



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:53 AM UTC

PDB ID : 4Q4X / pdb_00004q4x
Title : Crystal structure of Cocksackievirus A24v soaked with 6'-Sialyllactose (6SL)
Authors : Zocher, G.; Stehle, T.
Deposited on : 2014-04-15
Resolution : 1.65 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

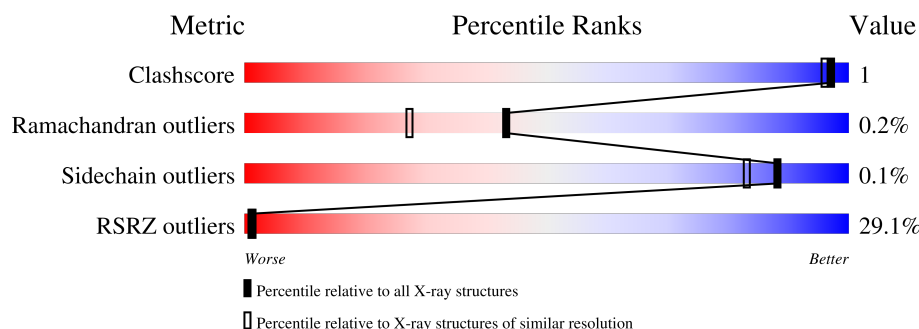
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	1	305	35% 90% 8%
2	2	271	24% 96% ..
3	3	240	18% 94% ..
4	4	69	39% 78% 19%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7443 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 Cocksackievirus capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	281	Total	C	N	O	S	0	8	0
			2281	1454	382	437	8			

- Molecule 2 is a protein called Cocksackievirus capsid protein VP2.

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

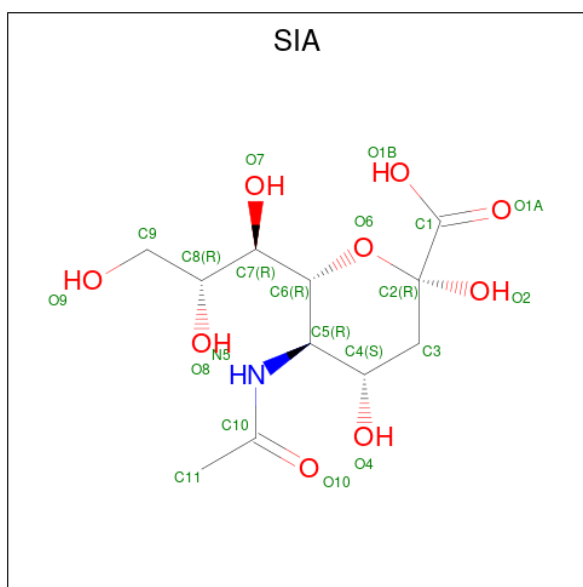
- Molecule 3 is a protein called Cocksackievirus capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	234	Total	C	N	O	S	0	9	0
			1844	1184	291	347	22			

- Molecule 4 is a protein called Cocksackievirus capsid protein VP4.

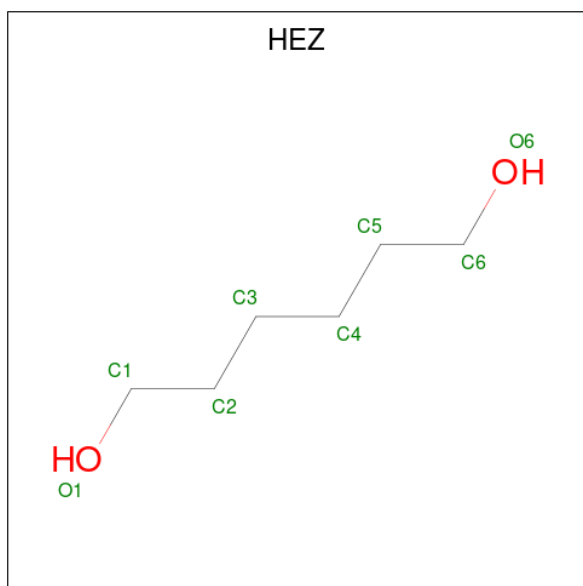
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	56	Total	C	N	O	S	0	1	0
			416	261	67	87	1			

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	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	1	1	Total	C	O	0	0
			8	6	2		
6	1	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1	1	Total Na 1 1	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1	3	Total Ca 3 3	0	0
8	2	1	Total Ca 1 1	0	0
8	3	1	Total Ca 1 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	1	3	Total Cl 3 3	0	0
9	2	1	Total Cl 1 1	0	0
9	3	1	Total Cl 1 1	0	0

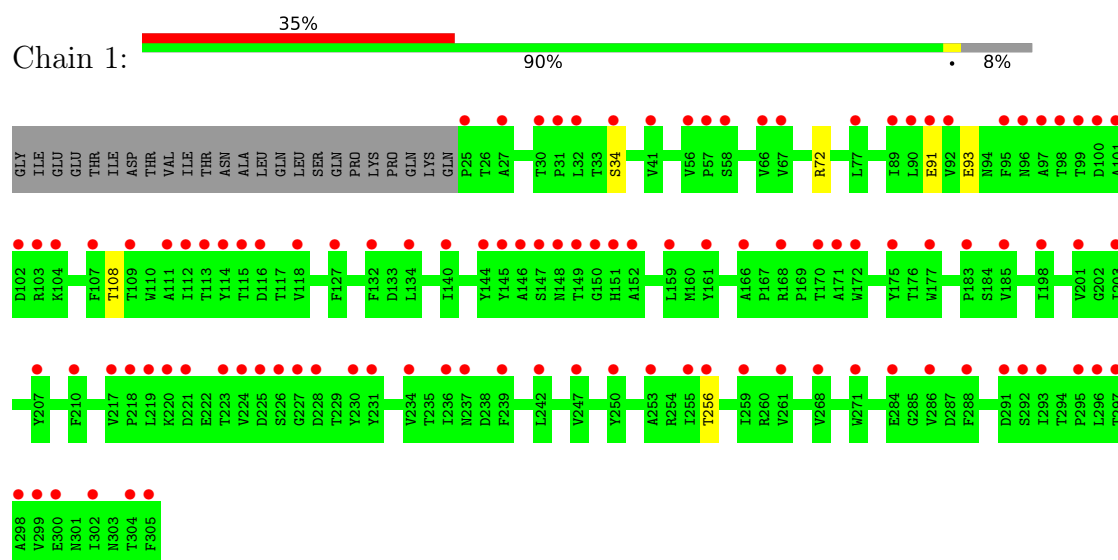
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	1	275	Total O 275 275	0	0
10	2	226	Total O 226 226	0	0
10	3	222	Total O 222 222	0	0
10	4	59	Total O 59 59	0	0

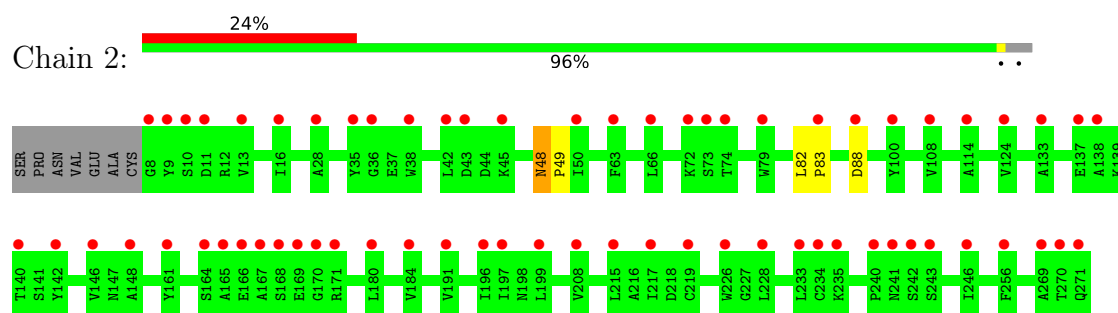
3 Residue-property plots [i](#)

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.

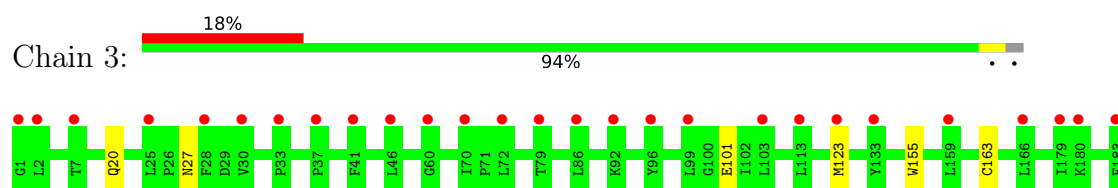
• Molecule 1: Cocksackievirus capsid protein VP1

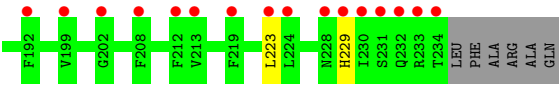


• Molecule 2: Cocksackievirus capsid protein VP2

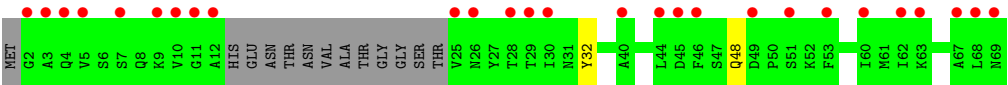
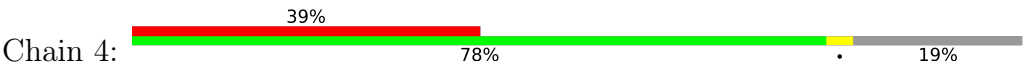


• Molecule 3: Cocksackievirus capsid protein VP3





● Molecule 4: Cocksackievirus 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	306.40Å 366.10Å 367.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 1.65 49.95 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.95-1.65) 99.3 (49.95-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.149 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	7443	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: CL, SIA, HEZ, NA, CA

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	1	0.44	1/2369 (0.0%)	0.65	0/3236
2	2	0.36	0/2143	0.66	0/2927
3	3	0.38	0/1921	0.63	0/2617
4	4	0.45	0/425	0.59	0/575
All	All	0.40	1/6858 (0.0%)	0.64	0/9355

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	2	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	34	SER	C-O	5.07	1.30	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	82	LEU	Mainchain,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	1	2281	0	2214	5	0
2	2	2072	0	2000	2	0
3	3	1844	0	1843	5	0
4	4	416	0	396	2	0
5	1	21	0	18	0	0
6	1	16	0	28	0	0
7	1	1	0	0	0	0
8	1	3	0	0	0	0
8	2	1	0	0	0	0
8	3	1	0	0	0	0
9	1	3	0	0	0	0
9	2	1	0	0	1	0
9	3	1	0	0	0	0
10	1	275	0	0	1	0
10	2	226	0	0	1	0
10	3	222	0	0	0	0
10	4	59	0	0	0	0
All	All	7443	0	6499	12	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 (12) 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)
3:3:20:GLN:HE22	4:4:32:TYR:H	1.34	0.76
1:1:91:GLU:O	1:1:108[B]:THR:HG21	1.98	0.64
3:3:101:GLU:OE1	3:3:229:HIS:HD2	1.82	0.62
1:1:256[B]:THR:HG22	10:1:6252:HOH:O	2.00	0.61
1:1:72:ARG:HH11	4:4:48:GLN:HE22	1.52	0.58
10:2:706:HOH:O	3:3:123[B]:MET:SD	2.58	0.54
2:2:48:ASN:HB3	2:2:49:PRO:CD	2.45	0.45
1:1:93:GLU:HG2	1:1:256[B]:THR:HG23	1.97	0.45
3:3:27[A]:ASN:HD22	3:3:27[A]:ASN:HA	1.70	0.43
3:3:155:TRP:CD1	3:3:163:CYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:91:GLU:O	1:1:108[B]:THR:CG2	2.67	0.41
2:2:88[B]:ASP:OD2	9:2:402:CL:CL	2.76	0.41

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	1	287/305 (94%)	280 (98%)	7 (2%)	0	100	100
2	2	267/271 (98%)	254 (95%)	11 (4%)	2 (1%)	18	6
3	3	241/240 (100%)	230 (95%)	11 (5%)	0	100	100
4	4	53/69 (77%)	51 (96%)	2 (4%)	0	100	100
All	All	848/885 (96%)	815 (96%)	31 (4%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	48	ASN
2	2	83	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	1	254/268 (95%)	254 (100%)	0	100	100
2	2	223/225 (99%)	223 (100%)	0	100	100
3	3	216/212 (102%)	215 (100%)	1 (0%)	81	72
4	4	44/57 (77%)	44 (100%)	0	100	100
All	All	737/762 (97%)	736 (100%)	1 (0%)	88	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	61	ASN
2	2	94	GLN
2	2	260	ASN
3	3	20	GLN
3	3	229	HIS
4	4	48	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	1	5002	-	7,7,7	0.22	0	6,6,6	0.61	0
5	SIA	1	5001	-	21,21,21	0.91	1 (4%)	24,31,31	0.92	1 (4%)
6	HEZ	1	5003	-	7,7,7	0.26	0	6,6,6	0.52	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
6	HEZ	1	5002	-	-	1/5/5/5	-
5	SIA	1	5001	-	-	7/20/38/38	0/1/1/1
6	HEZ	1	5003	-	-	3/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	5001	SIA	O2-C2	2.79	1.43	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	5001	SIA	O1A-C1-C2	-2.54	119.61	123.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	5003	HEZ	C4-C5-C6-O6
6	1	5002	HEZ	O1-C1-C2-C3
6	1	5003	HEZ	C2-C3-C4-C5
5	1	5001	SIA	C6-C7-C8-O8
5	1	5001	SIA	C7-C8-C9-O9

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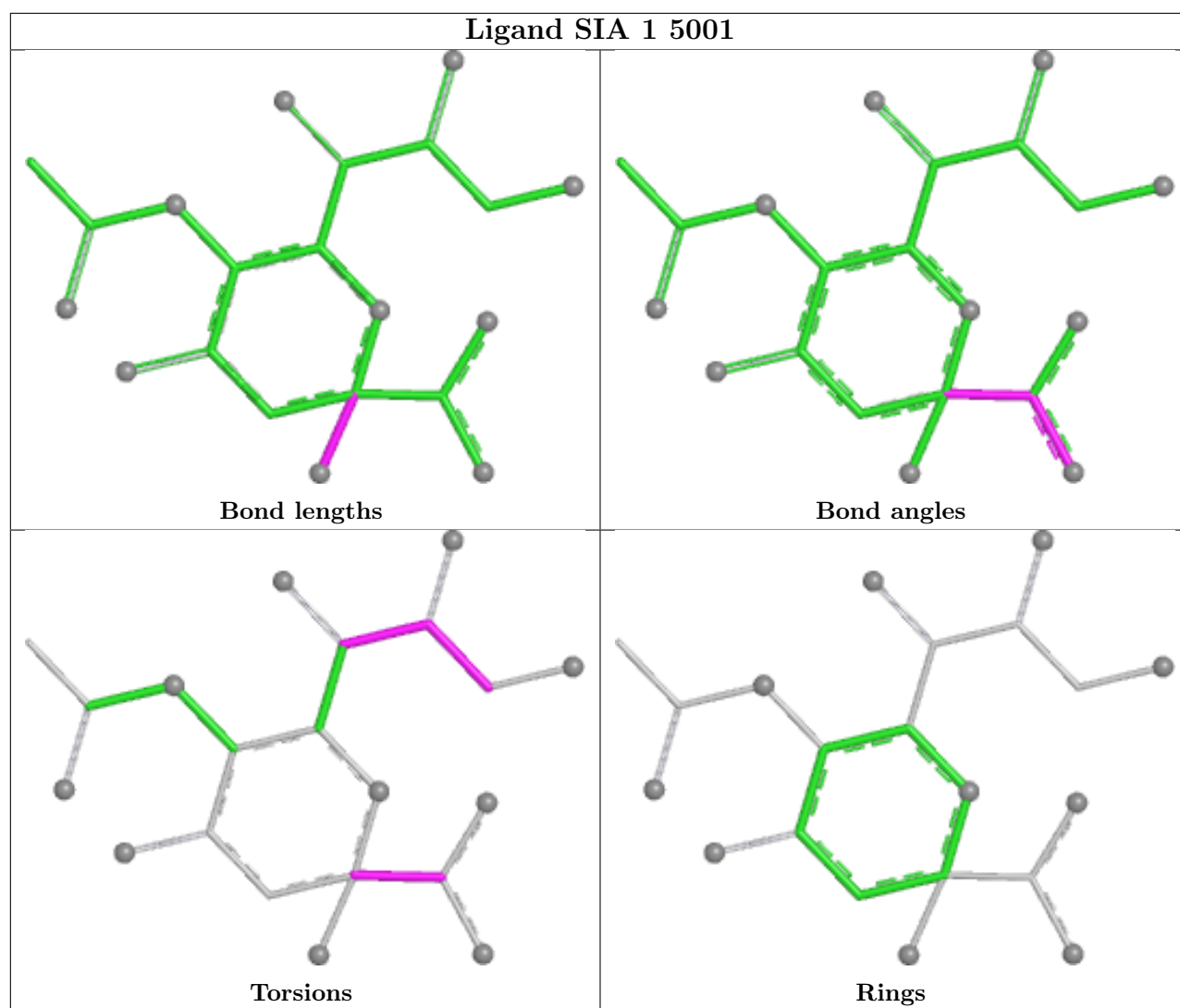
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Mol	Chain	Res	Type	Atoms
6	1	5003	HEZ	O1-C1-C2-C3
5	1	5001	SIA	O7-C7-C8-O8
5	1	5001	SIA	O7-C7-C8-C9
5	1	5001	SIA	O1B-C1-C2-O2
5	1	5001	SIA	O8-C8-C9-O9
5	1	5001	SIA	C6-C7-C8-C9

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	1	281/305 (92%)	1.85	107 (38%) 1 1	14, 22, 37, 54	8 (2%)
2	2	264/271 (97%)	1.58	66 (25%) 2 1	12, 21, 33, 57	5 (1%)
3	3	234/240 (97%)	1.45	43 (18%) 3 4	13, 21, 29, 58	9 (3%)
4	4	56/69 (81%)	2.28	27 (48%) 0 0	15, 28, 37, 51	1 (1%)
All	All	835/885 (94%)	1.68	243 (29%) 1 1	12, 22, 35, 58	23 (2%)

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	234	THR	8.0
1	1	224	VAL	6.7
1	1	223	THR	6.2
2	2	271	GLN	6.2
1	1	148	ASN	6.2
2	2	9	TYR	6.2
4	4	69	ASN	6.1
2	2	8	GLY	5.9
4	4	2	GLY	5.6
4	4	10	VAL	5.5
4	4	25	VAL	5.5
2	2	165	ALA	5.4
1	1	98	THR	5.3
2	2	167	ALA	5.1
1	1	161[A]	TYR	4.7
1	1	149	THR	4.7
1	1	145	TYR	4.7
2	2	166	GLU	4.6
1	1	104	LYS	4.6
1	1	151	HIS	4.5
4	4	60	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	1	225	ASP	4.5
1	1	114	TYR	4.4
1	1	297	THR	4.3
1	1	97	ALA	4.3
3	3	113	LEU	4.2
4	4	44	LEU	4.2
1	1	147	SER	4.2
2	2	242	SER	4.2
1	1	150	GLY	4.1
4	4	12	ALA	4.0
4	4	62	ILE	4.0
1	1	115	THR	4.0
3	3	233	ARG	3.9
3	3	86	LEU	3.9
4	4	68	LEU	3.9
2	2	233	LEU	3.7
1	1	146	ALA	3.7
3	3	232	GLN	3.6
2	2	243	SER	3.6
3	3	229	HIS	3.6
2	2	270	THR	3.6
1	1	268	VAL	3.6
4	4	3	ALA	3.5
3	3	99	LEU	3.5
1	1	103	ARG	3.5
1	1	227	GLY	3.5
1	1	66	VAL	3.5
1	1	41	VAL	3.4
4	4	5	VAL	3.4
1	1	250	TYR	3.4
1	1	89	ILE	3.4
1	1	159	LEU	3.4
1	1	237	ASN	3.4
1	1	101	ALA	3.4
1	1	100	ASP	3.3
1	1	220	LYS	3.3
1	1	112	ILE	3.3
1	1	299	VAL	3.3
2	2	74	THR	3.2
3	3	159	LEU	3.2
1	1	239	PHE	3.2
2	2	269	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	4	11	GLY	3.2
1	1	170	THR	3.2
2	2	11	ASP	3.2
1	1	90	LEU	3.2
1	1	304	THR	3.1
1	1	221	ASP	3.1
3	3	96	TYR	3.1
1	1	293	ILE	3.1
2	2	180	LEU	3.1
2	2	38	TRP	3.0
2	2	13	VAL	3.0
1	1	228	ASP	3.0
2	2	73	SER	3.0
1	1	77	LEU	3.0
2	2	235	LYS	3.0
2	2	83	PRO	3.0
3	3	230	ILE	3.0
1	1	99	THR	2.9
2	2	28	ALA	2.9
1	1	32	LEU	2.9
1	1	288	PHE	2.9
3	3	219	PHE	2.9
4	4	51	SER	2.9
2	2	88[A]	ASP	2.9
3	3	183	PHE	2.9
2	2	142	TYR	2.9
1	1	132	PHE	2.8
1	1	256[A]	THR	2.8
1	1	253	ALA	2.8
2	2	169	GLU	2.8
2	2	226	TRP	2.8
3	3	192	PHE	2.8
2	2	168	SER	2.8
1	1	255	ILE	2.8
1	1	292	SER	2.8
3	3	103	LEU	2.7
1	1	140	ILE	2.7
1	1	25	PRO	2.7
1	1	210	PHE	2.7
3	3	28	PHE	2.7
1	1	198	ILE	2.7
1	1	34	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	1	113	THR	2.7
1	1	234	VAL	2.7
2	2	140	THR	2.7
2	2	208	VAL	2.7
2	2	35	TYR	2.7
3	3	60	GLY	2.7
1	1	259	ILE	2.7
3	3	92	LYS	2.7
1	1	219	LEU	2.6
3	3	46	LEU	2.6
3	3	30	VAL	2.6
3	3	179	ILE	2.6
4	4	40	ALA	2.6
1	1	107	PHE	2.6
2	2	36	GLY	2.6
1	1	67	VAL	2.6
1	1	144	TYR	2.6
1	1	230	TYR	2.6
2	2	146	VAL	2.6
4	4	30	ILE	2.6
1	1	152	ALA	2.6
2	2	199	LEU	2.6
3	3	2	LEU	2.6
1	1	236	ILE	2.6
1	1	27	ALA	2.6
1	1	291	ASP	2.5
3	3	41	PHE	2.5
2	2	50	ILE	2.5
1	1	116	ASP	2.5
1	1	271	TRP	2.5
2	2	72	LYS	2.5
1	1	58	SER	2.5
3	3	123[A]	MET	2.5
1	1	95	PHE	2.5
3	3	166	LEU	2.5
1	1	111	ALA	2.5
1	1	166	ALA	2.5
1	1	295	PRO	2.5
2	2	197	ILE	2.5
1	1	300	GLU	2.5
2	2	217	ILE	2.5
2	2	43	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	296	LEU	2.4
1	1	134	LEU	2.4
3	3	212	PHE	2.4
1	1	302	ILE	2.4
2	2	196	ILE	2.4
3	3	180	LYS	2.4
3	3	1	GLY	2.4
3	3	7	THR	2.4
4	4	63	LYS	2.4
1	1	92[A]	VAL	2.4
1	1	185	VAL	2.4
2	2	191	VAL	2.4
4	4	26	ASN	2.3
1	1	177	TRP	2.3
2	2	79	TRP	2.3
2	2	164	SER	2.3
2	2	137	GLU	2.3
1	1	168	ARG	2.3
2	2	138	ALA	2.3
4	4	67	ALA	2.3
2	2	228	LEU	2.3
2	2	63	PHE	2.3
1	1	284	GLU	2.3
2	2	124	VAL	2.3
2	2	184	VAL	2.3
3	3	37	PRO	2.3
2	2	241	ASN	2.3
1	1	305	PHE	2.3
2	2	171	ARG	2.2
1	1	242	LEU	2.2
3	3	224	LEU	2.2
4	4	46	PHE	2.2
1	1	175	TYR	2.2
1	1	231	TYR	2.2
2	2	16	ILE	2.2
1	1	201	VAL	2.2
1	1	218	PRO	2.2
3	3	79[A]	THR	2.2
4	4	29	THR	2.2
1	1	226	SER	2.2
4	4	45	ASP	2.2
1	1	109	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	1	183	PRO	2.2
3	3	231	SER	2.2
1	1	96	ASN	2.2
1	1	203	ILE	2.2
2	2	246	ILE	2.2
2	2	114	ALA	2.1
2	2	170	GLY	2.1
4	4	7	SER	2.1
1	1	57	PRO	2.1
1	1	127	PHE	2.1
2	2	256	PHE	2.1
1	1	207	TYR	2.1
1	1	118	VAL	2.1
3	3	202	GLY	2.1
2	2	234	CYS	2.1
2	2	45	LYS	2.1
3	3	228	ASN	2.1
2	2	66	LEU	2.1
3	3	25	LEU	2.1
1	1	102	ASP	2.1
1	1	172	TRP	2.1
4	4	49	ASP	2.1
3	3	33	PRO	2.1
2	2	161	TYR	2.1
3	3	70	ILE	2.1
1	1	56	VAL	2.1
1	1	217	VAL	2.1
1	1	261	VAL	2.1
1	1	286	VAL	2.1
3	3	199	VAL	2.1
3	3	213	VAL	2.1
2	2	219[A]	CYS	2.1
2	2	42	LEU	2.1
2	2	215	LEU	2.1
3	3	223	LEU	2.1
4	4	28	THR	2.1
2	2	100	TYR	2.1
1	1	171	ALA	2.0
2	2	148	ALA	2.0
4	4	4	GLN	2.0
2	2	108	VAL	2.0
3	3	72	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	1	30	THR	2.0
1	1	31	PRO	2.0
2	2	240	PRO	2.0
1	1	91	GLU	2.0
3	3	133	TYR	2.0
3	3	208	PHE	2.0
4	4	53	PHE	2.0
1	1	298	ALA	2.0
2	2	133	ALA	2.0
2	2	10	SER	2.0
1	1	247	VAL	2.0
4	4	9	LYS	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
8	CA	3	601	1/1	0.73	0.20	43,43,43,43	1
6	HEZ	1	5003	8/8	0.83	0.30	54,59,64,71	0
5	SIA	1	5001	21/21	0.84	0.26	33,45,53,65	0
6	HEZ	1	5002	8/8	0.86	0.25	38,39,49,53	0
9	CL	2	402	1/1	0.94	0.15	36,36,36,36	0
9	CL	1	5010	1/1	0.95	0.18	50,50,50,50	0
8	CA	2	401	1/1	0.96	0.24	27,27,27,27	1
9	CL	3	602	1/1	0.96	0.26	38,38,38,38	0
7	NA	1	5004	1/1	0.97	0.15	27,27,27,27	0
9	CL	1	5009	1/1	0.99	0.10	27,27,27,27	0
8	CA	1	5006	1/1	0.99	0.09	27,27,27,27	0

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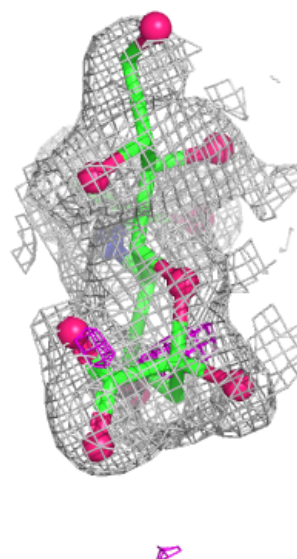
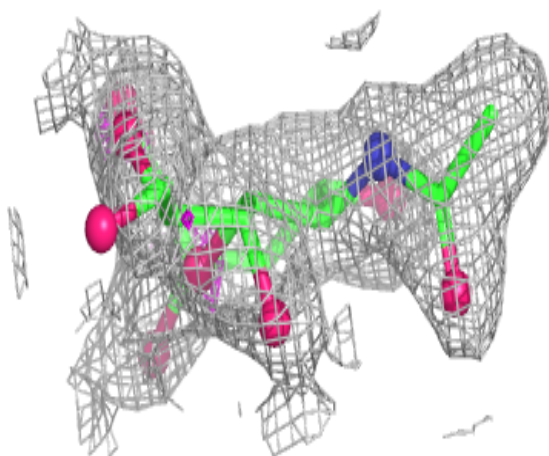
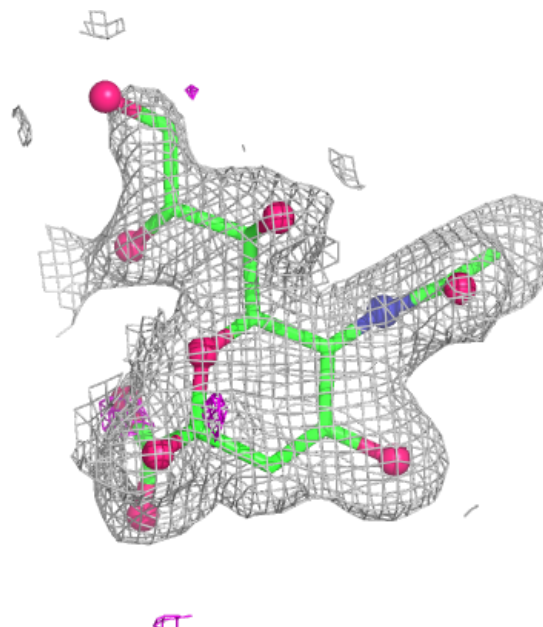
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	1	5007	1/1	0.99	0.08	25,25,25,25	0
9	CL	1	5008	1/1	0.99	0.06	24,24,24,24	0
8	CA	1	5005	1/1	1.00	0.08	23,23,23,23	0

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 1 5001:

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.