



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 6TSD / pdb_00006tsd
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 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

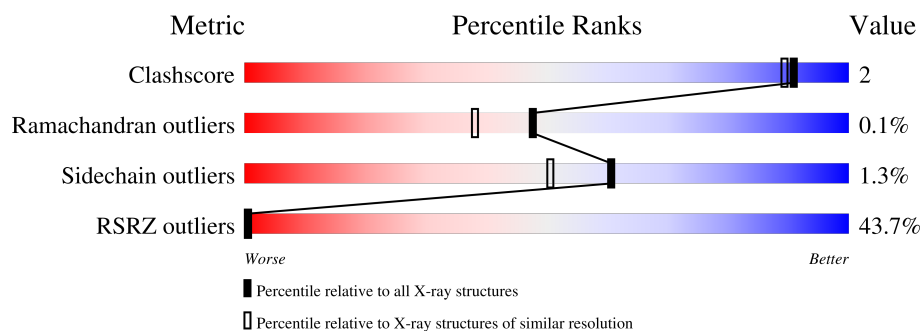
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	43% 89% 8%
2	222	271	41% 94%
3	333	240	32% 94%
4	444	69	65% 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

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
1	111	281	Total	C	N	O	S	0	8	0
			2275	1450	382	435	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	3	0
			2062	1315	342	391	14			

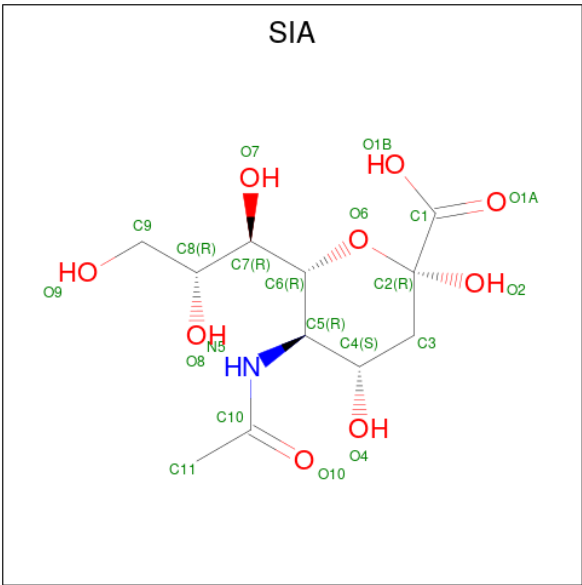
- Molecule 3 is a protein called Capsid protein VP3.

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

- Molecule 4 is a protein called Capsid protein VP4.

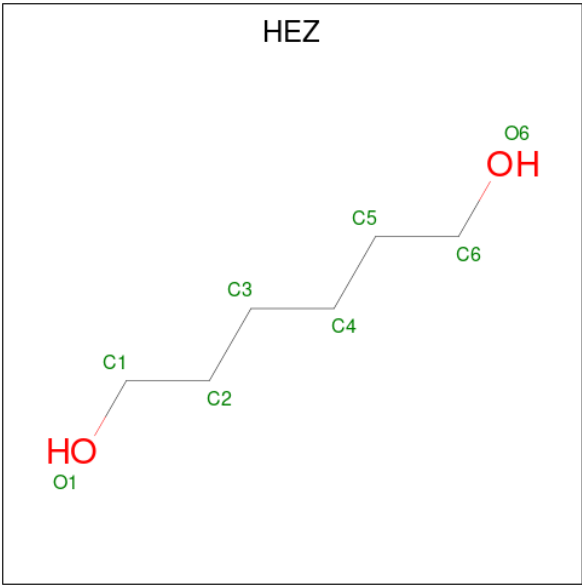
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	444	57	Total	C	N	O	S	0	2	0
			431	271	70	89	1			

- 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		
6	111	1	Total	C	O	0	0
			8	6	2		
6	222	1	Total	C	O	0	0
			8	6	2		

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is water.

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

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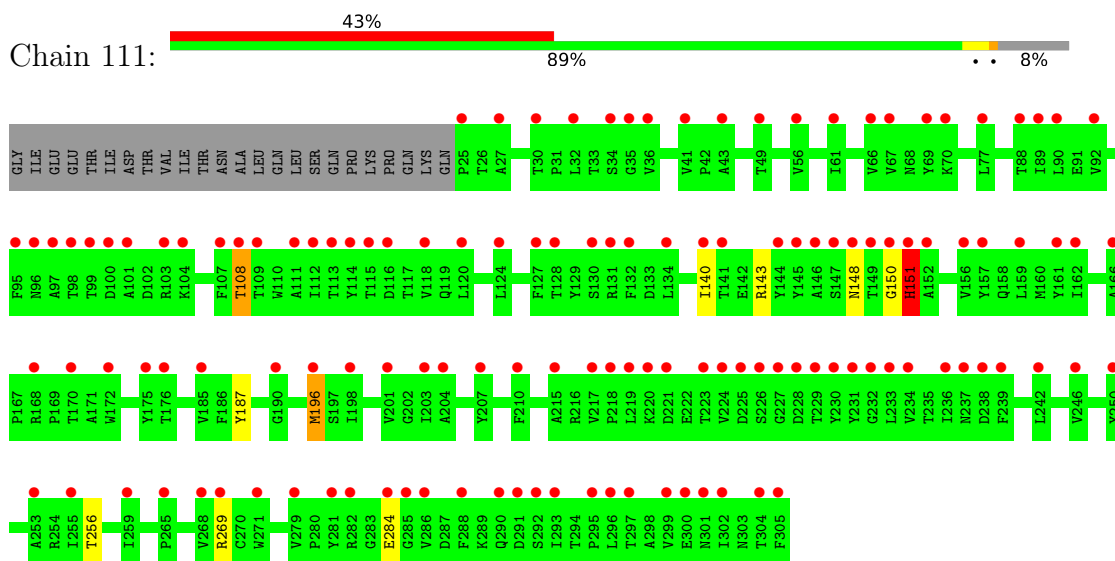
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	333	225	Total 225	O 225	0	0
11	444	70	Total 70	O 70	0	0

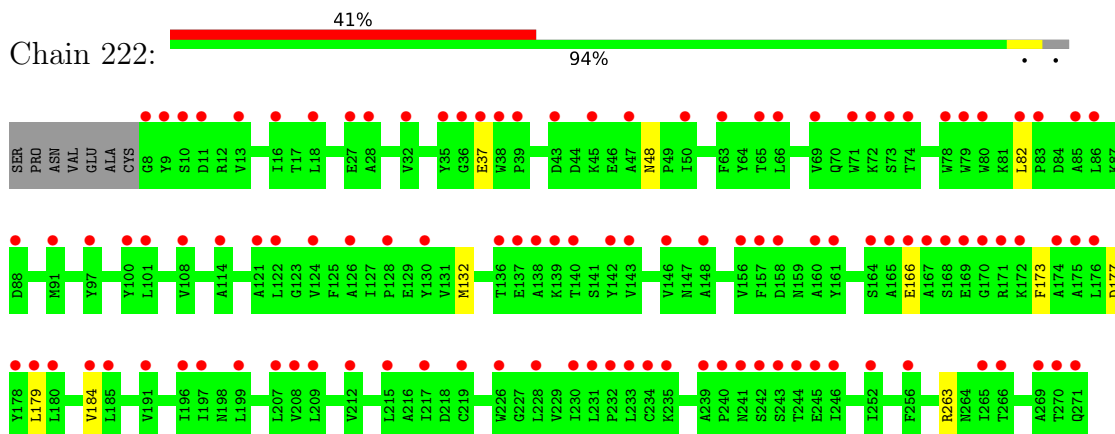
3 Residue-property plots

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

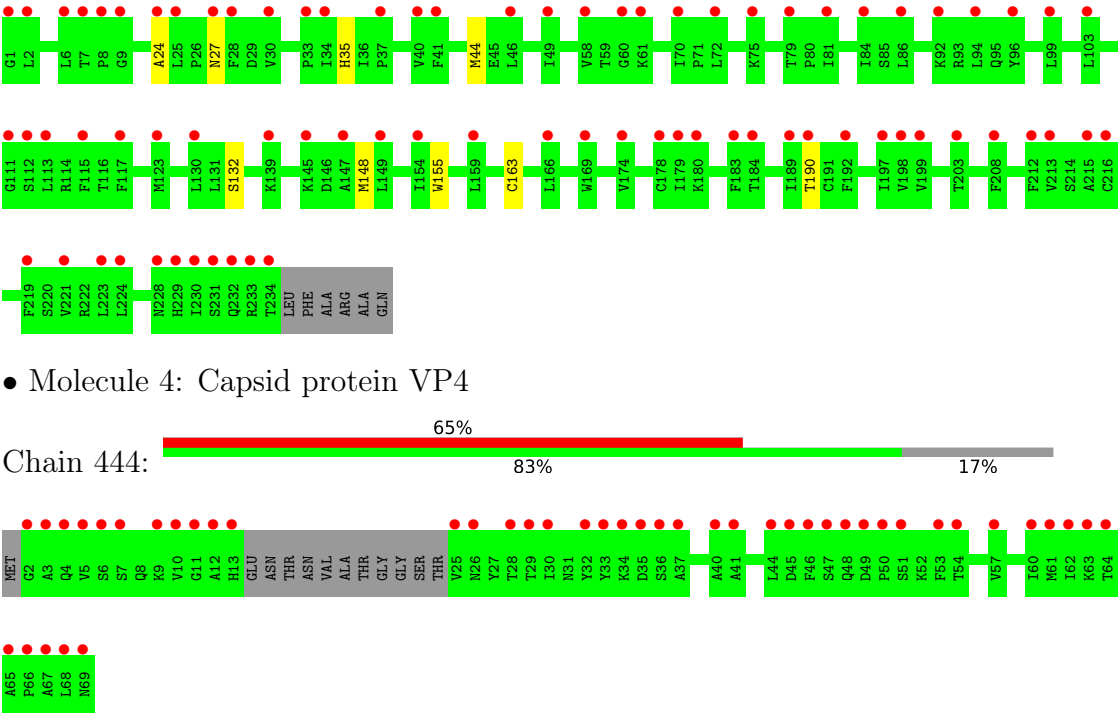


• Molecule 2: Capsid protein VP2



• Molecule 3: Capsid protein VP3





● Molecule 4: Capsid protein VP4

Chain 444:

65%

83%

17%

4 Data and refinement statistics

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) 99.8 (49.95-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0232 2018/13/08	Depositor
R, R_{free}	0.150 , (Not available) (Not available) , (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)	0.41 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.48	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.*

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: NA, SIA, CL, HEZ, MG, 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	111	0.93	1/2362 (0.0%)	1.12	0/3228
2	222	0.90	0/2127	1.14	1/2905 (0.0%)
3	333	0.92	0/1919	1.11	0/2613
4	444	0.98	0/444	1.21	0/601
All	All	0.92	1/6852 (0.0%)	1.13	1/9347 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	111	151	HIS	CE1-NE2	6.02	1.38	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	222	177	ASP	CA-CB-CG	5.60	118.20	112.60

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	8	0
2	222	2062	0	1985	3	0
3	333	1842	0	1841	6	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	22	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 2.

All (22) 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
1:111:150:GLY:C	1:111:151:HIS:ND1	2.63	0.56
3:333:27:ASN:ND2	11:333:402:HOH:O	2.32	0.55
6:111:502:HEZ:C4	6:111:503:HEZ:H41	2.39	0.53
1:111:151:HIS:ND1	1:111:151:HIS:N	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:333:132[A]:SER:OG	3:333:190[A]:THR:OG1	2.28	0.51
1:111:196:MET:HG3	3:333:24:ALA:HB2	1.92	0.51
1:111:108[A]:THR:HG23	11:111:606:HOH:O	2.11	0.50
1:111:140[B]:ILE:HD12	1:111:187:TYR:CD2	2.47	0.49
3:333:44[B]:MET:HE2	3:333:44[B]:MET:HA	1.97	0.47
2:222:179:LEU:HA	2:222:184:VAL:O	2.16	0.45
3:333:155:TRP:CD1	3:333:163:CYS:HB2	2.52	0.45
6:111:502:HEZ:C5	6:111:503:HEZ:H41	2.49	0.42
5:111:501:SIA:O1A	5:111:501:SIA:O9	2.35	0.42
6:111:502:HEZ:H61	6:111:503:HEZ:C4	2.49	0.42
1:111:269:ARG:NH1	11:111:609:HOH:O	2.53	0.42
2:222:37:GLU:CD	3:333:35:HIS:HE2	2.27	0.41
1:111:196:MET:HE3	1:111:196:MET:HB3	1.96	0.41
2:222:132[B]:MET:HB2	2:222:173:PHE:CD1	2.56	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	111	287/305 (94%)	276 (96%)	11 (4%)	0	100	100
2	222	265/271 (98%)	250 (94%)	14 (5%)	1 (0%)	30	19
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%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	222	48	ASN

5.3.2 Protein sidechains ⓘ

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%)	38	21
2	222	221/225 (98%)	219 (99%)	2 (1%)	70	62
3	333	215/212 (101%)	214 (100%)	1 (0%)	81	77
4	444	47/57 (82%)	47 (100%)	0	100	100
All	All	737/762 (97%)	727 (99%)	10 (1%)	61	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	111	108[A]	THR
1	111	108[B]	THR
1	111	143	ARG
1	111	148	ASN
1	111	151	HIS
1	111	196	MET
1	111	284	GLU
2	222	166	GLU
2	222	263	ARG
3	333	148	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 [i](#)

There are no oligosaccharides 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
6	HEZ	222	4102	-	7,7,7	0.07	0	6,6,6	0.07	0
6	HEZ	111	503	-	7,7,7	2.02	3 (42%)	6,6,6	0.96	0
5	SIA	111	501	-	21,21,21	0.96	1 (4%)	24,31,31	1.34	3 (12%)
6	HEZ	111	502	-	7,7,7	1.55	2 (28%)	6,6,6	0.93	0
6	HEZ	222	4101	-	7,7,7	0.18	0	6,6,6	0.10	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	222	4102	-	-	3/5/5/5	-
6	HEZ	111	503	-	-	4/5/5/5	-
5	SIA	111	501	-	-	4/20/38/38	0/1/1/1
6	HEZ	111	502	-	-	2/5/5/5	-
6	HEZ	222	4101	-	-	3/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	111	503	HEZ	C5-C4	3.39	1.68	1.51
6	111	502	HEZ	C5-C4	3.27	1.68	1.51
5	111	501	SIA	O2-C2	2.59	1.43	1.39
6	111	503	HEZ	C3-C2	2.44	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	111	503	HEZ	C5-C6	2.38	1.64	1.51
6	111	502	HEZ	C3-C2	2.23	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	111	501	SIA	O6-C6-C7	3.49	112.11	106.65
5	111	501	SIA	O2-C2-C1	-2.87	104.67	110.73
5	111	501	SIA	O1A-C1-C2	-2.14	120.28	123.85

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	111	503	HEZ	O1-C1-C2-C3
6	111	503	HEZ	C3-C4-C5-C6
6	222	4101	HEZ	C2-C3-C4-C5
6	222	4101	HEZ	C1-C2-C3-C4
6	111	502	HEZ	O1-C1-C2-C3
5	111	501	SIA	O8-C8-C9-O9
6	111	503	HEZ	C4-C5-C6-O6
6	111	503	HEZ	C2-C3-C4-C5
5	111	501	SIA	C6-C7-C8-C9
6	222	4102	HEZ	C3-C4-C5-C6
5	111	501	SIA	O1B-C1-C2-O2
6	222	4101	HEZ	C4-C5-C6-O6
6	111	502	HEZ	C3-C4-C5-C6
6	222	4102	HEZ	C1-C2-C3-C4
6	222	4102	HEZ	C4-C5-C6-O6
5	111	501	SIA	C7-C8-C9-O9

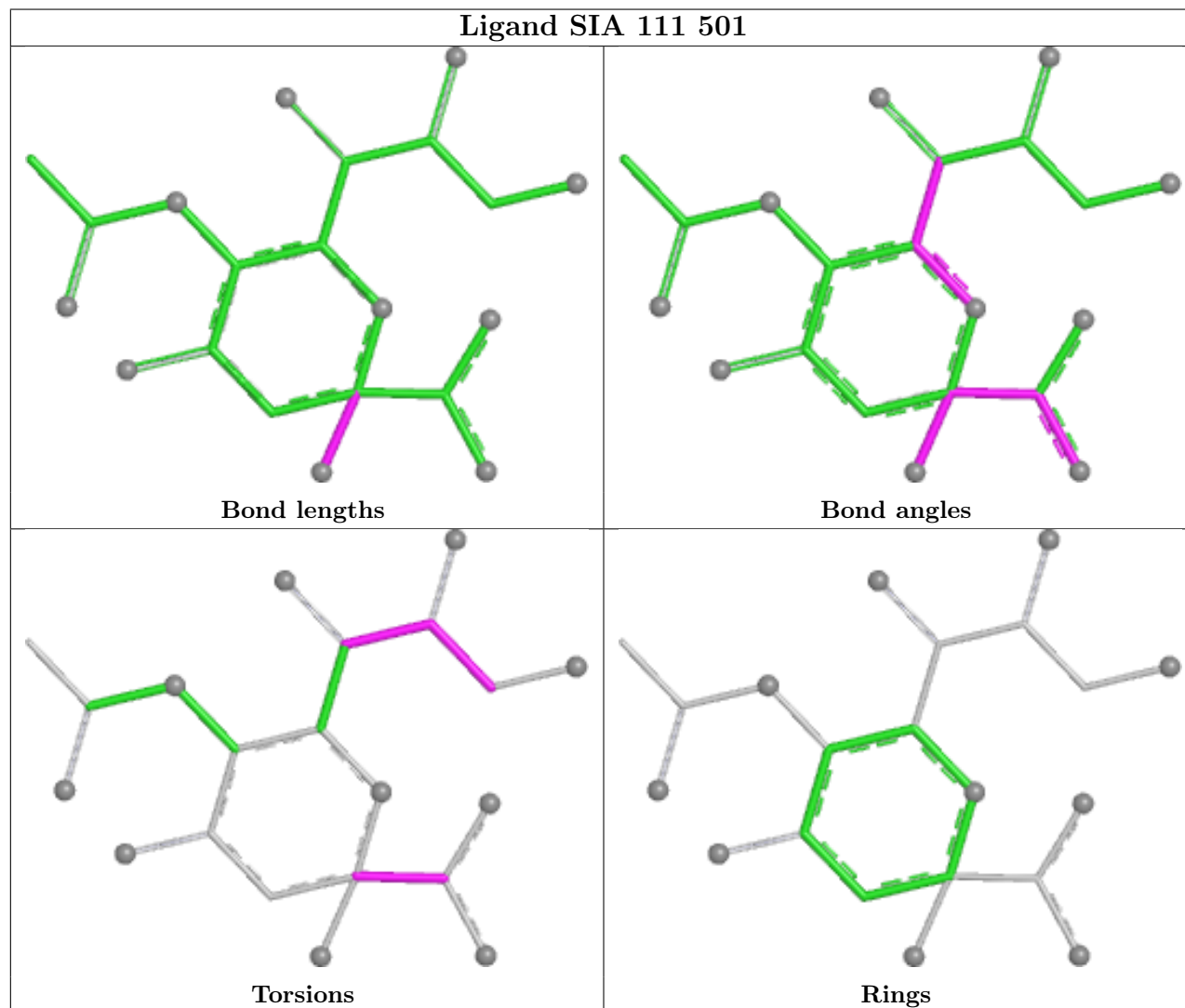
There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

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%)	2.16	131 (46%) 0 0	17, 29, 49, 82	8 (2%)
2	222	264/271 (97%)	1.97	112 (42%) 0 0	16, 28, 42, 76	3 (1%)
3	333	234/240 (97%)	1.77	77 (32%) 1 1	16, 28, 36, 47	10 (4%)
4	444	57/69 (82%)	2.96	45 (78%) 0 0	19, 35, 52, 73	2 (3%)
All	All	836/885 (94%)	2.04	365 (43%) 0 0	16, 28, 45, 82	23 (2%)

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	333	234[A]	THR	10.5
1	111	148	ASN	8.2
2	222	271	GLN	7.5
2	222	166	GLU	7.5
4	444	25	VAL	7.3
2	222	8	GLY	7.0
1	111	151	HIS	6.6
4	444	13	HIS	6.4
1	111	224	VAL	6.3
1	111	114	TYR	5.9
2	222	165	ALA	5.8
4	444	69	ASN	5.8
2	222	9	TYR	5.8
1	111	297	THR	5.8
4	444	10	VAL	5.6
1	111	223	THR	5.5
1	111	225	ASP	5.5
4	444	44	LEU	5.4
2	222	167	ALA	5.4
4	444	2	GLY	5.3
4	444	4	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	111	145	TYR	5.2
2	222	242	SER	5.0
1	111	104	LYS	4.9
4	444	60	ILE	4.7
1	111	98	THR	4.7
1	111	25	PRO	4.6
1	111	103	ARG	4.6
4	444	3	ALA	4.5
3	333	233	ARG	4.5
2	222	169	GLU	4.5
4	444	63	LYS	4.4
1	111	221	ASP	4.4
2	222	270	THR	4.4
1	111	147	SER	4.3
2	222	11	ASP	4.3
3	333	123	MET	4.3
1	111	34	SER	4.2
1	111	228	ASP	4.1
1	111	293	ILE	4.1
4	444	5	VAL	4.1
1	111	100[A]	ASP	4.1
1	111	170	THR	4.1
3	333	86	LEU	4.0
4	444	12	ALA	4.0
1	111	299	VAL	4.0
3	333	28	PHE	4.0
2	222	168	SER	3.9
1	111	227	GLY	3.9
1	111	291	ASP	3.9
1	111	168	ARG	3.9
3	333	159	LEU	3.9
2	222	74	THR	3.9
1	111	146	ALA	3.8
1	111	237	ASN	3.8
2	222	180	LEU	3.8
1	111	32	LEU	3.8
1	111	101	ALA	3.8
2	222	138	ALA	3.8
1	111	300	GLU	3.8
1	111	150	GLY	3.7
2	222	269	ALA	3.7
2	222	243	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	111	97	ALA	3.7
2	222	235	LYS	3.7
4	444	40	ALA	3.7
1	111	226	SER	3.7
1	111	268	VAL	3.7
1	111	149	THR	3.6
2	222	73	SER	3.6
1	111	255	ILE	3.6
1	111	108[A]	THR	3.6
2	222	72	LYS	3.6
3	333	99	LEU	3.6
3	333	113	LEU	3.6
1	111	230	TYR	3.5
2	222	43	ASP	3.5
1	111	190	GLY	3.5
1	111	27	ALA	3.5
1	111	134	LEU	3.5
1	111	90	LEU	3.4
2	222	233	LEU	3.4
3	333	46	LEU	3.4
1	111	115	THR	3.4
4	444	30	ILE	3.4
2	222	36	GLY	3.4
1	111	288	PHE	3.4
4	444	28	THR	3.4
4	444	29	THR	3.4
4	444	11	GLY	3.3
1	111	89	ILE	3.3
2	222	50	ILE	3.3
4	444	47	SER	3.3
2	222	114	ALA	3.3
1	111	239	PHE	3.3
1	111	152	ALA	3.3
1	111	290	GLN	3.3
3	333	41	PHE	3.3
2	222	148	ALA	3.2
2	222	146	VAL	3.2
3	333	198	VAL	3.2
4	444	46	PHE	3.2
2	222	35	TYR	3.2
4	444	68	LEU	3.2
3	333	183	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	111	112	ILE	3.2
2	222	142	TYR	3.2
2	222	217	ILE	3.1
4	444	62	ILE	3.1
1	111	66	VAL	3.1
1	111	253	ALA	3.1
1	111	77	LEU	3.1
3	333	75	LYS	3.1
2	222	83	PRO	3.1
1	111	144	TYR	3.1
1	111	233	LEU	3.1
2	222	228	LEU	3.1
1	111	41	VAL	3.1
1	111	185	VAL	3.0
1	111	201	VAL	3.0
1	111	234	VAL	3.0
2	222	212	VAL	3.0
1	111	296	LEU	3.0
1	111	281	TYR	3.0
4	444	51[A]	SER	3.0
2	222	124	VAL	3.0
1	111	271	TRP	3.0
3	333	92	LYS	3.0
2	222	234	CYS	3.0
3	333	34	ILE	3.0
2	222	66	LEU	2.9
1	111	35	GLY	2.9
2	222	136	THR	2.9
4	444	67	ALA	2.9
1	111	292	SER	2.9
3	333	58	VAL	2.9
2	222	160	ALA	2.9
1	111	220	LYS	2.9
1	111	140[A]	ILE	2.9
2	222	246	ILE	2.9
3	333	49	ILE	2.9
1	111	219	LEU	2.9
2	222	207	LEU	2.9
1	111	250	TYR	2.9
3	333	229	HIS	2.9
4	444	53	PHE	2.9
2	222	172	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	111	118	VAL	2.8
1	111	304	THR	2.8
3	333	96	TYR	2.8
2	222	45	LYS	2.8
1	111	127	PHE	2.8
2	222	196	ILE	2.8
1	111	286	VAL	2.8
1	111	161	TYR	2.8
3	333	27	ASN	2.8
2	222	185	LEU	2.8
3	333	72	LEU	2.8
2	222	244	THR	2.8
2	222	191	VAL	2.8
1	111	111	ALA	2.8
2	222	231	LEU	2.8
3	333	94	LEU	2.8
1	111	236	ILE	2.8
1	111	67	VAL	2.8
4	444	57	VAL	2.8
3	333	1	GLY	2.7
3	333	25	LEU	2.7
3	333	179	ILE	2.7
1	111	130	SER	2.7
1	111	246	VAL	2.7
2	222	85	ALA	2.7
1	111	305	PHE	2.7
1	111	99	THR	2.7
4	444	45	ASP	2.7
2	222	27	GLU	2.7
2	222	13	VAL	2.7
2	222	208	VAL	2.7
2	222	38	TRP	2.7
1	111	132	PHE	2.7
1	111	218	PRO	2.7
3	333	180	LYS	2.6
2	222	122	LEU	2.6
1	111	204	ALA	2.6
2	222	121	ALA	2.6
2	222	63	PHE	2.6
3	333	2	LEU	2.6
3	333	130	LEU	2.6
1	111	198	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	111	36	VAL	2.6
1	111	92[A]	VAL	2.6
1	111	284	GLU	2.6
2	222	137	GLU	2.6
3	333	199	VAL	2.6
3	333	115	PHE	2.6
1	111	159	LEU	2.6
2	222	139	LYS	2.6
1	111	279	VAL	2.6
3	333	40	VAL	2.6
4	444	65	ALA	2.6
1	111	96	ASN	2.6
4	444	6	SER	2.6
2	222	140	THR	2.6
1	111	175	TYR	2.5
2	222	179	LEU	2.5
1	111	61	ILE	2.5
2	222	126	ALA	2.5
4	444	26	ASN	2.5
1	111	231	TYR	2.5
1	111	95	PHE	2.5
3	333	219	PHE	2.5
3	333	60	GLY	2.5
4	444	41	ALA	2.5
3	333	184	THR	2.5
4	444	54	THR	2.5
3	333	33	PRO	2.5
4	444	49	ASP	2.5
2	222	82	LEU	2.5
2	222	86	LEU	2.5
2	222	176	LEU	2.5
3	333	223	LEU	2.5
3	333	154[A]	ILE	2.5
1	111	43	ALA	2.5
2	222	28	ALA	2.5
3	333	79	THR	2.5
4	444	50	PRO	2.5
2	222	100	TYR	2.4
1	111	210	PHE	2.4
1	111	242	LEU	2.4
3	333	231	SER	2.4
1	111	88	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	111	128	THR	2.4
1	111	229	THR	2.4
1	111	238	ASP	2.4
2	222	199	LEU	2.4
3	333	166	LEU	2.4
4	444	32	TYR	2.4
2	222	230	ILE	2.4
2	222	240	PRO	2.4
2	222	69	VAL	2.4
2	222	226	TRP	2.4
4	444	48	GLN	2.4
1	111	124	LEU	2.4
1	111	116	ASP	2.4
2	222	158	ASP	2.4
3	333	192	PHE	2.4
1	111	215	ALA	2.4
3	333	228	ASN	2.4
2	222	10	SER	2.4
2	222	101	LEU	2.3
1	111	69	TYR	2.3
1	111	49	THR	2.3
3	333	7	THR	2.3
1	111	166	ALA	2.3
3	333	197	ILE	2.3
3	333	230	ILE	2.3
4	444	66	PRO	2.3
2	222	108	VAL	2.3
1	111	172	TRP	2.3
1	111	109	THR	2.3
1	111	141	THR	2.3
3	333	190[A]	THR	2.3
4	444	64	THR	2.3
3	333	212	PHE	2.3
1	111	259	ILE	2.3
3	333	189	ILE	2.3
1	111	285	GLY	2.3
3	333	9	GLY	2.3
4	444	36[A]	SER	2.3
3	333	232	GLN	2.3
2	222	215	LEU	2.3
3	333	169	TRP	2.3
2	222	241	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	222	97	TYR	2.3
2	222	157	PHE	2.3
4	444	33	TYR	2.3
2	222	128	PRO	2.3
3	333	8	PRO	2.3
1	111	203	ILE	2.3
2	222	252	ILE	2.3
2	222	265	ILE	2.3
1	111	56	VAL	2.3
3	333	213	VAL	2.3
3	333	221	VAL	2.3
3	333	216	CYS	2.3
1	111	176	THR	2.3
4	444	61	MET	2.3
3	333	145	LYS	2.3
2	222	130	TYR	2.2
2	222	170	GLY	2.2
2	222	175	ALA	2.2
2	222	178	TYR	2.2
2	222	245	GLU	2.2
2	222	209	LEU	2.2
2	222	232	PRO	2.2
1	111	302	ILE	2.2
2	222	16	ILE	2.2
2	222	197	ILE	2.2
3	333	84	ILE	2.2
1	111	301[A]	ASN	2.2
4	444	9	LYS	2.2
2	222	171	ARG	2.2
1	111	217	VAL	2.2
2	222	143	VAL	2.2
2	222	184	VAL	2.2
1	111	120	LEU	2.2
2	222	18	LEU	2.2
3	333	6	LEU	2.2
3	333	149	LEU	2.2
3	333	111	GLY	2.2
4	444	35	ASP	2.2
1	111	107	PHE	2.2
1	111	207	TYR	2.2
3	333	81	ILE	2.2
2	222	79	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	222	91[A]	MET	2.2
1	111	156	VAL	2.2
2	222	156	VAL	2.2
3	333	30	VAL	2.2
1	111	113	THR	2.2
1	111	232	GLY	2.2
2	222	47	ALA	2.2
2	222	239	ALA	2.2
3	333	24	ALA	2.2
1	111	269	ARG	2.2
3	333	139	LYS	2.2
3	333	117	PHE	2.1
2	222	78	TRP	2.1
3	333	174	VAL	2.1
3	333	103	LEU	2.1
1	111	70	LYS	2.1
3	333	112	SER	2.1
3	333	203	THR	2.1
1	111	131	ARG	2.1
2	222	39	PRO	2.1
3	333	37	PRO	2.1
3	333	178	CYS	2.1
2	222	174	ALA	2.1
3	333	147	ALA	2.1
3	333	215	ALA	2.1
3	333	208	PHE	2.1
1	111	157	TYR	2.1
2	222	161	TYR	2.1
3	333	70	ILE	2.1
1	111	282	ARG	2.1
2	222	266	THR	2.1
2	222	32	VAL	2.1
2	222	80	TRP	2.1
1	111	295	PRO	2.1
2	222	219[A]	CYS	2.1
3	333	224	LEU	2.1
1	111	162	ILE	2.0
2	222	37	GLU	2.0
2	222	256	PHE	2.0
3	333	61	LYS	2.0
4	444	34	LYS	2.0
1	111	30	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	222	65	THR	2.0
1	111	265	PRO	2.0
2	222	71	TRP	2.0
4	444	37	ALA	2.0
2	222	88	ASP	2.0
2	222	164	SER	2.0
4	444	7	SER	2.0
1	111	196	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HEZ	111	502	8/8	0.79	0.20	103,119,134,136	8
6	HEZ	111	503	8/8	0.81	0.27	63,152,197,203	0
9	CA	333	303	1/1	0.83	0.71	35,35,35,35	1
5	SIA	111	501	21/21	0.84	0.26	32,43,55,62	21
6	HEZ	222	4102	8/8	0.86	0.26	58,76,80,80	0
6	HEZ	222	4101	8/8	0.87	0.21	38,42,46,50	0
10	MG	333	302	1/1	0.92	0.21	61,61,61,61	0
7	CL	333	304	1/1	0.93	0.28	45,45,45,45	0
7	CL	333	301	1/1	0.95	0.19	47,47,47,47	0
7	CL	111	504	1/1	0.96	0.14	42,42,42,42	0
7	CL	111	511	1/1	0.98	0.13	51,51,51,51	0
9	CA	111	507	1/1	0.98	0.09	34,34,34,34	0
9	CA	222	4103	1/1	0.98	0.13	35,35,35,35	1
7	CL	222	4104	1/1	0.98	0.10	40,40,40,40	0
7	CL	111	510	1/1	0.98	0.11	35,35,35,35	0

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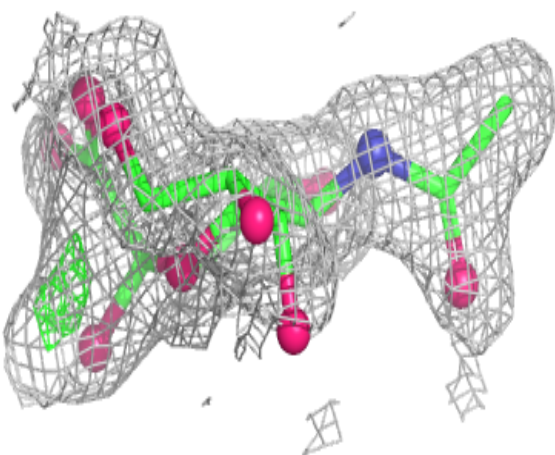
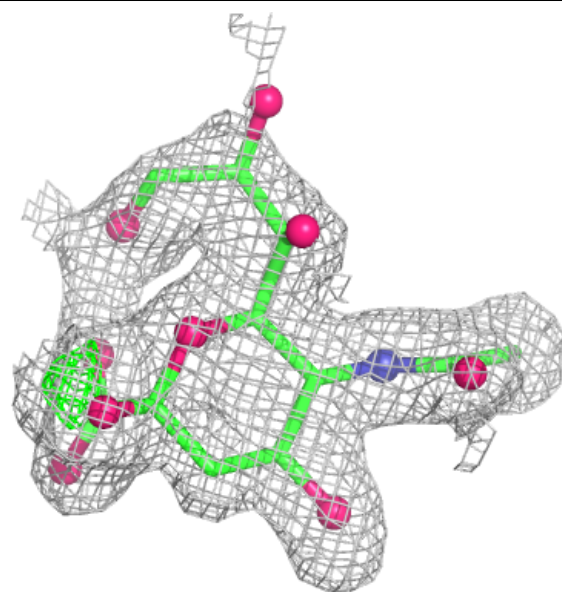
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CA	111	508	1/1	0.99	0.08	43,43,43,43	0
8	NA	111	505	1/1	0.99	0.09	29,29,29,29	0
9	CA	111	506	1/1	0.99	0.12	29,29,29,29	0
7	CL	111	509	1/1	0.99	0.08	30,30,30,30	0

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 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](#)

There are no such residues in this entry.