



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 09:30 PM EST

PDB ID : 4DJ8
Title : Structure of the hemagglutinin complexed with 6SLN from a highly pathogenic H7N7 influenza virus
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on : 2012-02-01
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

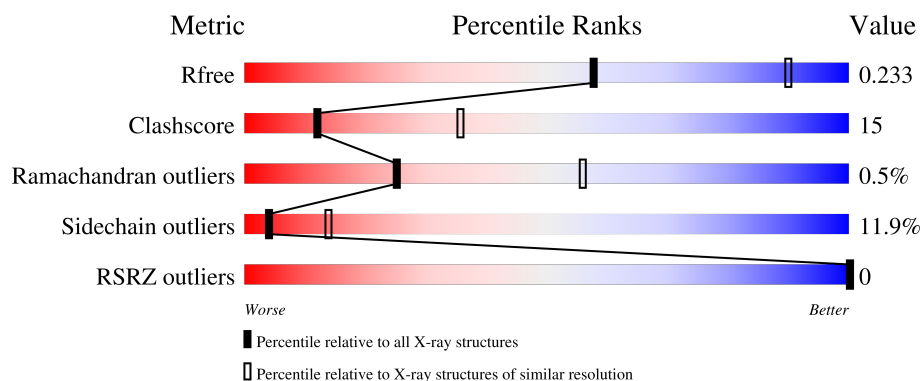
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	327	
1	C	327	
1	E	327	
2	B	177	
2	D	177	

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Mol	Chain	Length	Quality of chain
2	F	177	<div><div></div><div>66%</div><div>25%</div><div>• • 5%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11749 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	4	0	0
			2422	1502	435	471	14			
1	C	316	Total	C	N	O	S	4	0	0
			2422	1502	435	471	14			
1	E	317	Total	C	N	O	S	3	1	0
			2437	1510	440	473	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q6VMK1
A	-2	ASP	-	expression tag	UNP Q6VMK1
A	-1	PRO	-	expression tag	UNP Q6VMK1
A	0	GLY	-	expression tag	UNP Q6VMK1
C	-3	ALA	-	expression tag	UNP Q6VMK1
C	-2	ASP	-	expression tag	UNP Q6VMK1
C	-1	PRO	-	expression tag	UNP Q6VMK1
C	0	GLY	-	expression tag	UNP Q6VMK1
E	-3	ALA	-	expression tag	UNP Q6VMK1
E	-2	ASP	-	expression tag	UNP Q6VMK1
E	-1	PRO	-	expression tag	UNP Q6VMK1
E	0	GLY	-	expression tag	UNP Q6VMK1

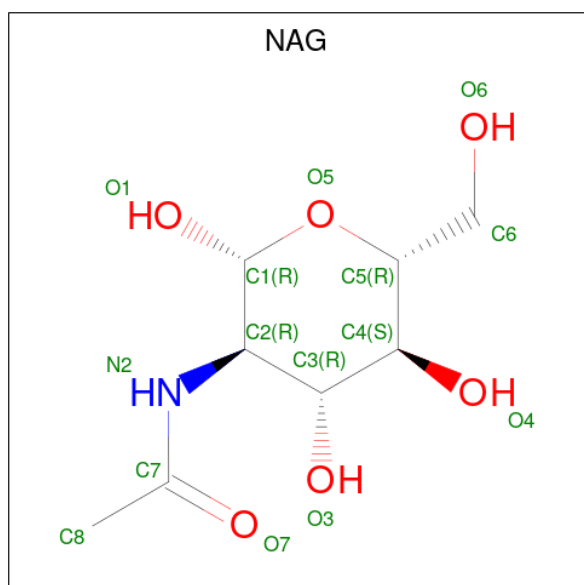
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	4	0	0
			1380	851	243	279	7			
2	D	171	Total	C	N	O	S	0	0	0
			1388	857	244	280	7			
2	F	169	Total	C	N	O	S	0	0	0
			1369	845	239	278	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6VMK1
B	176	GLY	-	expression tag	UNP Q6VMK1
B	177	ARG	-	expression tag	UNP Q6VMK1
D	175	SER	-	expression tag	UNP Q6VMK1
D	176	GLY	-	expression tag	UNP Q6VMK1
D	177	ARG	-	expression tag	UNP Q6VMK1
F	175	SER	-	expression tag	UNP Q6VMK1
F	176	GLY	-	expression tag	UNP Q6VMK1
F	177	ARG	-	expression tag	UNP Q6VMK1

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



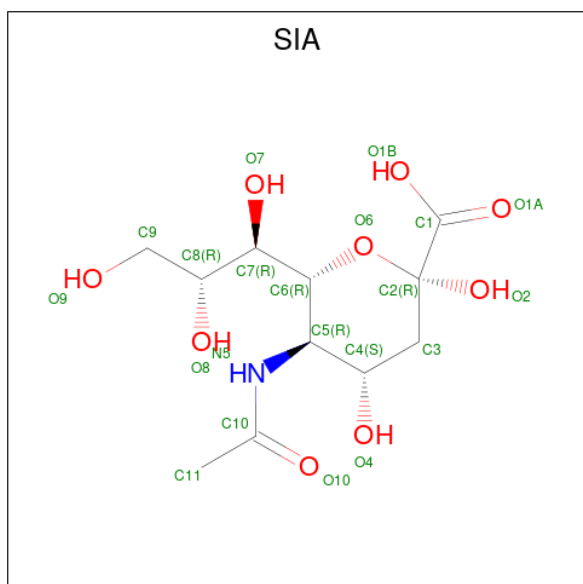
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- 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
4	A	1	Total	C	N	O	0	0
			20	11	1	8		
4	C	1	Total	C	N	O	0	0
			20	11	1	8		
4	E	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 5 is water.

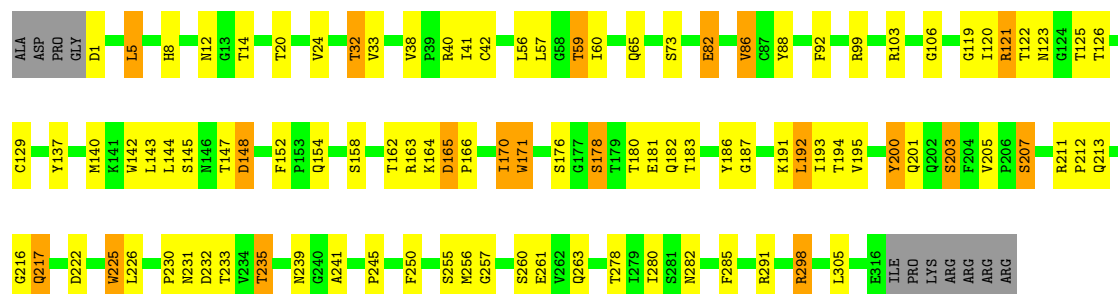
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	14	Total 14	O 14	0	0
5	C	25	Total 25	O 25	0	0
5	D	11	Total 11	O 11	0	0
5	E	18	Total 18	O 18	0	0
5	F	13	Total 13	O 13	0	0

3 Residue-property plots

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

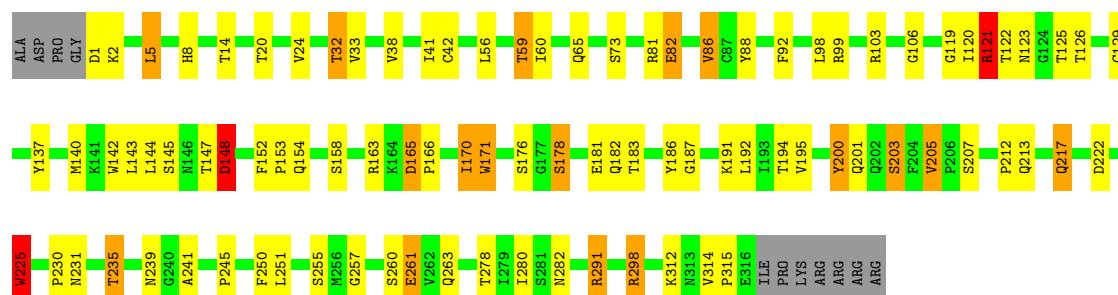
• Molecule 1: Hemagglutinin

Chain A: 



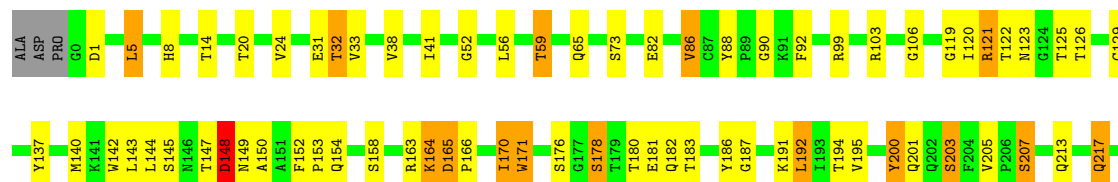
• Molecule 1: Hemagglutinin

Chain C: 



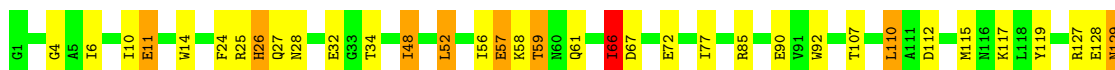
• Molecule 1: Hemagglutinin

Chain E: 

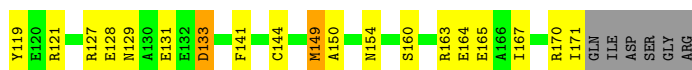
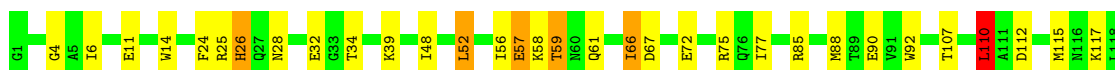




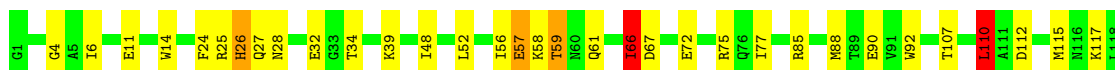
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.77Å 117.60Å 120.46Å 90.00° 124.15° 90.00°	Depositor
Resolution (Å)	48.23 – 2.80 48.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.23-2.80) 99.2 (48.23-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.235 0.190 , 0.233	Depositor DCC
R_{free} test set	2934 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2* *h+1/2*k 0.000 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1 /2*h+1/2*k-l 0.010 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1 /2*h-1/2*k-l 0.003 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1 /2*h-1/2*k 0.000 for -h-k-l,l,k 0.013 for -h+k-l,-l,-k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2* *h-1/2*k 0.012 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1 /2*h+1/2*k 0.438 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.448 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l 0.010 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.91	4/2468 (0.2%)	0.93	2/3337 (0.1%)
1	C	0.99	8/2468 (0.3%)	1.04	8/3337 (0.2%)
1	E	0.96	4/2483 (0.2%)	0.93	3/3356 (0.1%)
2	B	0.87	1/1404 (0.1%)	0.85	1/1892 (0.1%)
2	D	0.87	1/1412 (0.1%)	0.86	1/1903 (0.1%)
2	F	0.90	1/1393 (0.1%)	0.84	1/1878 (0.1%)
All	All	0.93	19/11628 (0.2%)	0.93	16/15703 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
All	All	0	2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	164	LYS	CG-CD	-11.97	1.11	1.52
1	C	148	ASP	CA-CB	-10.29	1.31	1.53
1	C	225	TRP	CD2-CE2	10.07	1.53	1.41
1	C	148	ASP	CB-CG	7.50	1.67	1.51
1	E	171	TRP	CD2-CE2	7.07	1.49	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ASP	CB-CG-OD2	-15.69	104.18	118.30
1	C	225	TRP	CE2-CD2-CG	-12.13	97.60	107.30
1	C	148	ASP	CB-CG-OD1	12.03	129.13	118.30
1	C	225	TRP	CG-CD2-CE3	8.81	141.83	133.90
1	E	148	ASP	C-N-CA	7.57	140.62	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	66	ILE	Peptide
2	F	66	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2422	0	2369	80	0
1	C	2422	0	2369	81	0
1	E	2437	0	2384	72	0
2	B	1380	0	1283	54	0
2	D	1388	0	1294	51	0
2	F	1369	0	1270	52	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
3	D	14	0	13	2	0
3	E	42	0	39	0	0
3	F	14	0	13	2	0
4	A	20	0	17	0	0
4	C	20	0	17	0	0
4	E	20	0	17	0	0
5	A	22	0	0	3	0
5	B	14	0	0	1	0
5	C	25	0	0	4	0
5	D	11	0	0	1	0
5	E	18	0	0	0	0
5	F	13	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11749	0	11176	351	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 15.

The worst 5 of 351 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:98:LEU:HD13	1:C:225:TRP:CE3	1.79	1.17
1:C:98:LEU:HD13	1:C:225:TRP:HE3	1.13	1.07
2:B:165:GLU:HG2	5:B:313:HOH:O	1.59	1.02
2:B:59:THR:HG23	2:B:61:GLN:H	1.21	1.02
1:C:225:TRP:O	1:C:225:TRP:CD1	2.12	1.01

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	314/327 (96%)	287 (91%)	26 (8%)	1 (0%)	37	67
1	C	314/327 (96%)	285 (91%)	28 (9%)	1 (0%)	37	67
1	E	316/327 (97%)	288 (91%)	26 (8%)	2 (1%)	22	51
2	B	168/177 (95%)	158 (94%)	9 (5%)	1 (1%)	22	51
2	D	169/177 (96%)	157 (93%)	11 (6%)	1 (1%)	22	51
2	F	167/177 (94%)	155 (93%)	11 (7%)	1 (1%)	22	51
All	All	1448/1512 (96%)	1330 (92%)	111 (8%)	7 (0%)	25	56

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	127	ARG
1	C	148	ASP
1	A	148	ASP
2	B	127	ARG
1	E	150	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/277 (97%)	236 (88%)	32 (12%)	4	14
1	C	268/277 (97%)	234 (87%)	34 (13%)	3	12
1	E	269/277 (97%)	235 (87%)	34 (13%)	3	12
2	B	145/151 (96%)	131 (90%)	14 (10%)	6	21
2	D	146/151 (97%)	129 (88%)	17 (12%)	4	15
2	F	144/151 (95%)	128 (89%)	16 (11%)	5	16
All	All	1240/1284 (97%)	1093 (88%)	147 (12%)	4	14

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	165	ASP
2	F	129	ASN
1	E	180	THR
1	E	312	LYS
1	C	14	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	NAG	B	201	2	14,14,15	0.60	0	17,19,21	2.20	5 (29%)
3	NAG	E	401	1	14,14,15	0.64	0	17,19,21	1.53	3 (17%)
3	NAG	A	402	1	14,14,15	0.51	0	17,19,21	2.56	5 (29%)
3	NAG	A	401	1	14,14,15	0.47	0	17,19,21	1.10	1 (5%)
3	NAG	C	402	1	14,14,15	0.53	0	17,19,21	2.29	4 (23%)
4	SIA	C	404	-	20,20,21	1.16	2 (10%)	21,28,31	2.21	9 (42%)
4	SIA	E	404	-	20,20,21	1.20	1 (5%)	21,28,31	2.07	7 (33%)
3	NAG	D	201	2	14,14,15	0.59	0	17,19,21	2.08	5 (29%)
3	NAG	C	403	1	14,14,15	0.57	0	17,19,21	1.52	5 (29%)
3	NAG	E	403	1	14,14,15	0.50	0	17,19,21	1.17	1 (5%)
3	NAG	A	403	1	14,14,15	0.68	0	17,19,21	1.97	3 (17%)
4	SIA	A	404	-	20,20,21	1.16	1 (5%)	21,28,31	1.90	4 (19%)
3	NAG	F	201	2	14,14,15	0.73	1 (7%)	17,19,21	1.86	4 (23%)
3	NAG	E	402	1	14,14,15	0.53	0	17,19,21	2.24	3 (17%)
3	NAG	C	401	1	14,14,15	0.50	0	17,19,21	2.11	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
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
4	SIA	C	404	-	-	5/18/34/38	0/1/1/1
4	SIA	E	404	-	-	5/18/34/38	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	C	403	1	-	2/6/23/26	0/1/1/1
3	NAG	E	403	1	-	2/6/23/26	0/1/1/1
3	NAG	A	403	1	-	3/6/23/26	0/1/1/1
4	SIA	A	404	-	-	4/18/34/38	0/1/1/1
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	404	SIA	C7-C6	3.36	1.57	1.52
4	A	404	SIA	C7-C6	3.26	1.57	1.52
4	C	404	SIA	C7-C6	2.93	1.56	1.52
4	C	404	SIA	C8-C7	2.08	1.57	1.53
3	F	201	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	C1-O5-C5	7.59	122.35	112.19
3	E	402	NAG	C1-O5-C5	7.27	121.94	112.19
3	C	402	NAG	C1-O5-C5	7.08	121.68	112.19
3	B	201	NAG	C1-O5-C5	6.60	121.03	112.19
3	D	201	NAG	C1-O5-C5	5.28	119.26	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	SIA	O8-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
4	A	404	SIA	C11-C10-N5-C5
4	A	404	SIA	O10-C10-N5-C5
4	C	404	SIA	C7-C8-C9-O9
4	C	404	SIA	O8-C8-C9-O9

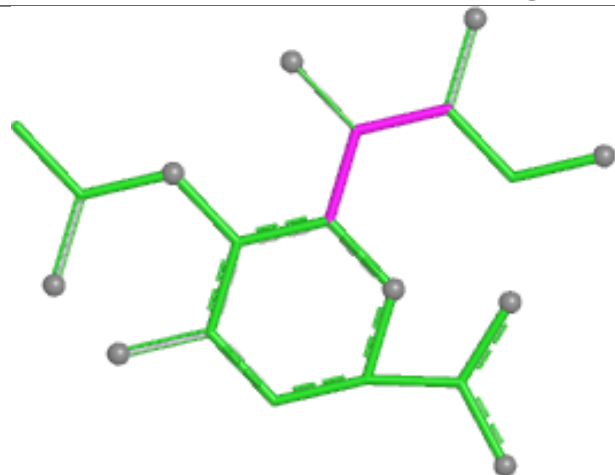
There are no ring outliers.

2 monomers are involved in 4 short contacts:

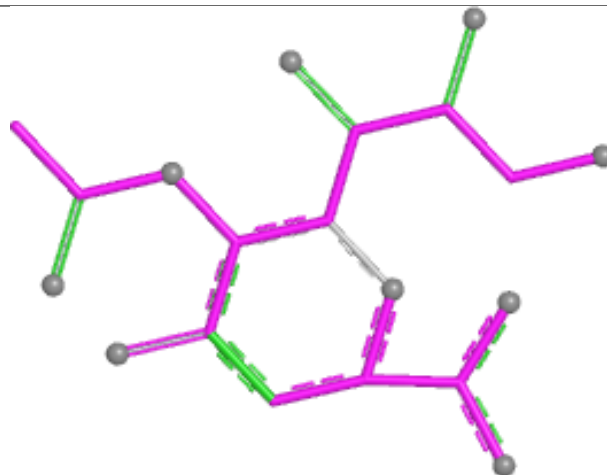
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	NAG	2	0
3	F	201	NAG	2	0

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

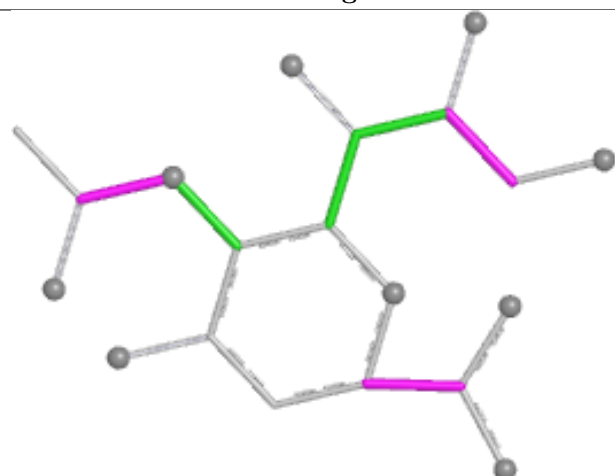
Ligand SIA C 404



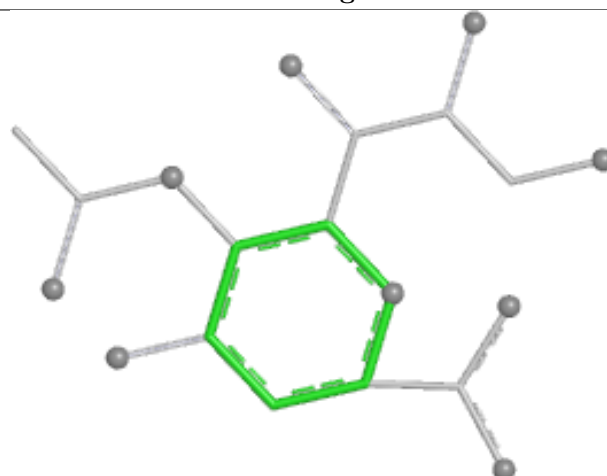
Bond lengths



Bond angles

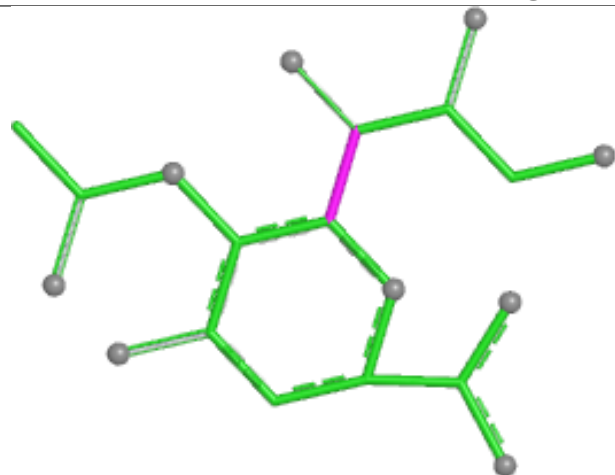


Torsions

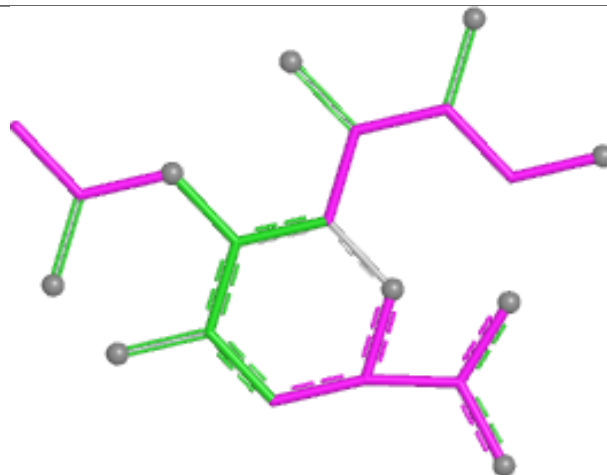


Rings

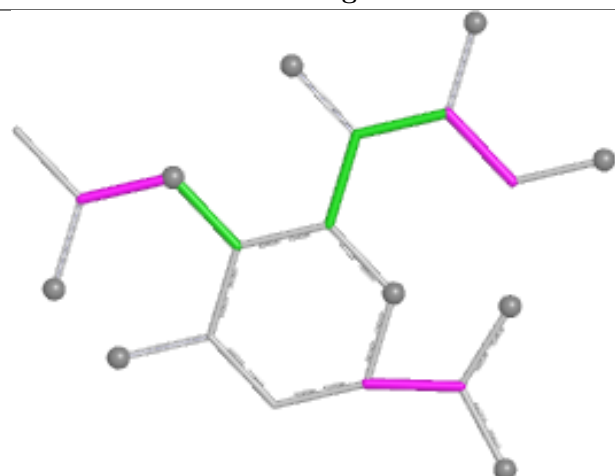
Ligand SIA E 404



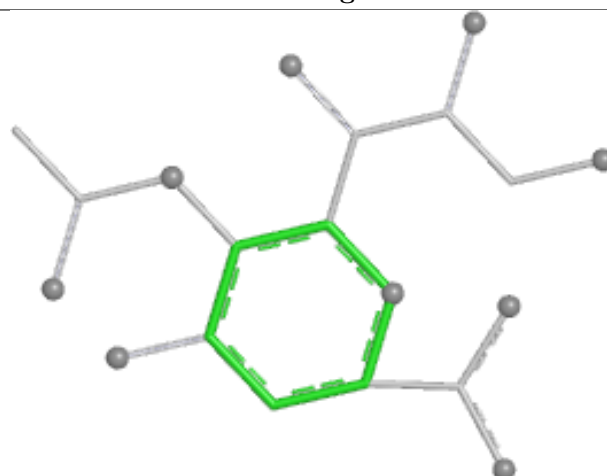
Bond lengths



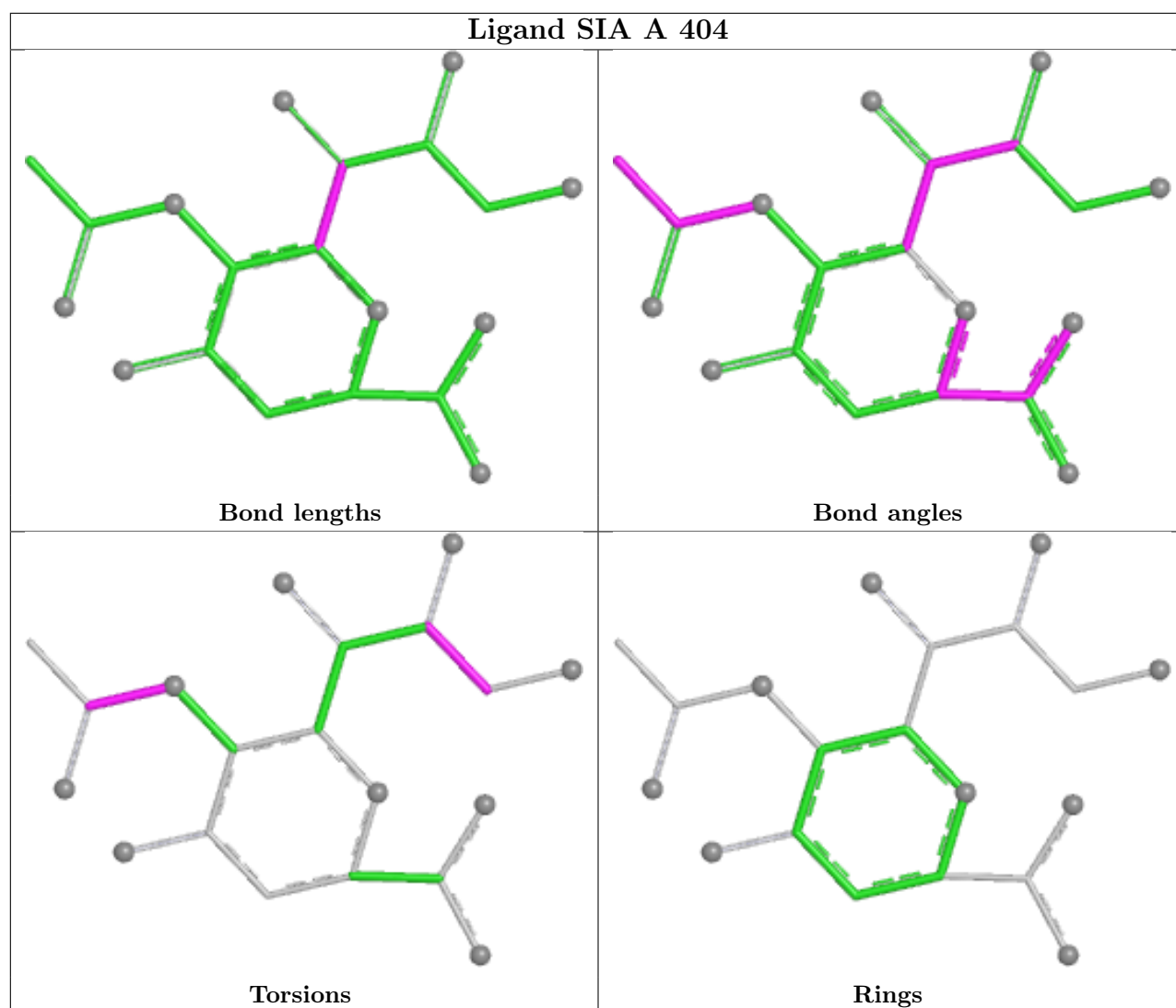
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	316/327 (96%)	-1.43	0 100 100	19, 46, 88, 114	1 (0%)
1	C	316/327 (96%)	-1.44	0 100 100	19, 47, 89, 112	3 (0%)
1	E	317/327 (96%)	-1.50	0 100 100	18, 44, 86, 115	3 (0%)
2	B	170/177 (96%)	-1.03	0 100 100	17, 64, 107, 118	1 (0%)
2	D	171/177 (96%)	-1.04	0 100 100	17, 64, 106, 118	0
2	F	169/177 (95%)	-1.02	0 100 100	18, 62, 108, 113	0
All	All	1459/1512 (96%)	-1.31	0 100 100	17, 52, 98, 118	8 (0%)

There are no RSRZ outliers to report.

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](#)

There are no monosaccharides in this entry.

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
3	NAG	C	403	14/15	0.94	0.08	103,126,148,157	0

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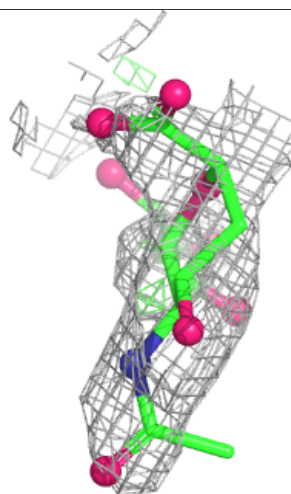
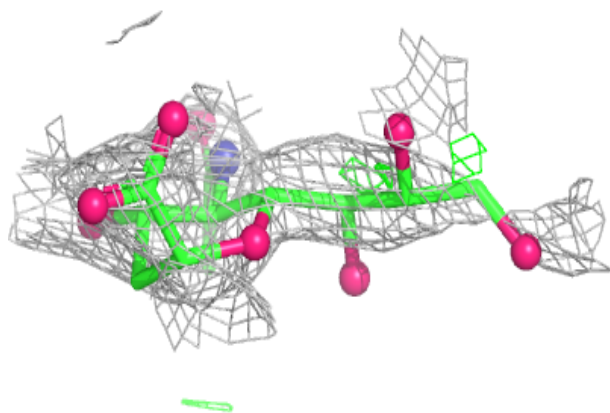
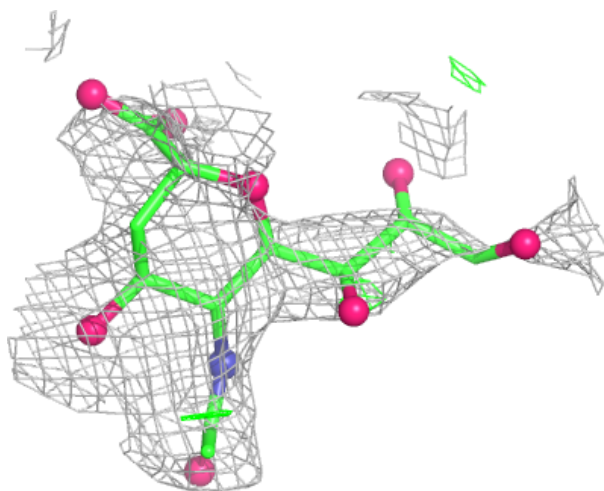
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	403	14/15	0.94	0.08	96,128,156,157	0
3	NAG	A	401	14/15	0.95	0.09	103,123,143,145	0
3	NAG	A	403	14/15	0.96	0.07	92,129,157,166	0
3	NAG	E	402	14/15	0.96	0.11	84,121,148,151	0
3	NAG	C	401	14/15	0.96	0.09	98,123,145,154	0
3	NAG	E	401	14/15	0.97	0.07	94,114,131,138	0
3	NAG	C	402	14/15	0.97	0.08	83,114,141,143	0
3	NAG	A	402	14/15	0.97	0.08	76,118,143,150	0
3	NAG	D	201	14/15	0.98	0.06	61,83,94,97	0
3	NAG	B	201	14/15	0.98	0.05	57,74,98,107	0
4	SIA	A	404	20/21	0.98	0.10	119,147,190,237	0
4	SIA	C	404	20/21	0.98	0.10	111,138,176,195	0
4	SIA	E	404	20/21	0.98	0.10	99,130,177,200	0
3	NAG	F	201	14/15	0.99	0.05	58,80,95,101	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.

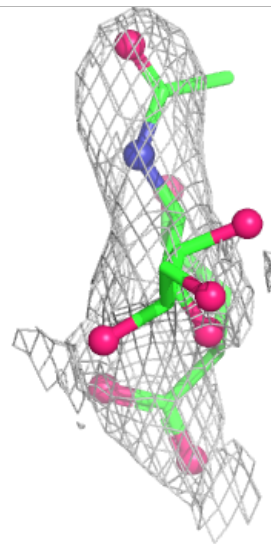
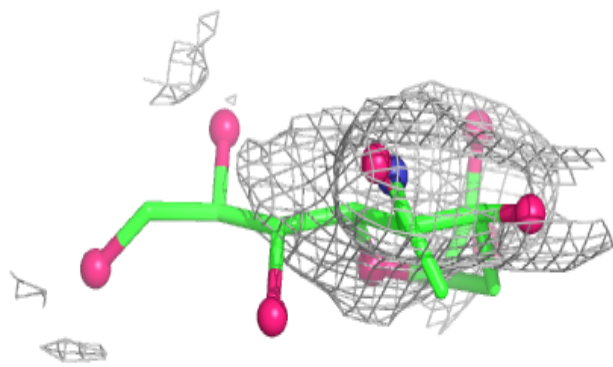
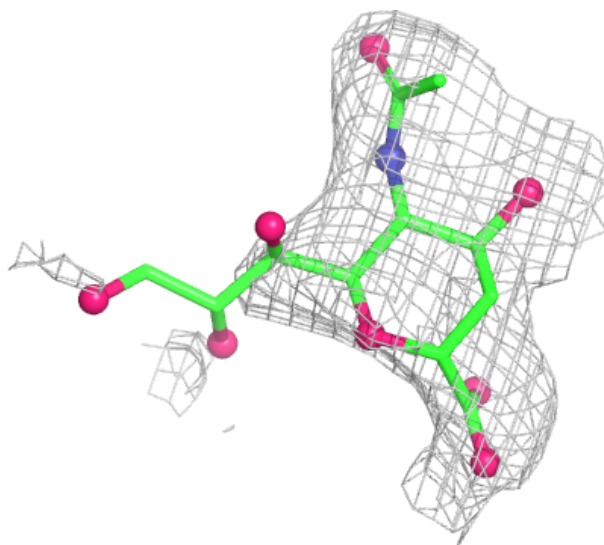
Electron density around SIA A 404:

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



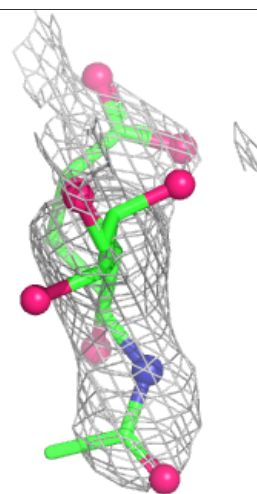
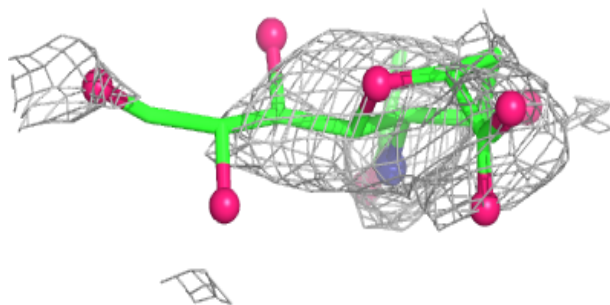
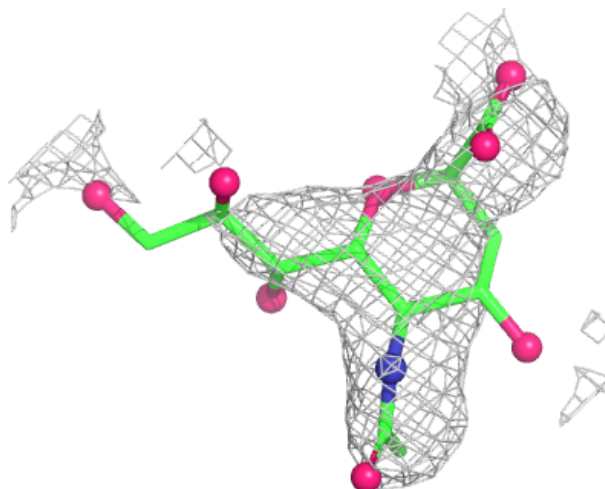
Electron density around SIA C 404:

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



Electron density around SIA E 404:

$2mF_o-DF_c$ (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.