



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 8I3P / pdb_00008i3p
Title : crystal structure of yeast cytosine deaminase mutant yCD-RQ-1/8SAH in complex with (R)-4-hydroxy-3,4-dihydropyrimidin-2(1H)-one
Authors : Qin, M.M.; Deng, H.Z.; Yao, L.S.
Deposited on : 2023-01-17
Resolution : 1.30 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

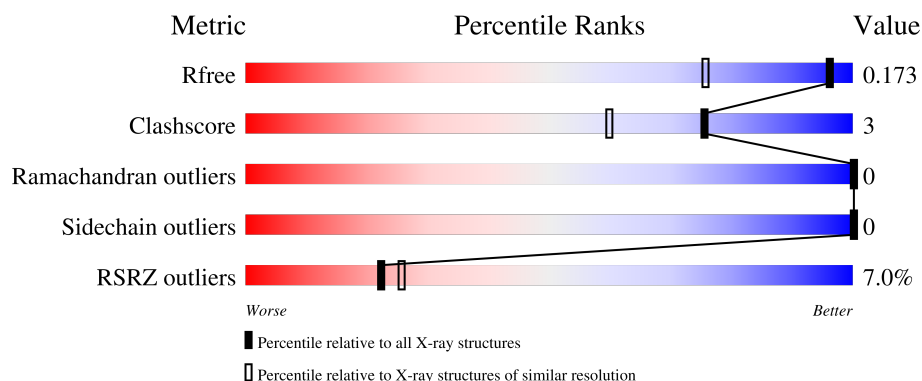
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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))
R_{free}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	A	198	5% 77% 6% • 17%
1	B	198	7% 78% 5% • 16%

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
4	EDO	B	603	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2885 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 Cytosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1247	776	217	243	11			
1	B	166	Total	C	N	O	S	0	2	0
			1263	788	219	244	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q12178
A	159	ARG	-	expression tag	UNP Q12178
A	160	ILE	-	expression tag	UNP Q12178
A	161	GLU	-	expression tag	UNP Q12178
A	162	LEU	-	expression tag	UNP Q12178
A	163	GLN	-	expression tag	UNP Q12178
A	164	LYS	-	expression tag	UNP Q12178
A	165	GLN	-	expression tag	UNP Q12178
A	166	GLN	-	expression tag	UNP Q12178
A	167	GLU	-	expression tag	UNP Q12178
A	168	GLU	-	expression tag	UNP Q12178
A	169	GLU	-	expression tag	UNP Q12178
A	170	ALA	-	expression tag	UNP Q12178
A	171	GLU	-	expression tag	UNP Q12178
A	172	ARG	-	expression tag	UNP Q12178
A	173	LEU	-	expression tag	UNP Q12178
A	174	ARG	-	expression tag	UNP Q12178
A	175	ARG	-	expression tag	UNP Q12178
A	176	ILE	-	expression tag	UNP Q12178
A	177	GLN	-	expression tag	UNP Q12178
A	178	GLU	-	expression tag	UNP Q12178
A	179	GLU	-	expression tag	UNP Q12178
A	180	MET	-	expression tag	UNP Q12178
A	181	GLU	-	expression tag	UNP Q12178
A	182	LYS	-	expression tag	UNP Q12178

Continued on next page...

Continued from previous page...

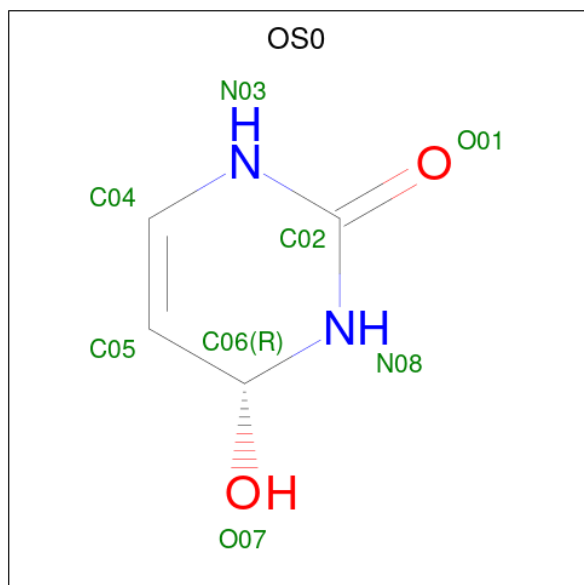
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	-	expression tag	UNP Q12178
A	184	ARG	-	expression tag	UNP Q12178
A	185	LYS	-	expression tag	UNP Q12178
A	186	ARG	-	expression tag	UNP Q12178
A	187	ARG	-	expression tag	UNP Q12178
A	188	GLU	-	expression tag	UNP Q12178
A	189	GLU	-	expression tag	UNP Q12178
A	190	ASP	-	expression tag	UNP Q12178
A	191	GLU	-	expression tag	UNP Q12178
A	192	GLN	-	expression tag	UNP Q12178
A	193	ARG	-	expression tag	UNP Q12178
A	194	ARG	-	expression tag	UNP Q12178
A	195	ARG	-	expression tag	UNP Q12178
A	196	LYS	-	expression tag	UNP Q12178
A	197	GLU	-	expression tag	UNP Q12178
B	0	GLY	-	expression tag	UNP Q12178
B	159	ARG	-	expression tag	UNP Q12178
B	160	ILE	-	expression tag	UNP Q12178
B	161	GLU	-	expression tag	UNP Q12178
B	162	LEU	-	expression tag	UNP Q12178
B	163	GLN	-	expression tag	UNP Q12178
B	164	LYS	-	expression tag	UNP Q12178
B	165	GLN	-	expression tag	UNP Q12178
B	166	GLN	-	expression tag	UNP Q12178
B	167	GLU	-	expression tag	UNP Q12178
B	168	GLU	-	expression tag	UNP Q12178
B	169	GLU	-	expression tag	UNP Q12178
B	170	ALA	-	expression tag	UNP Q12178
B	171	GLU	-	expression tag	UNP Q12178
B	172	ARG	-	expression tag	UNP Q12178
B	173	LEU	-	expression tag	UNP Q12178
B	174	ARG	-	expression tag	UNP Q12178
B	175	ARG	-	expression tag	UNP Q12178
B	176	ILE	-	expression tag	UNP Q12178
B	177	GLN	-	expression tag	UNP Q12178
B	178	GLU	-	expression tag	UNP Q12178
B	179	GLU	-	expression tag	UNP Q12178
B	180	MET	-	expression tag	UNP Q12178
B	181	GLU	-	expression tag	UNP Q12178
B	182	LYS	-	expression tag	UNP Q12178
B	183	GLU	-	expression tag	UNP Q12178
B	184	ARG	-	expression tag	UNP Q12178

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	185	LYS	-	expression tag	UNP Q12178
B	186	ARG	-	expression tag	UNP Q12178
B	187	ARG	-	expression tag	UNP Q12178
B	188	GLU	-	expression tag	UNP Q12178
B	189	GLU	-	expression tag	UNP Q12178
B	190	ASP	-	expression tag	UNP Q12178
B	191	GLU	-	expression tag	UNP Q12178
B	192	GLN	-	expression tag	UNP Q12178
B	193	ARG	-	expression tag	UNP Q12178
B	194	ARG	-	expression tag	UNP Q12178
B	195	ARG	-	expression tag	UNP Q12178
B	196	LYS	-	expression tag	UNP Q12178
B	197	GLU	-	expression tag	UNP Q12178

- Molecule 2 is 4-oxidanyl-3,4-dihydro-1H-pyrimidin-2-one (CCD ID: OS0) (formula: $C_4H_6N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	2	2		
2	B	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	175	Total	O	0	0
			175	175		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.17Å 68.90Å 49.42Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	33.41 – 1.30 33.41 – 1.30	Depositor EDS
% Data completeness (in resolution range)	86.0 (33.41-1.30) 85.9 (33.41-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.141 , 0.161 0.161 , 0.173	Depositor DCC
R_{free} test set	2022 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.051 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2885	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, OSO

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	A	0.92	4/1266 (0.3%)	0.84	0/1704
1	B	0.94	6/1289 (0.5%)	0.90	5/1732 (0.3%)
All	All	0.93	10/2555 (0.4%)	0.87	5/3436 (0.1%)

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
1	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	LYS	C-O	-7.86	1.14	1.24
1	B	7	ALA	C-O	-5.84	1.17	1.24
1	A	155	ASP	C-O	-5.82	1.16	1.24
1	B	132[A]	VAL	C-O	5.17	1.30	1.24
1	B	132[B]	VAL	C-O	5.17	1.30	1.24
1	A	151	ASP	C-O	-5.16	1.18	1.24
1	B	8	SER	C-O	-5.16	1.17	1.24
1	A	153	PHE	C-O	-5.14	1.17	1.24
1	B	36	CYS	C-O	-5.11	1.17	1.23
1	A	141	MET	C-O	-5.05	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	MET	CA-C-O	-6.80	113.27	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132[A]	VAL	CA-C-O	6.50	127.04	119.36
1	B	132[B]	VAL	CA-C-O	6.50	127.04	119.36
1	B	132[A]	VAL	N-CA-C	5.25	120.26	113.07
1	B	132[B]	VAL	N-CA-C	5.25	120.26	113.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLU	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	A	1247	0	1178	8	0
1	B	1263	0	1210	7	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	6	3	0
4	B	4	0	6	4	0
5	A	174	0	0	2	0
5	B	175	0	0	2	0
All	All	2885	0	2400	15	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 3.

All (15) 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:B:125:ARG:HE	4:B:603:EDO:H12	1.06	1.13
1:B:125:ARG:NE	4:B:603:EDO:H12	1.89	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HE	4:A:603:EDO:H21	1.40	0.85
1:B:125:ARG:HE	4:B:603:EDO:C1	1.90	0.84
1:B:4:GLY:HA3	5:B:827:HOH:O	1.86	0.74
1:A:4:GLY:N	5:A:701:HOH:O	2.20	0.73
1:B:12:GLN:HG2	5:B:866:HOH:O	1.97	0.64
1:B:147:GLU:HG3	1:B:148:ARG:HG3	1.83	0.60
1:A:125:ARG:HE	4:A:603:EDO:C2	2.14	0.59
1:A:54:PHE:CZ	1:A:151:ASP:HB3	2.47	0.49
1:A:162:LEU:O	1:A:166:GLN:HB2	2.15	0.47
1:A:125:ARG:NE	4:A:603:EDO:H21	2.21	0.44
1:A:117:LYS:NZ	4:B:603:EDO:H21	2.33	0.43
1:A:150:GLN:HG2	5:A:812:HOH:O	2.17	0.43
1:B:6:MET:O	1:B:9:LYS:HG2	2.20	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	A	162/198 (82%)	160 (99%)	2 (1%)	0	100	100
1	B	166/198 (84%)	163 (98%)	3 (2%)	0	100	100
All	All	328/396 (83%)	323 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	126/169 (75%)	126 (100%)	0	100	100
1	B	130/169 (77%)	130 (100%)	0	100	100
All	All	256/338 (76%)	256 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
4	EDO	B	603	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	603	-	3,3,3	0.33	0	2,2,2	0.23	0
2	OS0	A	601	3	7,8,8	2.93	3 (42%)	6,10,10	3.15	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OS0	B	601	3	7,8,8	2.98	3 (42%)	6,10,10	2.23	3 (50%)

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
4	EDO	B	603	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
2	OS0	A	601	3	-	-	0/1/1/1
2	OS0	B	601	3	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OS0	C02-N03	5.55	1.43	1.36
2	B	601	OS0	C04-N03	5.30	1.43	1.36
2	B	601	OS0	C02-N08	4.57	1.43	1.34
2	A	601	OS0	C02-N08	3.52	1.41	1.34
2	A	601	OS0	C04-N03	2.95	1.40	1.36
2	B	601	OS0	C02-N03	2.78	1.40	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	OS0	O01-C02-N03	-5.70	116.92	122.79
2	A	601	OS0	N03-C02-N08	4.50	120.56	116.06
2	B	601	OS0	N03-C02-N08	3.30	119.36	116.06
2	B	601	OS0	C04-N03-C02	-2.65	120.77	122.40
2	B	601	OS0	O01-C02-N03	-2.58	120.13	122.79

There are no chirality outliers.

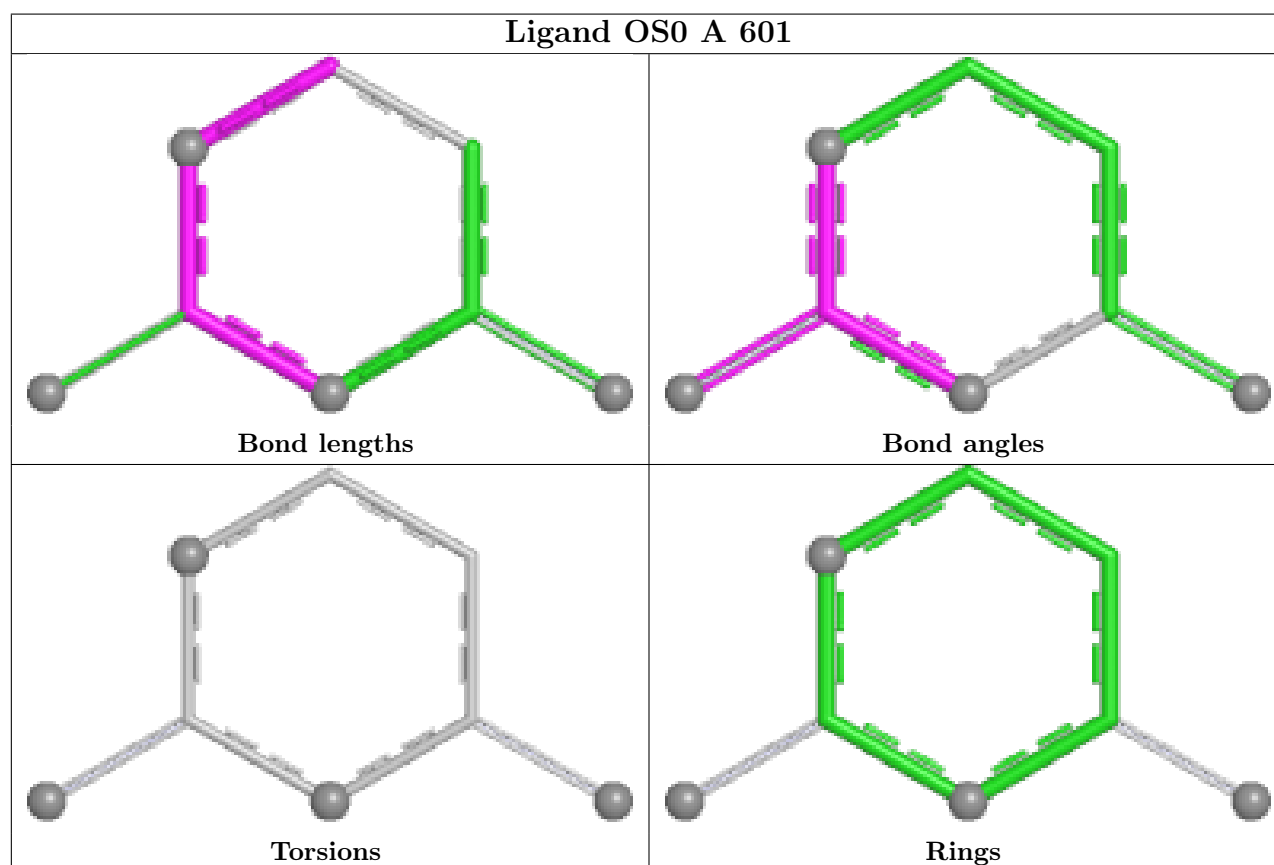
There are no torsion outliers.

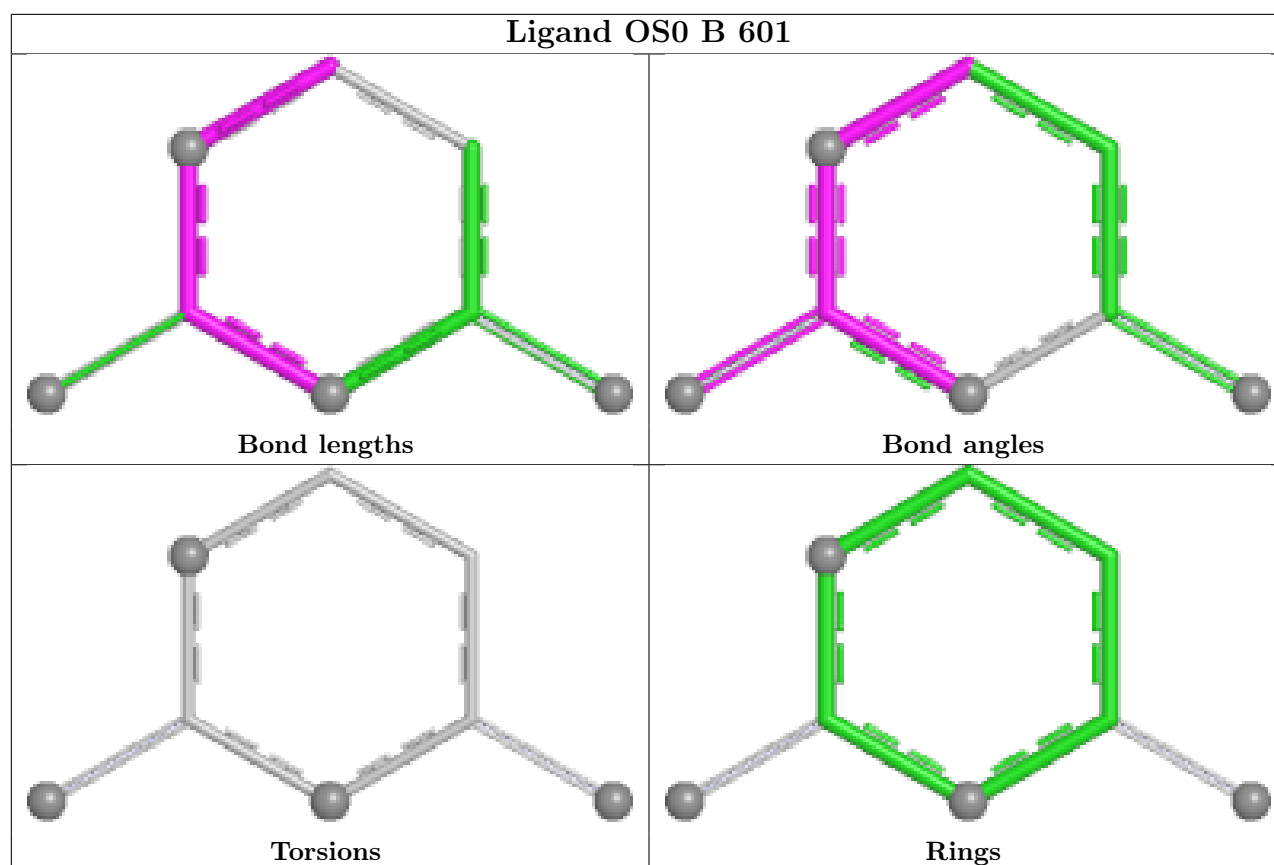
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	EDO	4	0
4	A	603	EDO	3	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 [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	A	164/198 (82%)	0.43	10 (6%) 27 31	10, 13, 24, 28	7 (4%)
1	B	166/198 (83%)	0.53	13 (7%) 19 21	7, 13, 26, 34	5 (3%)
All	All	330/396 (83%)	0.48	23 (6%) 22 26	7, 13, 25, 34	12 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	8.4
1	B	5	GLY	7.1
1	A	167	GLU	5.1
1	A	4	GLY	5.1
1	B	160	ILE	4.9
1	B	4	GLY	4.5
1	A	6	MET	4.1
1	B	6	MET	4.1
1	B	164	LYS	3.8
1	A	162	LEU	3.6
1	B	169	GLU	3.5
1	A	166	GLN	3.0
1	B	167	GLU	2.7
1	A	160	ILE	2.6
1	B	161	GLU	2.6
1	B	162	LEU	2.5
1	B	165	GLN	2.5
1	B	26	TYR	2.5
1	A	161	GLU	2.3
1	A	81	ASP	2.3
1	A	153	PHE	2.3
1	B	168	GLU	2.3
1	B	163	GLN	2.2

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](#)

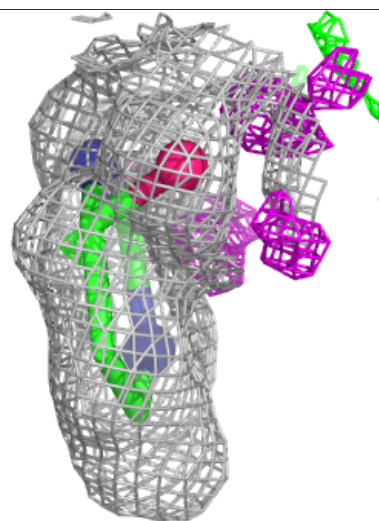
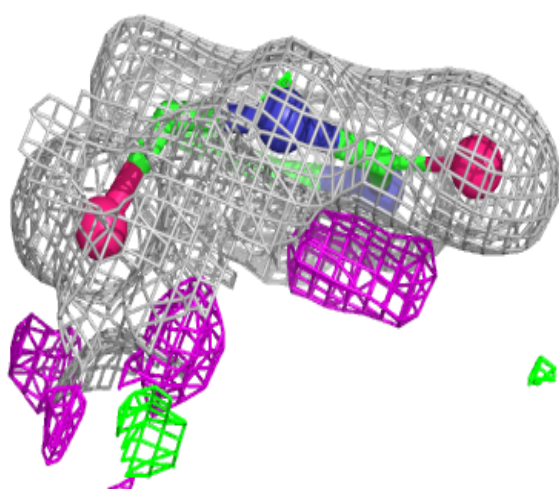
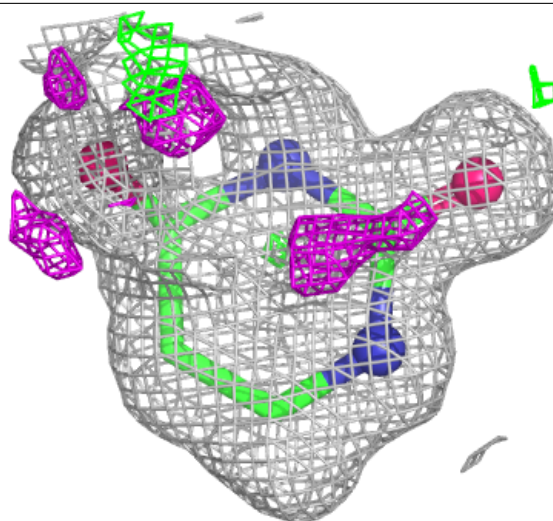
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	B	603	4/4	0.62	0.21	28,28,28,28	0
4	EDO	A	603	4/4	0.76	0.16	27,27,28,28	0
2	OS0	A	601	8/8	0.97	0.06	9,10,10,11	0
2	OS0	B	601	8/8	0.99	0.05	8,9,10,10	0
3	ZN	A	602	1/1	1.00	0.02	10,10,10,10	0
3	ZN	B	602	1/1	1.00	0.01	10,10,10,10	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.

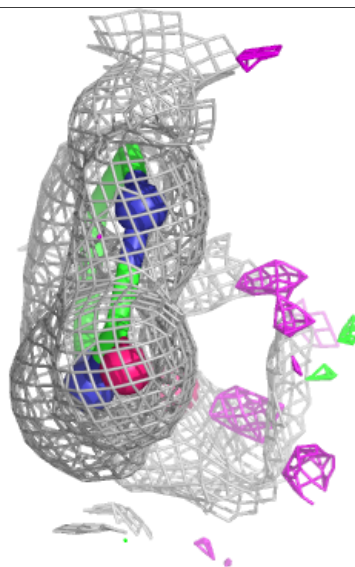
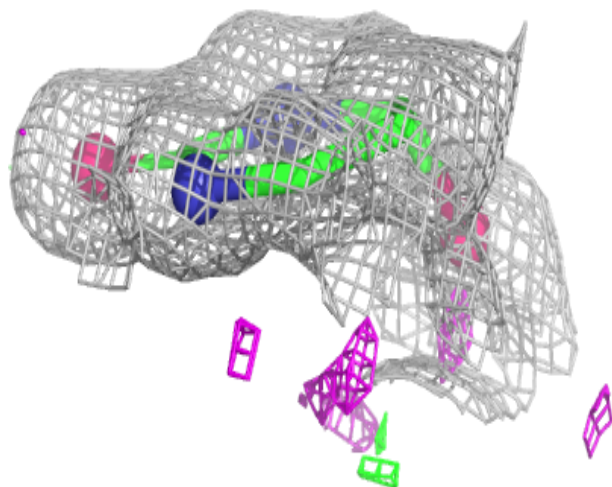
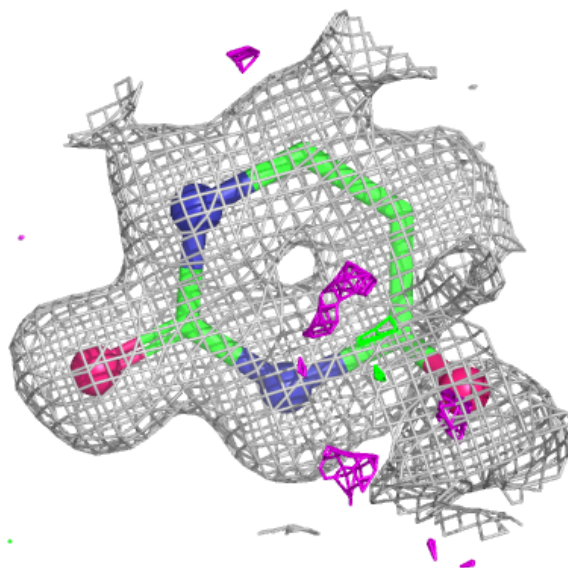
Electron density around OS0 A 601:

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



Electron density around OS0 B 601:

$2mF_o-DF_c$ (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.