA	B	2603	-	21,21,21	0.96	1 (4%)	24,31,31	1.19	3 (12%)
5	SIA	C	3604	-	21,21,21	0.80	0	24,31,31	1.10	2 (8%)
4	NAG	A	1602	1	14,14,15	0.64	0	17,19,21	0.90	1 (5%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NTJ	C	3601	1	-	0/1/7/7	-
4	NAG	B	2602	1	-	2/6/23/26	0/1/1/1
3	NTJ	A	1601	1	-	0/1/7/7	-
4	NAG	C	3603	1	-	2/6/23/26	0/1/1/1
5	SIA	A	1603	-	-	13/20/38/38	0/1/1/1
3	NTJ	B	2601	1	-	0/1/7/7	-
5	SIA	B	2603	-	-	8/20/38/38	0/1/1/1
5	SIA	C	3604	-	-	15/20/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1602	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2603	SIA	C7-C6	2.15	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2603	SIA	O6-C6-C7	3.10	111.49	106.65
5	A	1603	SIA	O1A-C1-C2	-3.05	118.76	123.85
3	B	2601	NTJ	C1-N1-C2	-2.97	108.88	113.60
5	B	2603	SIA	O1A-C1-C2	-2.97	118.90	123.85
5	C	3604	SIA	O1A-C1-C2	-2.95	118.92	123.85
5	C	3604	SIA	O6-C6-C7	2.88	111.15	106.65
3	C	3601	NTJ	C1-N1-C2	-2.88	109.03	113.60
3	A	1601	NTJ	C1-N1-C2	-2.82	109.12	113.60
3	A	1601	NTJ	P1-N1-C2	-2.73	108.97	121.78
3	B	2601	NTJ	P1-N1-C2	-2.64	109.41	121.78
3	B	2601	NTJ	P1-N1-C1	-2.64	109.41	121.78
3	C	3601	NTJ	P1-N1-C2	-2.62	109.51	121.78
3	C	3601	NTJ	P1-N1-C1	-2.57	109.76	121.78
3	A	1601	NTJ	P1-N1-C1	-2.52	109.97	121.78
5	A	1603	SIA	O6-C6-C7	2.22	110.12	106.65
4	A	1602	NAG	O5-C1-C2	-2.06	108.10	111.29
4	B	2602	NAG	C2-N2-C7	-2.05	120.16	122.90
5	B	2603	SIA	C3-C2-C1	-2.02	109.08	112.84

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1602	NAG	C3-C2-N2-C7
4	A	1602	NAG	C8-C7-N2-C2
4	A	1602	NAG	O7-C7-N2-C2
4	B	2602	NAG	C8-C7-N2-C2
4	B	2602	NAG	O7-C7-N2-C2
5	A	1603	SIA	C5-C6-C7-C8
5	A	1603	SIA	C5-C6-C7-O7
5	A	1603	SIA	O6-C6-C7-C8

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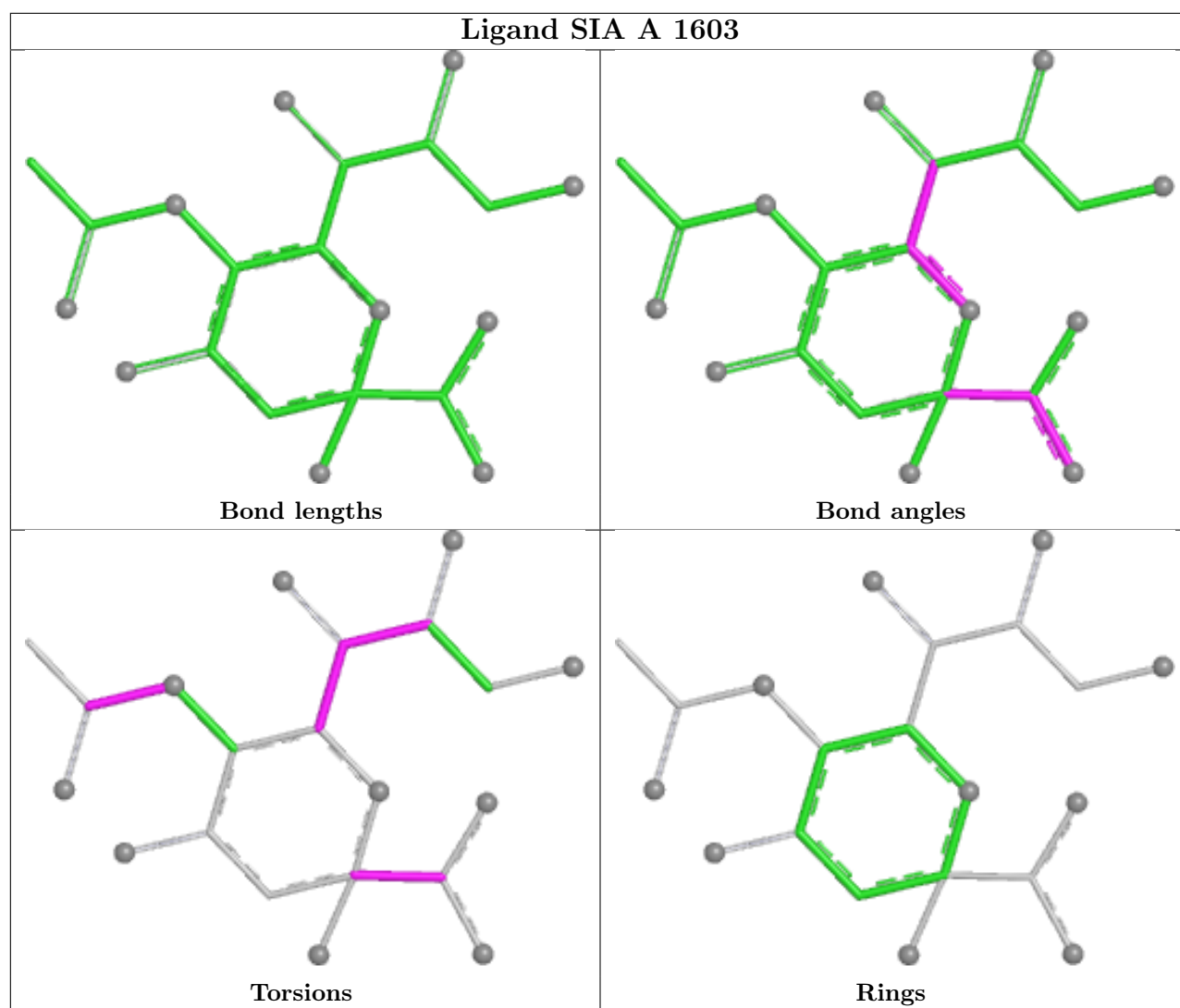
Mol	Chain	Res	Type	Atoms
5	A	1603	SIA	O6-C6-C7-O7
5	A	1603	SIA	C6-C7-C8-C9
5	A	1603	SIA	C6-C7-C8-O8
5	A	1603	SIA	O7-C7-C8-C9
5	A	1603	SIA	O7-C7-C8-O8
5	A	1603	SIA	C11-C10-N5-C5
5	A	1603	SIA	O10-C10-N5-C5
5	B	2603	SIA	C4-C5-N5-C10
5	B	2603	SIA	C5-C6-C7-C8
5	B	2603	SIA	C5-C6-C7-O7
5	B	2603	SIA	O6-C6-C7-C8
5	B	2603	SIA	O6-C6-C7-O7
5	B	2603	SIA	C11-C10-N5-C5
5	B	2603	SIA	O10-C10-N5-C5
5	C	3604	SIA	O1A-C1-C2-O2
5	C	3604	SIA	O1B-C1-C2-O2
5	C	3604	SIA	C5-C6-C7-C8
5	C	3604	SIA	O6-C6-C7-C8
5	C	3604	SIA	C11-C10-N5-C5
5	C	3604	SIA	O10-C10-N5-C5
4	C	3603	NAG	C8-C7-N2-C2
4	A	1602	NAG	O5-C5-C6-O6
5	C	3604	SIA	O7-C7-C8-C9
4	A	1602	NAG	C4-C5-C6-O6
4	C	3603	NAG	O7-C7-N2-C2
5	C	3604	SIA	C6-C7-C8-C9
5	C	3604	SIA	O7-C7-C8-O8
5	C	3604	SIA	C6-C7-C8-O8
5	C	3604	SIA	C7-C8-C9-O9
5	C	3604	SIA	O8-C8-C9-O9
5	C	3604	SIA	C5-C6-C7-O7
5	A	1603	SIA	O1A-C1-C2-O6
5	A	1603	SIA	O1B-C1-C2-O2
5	A	1603	SIA	O1B-C1-C2-O6
5	C	3604	SIA	O1B-C1-C2-O6
5	C	3604	SIA	C4-C5-N5-C10
5	B	2603	SIA	C6-C5-N5-C10

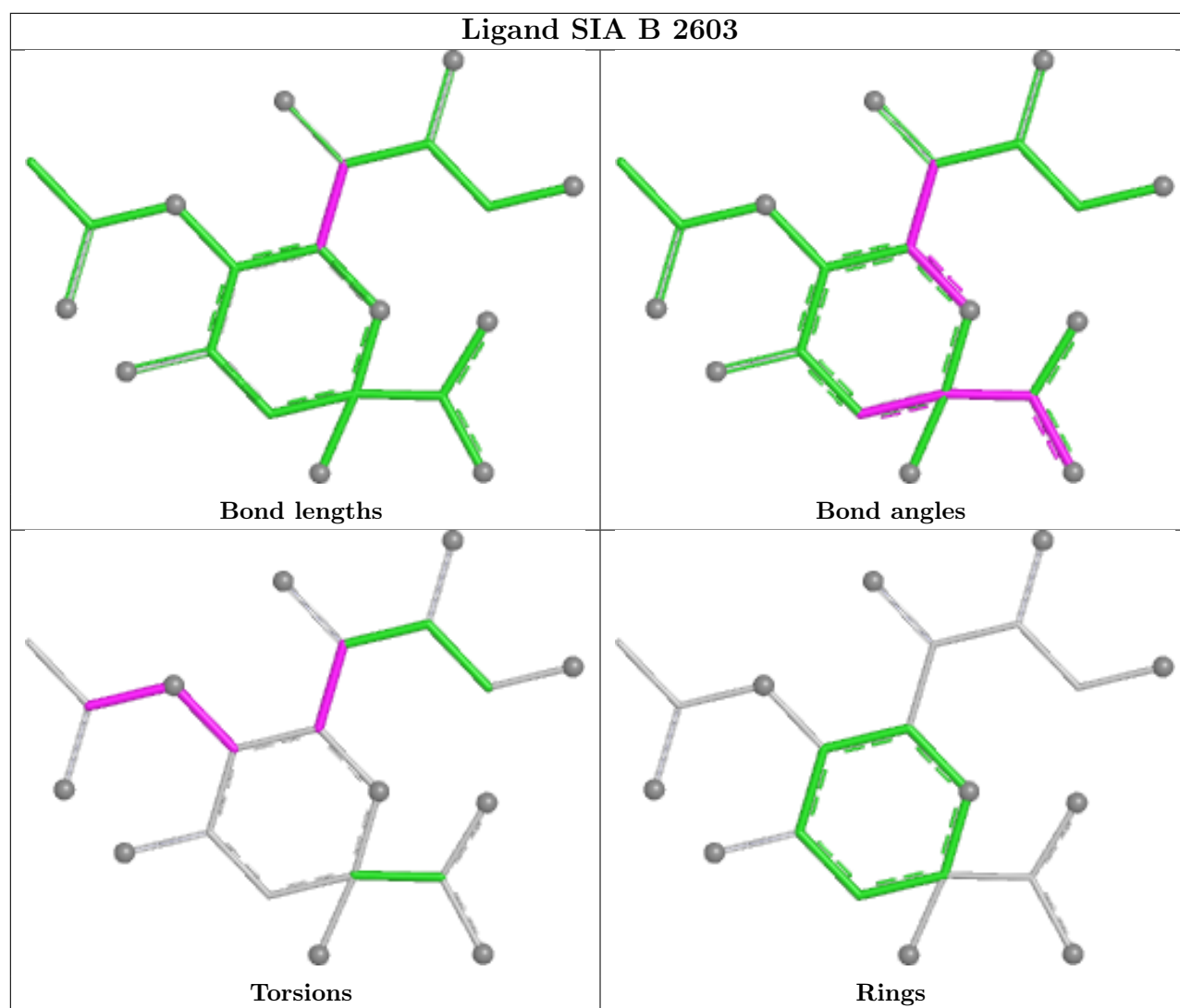
There are no ring outliers.

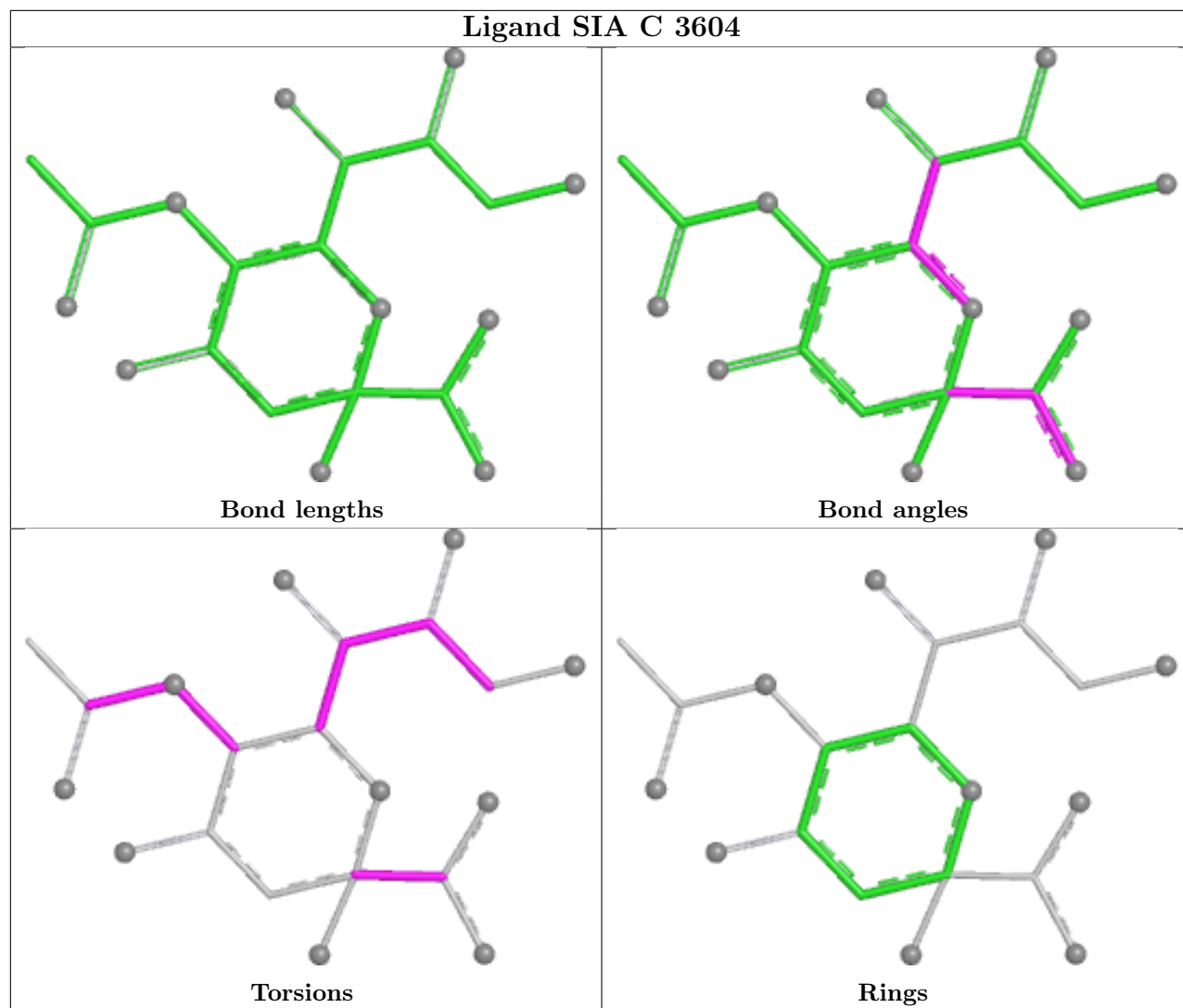
8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2602	NAG	1	0
3	A	1601	NTJ	1	0
5	A	1603	SIA	3	0
6	A	1605	SO4	1	0
6	C	3602	SO4	1	0
6	A	1604	SO4	2	0
5	B	2603	SIA	6	0
5	C	3604	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	532/532 (100%)	-0.30	11 (2%) 63 61	6, 23, 67, 86	0
1	B	531/532 (99%)	-0.24	9 (1%) 69 67	6, 28, 69, 83	0
1	C	531/532 (99%)	-0.47	4 (0%) 82 81	3, 21, 45, 79	0
All	All	1594/1596 (99%)	-0.33	24 (1%) 72 70	3, 24, 64, 86	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2342	HIS	3.8
1	A	1342	HIS	3.7
1	A	1370	GLU	3.5
1	C	3342	HIS	3.3
1	A	1341	PHE	3.1
1	A	1371	GLY	3.0
1	A	1307	ASP	2.8
1	B	2371	GLY	2.8
1	A	1316	GLN	2.5
1	C	3340	ASN	2.4
1	B	2406	GLY	2.4
1	B	2409	ASP	2.4
1	B	2407	THR	2.3
1	A	1459	MET	2.3
1	B	2310	GLY	2.3
1	C	3341	PHE	2.3
1	A	1406	GLY	2.2
1	A	1409	ASP	2.2
1	C	3027	ASP	2.2
1	A	1315	SER	2.2
1	A	1407	THR	2.0
1	B	2340	ASN	2.0
1	B	2411	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	2398	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

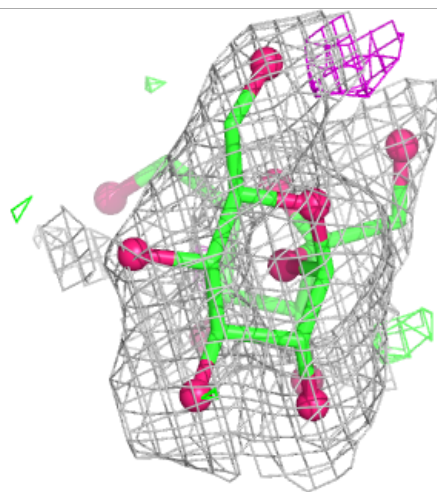
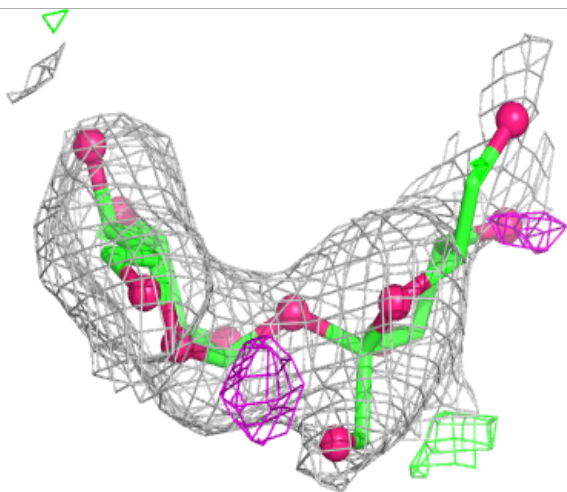
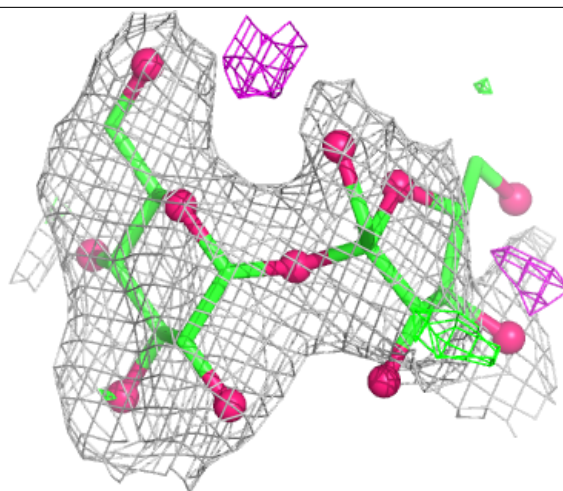
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	D	2	12/12	0.75	0.17	59,64,67,70	0
2	FRU	E	2	12/12	0.85	0.11	58,60,61,62	0
2	GLC	E	1	11/12	0.88	0.11	61,62,63,64	0
2	GLC	D	1	11/12	0.89	0.11	47,51,52,54	0
2	FRU	F	2	12/12	0.92	0.10	31,33,35,38	0
2	GLC	F	1	11/12	0.96	0.07	26,29,32,38	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

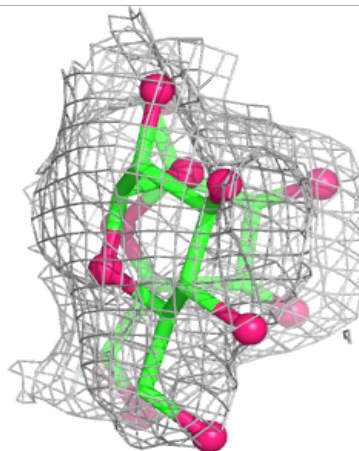
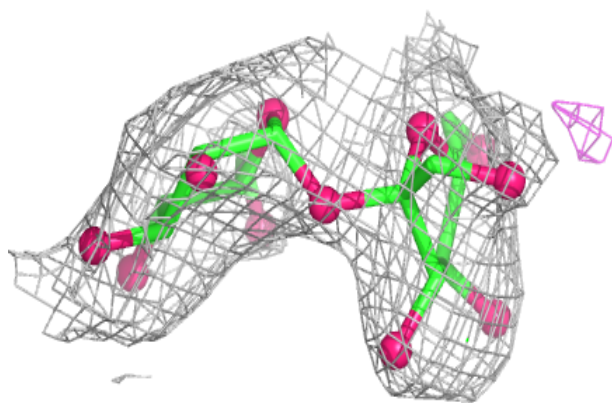
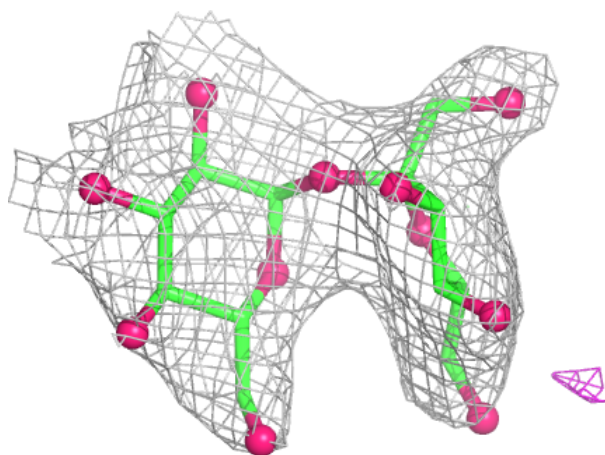
Electron density around Chain D:

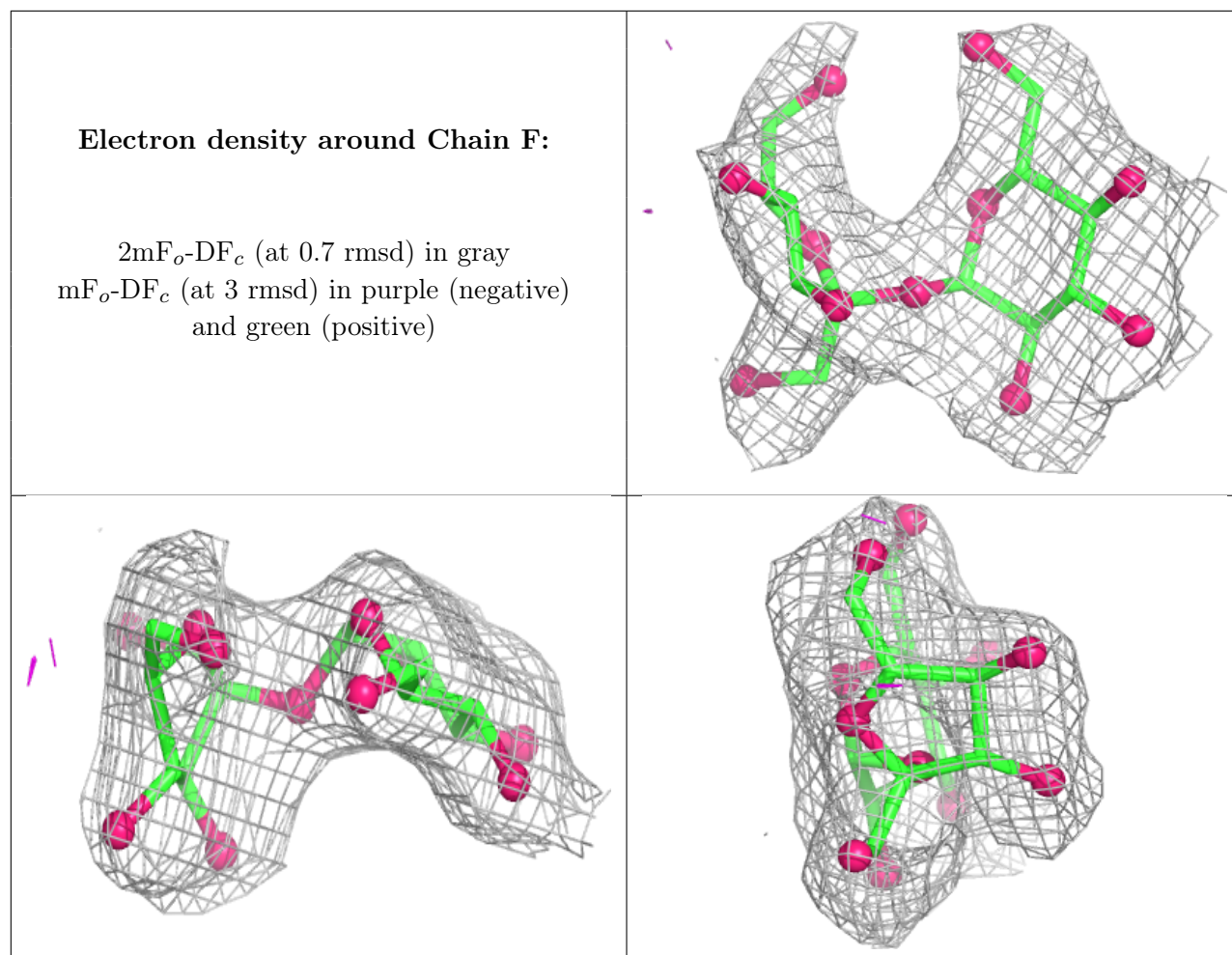
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

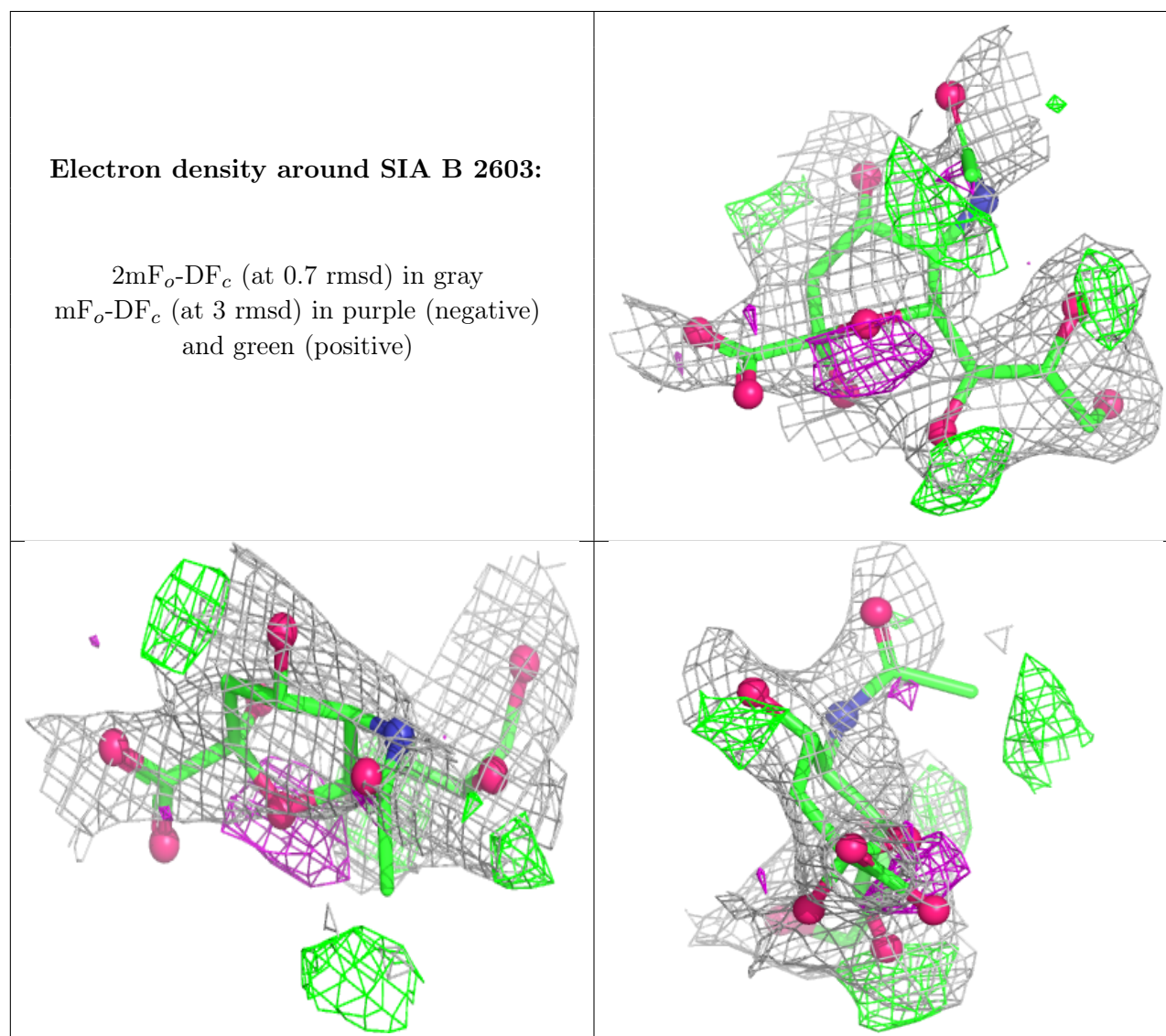
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1602	14/15	0.34	0.26	55,59,62,62	0
4	NAG	B	2602	14/15	0.73	0.14	64,69,71,71	0
5	SIA	B	2603	21/21	0.74	0.19	42,61,65,66	0
5	SIA	C	3604	21/21	0.78	0.24	75,79,83,85	0
4	NAG	C	3603	14/15	0.79	0.17	61,66,69,69	0
6	SO4	A	1605	5/5	0.79	0.21	144,144,144,144	0
5	SIA	A	1603	21/21	0.80	0.19	72,83,88,89	0
6	SO4	C	3602	5/5	0.83	0.29	165,166,166,166	0
6	SO4	B	2604	5/5	0.87	0.24	149,149,149,149	0
6	SO4	C	3605	5/5	0.91	0.22	140,140,141,141	0

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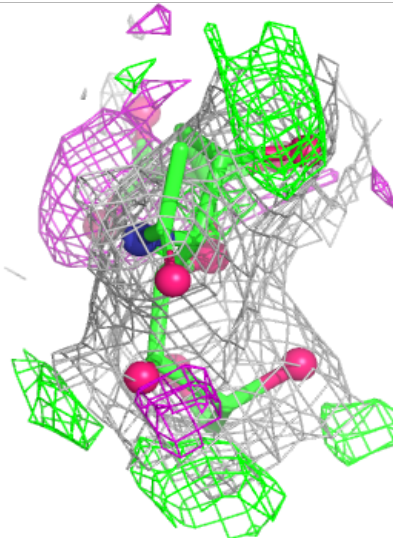
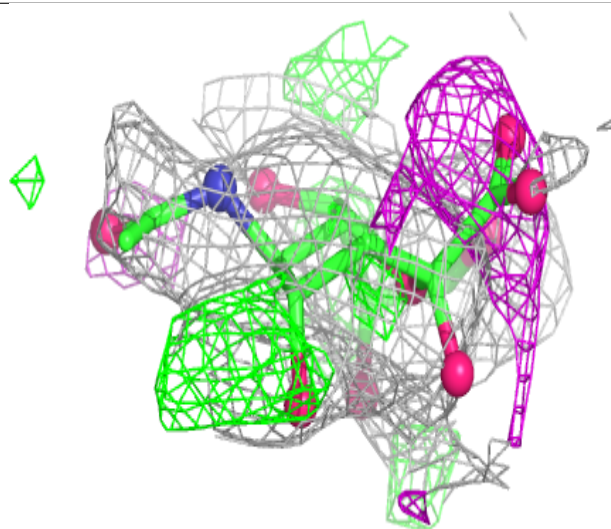
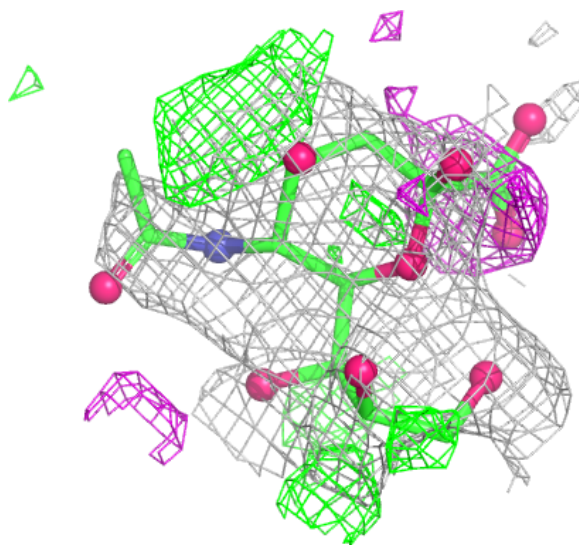
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	1604	5/5	0.92	0.18	147,147,147,148	0
3	NTJ	C	3601	8/8	0.96	0.11	36,40,42,45	0
3	NTJ	A	1601	8/8	0.97	0.10	38,39,42,43	0
3	NTJ	B	2601	8/8	0.97	0.10	39,39,41,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



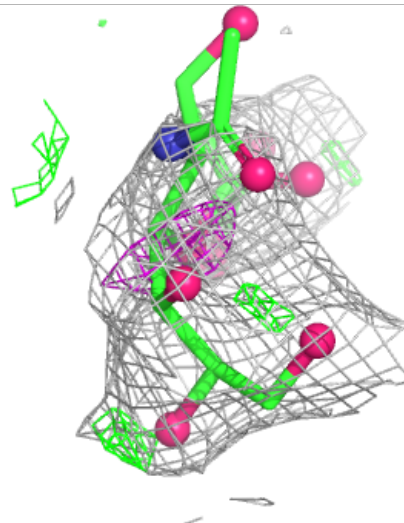
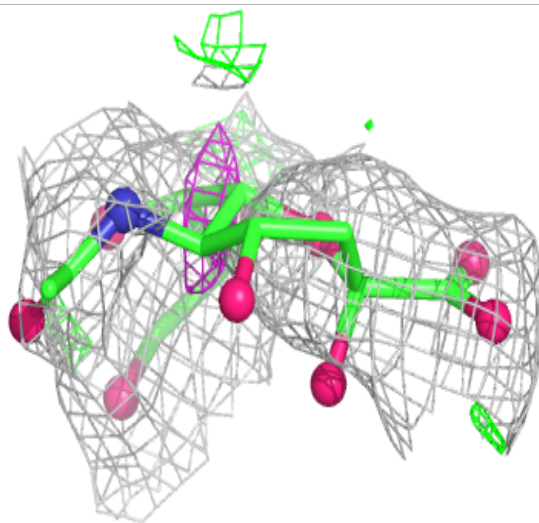
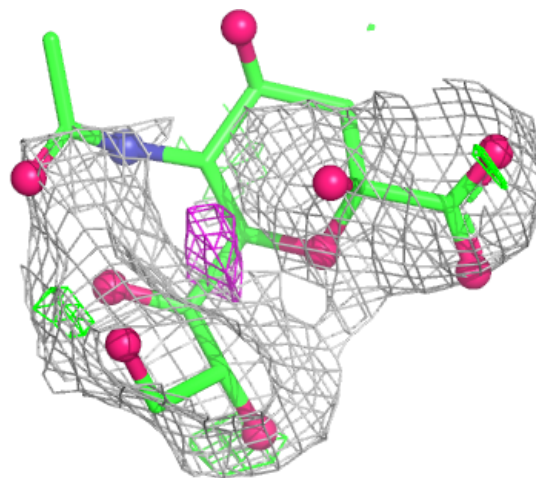
Electron density around SIA C 3604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SIA A 1603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.