wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2022 – 07:04 am GMT

PDB ID	:	6TSD
Title	:	Crystal structure of human coxsackievirus A24v in complex with pentavalent inhibitor ME0752
Authors	:	Zocher, G.; Stehle, T.
Deposited on	:	2019-12-20
Resolution	:	1.81 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 (i) 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 (i)) were used in the production of this report:

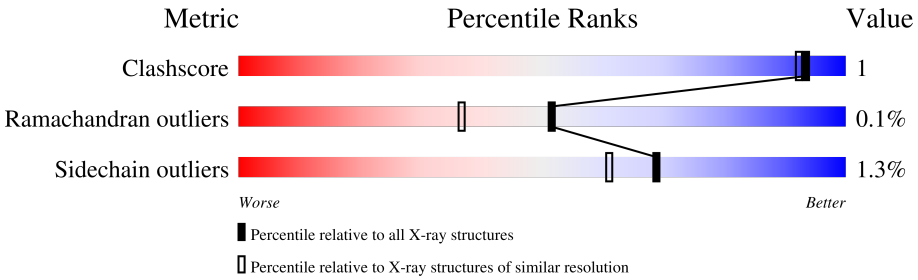
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	111	305	89% 8%
2	222	271	94%
3	333	240	95%
4	444	69	83% 17%

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	HEZ	111	502	-	-	X	-
6	HEZ	111	503	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7493 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	111	281	2275	1450	382	435	8	0	8	0

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	222	264	2062	1315	342	391	14	0	3	0

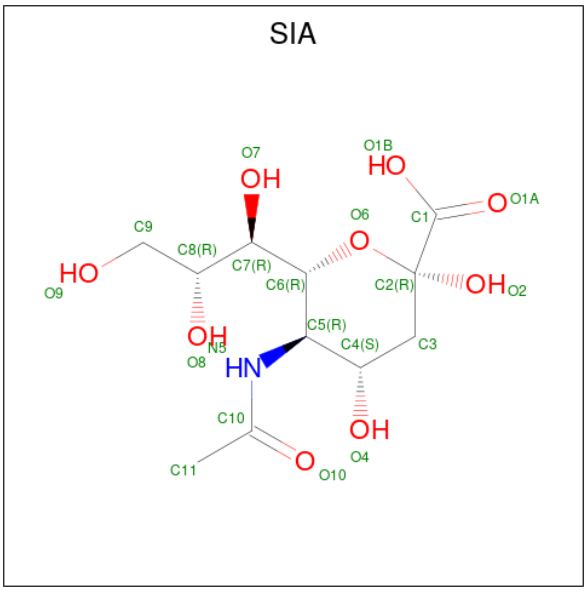
- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	333	234	1842	1185	289	346	22	0	10	0

- Molecule 4 is a protein called Capsid protein VP4.

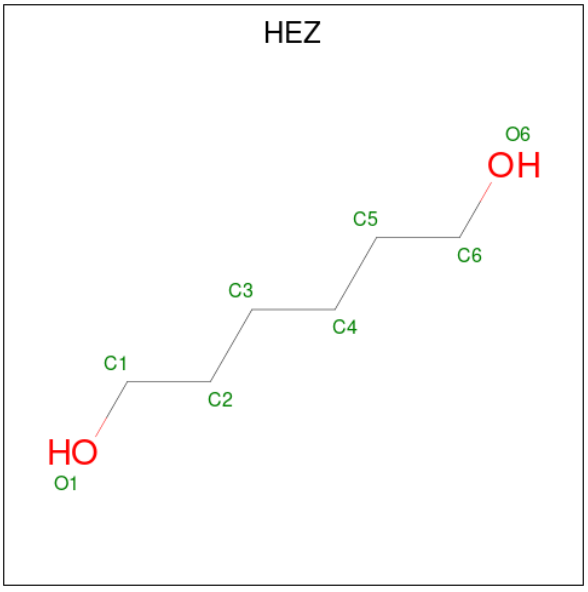
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	444	57	431	271	70	89	1	0	2	0

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	111	1	Total C N O 21 11 1 9	0	0

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	111	1	Total C O 8 6 2	0	0
6	111	1	Total C O 8 6 2	0	0
6	222	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	222	1	Total C O 8 6 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	111	4	Total Cl 4 4	0	0
7	222	1	Total Cl 1 1	0	0
7	333	2	Total Cl 2 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	111	1	Total Na 1 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	111	3	Total Ca 3 3	0	0
9	222	1	Total Ca 1 1	0	0
9	333	1	Total Ca 1 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	333	1	Total Mg 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	111	287	Total O 287 287	0	0
11	222	234	Total O 234 234	0	0

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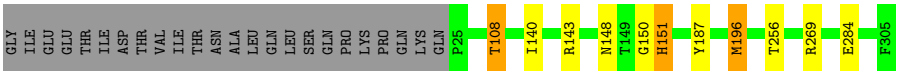
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	333	225	Total O 225 225	0	0
11	444	70	Total O 70 70	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

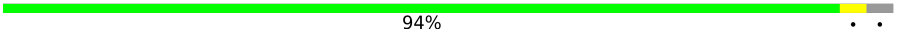
- Molecule 1: Capsid protein VP1

Chain 111:



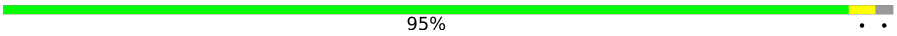
- Molecule 2: Capsid protein VP2

Chain 222:



- Molecule 3: Capsid protein VP3

Chain 333:



- Molecule 4: Capsid protein VP4

Chain 444:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	305.48Å 365.35Å 366.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 1.81 49.95 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.95-1.81) 99.9 (49.95-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0232 2018/13/08	Depositor
R, R_{free}	0.150 , (Not available) 0.410 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, CL, CA, HEZ, SIA, NA

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	111	0.60	0/2362	0.76	0/3228
2	222	0.60	0/2127	0.77	0/2905
3	333	0.60	0/1919	0.75	0/2613
4	444	0.65	0/444	0.72	0/601
All	All	0.60	0/6852	0.76	0/9347

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	222	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	222	82	LEU	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	111	2275	0	2216	7	0
2	222	2062	0	1985	2	0
3	333	1842	0	1841	4	0
4	444	431	0	415	0	0
5	111	21	0	18	1	0
6	111	16	0	28	6	0
6	222	16	0	28	0	0
7	111	4	0	0	0	0
7	222	1	0	0	0	0
7	333	2	0	0	0	0
8	111	1	0	0	0	0
9	111	3	0	0	0	0
9	222	1	0	0	0	0
9	333	1	0	0	0	0
10	333	1	0	0	0	0
11	111	287	0	0	3	0
11	222	234	0	0	0	0
11	333	225	0	0	1	0
11	444	70	0	0	0	0
All	All	7493	0	6531	19	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 1.

The worst 5 of 19 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)
1:111:256[B]:THR:HG22	11:111:676:HOH:O	1.94	0.67
6:111:502:HEZ:H61	6:111:503:HEZ:C5	2.31	0.61
6:111:502:HEZ:H41	6:111:503:HEZ:H41	1.83	0.59
6:111:502:HEZ:H61	6:111:503:HEZ:H52	1.86	0.58
3:333:27:ASN:ND2	11:333:402:HOH:O	2.32	0.55

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	111	287/305 (94%)	276 (96%)	11 (4%)	0	100 100
2	222	265/271 (98%)	250 (94%)	14 (5%)	1 (0%)	34 21
3	333	241/240 (100%)	230 (95%)	11 (5%)	0	100 100
4	444	55/69 (80%)	53 (96%)	2 (4%)	0	100 100
All	All	848/885 (96%)	809 (95%)	38 (4%)	1 (0%)	51 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	222	48	ASN

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	111	254/268 (95%)	247 (97%)	7 (3%)	43 29
2	222	221/225 (98%)	219 (99%)	2 (1%)	78 74
3	333	215/212 (101%)	214 (100%)	1 (0%)	88 87
4	444	47/57 (82%)	47 (100%)	0	100 100
All	All	737/762 (97%)	727 (99%)	10 (1%)	69 58

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	222	166	GLU
2	222	263	ARG
3	333	148	MET
1	111	148	ASN
1	111	151	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	SIA	111	501	-	21,21,21	0.98	1 (4%)	25,31,31	1.28	3 (12%)
6	HEZ	111	503	-	7,7,7	1.86	3 (42%)	6,6,6	0.89	0
6	HEZ	222	4102	-	7,7,7	0.08	0	6,6,6	0.08	0
6	HEZ	111	502	-	7,7,7	1.40	2 (28%)	6,6,6	0.87	0
6	HEZ	222	4101	-	7,7,7	0.17	0	6,6,6	0.09	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
5	SIA	111	501	-	-	3/20/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEZ	111	503	-	-	4/5/5/5	-
6	HEZ	222	4102	-	-	2/5/5/5	-
6	HEZ	111	502	-	-	2/5/5/5	-
6	HEZ	222	4101	-	-	3/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	111	503	HEZ	C5-C4	3.04	1.68	1.51
6	111	502	HEZ	C5-C4	2.93	1.68	1.51
5	111	501	SIA	O2-C2	2.86	1.43	1.39
6	111	503	HEZ	C5-C6	2.35	1.64	1.50
6	111	503	HEZ	C3-C2	2.20	1.63	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	111	501	SIA	O6-C6-C7	3.12	112.11	107.29
5	111	501	SIA	O2-C2-C1	-3.00	104.67	110.76
5	111	501	SIA	O1A-C1-C2	-2.18	120.28	123.59

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	111	501	SIA	O1B-C1-C2-O2
6	111	503	HEZ	O1-C1-C2-C3
6	222	4101	HEZ	C2-C3-C4-C5
6	111	503	HEZ	C3-C4-C5-C6
6	222	4101	HEZ	C1-C2-C3-C4

There are no ring outliers.

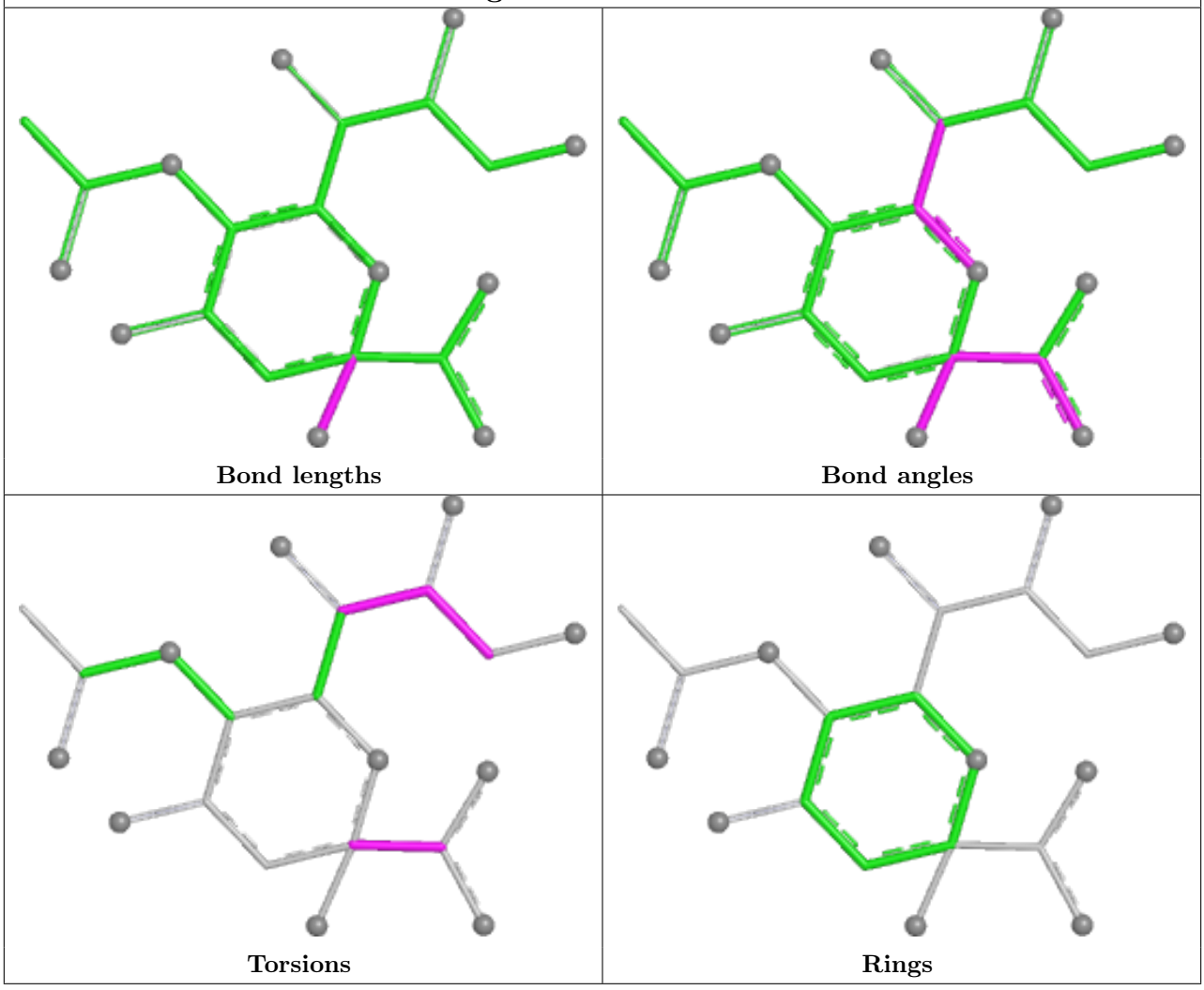
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	111	501	SIA	1	0
6	111	503	HEZ	6	0
6	111	502	HEZ	6	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 then 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 111 501



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

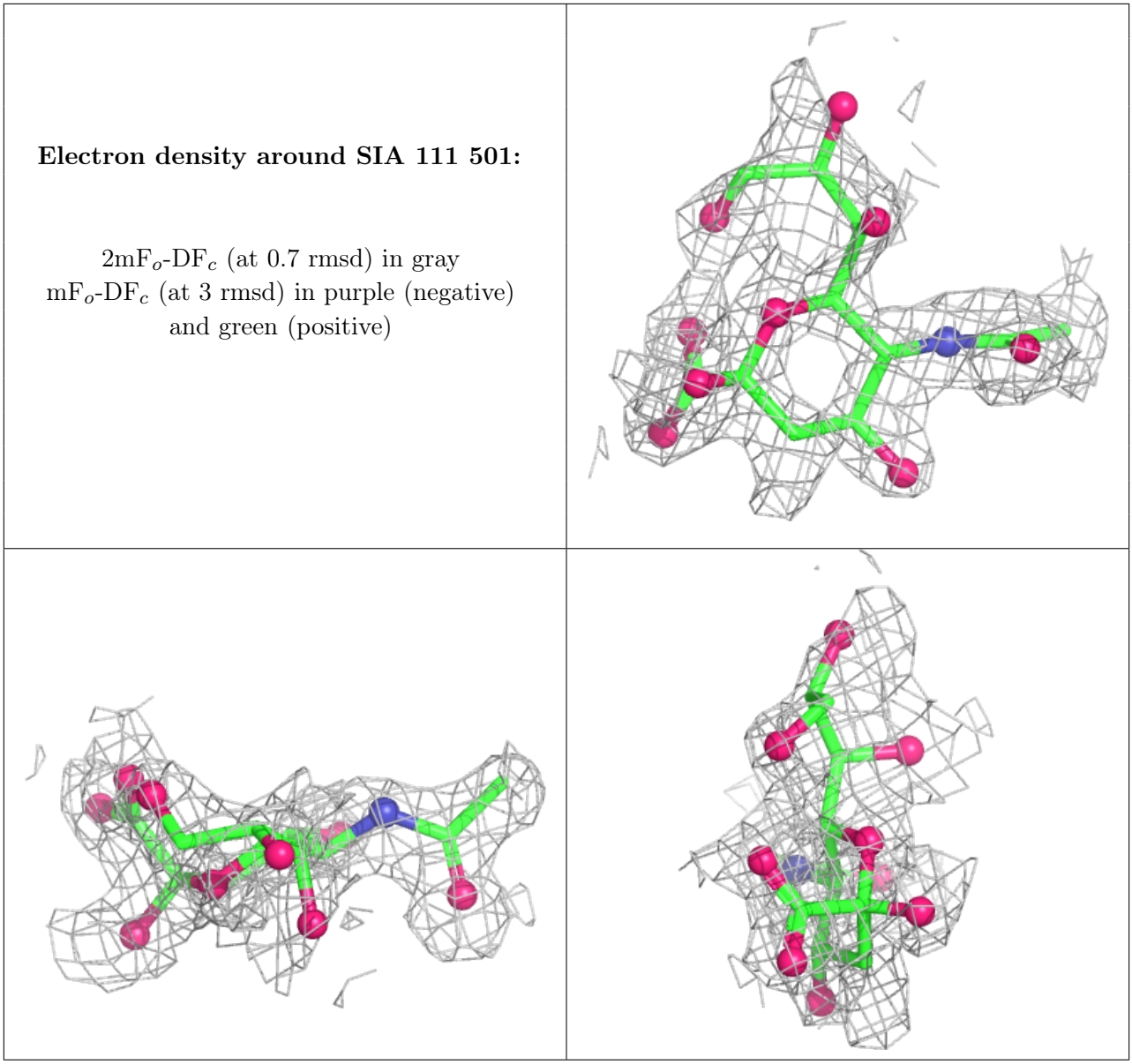
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 111 501:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.