



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:22 PM UTC

PDB ID : 7OJ7 / pdb_00007oj7
Title : Crystal structure of human coxsackievirus A24v in complex with a pentavalent N-acetylneuraminic acid conjugate
Authors : Zocher, G.; Stehle, T.
Deposited on : 2021-05-14
Resolution : 1.78 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

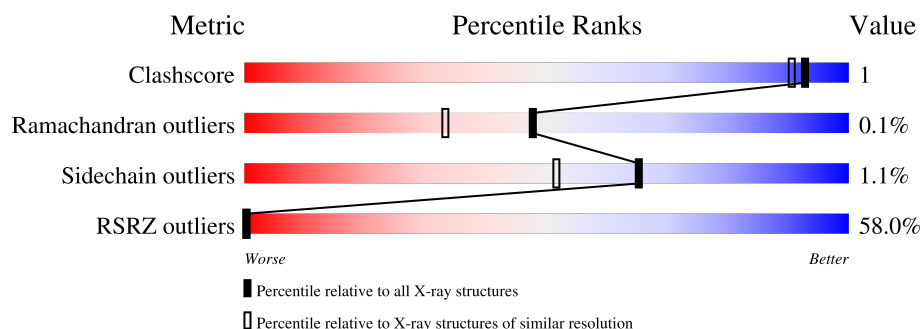
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	58% 88% 8%
2	222	271	51% 93% . .
3	333	240	51% 92% 5% .
4	444	69	65% 80% . 17%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7478 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	6	0
			2267	1442	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	4	0
			2068	1318	343	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	12	0
			1855	1193	293	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
			438	274	72	91	1			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	111	3	Total	Ca	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

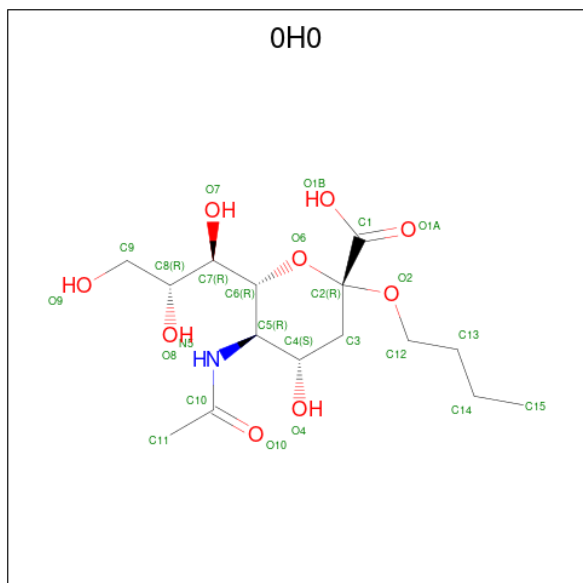
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	111	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	222	3	Total	Cl	0	0
			3	3		
6	333	1	Total	Cl	0	0
			1	1		

- Molecule 7 is Carbohydrate component from a pentavalent N-acetylneuraminic acid conjugate (CCD ID: 0H0) (formula: $C_{15}H_{27}NO_9$).



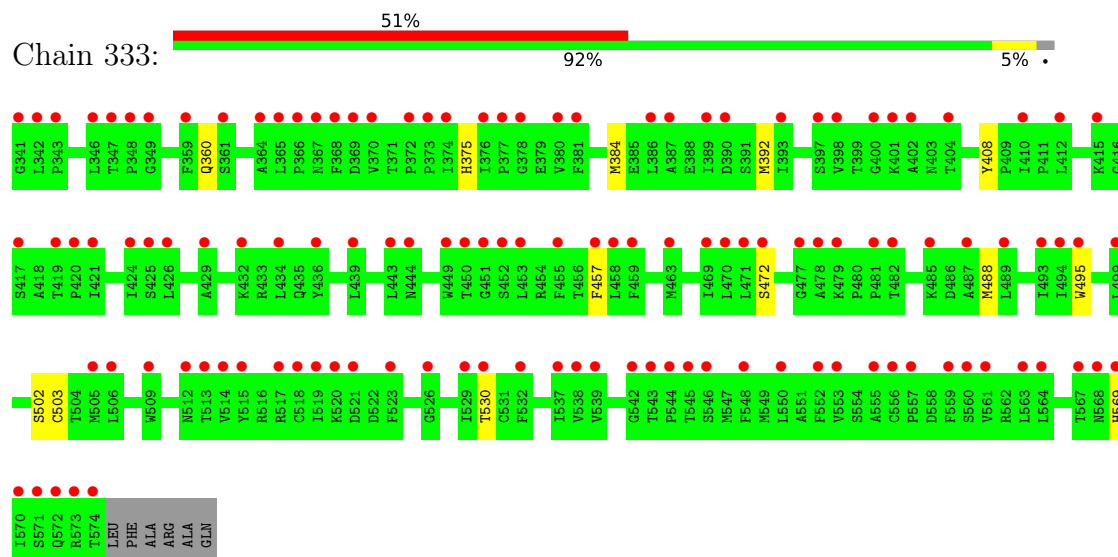
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	111	1	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	111	286	Total	O	0	0
			286	286		
8	222	238	Total	O	0	0
			238	238		
8	333	226	Total	O	0	0
			226	226		
8	444	66	Total	O	0	0
			66	66		

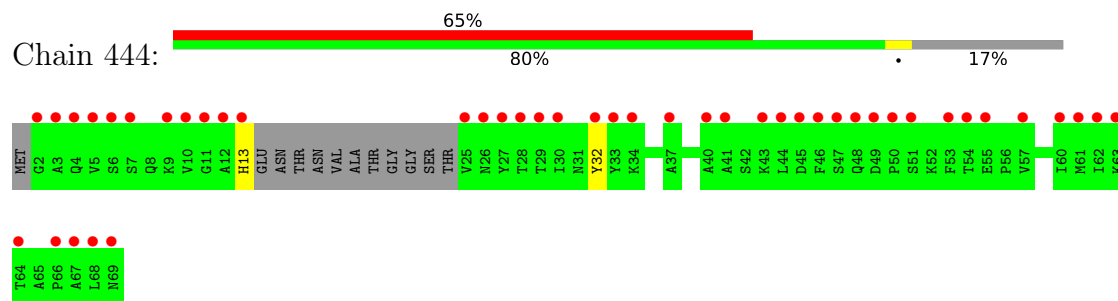
• Molecule 3: Capsid protein VP3

Chain 333:



• Molecule 4: Capsid protein VP4

Chain 444:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	305.52Å 365.55Å 366.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 1.78 49.96 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.96-1.78) 99.9 (49.96-1.78)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0232 2018/13/08	Depositor
R, R_{free}	0.158 , (Not available) 0.401 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.53	EDS
Total number of atoms	7478	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.25% 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: OH0, CL, 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	0.92	1/2348 (0.0%)	1.12	0/3207
2	222	0.89	0/2136	1.13	1/2917 (0.0%)
3	333	0.91	0/1939	1.09	0/2640
4	444	0.95	0/451	1.17	0/608
All	All	0.91	1/6874 (0.0%)	1.12	1/9372 (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	731	HIS	CE1-NE2	5.12	1.37	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	222	246	ASP	CA-CB-CG	5.53	118.13	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	2267	0	2198	7	0
2	222	2068	0	1994	4	0
3	333	1855	0	1856	10	0
4	444	438	0	428	1	0
5	111	3	0	0	0	0
6	111	3	0	0	0	0
6	222	3	0	0	0	0
6	333	1	0	0	0	0
7	111	24	0	0	0	0
8	111	286	0	0	2	0
8	222	238	0	0	0	0
8	333	226	0	0	0	0
8	444	66	0	0	0	0
All	All	7478	0	6476	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:333:360:GLN:HE22	4:444:32:TYR:H	1.31	0.79
1:111:836[B]:THR:HG22	8:111:1116:HOH:O	2.05	0.55
1:111:858:ALA:HA	3:333:569[A]:HIS:CE1	2.43	0.53
1:111:728:ASN:HD22	1:111:728:ASN:H	1.60	0.50
3:333:384[B]:MET:HE2	3:333:384[B]:MET:HA	1.93	0.50
3:333:472[A]:SER:OG	3:333:530[A]:THR:OG1	2.29	0.49
3:333:392:MET:HE3	3:333:408:TYR:CG	2.50	0.47
1:111:881[B]:ASN:HD22	1:111:883:ASN:H	1.63	0.46
2:222:106:GLU:CD	3:333:375:HIS:HE2	2.23	0.46
3:333:495:TRP:CD1	3:333:503:CYS:HB2	2.51	0.46
2:222:248:LEU:HA	2:222:253:VAL:O	2.17	0.45
1:111:849:ARG:NH1	8:111:1010:HOH:O	2.51	0.43
2:222:201[B]:MET:HB2	2:222:242:PHE:CD1	2.54	0.42
2:222:168:HIS:CG	2:222:328:PHE:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:111:730:GLY:C	1:111:731:HIS:HD2	2.28	0.41
3:333:457:PHE:O	3:333:502:SER:HA	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	111	285/305 (93%)	274 (96%)	11 (4%)	0	100	100
2	222	266/271 (98%)	251 (94%)	14 (5%)	1 (0%)	30	16
3	333	243/240 (101%)	232 (96%)	11 (4%)	0	100	100
4	444	55/69 (80%)	53 (96%)	2 (4%)	0	100	100
All	All	849/885 (96%)	810 (95%)	38 (4%)	1 (0%)	48	33

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	252/268 (94%)	247 (98%)	5 (2%)	48	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	222	223/225 (99%)	222 (100%)	1 (0%)	84	78
3	333	218/212 (103%)	217 (100%)	1 (0%)	81	73
4	444	49/57 (86%)	48 (98%)	1 (2%)	48	29
All	All	742/762 (97%)	734 (99%)	8 (1%)	65	51

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

Mol	Chain	Res	Type
1	111	723	ARG
1	111	728	ASN
1	111	776	MET
1	111	813	LEU
1	111	864	GLU
2	222	332	ARG
3	333	488	MET
4	444	13	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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
7	OH0	111	907	-	24,24,25	2.27	8 (33%)	29,34,35	0.92	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
7	OH0	111	907	-	-	5/25/43/44	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	111	907	OH0	O6-C2	5.35	1.49	1.42
7	111	907	OH0	C4-C5	-4.05	1.49	1.53
7	111	907	OH0	O2-C2	3.93	1.46	1.40
7	111	907	OH0	C10-N5	3.70	1.46	1.34
7	111	907	OH0	C5-N5	3.41	1.51	1.45
7	111	907	OH0	O6-C6	3.02	1.48	1.44
7	111	907	OH0	C11-C10	2.86	1.56	1.50
7	111	907	OH0	O1A-C1	2.07	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

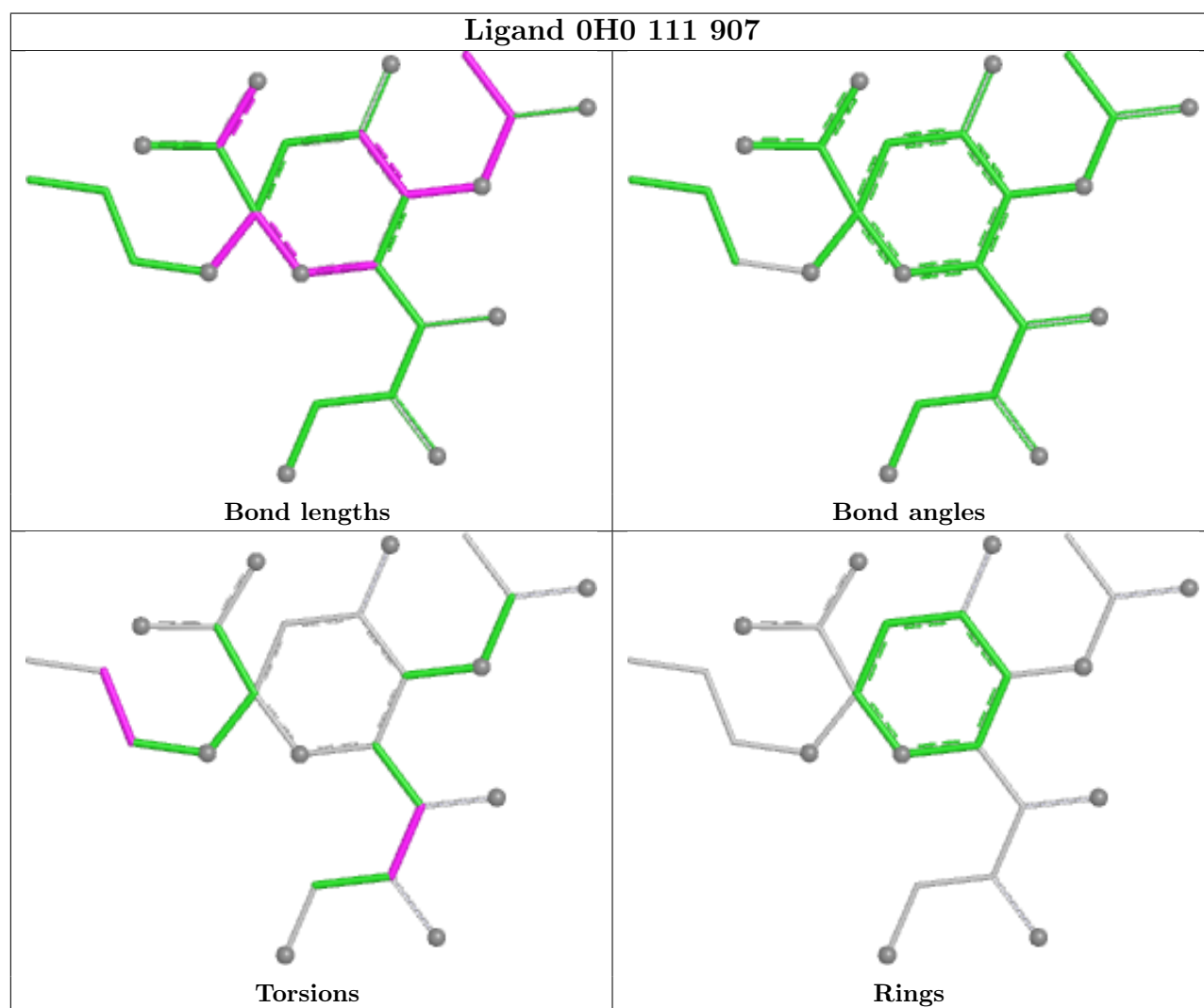
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	111	907	OH0	O2-C12-C13-C14
7	111	907	OH0	O7-C7-C8-C9
7	111	907	OH0	C6-C7-C8-C9
7	111	907	OH0	C6-C7-C8-O8
7	111	907	OH0	O7-C7-C8-O8

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 ⓘ

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%)	2.52	178 (63%) 0 0	20, 32, 54, 84	6 (2%)
2	222	264/271 (97%)	2.36	139 (52%) 0 0	18, 30, 47, 83	4 (1%)
3	333	234/240 (97%)	2.18	123 (52%) 0 0	18, 30, 39, 59	12 (5%)
4	444	57/69 (82%)	3.32	45 (78%) 0 0	21, 38, 61, 81	2 (3%)
All	All	836/885 (94%)	2.43	485 (58%) 0 0	18, 31, 49, 84	24 (2%)

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	111	804	VAL	9.9
3	333	574[A]	THR	9.1
2	222	340	GLN	8.3
1	111	805	ASP	8.3
2	222	234	ALA	8.2
1	111	803	THR	8.1
4	444	25	VAL	7.8
4	444	69	ASN	7.3
2	222	235	GLU	7.0
1	111	728	ASN	7.0
4	444	13	HIS	6.8
1	111	731	HIS	6.8
4	444	2	GLY	6.7
1	111	877	THR	6.4
2	222	236	ALA	6.3
3	333	426	LEU	6.3
4	444	4	GLN	6.0
2	222	78	TYR	5.9
1	111	678	THR	5.8
2	222	77	GLY	5.8
1	111	806	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	111	879	VAL	5.6
4	444	43	LYS	5.6
4	444	44	LEU	5.6
4	444	11	GLY	5.5
4	444	10	VAL	5.5
4	444	60	ILE	5.4
3	333	569[A]	HIS	5.4
1	111	694	TYR	5.2
2	222	260	VAL	5.0
4	444	5	VAL	5.0
2	222	80	ASP	4.8
1	111	801	ASP	4.8
1	111	739	LEU	4.8
2	222	238	GLU	4.8
1	111	725	TYR	4.7
2	222	143	THR	4.7
2	222	237	SER	4.7
2	222	311	SER	4.7
1	111	621	VAL	4.6
2	222	338	ALA	4.6
4	444	12	ALA	4.6
2	222	339	THR	4.5
1	111	605	PRO	4.5
4	444	30	ILE	4.4
3	333	453	LEU	4.4
1	111	727	SER	4.4
2	222	152	PRO	4.3
1	111	695	THR	4.3
1	111	833	ALA	4.3
2	222	281	VAL	4.3
2	222	304	LYS	4.3
1	111	807	GLY	4.3
3	333	572	GLN	4.3
1	111	750	THR	4.3
2	222	249	LEU	4.3
4	444	3	ALA	4.2
2	222	297	LEU	4.2
3	333	386	LEU	4.2
1	111	848	VAL	4.2
2	222	119	ILE	4.2
1	111	808	ASP	4.2
4	444	40	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	444	62	ILE	4.2
1	111	729	THR	4.2
3	333	463	MET	4.2
3	333	523	PHE	4.2
3	333	573	ARG	4.1
4	444	53	PHE	4.1
1	111	683	ARG	4.1
1	111	720	ILE	4.1
1	111	816	ILE	4.1
1	111	607	ALA	4.1
1	111	677	ALA	4.1
2	222	276	LEU	4.1
4	444	68	LEU	4.0
1	111	681	ALA	4.0
1	111	726	ALA	4.0
1	111	684	LYS	4.0
2	222	155	LEU	4.0
3	333	499	LEU	4.0
2	222	217	ALA	4.0
1	111	614	SER	4.0
1	111	612	LEU	4.0
2	222	253	VAL	4.0
1	111	864	GLU	3.9
1	111	748	ARG	3.9
1	111	724	TYR	3.9
1	111	741	TYR	3.9
2	222	211	TYR	3.9
2	222	312	SER	3.9
2	222	268	LEU	3.9
2	222	142	SER	3.9
2	222	104	TYR	3.9
3	333	559	PHE	3.9
3	333	570	ILE	3.9
4	444	63	LYS	3.9
1	111	817	ASN	3.9
1	111	884	THR	3.8
1	111	669	ILE	3.8
3	333	469	ILE	3.8
2	222	97	ALA	3.8
2	222	183	ALA	3.8
1	111	873	ILE	3.8
2	222	315	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	222	277	VAL	3.8
2	222	241	LYS	3.8
2	222	207	ALA	3.8
1	111	851	TRP	3.7
2	222	105	GLY	3.7
1	111	616	VAL	3.7
1	111	675	PHE	3.6
3	333	368	PHE	3.6
3	333	519	ILE	3.6
2	222	215	VAL	3.6
2	222	112	ASP	3.6
3	333	532	PHE	3.6
2	222	302	LEU	3.6
1	111	810	TYR	3.6
1	111	830	TYR	3.6
1	111	868	PHE	3.5
3	333	398	VAL	3.5
1	111	872	SER	3.5
2	222	295	TRP	3.5
2	222	135	LEU	3.5
3	333	434	LEU	3.5
3	333	506	LEU	3.5
1	111	783	ILE	3.4
4	444	46	PHE	3.4
1	111	799	LEU	3.4
4	444	49	ASP	3.4
1	111	819	PHE	3.4
3	333	470	LEU	3.4
2	222	85	ILE	3.4
2	222	157[A]	ASP	3.4
3	333	381	PHE	3.4
1	111	730	GLY	3.4
3	333	347	THR	3.4
3	333	539	VAL	3.4
1	111	755	TYR	3.3
3	333	389	ILE	3.3
2	222	239	GLY	3.3
1	111	640	VAL	3.3
1	111	646	VAL	3.3
3	333	374	ILE	3.3
1	111	693	THR	3.3
1	111	670	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	444	67	ALA	3.3
3	333	436	TYR	3.3
1	111	882	ILE	3.3
3	333	424	ILE	3.3
1	111	876	LEU	3.3
3	333	564	LEU	3.3
1	111	680[A]	ASP	3.3
1	111	712	PHE	3.3
1	111	809	THR	3.2
2	222	92	ILE	3.2
1	111	790	PHE	3.2
3	333	568	ASN	3.2
1	111	732	ALA	3.2
3	333	393	ILE	3.2
1	111	752	TRP	3.2
2	222	107	TRP	3.2
2	222	191	LEU	3.2
2	222	132	PHE	3.2
2	222	303	CYS	3.2
1	111	765	VAL	3.2
1	111	826	VAL	3.2
4	444	28	THR	3.2
1	111	813	LEU	3.2
2	222	331	LEU	3.2
2	222	154	ALA	3.2
1	111	870	GLN	3.1
3	333	485	LYS	3.1
4	444	51[A]	SER	3.1
2	222	98	ALA	3.1
1	111	698	VAL	3.1
3	333	412	LEU	3.1
4	444	45	ASP	3.1
2	222	208	LYS	3.1
3	333	415	LYS	3.1
4	444	26	ASN	3.1
3	333	556	CYS	3.1
1	111	647	VAL	3.0
1	111	714	LEU	3.0
1	111	839	ILE	3.0
1	111	751	ALA	3.0
2	222	141	LYS	3.0
2	222	101	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	333	538	VAL	3.0
2	222	86	THR	3.0
2	222	313	THR	3.0
3	333	530[A]	THR	3.0
1	111	871	ASP	3.0
3	333	377	PRO	3.0
3	333	367[A]	ASN	3.0
1	111	737	TYR	3.0
1	111	778	ILE	3.0
2	222	96	GLU	3.0
1	111	707	PHE	3.0
1	111	885	PHE	3.0
3	333	459	PHE	3.0
1	111	797	VAL	2.9
1	111	866	VAL	2.9
2	222	233	SER	2.9
1	111	625	THR	2.9
3	333	432	LYS	2.9
2	222	151	LEU	2.9
3	333	443	LEU	2.9
1	111	641	ILE	2.9
1	111	835	ILE	2.9
2	222	265	ILE	2.9
3	333	529	ILE	2.9
2	222	259	PHE	2.9
4	444	47	SER	2.9
3	333	479	LYS	2.9
1	111	691	ALA	2.9
1	111	746	ALA	2.9
1	111	657	LEU	2.9
2	222	286	ILE	2.9
3	333	493	ILE	2.9
1	111	721	THR	2.9
2	222	169	TYR	2.9
1	111	812	GLY	2.9
3	333	349	GLY	2.9
1	111	679	THR	2.8
4	444	54	THR	2.8
1	111	672[A]	VAL	2.8
1	111	814	VAL	2.8
1	111	829	GLU	2.8
2	222	138	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	222	225	VAL	2.8
2	222	309	PRO	2.8
3	333	410	ILE	2.8
1	111	689	THR	2.8
1	111	880	GLU	2.8
2	222	206	GLU	2.8
1	111	623	ALA	2.8
3	333	370	VAL	2.8
1	111	811	TYR	2.8
3	333	373	PRO	2.8
2	222	254	LEU	2.8
3	333	439	LEU	2.8
4	444	48	GLN	2.8
2	222	240	ARG	2.8
3	333	380	VAL	2.8
2	222	261	TYR	2.8
2	222	299	ILE	2.8
2	222	321	ILE	2.8
3	333	376	ILE	2.8
2	222	202	ALA	2.7
2	222	229	ALA	2.7
3	333	387	ALA	2.7
2	222	124	GLU	2.7
2	222	148	TRP	2.7
4	444	50	PRO	2.7
2	222	170	LEU	2.7
4	444	33	TYR	2.7
1	111	742	ILE	2.7
2	222	81	ARG	2.7
1	111	763	PRO	2.7
1	111	798	PRO	2.7
3	333	481	PRO	2.7
2	222	205	THR	2.7
2	222	318	THR	2.7
3	333	543	THR	2.7
1	111	865	GLY	2.7
3	333	400	GLY	2.7
3	333	512	ASN	2.7
1	111	784	ALA	2.7
4	444	41	ALA	2.7
1	111	696	ASP	2.7
1	111	818	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	222	82	VAL	2.7
2	222	111	LEU	2.7
2	222	212	VAL	2.7
3	333	561	VAL	2.7
4	444	27	TYR	2.7
3	333	520	LYS	2.7
4	444	34	LYS	2.7
1	111	631	ALA	2.7
2	222	108	PRO	2.6
3	333	417	SER	2.6
2	222	325	PHE	2.6
3	333	450	THR	2.6
2	222	248	LEU	2.6
3	333	515	TYR	2.6
1	111	757	TRP	2.6
1	111	608	GLN	2.6
2	222	114	LYS	2.6
1	111	687	PHE	2.6
1	111	688	THR	2.6
2	222	335	THR	2.6
3	333	341	GLY	2.6
3	333	419	THR	2.6
1	111	636	VAL	2.6
1	111	710	SER	2.6
1	111	795	ALA	2.6
4	444	66	PRO	2.6
3	333	369	ASP	2.6
3	333	552	PHE	2.6
3	333	458	LEU	2.6
1	111	827	VAL	2.6
4	444	6	SER	2.6
2	222	147	TRP	2.6
3	333	509	TRP	2.6
2	222	134	THR	2.5
2	222	87	LEU	2.5
2	222	300	LEU	2.5
2	222	305	LEU	2.5
3	333	571	SER	2.5
2	222	230	TYR	2.5
2	222	247	TYR	2.5
1	111	736	VAL	2.5
2	222	127	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	222	193	VAL	2.5
2	222	334	ILE	2.5
1	111	875	PRO	2.5
1	111	615	GLY	2.5
3	333	526	GLY	2.5
2	222	209	THR	2.5
2	222	79	SER	2.5
3	333	452	SER	2.5
3	333	548	PHE	2.5
1	111	822	LEU	2.5
1	111	649	TYR	2.5
1	111	787	TYR	2.5
1	111	682	ASP	2.5
1	111	626	ALA	2.5
3	333	514	VAL	2.5
2	222	196	ILE	2.5
3	333	482	THR	2.5
1	111	838	LYS	2.5
1	111	834	ARG	2.5
4	444	7	SER	2.5
1	111	881[A]	ASN	2.5
2	222	294	ASN	2.5
1	111	704	LEU	2.5
1	111	766	PHE	2.5
2	222	186	PHE	2.5
3	333	390	ASP	2.5
2	222	195	ALA	2.5
2	222	319	VAL	2.5
1	111	651	THR	2.5
1	111	708	THR	2.5
3	333	513	THR	2.5
3	333	567	THR	2.5
1	111	800	LYS	2.4
1	111	671	GLU	2.4
2	222	161	PHE	2.4
3	333	342	LEU	2.4
3	333	489	LEU	2.4
3	333	563	LEU	2.4
1	111	770	GLY	2.4
2	222	308	ALA	2.4
3	333	478	ALA	2.4
1	111	606	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	111	781	VAL	2.4
3	333	472[A]	SER	2.4
3	333	553	VAL	2.4
4	444	57	VAL	2.4
2	222	284	LEU	2.4
3	333	365	LEU	2.4
3	333	449	TRP	2.4
3	333	544	PRO	2.4
3	333	429	ALA	2.4
1	111	610	THR	2.4
1	111	756	THR	2.4
3	333	404	THR	2.4
2	222	166	TYR	2.4
2	222	314	GLU	2.4
4	444	55	GLU	2.4
1	111	650	LYS	2.4
1	111	849	ARG	2.4
1	111	788	SER	2.4
3	333	346	LEU	2.4
2	222	258	ALA	2.4
1	111	629	THR	2.4
3	333	457	PHE	2.4
3	333	521	ASP	2.4
1	111	861	TYR	2.4
1	111	676	ASN	2.3
1	111	764	SER	2.3
1	111	856	PRO	2.3
3	333	366	PRO	2.3
1	111	821	THR	2.3
4	444	29	THR	2.3
2	222	149	TRP	2.3
2	222	199	TYR	2.3
3	333	495	TRP	2.3
3	333	421	ILE	2.3
1	111	841	VAL	2.3
3	333	477	GLY	2.3
2	222	106	GLU	2.3
1	111	832	PRO	2.3
1	111	869	LYS	2.3
3	333	372	PRO	2.3
2	222	317	ILE	2.3
3	333	537	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	111	667	VAL	2.3
1	111	824	VAL	2.3
3	333	348	PRO	2.3
1	111	613	THR	2.3
2	222	290	ALA	2.3
1	111	624	LEU	2.3
1	111	700	LEU	2.3
1	111	791	TYR	2.3
1	111	692	ILE	2.3
1	111	847	HIS	2.2
1	111	874	THR	2.2
2	222	326	THR	2.2
3	333	361	SER	2.2
2	222	185	LYS	2.2
3	333	542	GLY	2.2
4	444	61	MET	2.2
2	222	307	TYR	2.2
4	444	32	TYR	2.2
1	111	637	PRO	2.2
1	111	668	THR	2.2
1	111	711	ARG	2.2
2	222	270	THR	2.2
2	222	244	ALA	2.2
1	111	850	CYS	2.2
4	444	9	LYS	2.2
3	333	471	LEU	2.2
3	333	550	LEU	2.2
3	333	378	GLY	2.2
3	333	455	PHE	2.2
2	222	266	ILE	2.2
3	333	420	PRO	2.2
2	222	177	VAL	2.2
2	222	255	ALA	2.2
1	111	793	GLY	2.2
1	111	706	PHE	2.2
3	333	444	ASN	2.2
1	111	611	PRO	2.2
3	333	494[A]	ILE	2.2
1	111	836[A]	THR	2.2
1	111	638	SER	2.2
3	333	364	ALA	2.1
3	333	555	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	111	831	ASN	2.1
2	222	310	ASN	2.1
3	333	546[A]	SER	2.1
2	222	91	THR	2.1
2	222	242	PHE	2.1
3	333	557	PRO	2.1
1	111	769	TYR	2.1
1	111	859	VAL	2.1
1	111	828	ASN	2.1
3	333	505	MET	2.1
1	111	653	SER	2.1
1	111	802	GLU	2.1
3	333	560	SER	2.1
1	111	697	THR	2.1
3	333	545	THR	2.1
1	111	718	PHE	2.1
2	222	100	ALA	2.1
2	222	243	ALA	2.1
4	444	37	ALA	2.1
3	333	518	CYS	2.1
4	444	64	THR	2.1
3	333	343	PRO	2.1
1	111	690	TRP	2.1
1	111	685	LYS	2.1
3	333	401	LYS	2.1
2	222	214	TYR	2.1
2	222	226	PHE	2.1
2	222	328	PHE	2.1
3	333	451	GLY	2.0
2	222	121	ALA	2.0
3	333	402	ALA	2.0
2	222	227	ASP	2.0
1	111	771	SER	2.0
3	333	397[A]	SER	2.0
3	333	425	SER	2.0
2	222	245	LEU	2.0
2	222	291	LYS	2.0
1	111	820	GLY	2.0
2	222	289	MET	2.0
1	111	862	ARG	2.0
2	222	194	PHE	2.0
3	333	359	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
3	333	517	ARG	2.0
3	333	487	ALA	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](#)

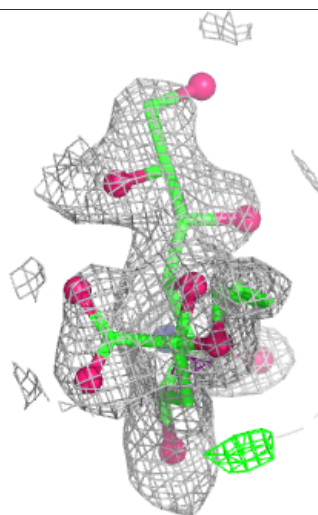
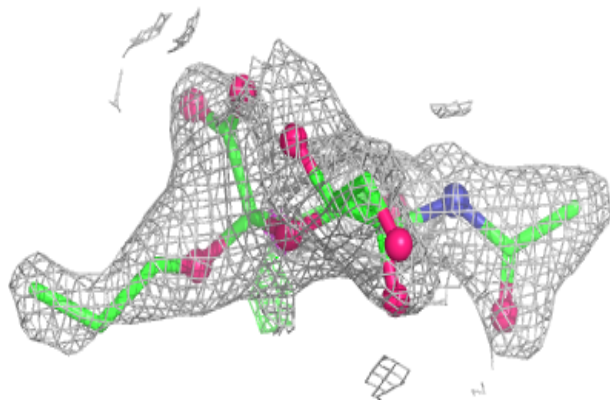
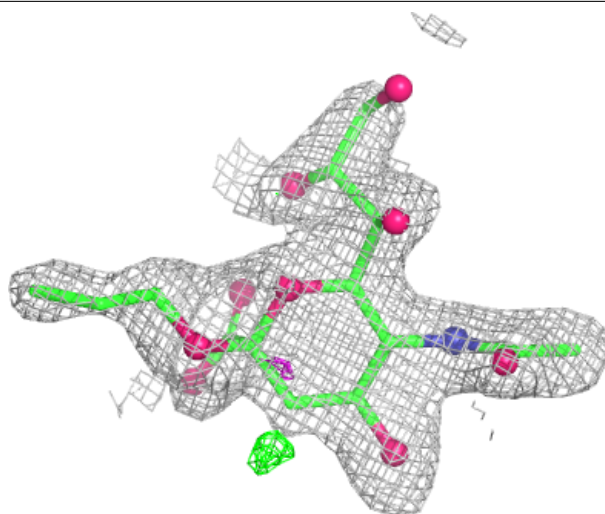
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	CL	333	601	1/1	0.80	0.52	35,35,35,35	1
7	OH0	111	907	24/25	0.87	0.27	37,54,70,74	24
6	CL	222	403	1/1	0.91	0.38	53,53,53,53	0
6	CL	222	401	1/1	0.95	0.15	48,48,48,48	0
6	CL	111	906	1/1	0.96	0.17	59,59,59,59	0
6	CL	222	402	1/1	0.97	0.32	37,37,37,37	1
5	CA	111	901	1/1	0.98	0.18	45,45,45,45	0
5	CA	111	903	1/1	0.98	0.12	37,37,37,37	0
6	CL	111	905	1/1	0.98	0.13	41,41,41,41	0
6	CL	111	904	1/1	0.99	0.07	34,34,34,34	0
5	CA	111	902	1/1	1.00	0.10	32,32,32,32	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 OH0 111 907:

$2mF_o-DF_c$ (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.