



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 01:57 PM EST

PDB ID : 5EGC
Title : Structure of the Adeno-Associated Virus Serotype 1 sialic acid complex
Authors : Huang, L.Y.; Agbandje-McKenna, M.
Deposited on : 2015-10-27
Resolution : 3.01 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

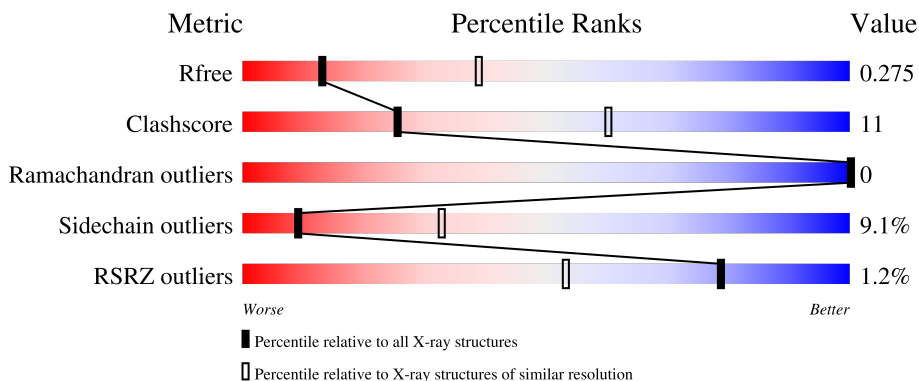
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	520	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SIA	A	801	-	-	-	X

2 Entry composition [i](#)

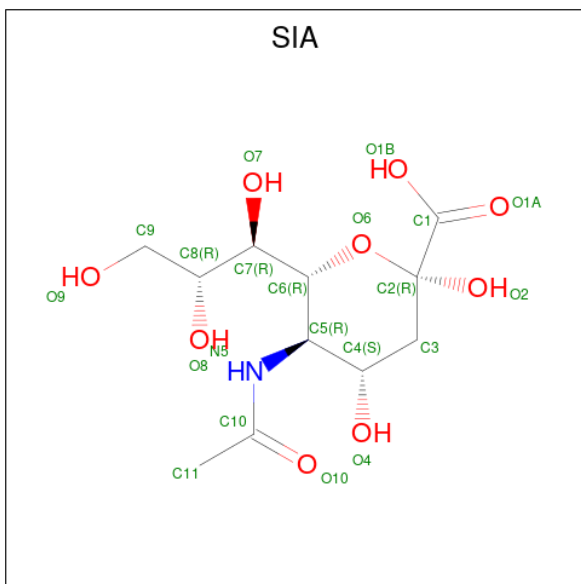
There are 4 unique types of molecules in this entry. The entry contains 4161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	520	4138	2617	714	791	16	0	2	0

- Molecule 2 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		
2	A	1	21	11	1	9	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

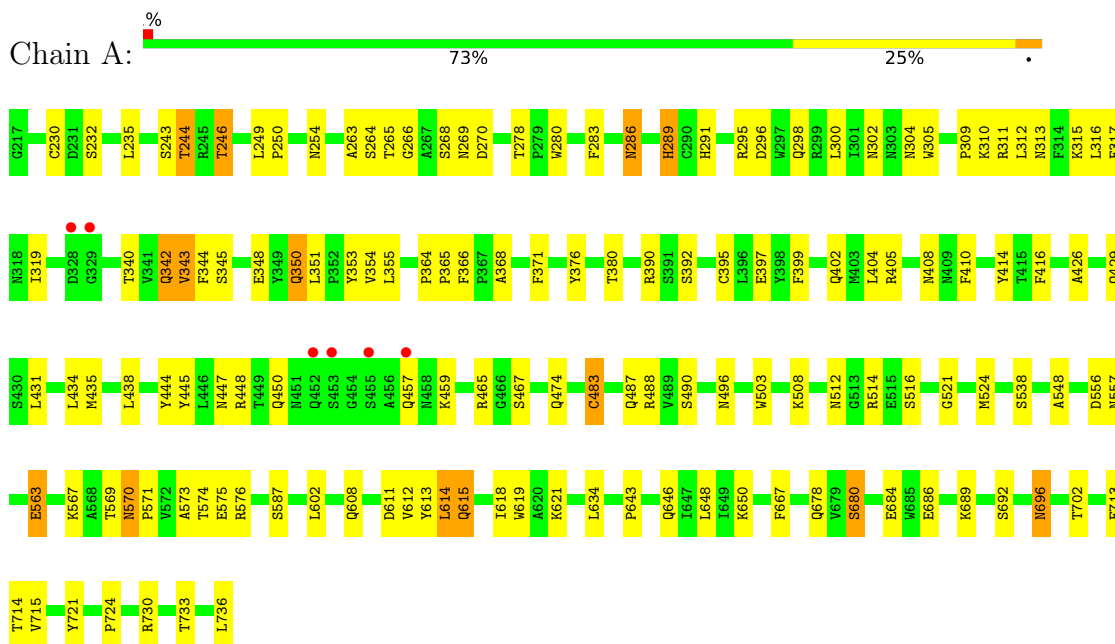
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

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



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	455.63Å 261.75Å 450.98Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	49.92 – 3.01 49.92 – 3.01	Depositor EDS
% Data completeness (in resolution range)	60.5 (49.92-3.01) 47.1 (49.92-3.01)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.269 , 0.276 0.273 , 0.275	Depositor DCC
R_{free} test set	2015 reflections (0.34%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.000 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-1$ 0.000 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-1$	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9387e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.44	0/4264	0.63	0/5813

There are no bond length outliers.

There are no bond angle outliers.

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	4138	0	3903	86	0
2	A	21	0	18	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	4161	0	3921	86	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 11.

All (86) 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:246:THR:HB	1:A:678:GLN:HE21	1.36	0.90
1:A:490:SER:H	1:A:496:ASN:HD21	1.22	0.87
1:A:286:ASN:HD21	1:A:619:TRP:H	1.26	0.83
1:A:278:THR:HG22	1:A:280:TRP:H	1.46	0.78
1:A:263:ALA:O	1:A:264:SER:HB3	1.87	0.75
1:A:570:ASN:HD21	1:A:608:GLN:H	1.37	0.70
1:A:696:ASN:H	1:A:696:ASN:HD22	1.41	0.69
1:A:289:HIS:CE1	1:A:365:PRO:HG3	2.32	0.65
1:A:615:GLN:HE21	1:A:615:GLN:H	1.44	0.65
1:A:278:THR:HB	1:A:376:TYR:O	1.96	0.64
1:A:429:GLN:HE21	1:A:736:LEU:H	1.47	0.61
1:A:230:CYS:HB2	1:A:244:THR:HG22	1.83	0.60
1:A:503:TRP:O	1:A:508:LYS:NZ	2.33	0.60
1:A:312:LEU:HD22	1:A:414:TYR:HB3	1.83	0.60
1:A:264:SER:OG	1:A:265:THR:N	2.35	0.60
1:A:295:ARG:HH11	1:A:298:GLN:HE21	1.50	0.59
1:A:380:THR:HG21	1:A:392:SER:H	1.68	0.59
1:A:278:THR:HG22	1:A:280:TRP:N	2.17	0.59
1:A:621:LYS:HB2	1:A:643:PRO:HG3	1.85	0.58
1:A:249:LEU:HD12	1:A:250:PRO:HD2	1.87	0.57
1:A:310:LYS:HD2	1:A:686:GLU:HB2	1.88	0.56
1:A:444:TYR:CZ	1:A:465:ARG:HB3	2.41	0.56
1:A:316:LEU:HD12	1:A:343:VAL:HG21	1.89	0.55
1:A:435:MET:HG3	1:A:474:GLN:HE22	1.71	0.55
1:A:364:PRO:HG3	1:A:371:PHE:HB3	1.89	0.54
1:A:696:ASN:H	1:A:696:ASN:ND2	2.02	0.54
1:A:615:GLN:H	1:A:615:GLN:NE2	2.06	0.53
1:A:344:PHE:CE2	1:A:648:LEU:HD23	2.43	0.53
1:A:353:TYR:CE2	1:A:355:LEU:HB2	2.44	0.53
1:A:295:ARG:HD2	1:A:298:GLN:HE21	1.74	0.53
1:A:317:PHE:HE1	1:A:680:SER:HB2	1.75	0.52
1:A:283:PHE:CZ	1:A:316:LEU:HD21	2.44	0.52
1:A:563:GLU:OE2	1:A:613:TYR:OH	2.21	0.51
1:A:311:ARG:HG2	1:A:684:GLU:HB3	1.92	0.51
1:A:611:ASP:OD1	1:A:612:VAL:N	2.43	0.51
1:A:444:TYR:CE1	1:A:465:ARG:HB3	2.48	0.49
1:A:487:GLN:NE2	1:A:488:ARG:H	2.11	0.49
1:A:434:LEU:HD21	1:A:736:LEU:HD23	1.95	0.48
1:A:611:ASP:HB2	1:A:730:ARG:NH1	2.28	0.48
1:A:355:LEU:HD12	1:A:646:GLN:HG2	1.96	0.48
1:A:488:ARG:HB2	1:A:574:THR:HB	1.95	0.48
1:A:395:CYS:SG	1:A:397:GLU:HB2	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HB2	1:A:410:PHE:HB3	1.97	0.46
1:A:426:ALA:O	1:A:733:THR:HA	2.15	0.46
1:A:270:ASP:HA	1:A:514:ARG:CG	2.45	0.46
1:A:524:MET:HB2	1:A:573:ALA:HB2	1.97	0.46
1:A:315[B]:LYS:HG3	1:A:410:PHE:O	2.16	0.46
1:A:264:SER:O	1:A:265:THR:OG1	2.20	0.46
1:A:230:CYS:SG	1:A:243:SER:HA	2.56	0.46
1:A:295:ARG:HH11	1:A:298:GLN:NE2	2.14	0.46
1:A:405:ARG:N	1:A:408:ASN:OD1	2.45	0.46
1:A:634:LEU:HD23	1:A:634:LEU:HA	1.66	0.46
1:A:366:PHE:CE2	1:A:368:ALA:HB3	2.51	0.45
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.83	0.45
1:A:289:HIS:HB3	1:A:614:LEU:HD22	1.98	0.45
1:A:232:SER:OG	1:A:296:ASP:OD2	2.26	0.45
1:A:264:SER:C	1:A:265:THR:HG23	2.37	0.45
1:A:286:ASN:ND2	1:A:618:ILE:H	2.14	0.45
1:A:340:THR:HA	1:A:404:LEU:O	2.17	0.44
1:A:487:GLN:HE21	1:A:488:ARG:H	1.65	0.44
1:A:230:CYS:HB2	1:A:244:THR:CG2	2.46	0.44
1:A:348:GLU:HB2	1:A:350:GLN:NE2	2.33	0.44
1:A:714:THR:HG22	1:A:715:VAL:N	2.32	0.44
1:A:305:TRP:CZ2	1:A:692:SER:HB2	2.53	0.44
1:A:264:SER:O	1:A:266:GLY:N	2.46	0.43
1:A:278:THR:CG2	1:A:280:TRP:H	2.22	0.43
1:A:280:TRP:CD2	1:A:650:LYS:HB2	2.54	0.43
1:A:295:ARG:HD2	1:A:298:GLN:NE2	2.33	0.43
1:A:445:TYR:HE1	1:A:447:ASN:HD22	1.66	0.43
1:A:344:PHE:CZ	1:A:648:LEU:HD23	2.54	0.42
1:A:399:PHE:CD1	1:A:399:PHE:N	2.86	0.42
1:A:298:GLN:O	1:A:302:ASN:HB2	2.20	0.42
1:A:570:ASN:HD22	1:A:570:ASN:N	2.17	0.42
1:A:270:ASP:HA	1:A:514:ARG:HG2	2.02	0.41
1:A:521:GLY:O	1:A:634:LEU:HD22	2.20	0.41
1:A:524:MET:SD	1:A:573:ALA:HA	2.60	0.41
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.88	0.41
1:A:304:ASN:HD21	1:A:689:LYS:NZ	2.19	0.41
1:A:714:THR:O	1:A:721:TYR:HA	2.21	0.41
1:A:342:GLN:HA	1:A:402:GLN:O	2.21	0.41
1:A:459:LYS:NZ	1:A:587:SER:HB3	2.36	0.40
1:A:713:PHE:CE2	1:A:724:PRO:HD2	2.56	0.40
1:A:309:PRO:HB2	1:A:416:PHE:CD1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ALA:HB2	1:A:557:ASN:O	2.21	0.40
1:A:483:CYS:HB2	1:A:571:PRO:HG2	2.03	0.40
1:A:448:ARG:NH1	2:A:801:SIA:O1B	2.54	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	520/520 (100%)	484 (93%)	36 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	453/451 (100%)	412 (91%)	41 (9%)	9 33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	244	THR
1	A	246	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	254	ASN
1	A	268	SER
1	A	269	ASN
1	A	286	ASN
1	A	289	HIS
1	A	291	HIS
1	A	300	LEU
1	A	313	ASN
1	A	319	ILE
1	A	342	GLN
1	A	343	VAL
1	A	345	SER
1	A	350	GLN
1	A	354	VAL
1	A	390	ARG
1	A	431	LEU
1	A	438	LEU
1	A	450	GLN
1	A	457	GLN
1	A	467	SER
1	A	483	CYS
1	A	512	ASN
1	A	516	SER
1	A	538	SER
1	A	556	ASP
1	A	563	GLU
1	A	567	LYS
1	A	569	THR
1	A	570	ASN
1	A	575	GLU
1	A	576	ARG
1	A	602	LEU
1	A	614	LEU
1	A	615	GLN
1	A	667	PHE
1	A	680	SER
1	A	696	ASN
1	A	702	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	255	HIS
1	A	269	ASN
1	A	271	ASN
1	A	286	ASN
1	A	298	GLN
1	A	304	ASN
1	A	342	GLN
1	A	350	GLN
1	A	360	GLN
1	A	375	GLN
1	A	402	GLN
1	A	429	GLN
1	A	447	ASN
1	A	457	GLN
1	A	458	ASN
1	A	474	GLN
1	A	487	GLN
1	A	496	ASN
1	A	510	ASN
1	A	512	ASN
1	A	552	ASN
1	A	557	ASN
1	A	570	ASN
1	A	615	GLN
1	A	678	GLN
1	A	691	ASN
1	A	696	ASN

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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	SIA	A	801	-	21,21,21	1.54	3 (14%)	25,31,31	1.55	4 (16%)

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	SIA	A	801	-	-	3/20/38/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SIA	O6-C2	4.21	1.47	1.43
2	A	801	SIA	C2-C1	3.23	1.58	1.53
2	A	801	SIA	C7-C6	2.53	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	SIA	O1A-C1-C2	-4.65	116.55	123.59
2	A	801	SIA	C6-C5-N5	-2.12	107.38	110.91
2	A	801	SIA	C3-C2-C1	2.10	116.93	113.00
2	A	801	SIA	O1B-C1-O1A	2.07	130.41	123.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	SIA	O6-C6-C7-O7

Continued on next page...

Continued from previous page...

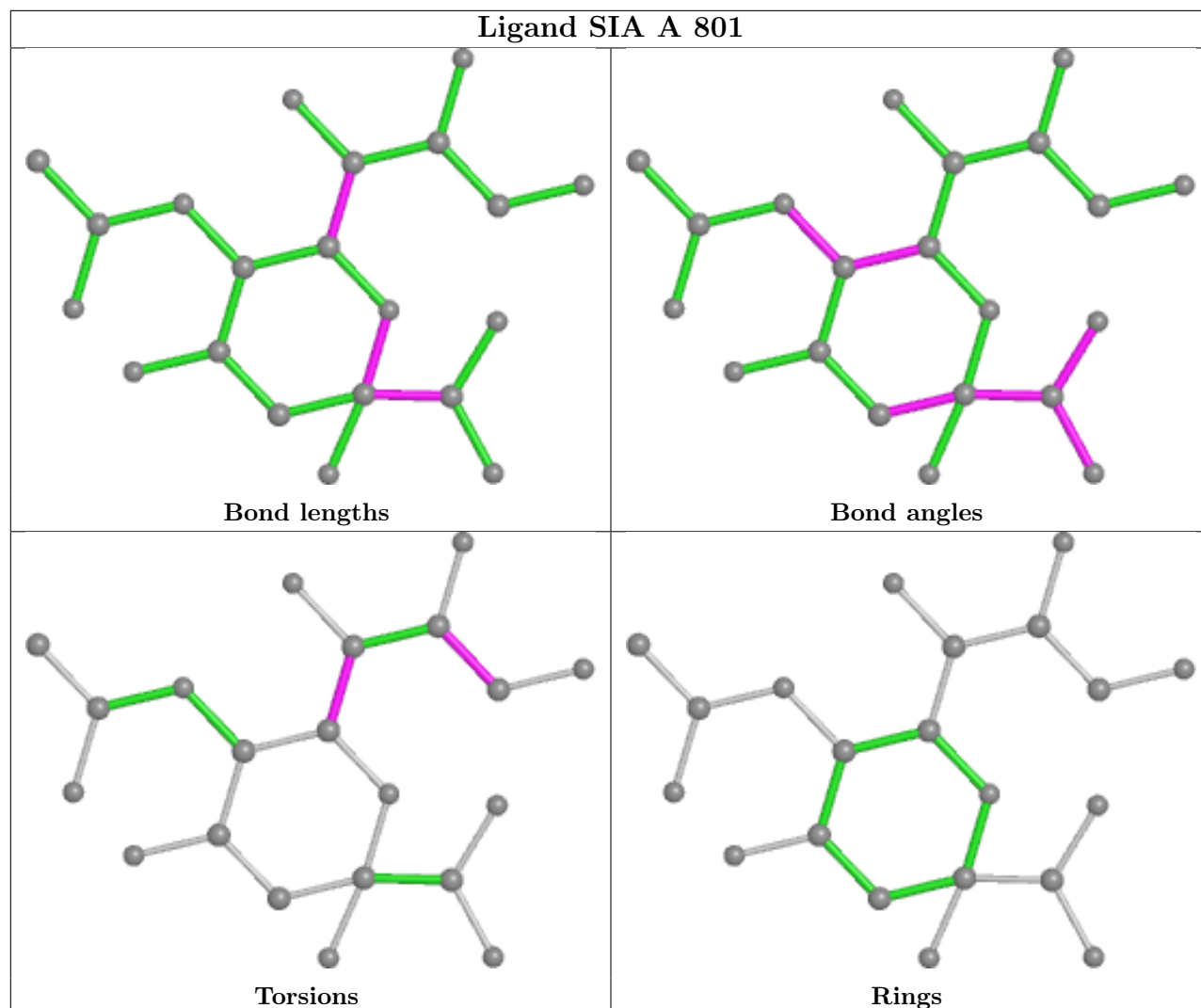
Mol	Chain	Res	Type	Atoms
2	A	801	SIA	C7-C8-C9-O9
2	A	801	SIA	O8-C8-C9-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SIA	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	520/520 (100%)	-0.66	6 (1%) 79 53	8, 19, 43, 89	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	SER	3.7
1	A	452[A]	GLN	3.2
1	A	328	ASP	3.1
1	A	329	GLY	2.6
1	A	457	GLN	2.4
1	A	455	SER	2.4

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](#)

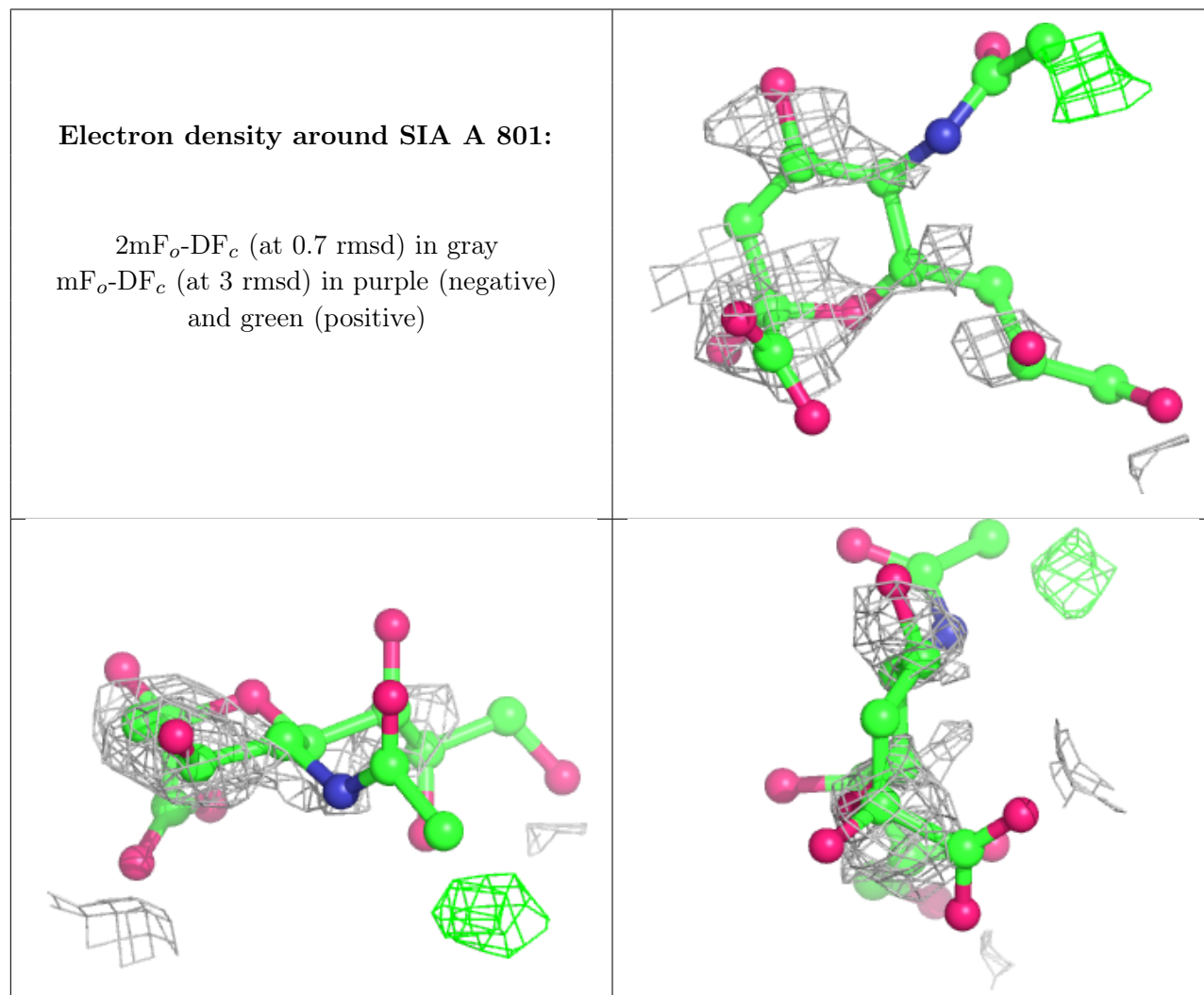
There are no monosaccharides in this entry.

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
2	SIA	A	801	21/21	0.69	0.66	19,32,35,39	21
3	MG	A	802	1/1	0.93	0.12	28,28,28,28	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.