



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 7QB5 / pdb_00007qb5
Title : Coxsackievirus A24v (CVA24v) in complex with a dimeric C2-C9-linked sialic acid inhibitor
Authors : Zocher, G.; Stehle, T.
Deposited on : 2021-11-18
Resolution : 1.73 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

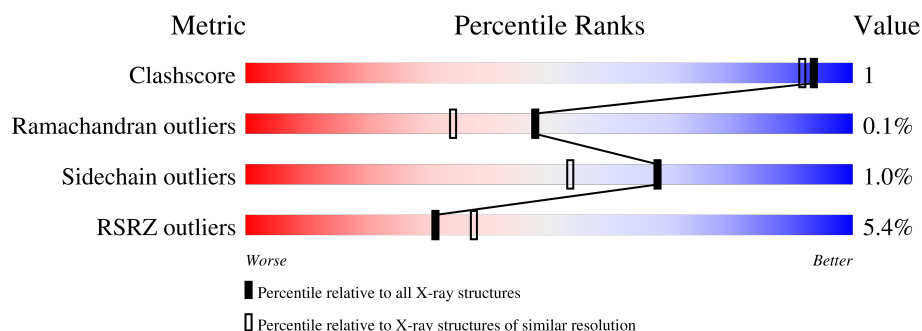
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	111	305	9% 89% 8%
2	222	271	3% 94%
3	333	240	2% 92% 5%
4	444	69	9% 78% 17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7489 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
1	111	281	Total	C	N	O	S	0	10	0
			2291	1462	382	439	8			

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	222	264	Total	C	N	O	S	0	5	0
			2072	1323	342	393	14			

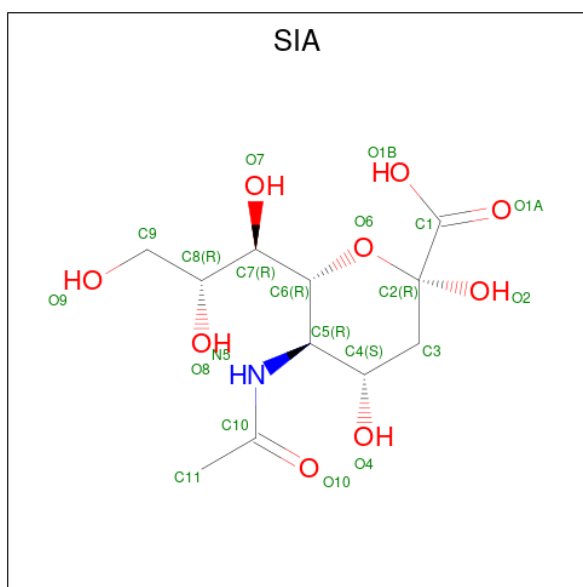
- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	333	234	Total	C	N	O	S	0	11	0
			1846	1188	289	347	22			

- Molecule 4 is a protein called Capsid protein VP4.

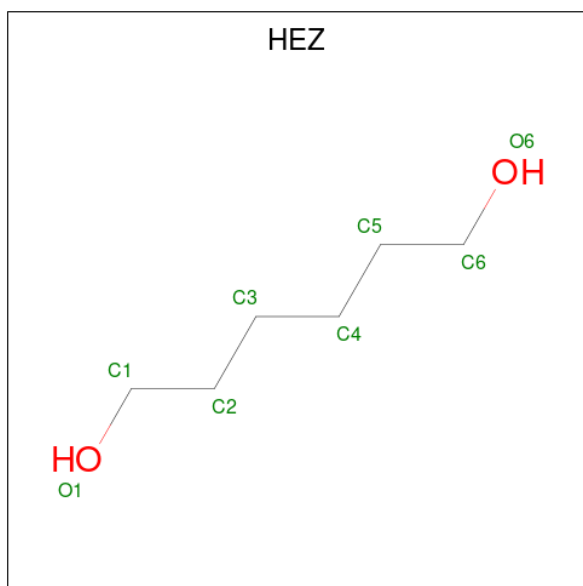
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	444	57	Total	C	N	O	S	0	2	0
			432	271	70	90	1			

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	111	3	Total 3	Ca 3	0	0
7	222	1	Total 1	Ca 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	111	3	Total 3	Cl 3	0	0
8	222	1	Total 1	Cl 1	0	0

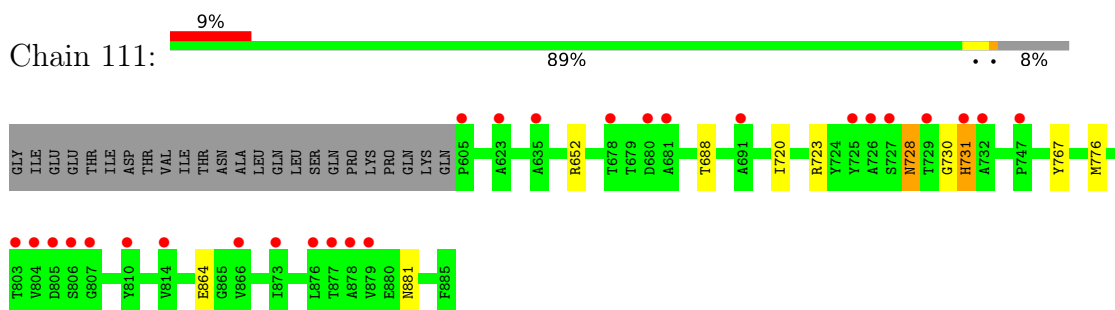
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	111	289	Total 289	O 289	0	0
9	222	238	Total 238	O 238	0	0
9	333	220	Total 220	O 220	0	0
9	444	64	Total 64	O 64	0	0

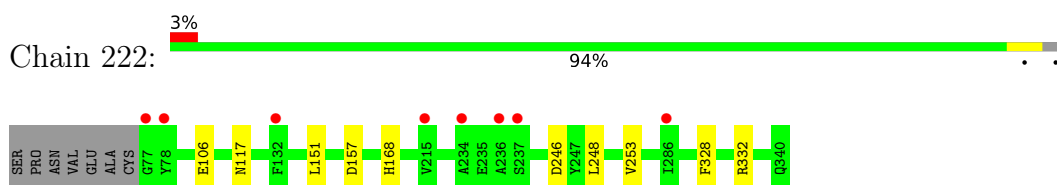
3 Residue-property plots [i](#)

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.

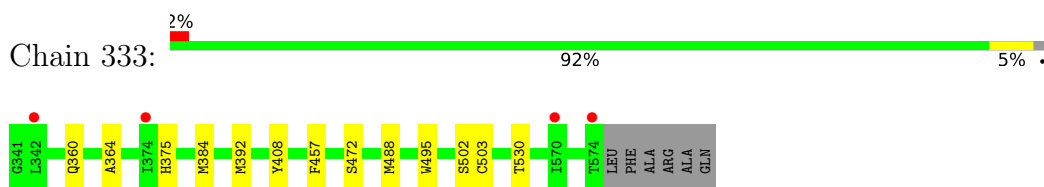
- Molecule 1: Capsid protein VP1



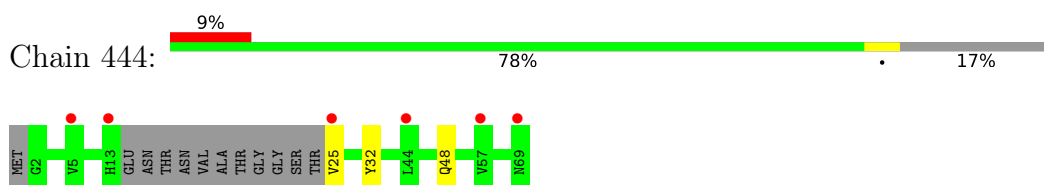
- Molecule 2: Capsid protein VP2



- Molecule 3: Capsid protein VP3



- Molecule 4: Capsid protein VP4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	305.76Å 365.71Å 366.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 1.73 49.92 – 1.73	Depositor EDS
% Data completeness (in resolution range)	90.9 (49.92-1.73) 90.5 (49.92-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.166 , (Not available) 0.404 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: SIA, HEZ, CA, CL

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	0.93	0/2385	1.12	0/3258
2	222	0.91	0/2143	1.14	1/2927 (0.0%)
3	333	0.93	0/1926	1.11	0/2624
4	444	0.97	0/445	1.19	0/601
All	All	0.92	0/6899	1.13	1/9410 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	222	246	ASP	CA-CB-CG	5.76	118.36	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	222	151	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	2291	0	2231	7	0
2	222	2072	0	2000	4	0
3	333	1846	0	1845	8	0
4	444	432	0	415	3	0
5	111	21	0	18	0	0
6	111	8	0	14	0	0
7	111	3	0	0	0	0
7	222	1	0	0	0	0
8	111	3	0	0	0	0
8	222	1	0	0	1	0
9	111	289	0	0	0	0
9	222	238	0	0	0	0
9	333	220	0	0	0	0
9	444	64	0	0	0	0
All	All	7489	0	6523	18	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.

All (18) 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)
3:333:360:GLN:HE22	4:444:32:TYR:H	1.32	0.78
1:111:652:ARG:HH11	4:444:48:GLN:HE22	1.43	0.66
4:444:25:VAL:O	4:444:25:VAL:HG12	2.01	0.59
3:333:384[B]:MET:HE2	3:333:384[B]:MET:HA	1.89	0.54
3:333:472[A]:SER:OG	3:333:530[A]:THR:OG1	2.26	0.53
1:111:728:ASN:HD22	1:111:728:ASN:H	1.58	0.52
1:111:731:HIS:ND1	1:111:731:HIS:N	2.61	0.48
1:111:730:GLY:C	1:111:731:HIS:ND1	2.73	0.47
3:333:392:MET:HE3	3:333:408:TYR:CG	2.50	0.46
1:111:776:MET:HG3	3:333:364:ALA:HB2	1.99	0.45
2:222:106:GLU:CD	3:333:375:HIS:HE2	2.25	0.45
3:333:495:TRP:CD1	3:333:503:CYS:HB2	2.52	0.44
1:111:720[B]:ILE:HD12	1:111:767:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:222:248:LEU:HA	2:222:253:VAL:O	2.17	0.44
2:222:157[B]:ASP:OD2	8:222:402:CL:CL	2.74	0.43
3:333:457:PHE:O	3:333:502:SER:HA	2.21	0.41
2:222:168:HIS:CG	2:222:328:PHE:HB3	2.57	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	111	289/305 (95%)	278 (96%)	11 (4%)	0	100	100
2	222	267/271 (98%)	253 (95%)	13 (5%)	1 (0%)	30	16
3	333	242/240 (101%)	230 (95%)	12 (5%)	0	100	100
4	444	55/69 (80%)	53 (96%)	2 (4%)	0	100	100
All	All	853/885 (96%)	814 (95%)	38 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	222	117	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	256/268 (96%)	250 (98%)	6 (2%)	44	21
2	222	223/225 (99%)	222 (100%)	1 (0%)	84	76
3	333	216/212 (102%)	215 (100%)	1 (0%)	81	71
4	444	47/57 (82%)	47 (100%)	0	100	100
All	All	742/762 (97%)	734 (99%)	8 (1%)	68	50

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	111	688[A]	THR
1	111	688[B]	THR
1	111	723	ARG
1	111	728	ASN
1	111	731	HIS
1	111	864	GLU
2	222	332	ARG
3	333	488	MET

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 ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
6	HEZ	111	902	-	7,7,7	0.67	0	6,6,6	0.41	0
5	SIA	111	901	-	21,21,21	1.00	1 (4%)	24,31,31	1.05	2 (8%)

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
6	HEZ	111	902	-	-	5/5/5/5	-
5	SIA	111	901	-	-	9/20/38/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	111	901	SIA	O2-C2	3.00	1.43	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	111	901	SIA	O1A-C1-C2	-3.37	118.23	123.85
5	111	901	SIA	O2-C2-C1	-2.07	106.36	110.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	111	901	SIA	O1A-C1-C2-O2
5	111	901	SIA	O1A-C1-C2-O6
5	111	901	SIA	O1B-C1-C2-O2
5	111	901	SIA	O1B-C1-C2-O6
6	111	902	HEZ	O1-C1-C2-C3
5	111	901	SIA	C6-C7-C8-O8
6	111	902	HEZ	C4-C5-C6-O6
6	111	902	HEZ	C3-C4-C5-C6

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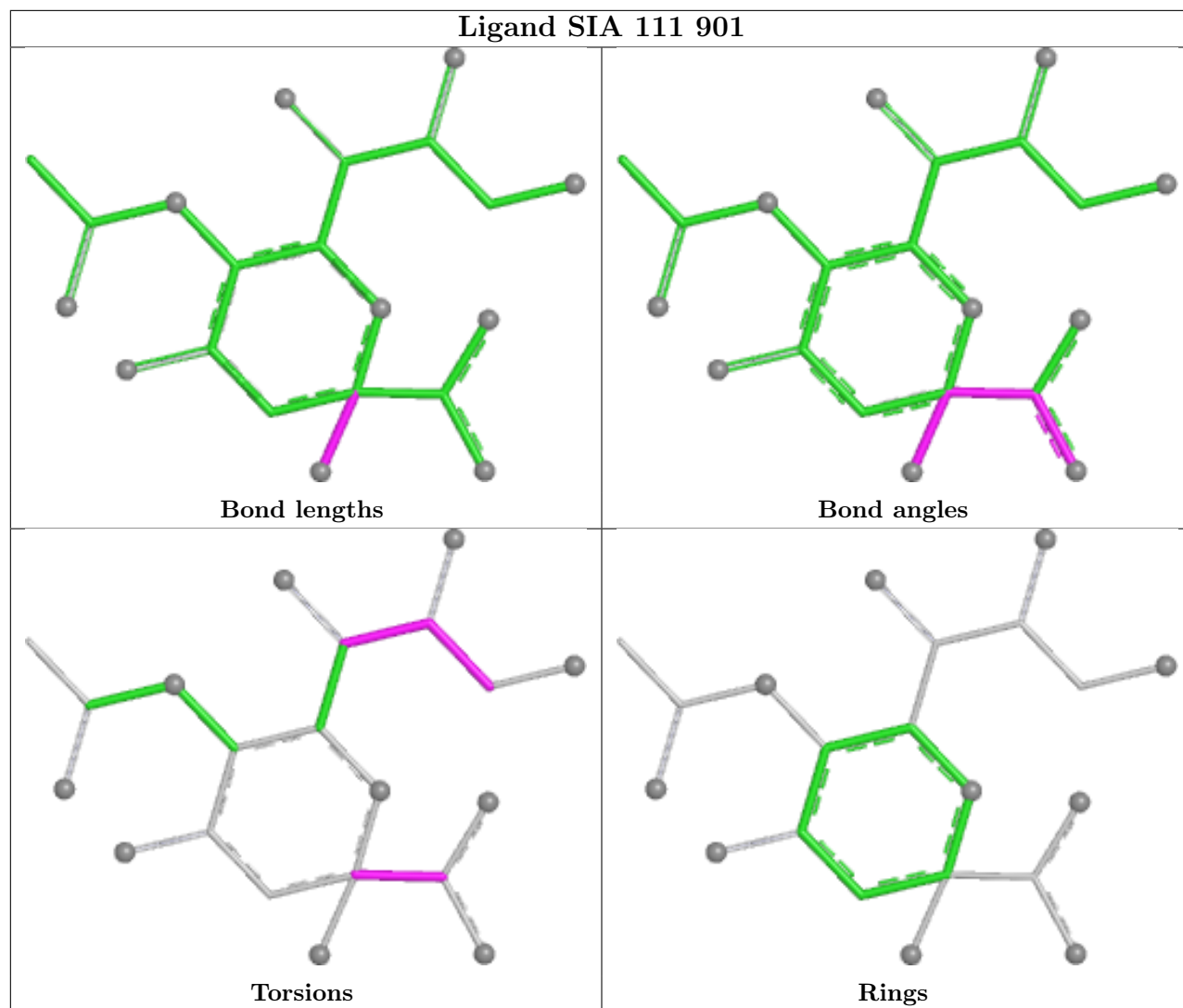
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Mol	Chain	Res	Type	Atoms
6	111	902	HEZ	C2-C3-C4-C5
5	111	901	SIA	O7-C7-C8-O8
5	111	901	SIA	O7-C7-C8-C9
5	111	901	SIA	C6-C7-C8-C9
6	111	902	HEZ	C1-C2-C3-C4
5	111	901	SIA	C7-C8-C9-O9

There are no ring outliers.

No monomer is involved in short contacts.

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	111	281/305 (92%)	1.01	27 (9%)	13 19	14, 24, 45, 65	10 (3%)
2	222	264/271 (97%)	0.85	8 (3%)	52 61	14, 23, 38, 67	5 (1%)
3	333	234/240 (97%)	0.80	4 (1%)	69 75	14, 23, 31, 44	11 (4%)
4	444	57/69 (82%)	1.23	6 (10%)	11 16	16, 30, 50, 72	2 (3%)
All	All	836/885 (94%)	0.91	45 (5%)	31 37	14, 24, 39, 72	28 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	222	234	ALA	4.4
4	444	25	VAL	3.9
2	222	236	ALA	3.5
3	333	574[A]	THR	3.5
4	444	5	VAL	3.3
4	444	44	LEU	3.1
1	111	806	SER	3.0
3	333	374	ILE	3.0
2	222	78	TYR	3.0
1	111	680[A]	ASP	2.9
1	111	803	THR	2.8
1	111	804	VAL	2.7
1	111	678	THR	2.7
2	222	77	GLY	2.7
1	111	729	THR	2.6
1	111	726	ALA	2.6
1	111	879	VAL	2.5
1	111	807	GLY	2.5
4	444	13	HIS	2.5
1	111	814	VAL	2.5
1	111	727	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	444	57	VAL	2.5
1	111	681	ALA	2.4
1	111	732	ALA	2.4
1	111	731	HIS	2.4
1	111	876	LEU	2.3
1	111	747	PRO	2.3
3	333	342	LEU	2.3
1	111	877	THR	2.3
1	111	805	ASP	2.3
1	111	725	TYR	2.2
1	111	635	ALA	2.2
1	111	605	PRO	2.2
2	222	237	SER	2.2
1	111	873	ILE	2.1
1	111	691	ALA	2.1
1	111	810	TYR	2.1
1	111	866	VAL	2.1
4	444	69	ASN	2.1
2	222	286	ILE	2.1
3	333	570	ILE	2.1
1	111	623	ALA	2.0
1	111	878	ALA	2.0
2	222	215	VAL	2.0
2	222	132	PHE	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

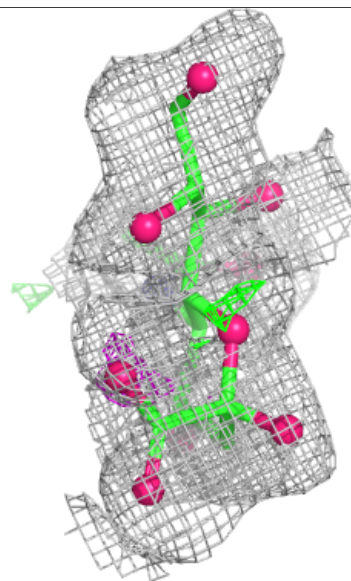
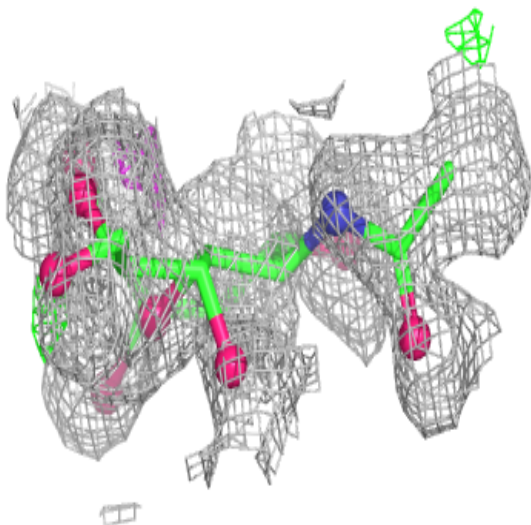
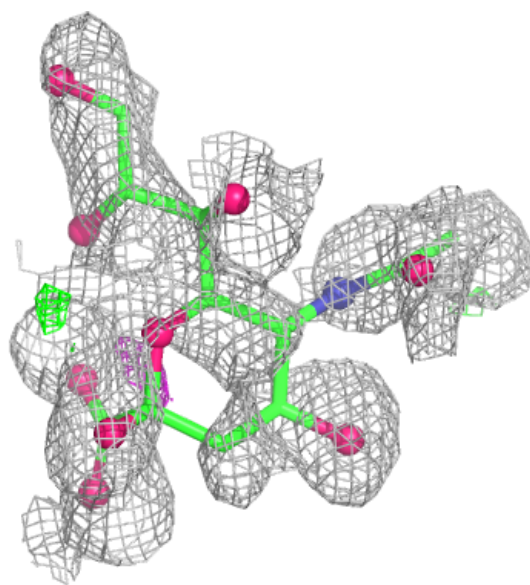
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	HEZ	111	902	8/8	0.95	0.17	58,71,94,95	0
5	SIA	111	901	21/21	0.96	0.15	34,48,59,76	0
7	CA	111	903	1/1	0.98	0.16	39,39,39,39	0
7	CA	222	401	1/1	0.98	0.11	33,33,33,33	1
7	CA	111	905	1/1	0.99	0.06	30,30,30,30	0
7	CA	111	904	1/1	0.99	0.06	25,25,25,25	0
8	CL	111	906	1/1	0.99	0.08	26,26,26,26	0
8	CL	111	907	1/1	0.99	0.08	31,31,31,31	0
8	CL	111	908	1/1	0.99	0.19	28,28,28,28	1
8	CL	222	402	1/1	0.99	0.08	37,37,37,37	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 111 901:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.