



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 07:51 PM EST

PDB ID : 4Q4Y  
Title : Crystal structure of Coxsackievirus A24v soaked with Disialyllacto-N-tetraose (DSLNT)  
Authors : Zocher, G.; Stehle, T.  
Deposited on : 2014-04-15  
Resolution : 1.88 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

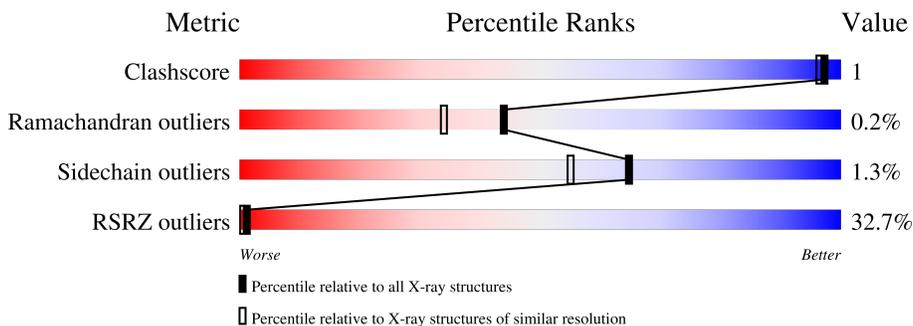
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

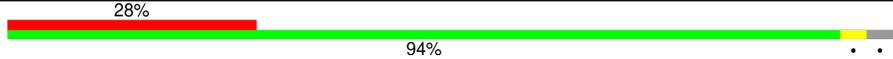
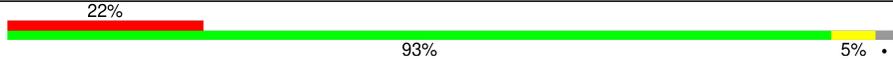
The reported resolution of this entry is 1.88 Å.

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	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1	305	
2	2	271	
3	3	240	
4	4	69	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7431 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 Coxsackievirus capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	281	2255	1433	382	432	8	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	264	2067	1320	342	391	14	0	4	0

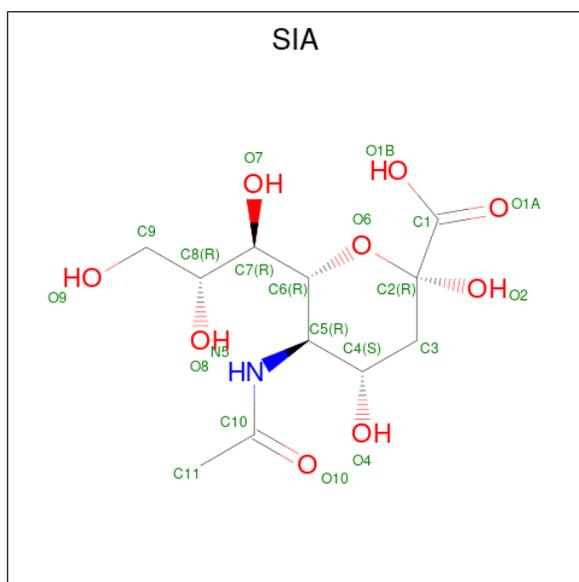
- Molecule 3 is a protein called Coxsackievirus capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	234	1830	1174	290	345	21	0	6	0

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

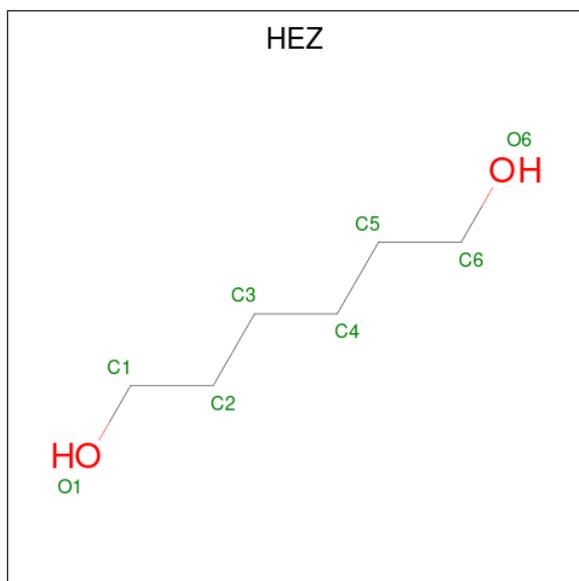
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	57	430	268	71	90	1	0	1	0

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1	3	Total Ca 3 3	0	0
7	2	1	Total Ca 1 1	0	0
7	3	1	Total Ca 1 1	0	0

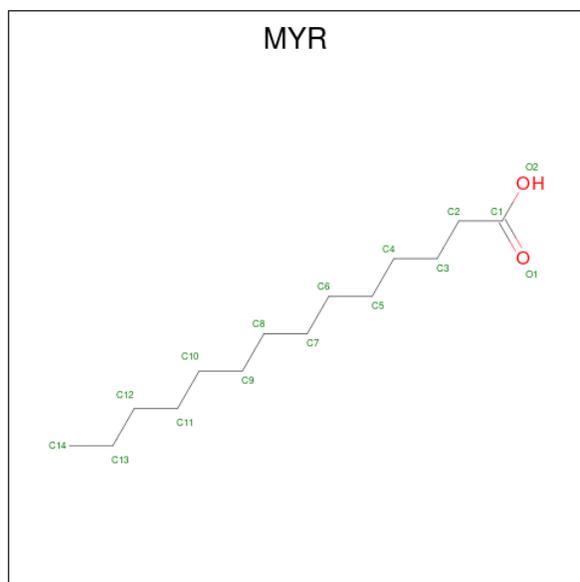
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1	4	Total Cl 4 4	0	0
8	2	1	Total Cl 1 1	0	0
8	3	2	Total Cl 2 2	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	2	1	Total Mg 1 1	0	0

- Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	4	1	Total	C	O	0	0
			6	5	1		

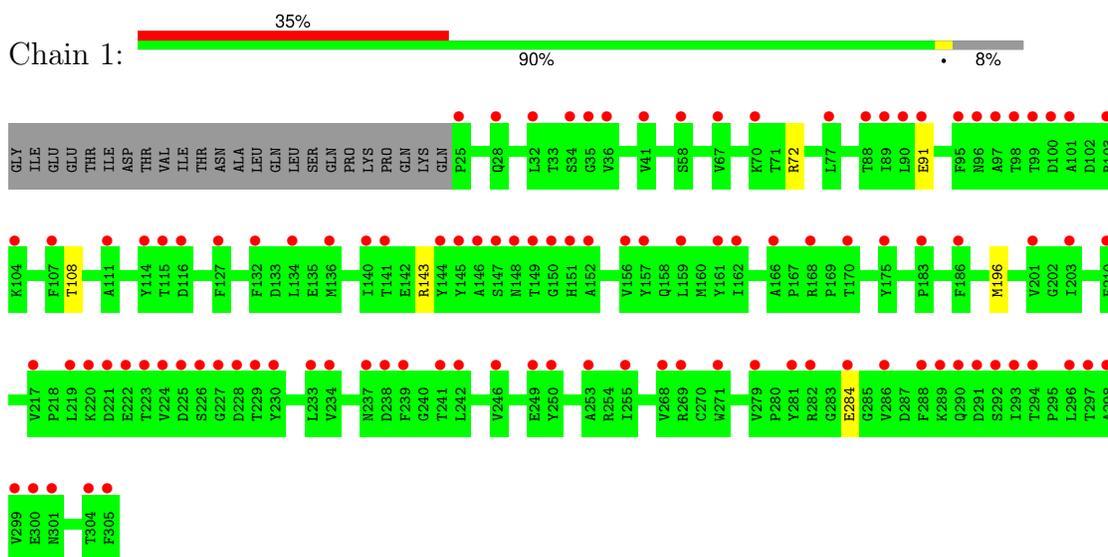
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	1	280	Total	O	0	0
			280	280		
11	2	229	Total	O	0	0
			229	229		
11	3	223	Total	O	0	0
			223	223		
11	4	61	Total	O	0	0
			61	61		

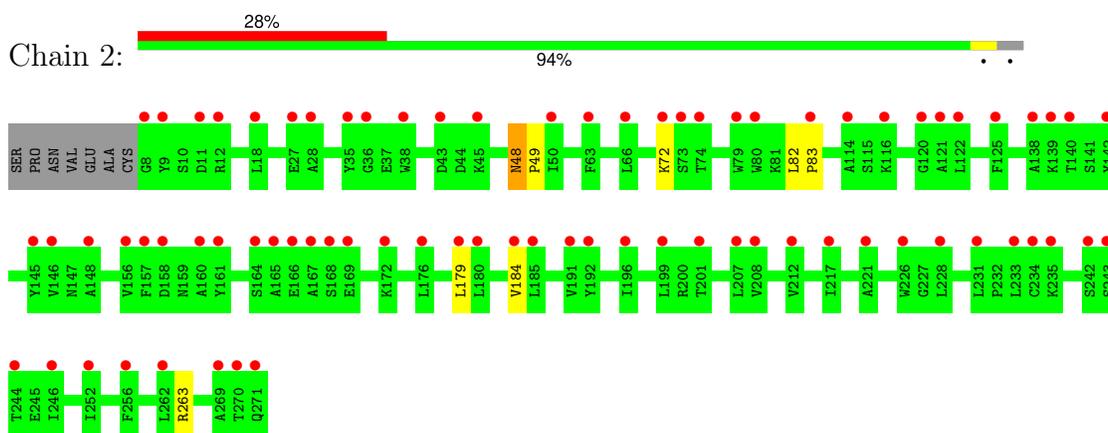
### 3 Residue-property plots [i](#)

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.

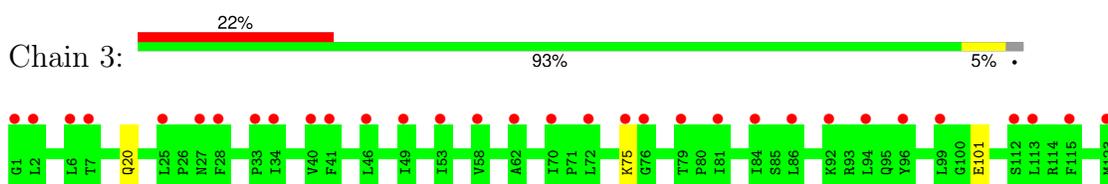
- Molecule 1: Cocksackievirus capsid protein VP1



- Molecule 2: Cocksackievirus capsid protein VP2

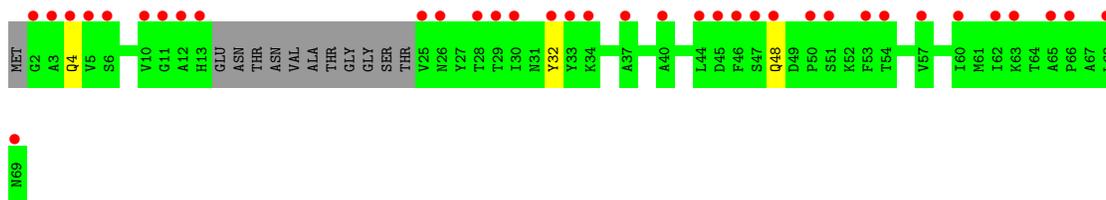
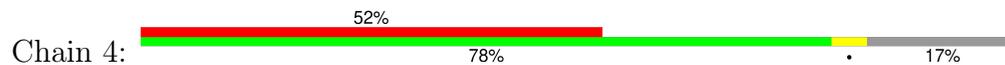


- Molecule 3: Cocksackievirus capsid protein VP3





- Molecule 4: Coxsackievirus capsid protein VP4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	304.48Å 365.30Å 366.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 1.88 49.78 – 1.88	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.78-1.88) 95.5 (49.78-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.157 , (Not available) 0.176 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.6	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.36	EDS
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, HEZ, CA, MG, SIA, MYR

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	0.36	0/2327	0.59	0/3178
2	2	0.30	0/2135	0.59	0/2916
3	3	0.31	0/1898	0.57	0/2585
4	4	0.36	0/440	0.51	0/594
All	All	0.33	0/6800	0.58	0/9273

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

There are no bond length outliers.

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	Peptide,Mainchain

### 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	2255	0	2178	4	0
2	2	2067	0	1996	2	0
3	3	1830	0	1821	5	0
4	4	430	0	407	2	0
5	1	21	0	18	0	0
6	1	16	0	28	0	0
7	1	3	0	0	0	0
7	2	1	0	0	0	0
7	3	1	0	0	0	0
8	1	4	0	0	0	0
8	2	1	0	0	0	0
8	3	2	0	0	0	0
9	2	1	0	0	0	0
10	4	6	0	6	0	0
11	1	280	0	0	1	0
11	2	229	0	0	0	0
11	3	223	0	0	1	0
11	4	61	0	0	0	0
All	All	7431	0	6454	11	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 (11) 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)
1:1:91:GLU:O	1:1:108[B]:THR:HG21	1.77	0.84
3:3:20:GLN:HE22	4:4:32:TYR:H	1.33	0.77
1:1:72:ARG:HH11	4:4:48:GLN:HE22	1.46	0.63
3:3:101:GLU:OE1	3:3:229:HIS:HD2	1.84	0.61
1:1:108[B]:THR:HG22	11:1:6105:HOH:O	2.06	0.55
1:1:91:GLU:O	1:1:108[B]:THR:CG2	2.52	0.52
2:2:48:ASN:HB3	2:2:49:PRO:CD	2.45	0.45
3:3:155:TRP:CD1	3:3:163:CYS:HB2	2.53	0.43
3:3:132[A]:SER:OG	3:3:190[A]:THR:OG1	2.38	0.41
3:3:139:LYS:NZ	11:3:819:HOH:O	2.53	0.41
2:2:179:LEU:HA	2:2:184:VAL:O	2.21	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	1	282/305 (92%)	273 (97%)	9 (3%)	0	100	100
2	2	266/271 (98%)	253 (95%)	11 (4%)	2 (1%)	16	6
3	3	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
4	4	54/69 (78%)	52 (96%)	2 (4%)	0	100	100
All	All	840/885 (95%)	805 (96%)	33 (4%)	2 (0%)	44	34

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	249/268 (93%)	246 (99%)	3 (1%)	67	58
2	2	222/225 (99%)	220 (99%)	2 (1%)	75	69
3	3	213/212 (100%)	210 (99%)	3 (1%)	62	52
4	4	46/57 (81%)	45 (98%)	1 (2%)	47	32
All	All	730/762 (96%)	721 (99%)	9 (1%)	65	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	143	ARG
1	1	196	MET
1	1	284	GLU
2	2	72	LYS
2	2	263	ARG
3	3	75	LYS
3	3	148	MET
3	3	223	LEU
4	4	4	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	65	HIS
2	2	61	ASN
2	2	94	GLN
2	2	225	ASN
3	3	20	GLN
3	3	27	ASN
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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 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	1	5001	-	21,21,21	0.89	1 (4%)	24,31,31	0.98	1 (4%)
10	MYR	4	101	4	4,5,15	0.63	0	3,4,15	0.67	0
6	HEZ	1	5002	-	7,7,7	0.22	0	6,6,6	0.55	0
6	HEZ	1	5003	-	7,7,7	0.32	0	6,6,6	0.36	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	1	5001	-	-	8/20/38/38	0/1/1/1
10	MYR	4	101	4	-	2/3/3/13	-
6	HEZ	1	5002	-	-	1/5/5/5	-
6	HEZ	1	5003	-	-	4/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	5001	SIA	O2-C2	2.67	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	-2.91	119.00	123.85

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	5001	SIA	O1A-C1-C2-O6
5	1	5001	SIA	O1B-C1-C2-O6
10	4	101	MYR	O1-C1-C2-C3
5	1	5001	SIA	O7-C7-C8-C9
5	1	5001	SIA	C6-C7-C8-O8

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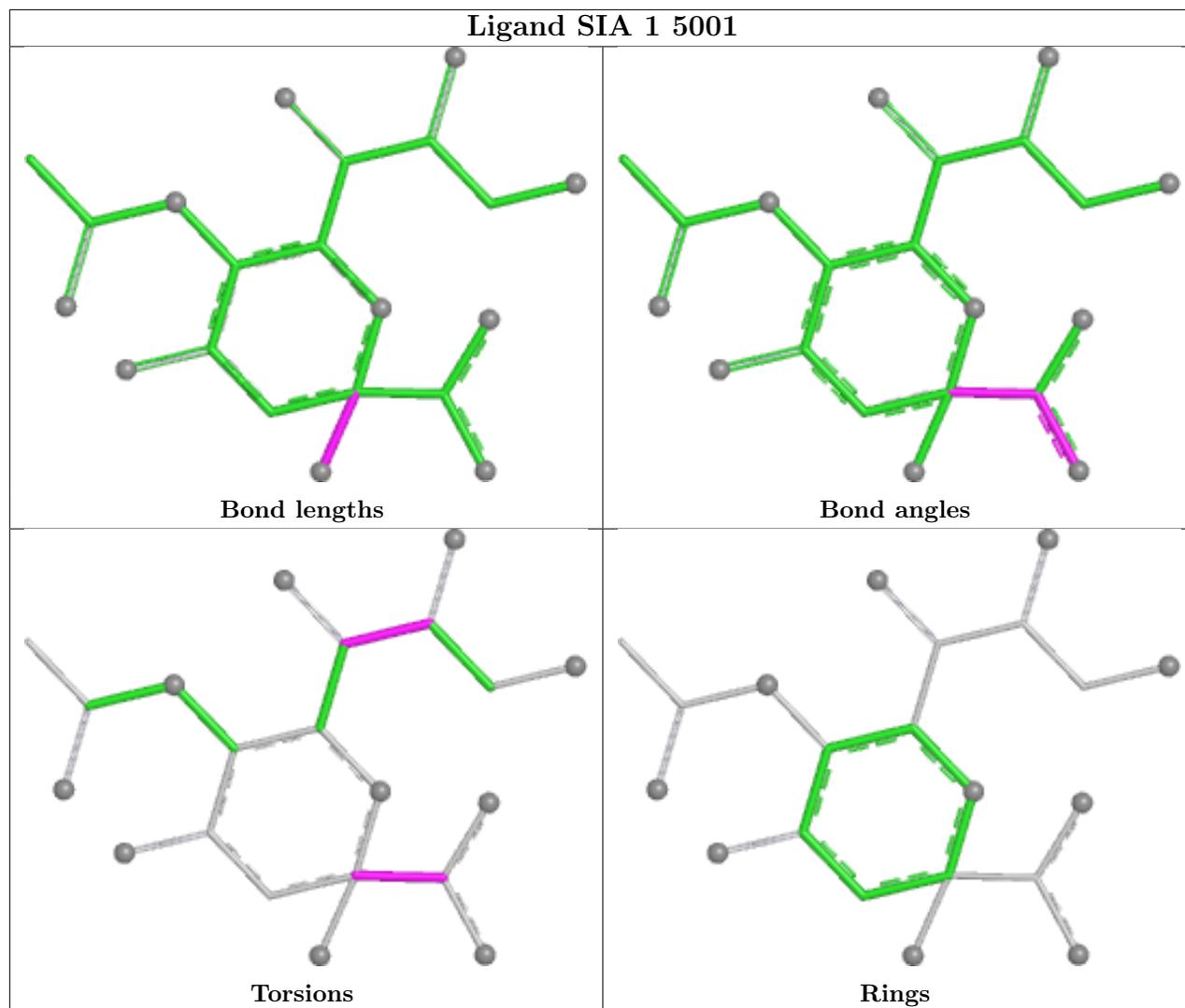
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Mol	Chain	Res	Type	Atoms
6	1	5002	HEZ	O1-C1-C2-C3
6	1	5003	HEZ	C4-C5-C6-O6
6	1	5003	HEZ	C3-C4-C5-C6
6	1	5003	HEZ	O1-C1-C2-C3
5	1	5001	SIA	O7-C7-C8-O8
5	1	5001	SIA	C6-C7-C8-C9
10	4	101	MYR	C1-C2-C3-C4
5	1	5001	SIA	O1A-C1-C2-O2
6	1	5003	HEZ	C1-C2-C3-C4
5	1	5001	SIA	O1B-C1-C2-O2

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 i

### 6.1 Protein, DNA and RNA chains i

**Warning:** The R factor obtained from EDS is 0.541, which does not match the depositor's R factor of 0.15652. Please interpret the results in this section carefully.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	281/305 (92%)	1.90	106 (37%) <span style="border: 1px solid red; padding: 1px;">1</span> <span style="border: 1px solid red; padding: 1px;">0</span>	14, 23, 42, 62	3 (1%)
2	2	264/271 (97%)	1.65	77 (29%) <span style="border: 1px solid red; padding: 1px;">1</span> <span style="border: 1px solid red; padding: 1px;">1</span>	12, 21, 35, 67	4 (1%)
3	3	234/240 (97%)	1.49	54 (23%) <span style="border: 1px solid red; padding: 1px;">2</span> <span style="border: 1px solid red; padding: 1px;">2</span>	13, 21, 28, 53	6 (2%)
4	4	57/69 (82%)	2.64	36 (63%) <span style="border: 1px solid red; padding: 1px;">0</span> <span style="border: 1px solid red; padding: 1px;">0</span>	14, 28, 40, 63	1 (1%)
All	All	836/885 (94%)	1.76	273 (32%) <span style="border: 1px solid red; padding: 1px;">1</span> <span style="border: 1px solid red; padding: 1px;">0</span>	12, 22, 37, 67	14 (1%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	148	ASN	8.2
2	2	165	ALA	7.9
4	4	13	HIS	7.6
2	2	9	TYR	7.4
2	2	271	GLN	6.8
1	1	225	ASP	6.7
1	1	223	THR	6.5
4	4	4	GLN	6.5
4	4	69	ASN	6.4
1	1	224	VAL	6.1
2	2	166	GLU	6.1
2	2	8	GLY	5.7
3	3	234	THR	5.7
2	2	167	ALA	5.3
4	4	3	ALA	5.2
1	1	103	ARG	5.2
1	1	145	TYR	4.9
2	2	169	GLU	4.8
1	1	98	THR	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	168	ARG	4.7
1	1	226	SER	4.7
4	4	60	ILE	4.6
1	1	114	TYR	4.6
1	1	101	ALA	4.5
4	4	25	VAL	4.4
1	1	146	ALA	4.4
4	4	2	GLY	4.3
1	1	228	ASP	4.3
1	1	293	ILE	4.2
2	2	242	SER	4.2
1	1	104	LYS	4.1
1	1	221	ASP	4.1
4	4	44	LEU	4.1
1	1	100	ASP	4.1
1	1	25	PRO	4.1
1	1	147	SER	4.0
1	1	297	THR	3.9
3	3	99	LEU	3.9
2	2	168	SER	3.8
1	1	151	HIS	3.7
1	1	150	GLY	3.7
1	1	34	SER	3.6
4	4	10	VAL	3.5
1	1	300	GLU	3.5
4	4	5	VAL	3.4
4	4	40	ALA	3.4
3	3	113	LEU	3.4
4	4	62	ILE	3.4
4	4	68	LEU	3.4
1	1	220	LYS	3.3
1	1	233	LEU	3.3
1	1	290	GLN	3.3
4	4	63	LYS	3.3
1	1	149	THR	3.3
1	1	170	THR	3.3
4	4	28	THR	3.3
2	2	11	ASP	3.3
3	3	159	LEU	3.3
1	1	36	VAL	3.2
4	4	12	ALA	3.2
3	3	123	MET	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	152	ALA	3.2
3	3	233	ARG	3.2
3	3	229	HIS	3.2
4	4	29	THR	3.1
1	1	140	ILE	3.1
4	4	30	ILE	3.1
2	2	138	ALA	3.1
3	3	41	PHE	3.1
1	1	41	VAL	3.1
2	2	180	LEU	3.1
2	2	212	VAL	3.1
3	3	199	VAL	3.1
1	1	227	GLY	3.0
1	1	90	LEU	3.0
1	1	234	VAL	3.0
2	2	228	LEU	3.0
2	2	233	LEU	3.0
1	1	291	ASP	3.0
1	1	253	ALA	3.0
1	1	292	SER	2.9
1	1	281	TYR	2.9
2	2	192	TYR	2.9
1	1	288	PHE	2.9
1	1	97	ALA	2.9
2	2	142	TYR	2.9
1	1	159	LEU	2.9
3	3	2	LEU	2.9
3	3	86	LEU	2.9
2	2	45	LYS	2.9
2	2	235	LYS	2.9
1	1	89	ILE	2.9
1	1	217	VAL	2.9
2	2	196	ILE	2.8
1	1	32	LEU	2.8
1	1	230	TYR	2.8
2	2	256	PHE	2.8
3	3	139	LYS	2.8
3	3	27	ASN	2.8
2	2	73	SER	2.8
4	4	57	VAL	2.8
3	3	180	LYS	2.8
4	4	51	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	134	LEU	2.8
3	3	25	LEU	2.7
1	1	127	PHE	2.7
1	1	67	VAL	2.7
1	1	299	VAL	2.7
2	2	270	THR	2.7
4	4	26	ASN	2.7
1	1	239	PHE	2.7
1	1	304	THR	2.7
3	3	92	LYS	2.7
3	3	115	PHE	2.7
3	3	197	ILE	2.7
2	2	139	LYS	2.7
2	2	38	TRP	2.6
4	4	11	GLY	2.6
2	2	140	THR	2.6
2	2	244	THR	2.6
4	4	47	SER	2.6
2	2	35	TYR	2.6
2	2	36	GLY	2.6
4	4	65	ALA	2.6
4	4	50	PRO	2.6
2	2	199	LEU	2.6
1	1	132	PHE	2.6
1	1	271	TRP	2.6
1	1	286	VAL	2.6
2	2	146	VAL	2.6
1	1	116	ASP	2.6
1	1	201	VAL	2.5
2	2	83	PRO	2.5
1	1	162	ILE	2.5
1	1	219	LEU	2.5
3	3	6	LEU	2.5
1	1	115	THR	2.5
2	2	160	ALA	2.5
2	2	157	PHE	2.5
1	1	255	ILE	2.5
1	1	99	THR	2.5
2	2	72	LYS	2.5
2	2	172	LYS	2.5
3	3	75	LYS	2.5
4	4	6	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	1	88	THR	2.5
3	3	28	PHE	2.5
1	1	77	LEU	2.4
3	3	70	ILE	2.4
1	1	268	VAL	2.4
2	2	164	SER	2.4
4	4	46	PHE	2.4
3	3	1	GLY	2.4
2	2	122	LEU	2.4
3	3	34	ILE	2.4
3	3	154	ILE	2.4
2	2	43	ASP	2.4
4	4	53	PHE	2.4
1	1	144	TYR	2.4
1	1	250	TYR	2.4
1	1	241	THR	2.4
1	1	35	GLY	2.4
1	1	157	TYR	2.4
1	1	161	TYR	2.4
4	4	32	TYR	2.4
1	1	282	ARG	2.3
2	2	185	LEU	2.3
2	2	207[A]	LEU	2.3
2	2	50	ILE	2.3
4	4	66	PRO	2.3
1	1	237	ASN	2.3
3	3	96	TYR	2.3
2	2	18	LEU	2.3
1	1	203	ILE	2.3
4	4	37	ALA	2.3
2	2	120	GLY	2.3
3	3	213	VAL	2.3
2	2	74	THR	2.3
3	3	183	PHE	2.3
4	4	54	THR	2.3
4	4	48	GLN	2.3
2	2	252	ILE	2.3
3	3	81	ILE	2.3
3	3	230	ILE	2.3
1	1	156	VAL	2.3
3	3	58	VAL	2.3
1	1	186	PHE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	2	179	LEU	2.3
1	1	111	ALA	2.2
1	1	28	GLN	2.2
1	1	91	GLU	2.2
2	2	63	PHE	2.2
3	3	208	PHE	2.2
2	2	243	SER	2.2
2	2	269	ALA	2.2
1	1	183	PRO	2.2
1	1	289	LYS	2.2
2	2	231	LEU	2.2
2	2	262	LEU	2.2
2	2	114	ALA	2.2
1	1	249	GLU	2.2
2	2	158	ASP	2.2
1	1	269	ARG	2.2
1	1	294	THR	2.2
3	3	7	THR	2.2
2	2	156	VAL	2.2
2	2	208	VAL	2.2
1	1	96	ASN	2.2
1	1	107	PHE	2.2
1	1	305	PHE	2.2
2	2	80	TRP	2.2
2	2	226	TRP	2.2
3	3	33	PRO	2.2
1	1	58	SER	2.1
1	1	246	VAL	2.1
1	1	222	GLU	2.1
3	3	192	PHE	2.1
1	1	296	LEU	2.1
2	2	221	ALA	2.1
3	3	46	LEU	2.1
3	3	72	LEU	2.1
2	2	79	TRP	2.1
2	2	12	ARG	2.1
3	3	49	ILE	2.1
1	1	229	THR	2.1
2	2	116	LYS	2.1
2	2	27	GLU	2.1
1	1	279	VAL	2.1
1	1	95	PHE	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	298	ALA	2.1
2	2	66	LEU	2.1
2	2	121	ALA	2.1
2	2	148	ALA	2.1
3	3	94	LEU	2.1
3	3	219	PHE	2.1
1	1	238	ASP	2.1
2	2	145	TYR	2.1
2	2	161	TYR	2.1
3	3	190[A]	THR	2.1
1	1	301[A]	ASN	2.1
3	3	76	GLY	2.1
2	2	184	VAL	2.1
2	2	234	CYS	2.1
3	3	216	CYS	2.1
1	1	166	ALA	2.1
4	4	45	ASP	2.1
2	2	246	ILE	2.1
3	3	53	ILE	2.1
3	3	84	ILE	2.1
3	3	112	SER	2.1
1	1	136[A]	MET	2.1
1	1	141	THR	2.1
1	1	284	GLU	2.1
3	3	198	VAL	2.0
2	2	28	ALA	2.0
3	3	62	ALA	2.0
1	1	242	LEU	2.0
2	2	176	LEU	2.0
1	1	210	PHE	2.0
3	3	212	PHE	2.0
4	4	34	LYS	2.0
2	2	201	THR	2.0
2	2	217	ILE	2.0
3	3	79	THR	2.0
3	3	129	ILE	2.0
3	3	179	ILE	2.0
1	1	175	TYR	2.0
4	4	33	TYR	2.0
1	1	70	LYS	2.0
2	2	191	VAL	2.0
3	3	40	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	3	174	VAL	2.0
2	2	125	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

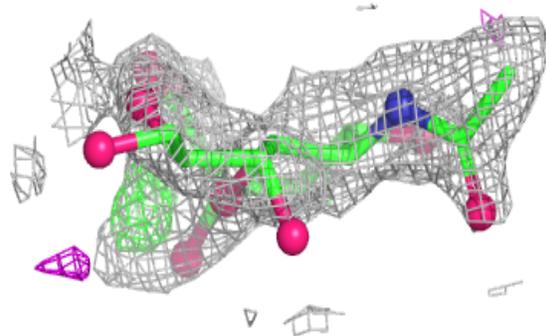
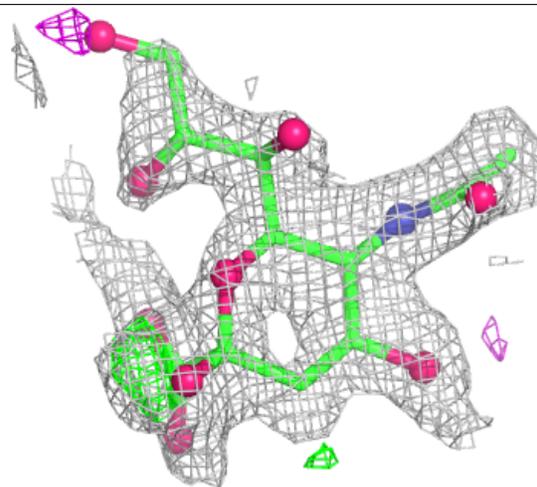
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	SIA	1	5001	21/21	0.79	0.31	26,38,44,55	21
7	CA	3	601	1/1	0.82	0.50	27,27,27,27	1
9	MG	2	402	1/1	0.83	0.26	42,42,42,42	0
6	HEZ	1	5002	8/8	0.85	0.28	39,42,56,60	0
6	HEZ	1	5003	8/8	0.86	0.29	57,63,65,67	0
10	MYR	4	101	6/16	0.91	0.21	46,49,57,58	0
8	CL	3	603	1/1	0.93	0.19	42,42,42,42	0
8	CL	3	602	1/1	0.95	0.25	39,39,39,39	0
7	CA	2	401	1/1	0.95	0.18	26,26,26,26	1
8	CL	1	5009	1/1	0.96	0.18	42,42,42,42	0
8	CL	1	5010	1/1	0.96	0.26	40,40,40,40	0
7	CA	1	5005	1/1	0.98	0.10	25,25,25,25	0
7	CA	1	5006	1/1	0.98	0.14	34,34,34,34	0
8	CL	1	5008	1/1	0.99	0.12	28,28,28,28	0
7	CA	1	5004	1/1	0.99	0.11	21,21,21,21	0
8	CL	1	5007	1/1	0.99	0.09	23,23,23,23	0
8	CL	2	403	1/1	0.99	0.06	30,30,30,30	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.