



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2024 – 11:49 am BST

PDB ID : 8RKR  
Title : Structure of human DELTA-1-PYRROLINE-5-CARBOXYLATE DEHYDROGENASE (ALDH4A1) complexed with a monophosphate-tweezer  
Authors : Porfetye, A.T.; Vetter, I.R.  
Deposited on : 2023-12-28  
Resolution : 1.20 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

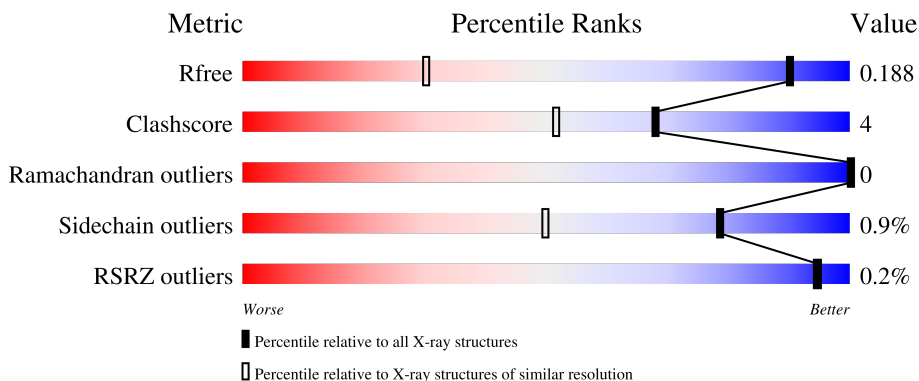
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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))
$R_{free}$	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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  $\leq 5\%$ . 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	567	
1	B	567	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9626 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4217	2697	716	787	17	0	22	0
1	B	532	4193	2683	712	782	16	0	16	0

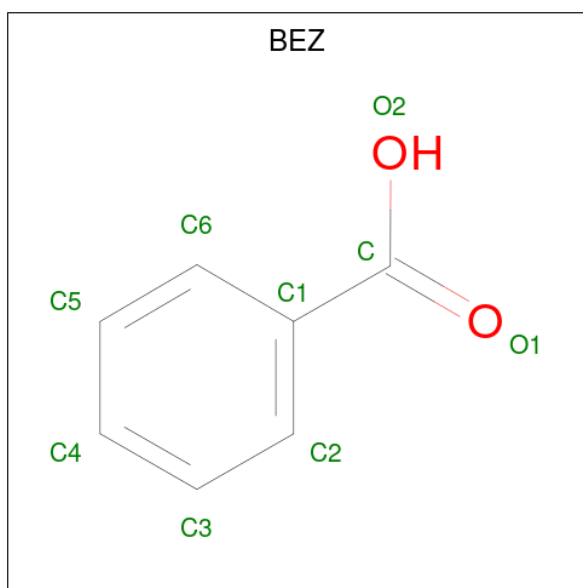
There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P30038
A	-2	GLY	-	expression tag	UNP P30038
A	-1	SER	-	expression tag	UNP P30038
A	0	SER	-	expression tag	UNP P30038
A	1	HIS	-	expression tag	UNP P30038
A	2	HIS	-	expression tag	UNP P30038
A	3	HIS	-	expression tag	UNP P30038
A	4	HIS	-	expression tag	UNP P30038
A	5	HIS	-	expression tag	UNP P30038
A	6	HIS	-	expression tag	UNP P30038
A	7	SER	-	expression tag	UNP P30038
A	8	SER	-	expression tag	UNP P30038
A	9	GLY	-	expression tag	UNP P30038
A	10	LEU	-	expression tag	UNP P30038
A	11	VAL	-	expression tag	UNP P30038
A	12	PRO	-	expression tag	UNP P30038
A	13	ARG	-	expression tag	UNP P30038
A	14	GLY	-	expression tag	UNP P30038
A	15	SER	-	expression tag	UNP P30038
A	16	HIS	-	expression tag	UNP P30038
A	17	MET	-	expression tag	UNP P30038
B	-3	MET	-	initiating methionine	UNP P30038
B	-2	GLY	-	expression tag	UNP P30038
B	-1	SER	-	expression tag	UNP P30038
B	0	SER	-	expression tag	UNP P30038

*Continued on next page...*



- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	597	Total O 597 597	0	0
4	B	535	Total O 535 535	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.91Å 85.16Å 85.61Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	48.47 – 1.20 48.47 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.47-1.20) 99.9 (48.47-1.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.165 , 0.188 0.166 , 0.188	Depositor DCC
$R_{free}$ test set	3279 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	9626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.53% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H1O, BEZ

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	0.72	2/4382 (0.0%)	0.86	4/5945 (0.1%)
1	B	0.76	4/4339 (0.1%)	0.90	8/5886 (0.1%)
All	All	0.74	6/8721 (0.1%)	0.88	12/11831 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314[A]	GLU	CD-OE1	8.04	1.34	1.25
1	B	314[B]	GLU	CD-OE1	8.04	1.34	1.25
1	B	314[A]	GLU	CD-OE2	7.24	1.33	1.25
1	B	314[B]	GLU	CD-OE2	7.24	1.33	1.25
1	A	314	GLU	CD-OE1	6.71	1.33	1.25
1	A	314	GLU	CD-OE2	5.50	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171[A]	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	B	171[B]	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	171[A]	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	A	171[B]	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	B	171[A]	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	171[B]	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	236	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	171[A]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	171[B]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	367	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	198	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	498	ARG	NE-CZ-NH1	5.02	122.81	120.30



There are no chirality outliers.

There are no planarity outliers.

## 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	4217	0	4205	32	0
1	B	4193	0	4176	33	0
2	A	48	0	0	0	0
3	A	18	0	10	1	0
3	B	18	0	10	0	0
4	A	597	0	0	20	0
4	B	535	0	0	4	0
All	All	9626	0	8401	64	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 4.

All (64) 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:301[B]:ASN:HD21	1:B:304:ARG:HD2	1.13	1.14
1:B:301[B]:ASN:OD1	1:B:304:ARG:NE	1.83	1.09
1:B:301[B]:ASN:HD21	1:B:304:ARG:CD	1.74	1.01
1:B:314[B]:GLU:OE2	1:B:315[B]:CYS:O	1.78	1.00
1:A:171[B]:ARG:NH2	4:A:701:HOH:O	1.74	0.99
1:A:315[B]:CYS:O	4:A:702:HOH:O	1.80	0.97
1:B:171[A]:ARG:NH2	4:B:701:HOH:O	1.81	0.94
1:B:288:VAL:CG2	1:B:289:PRO:HD3	1.98	0.93
1:A:348[A]:CYS:SG	4:A:1238:HOH:O	2.27	0.92
1:A:348[B]:CYS:SG	4:A:1066:HOH:O	2.33	0.86
1:A:55[B]:LYS:HE3	4:A:712:HOH:O	1.79	0.82
1:B:288:VAL:HG22	1:B:289:PRO:HD3	1.62	0.81
1:A:491[A]:GLN:OE1	4:A:703:HOH:O	1.99	0.81
1:B:301[B]:ASN:ND2	1:B:304:ARG:CD	2.47	0.76
1:B:288:VAL:HG23	1:B:289:PRO:HD3	1.68	0.74
1:B:301[B]:ASN:ND2	1:B:304:ARG:HD2	1.96	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301[B]:ASN:OD1	1:B:304:ARG:CZ	2.36	0.73
1:A:179:GLU:HG3	4:A:1062:HOH:O	1.92	0.69
1:A:363:GLN:OE1	4:A:705:HOH:O	2.12	0.68
1:A:461[A]:ASP:OD2	4:A:704:HOH:O	2.10	0.68
1:A:32:VAL:HG22	1:A:175:LYS:HD2	1.76	0.66
1:A:126:GLN:OE1	4:A:706:HOH:O	2.13	0.66
1:B:301[B]:ASN:ND2	1:B:304:ARG:HG2	2.12	0.65
1:B:370[A]:GLU:HG3	1:B:374[A]:ARG:NH2	2.12	0.65
1:A:288[A]:VAL:HG22	1:A:289:PRO:HD3	1.79	0.64
1:B:301[B]:ASN:ND2	1:B:304:ARG:CG	2.62	0.63
1:A:288[B]:VAL:HB	1:A:289:PRO:HD3	1.81	0.61
1:B:301[B]:ASN:HD21	1:B:304:ARG:CG	2.15	0.60
1:B:285:THR:HG23	1:B:314[B]:GLU:HG3	1.82	0.59
1:B:78:VAL:HG11	1:B:93:LYS:HE3	1.84	0.59
1:A:314:GLU:HB3	4:A:1005:HOH:O	2.07	0.54
1:B:288:VAL:CG2	1:B:289:PRO:CD	2.82	0.54
1:A:89:HIS:CE1	4:A:710:HOH:O	2.61	0.53
1:B:288:VAL:HG23	1:B:289:PRO:CD	2.37	0.52
1:A:165:GLU:OE2	4:A:707:HOH:O	2.19	0.51
1:A:186:ILE:HD12	4:B:819:HOH:O	2.10	0.50
1:A:288[A]:VAL:CG2	1:A:289:PRO:HD3	2.39	0.50
1:B:286:GLY:O	1:B:315[B]:CYS:HA	2.12	0.50
1:A:55[B]:LYS:HG3	4:A:712:HOH:O	2.13	0.49
1:B:56:ASP:O	1:B:60:ARG:HD3	2.12	0.49
1:A:179:GLU:CG	4:A:1062:HOH:O	2.58	0.48
1:A:546:VAL:HG11	1:B:518:GLN:HA	1.96	0.48
1:B:370[A]:GLU:OE2	1:B:374[A]:ARG:NH1	2.47	0.48
1:A:518:GLN:HA	1:B:546:VAL:HG11	1.94	0.48
1:B:370[A]:GLU:HG3	1:B:374[A]:ARG:HH22	1.78	0.48
1:B:107:GLU:HG3	4:B:1149:HOH:O	2.13	0.48
1:A:186:ILE:CD1	4:B:819:HOH:O	2.62	0.46
1:B:464:LYS:HG2	1:B:492:GLU:OE1	2.16	0.46
1:A:89:HIS:CE1	1:A:91:VAL:HG12	2.51	0.46
1:B:301[B]:ASN:CG	1:B:304:ARG:NE	2.64	0.45
1:B:301[B]:ASN:CG	1:B:304:ARG:HG2	2.37	0.44
1:A:288[A]:VAL:HG13	4:A:702:HOH:O	2.17	0.44
1:B:175:LYS:NZ	1:B:179:GLU:OE2	2.46	0.44
1:A:56:ASP:O	1:A:60:ARG:HD3	2.18	0.44
1:B:423:ASP:HA	1:B:426:GLY:O	2.17	0.44
1:B:190:PRO:HB3	1:B:552:LYS:HE3	1.99	0.43
1:B:288:VAL:HG12	1:B:315[A]:CYS:HB3	2.01	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288[A]:VAL:HG12	1:A:315[A]:CYS:CB	2.48	0.43
1:A:296:LYS:NZ	4:A:725:HOH:O	2.53	0.42
1:A:175:LYS:O	1:A:179:GLU:HG3	2.20	0.41
1:A:89:HIS:HE1	4:A:710:HOH:O	1.98	0.41
3:A:602:BEZ:C6	4:A:728:HOH:O	2.68	0.41
1:A:91:VAL:HG11	1:A:149:VAL:HG12	2.03	0.41
1:A:363:GLN:CG	4:A:713:HOH:O	2.69	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	552/567 (97%)	542 (98%)	10 (2%)	0	100	100
1	B	545/567 (96%)	532 (98%)	13 (2%)	0	100	100
All	All	1097/1134 (97%)	1074 (98%)	23 (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	457/465 (98%)	451 (99%)	6 (1%)	69	33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	451/465 (97%)	448 (99%)	3 (1%)	84	59
All	All	908/930 (98%)	899 (99%)	9 (1%)	78	47

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

Mol	Chain	Res	Type
1	A	55[A]	LYS
1	A	55[B]	LYS
1	A	181	GLU
1	A	449	PHE
1	A	460	ASP
1	A	487	LYS
1	B	420	LYS
1	B	449	PHE
1	B	563	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	GLN
1	A	363	GLN
1	A	563	GLN
1	B	300	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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$
3	BEZ	B	602	-	9,9,9	0.98	1 (11%)	11,11,11	0.90	1 (9%)
3	BEZ	A	602	-	9,9,9	0.90	1 (11%)	11,11,11	0.66	0
2	A1H1O	A	601	-	60,60,60	3.16	34 (56%)	97,101,101	3.22	39 (40%)
3	BEZ	A	603	-	9,9,9	1.16	1 (11%)	11,11,11	0.74	0
3	BEZ	B	601	-	9,9,9	0.63	0	11,11,11	0.91	1 (9%)

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
3	BEZ	B	602	-	-	0/4/4/4	0/1/1/1
3	BEZ	A	602	-	-	2/4/4/4	0/1/1/1
2	A1H1O	A	601	-	-	0/5/85/85	-
3	BEZ	A	603	-	-	0/4/4/4	0/1/1/1
3	BEZ	B	601	-	-	1/4/4/4	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1H1O	CAR-CAQ	-11.10	1.43	1.55
2	A	601	A1H1O	CBJ-CBI	-7.38	1.47	1.55
2	A	601	A1H1O	CBJ-CBK	-6.57	1.48	1.55
2	A	601	A1H1O	CAO-CAS	-5.60	1.46	1.52
2	A	601	A1H1O	CAG-CBK	-5.05	1.46	1.52
2	A	601	A1H1O	CBH-CAZ	-4.58	1.45	1.52
2	A	601	A1H1O	CBZ-CBR	-4.30	1.45	1.52
2	A	601	A1H1O	CBS-CBT	-4.24	1.50	1.55
2	A	601	A1H1O	CBC-CBB	-3.66	1.46	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1H1O	CAW-CAZ	-3.65	1.46	1.52
2	A	601	A1H1O	PAB-OAE	-3.63	1.53	1.59
2	A	601	A1H1O	CBQ-CBL	-3.53	1.33	1.40
2	A	601	A1H1O	CAY-CAQ	-3.52	1.46	1.52
2	A	601	A1H1O	CBN-CBT	-3.22	1.47	1.52
2	A	601	A1H1O	CBY-CBZ	-3.20	1.35	1.39
2	A	601	A1H1O	CAT-CAS	-3.07	1.47	1.52
2	A	601	A1H1O	CBS-CBR	-3.05	1.52	1.55
2	A	601	A1H1O	CAV-CBB	-3.04	1.47	1.52
2	A	601	A1H1O	CAP-CAO	-2.99	1.35	1.40
2	A	601	A1H1O	CBG-CBH	-2.95	1.35	1.39
2	A	601	A1H1O	CAP-CAQ	-2.93	1.49	1.52
2	A	601	A1H1O	CBA-CAZ	-2.90	1.52	1.55
2	A	601	A1H1O	CAY-CAT	-2.86	1.35	1.40
2	A	601	A1H1O	CBD-CBC	-2.80	1.36	1.39
3	A	603	BEZ	C1-C	2.69	1.55	1.49
2	A	601	A1H1O	CBM-CBL	-2.58	1.35	1.39
2	A	601	A1H1O	CBU-CBT	-2.57	1.48	1.52
2	A	601	A1H1O	CBZ-CBU	-2.55	1.35	1.40
3	B	602	BEZ	C1-C	2.54	1.54	1.49
2	A	601	A1H1O	PAB-OAD	2.49	1.64	1.54
2	A	601	A1H1O	CBL-CBK	-2.44	1.48	1.52
2	A	601	A1H1O	CAF-CAG	2.43	1.43	1.39
2	A	601	A1H1O	CBQ-CBI	-2.39	1.48	1.52
2	A	601	A1H1O	CBO-CBN	-2.22	1.36	1.40
2	A	601	A1H1O	PAB-OAC	2.20	1.63	1.54
3	A	602	BEZ	O2-C	-2.10	1.24	1.30
2	A	601	A1H1O	CAV-CAW	-2.01	1.36	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1H1O	CBR-CBS-CBT	-11.01	88.76	94.43
2	A	601	A1H1O	CBB-CBA-CAZ	-10.72	88.91	94.43
2	A	601	A1H1O	CAO-CAS-CAT	9.97	112.64	104.53
2	A	601	A1H1O	CAS-CAR-CAQ	-9.28	89.65	94.43
2	A	601	A1H1O	CAP-CAQ-CAY	8.45	111.41	104.53
2	A	601	A1H1O	CBI-CBJ-CBK	-8.21	90.21	94.43
2	A	601	A1H1O	CBS-CBR-CBO	4.86	103.54	99.28
2	A	601	A1H1O	OAE-CAF-CAG	4.53	123.66	118.34
2	A	601	A1H1O	CAG-CBK-CBL	4.52	108.21	104.53
2	A	601	A1H1O	CAH-CBI-CBQ	4.38	108.10	104.53

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1H1O	CBS-CBT-CBN	4.37	103.11	99.28
2	A	601	A1H1O	CAY-CAT-CAS	-4.31	102.13	106.58
2	A	601	A1H1O	CBJ-CBK-CBL	4.18	102.94	99.28
2	A	601	A1H1O	CBP-CBO-CBR	4.16	137.65	130.88
2	A	601	A1H1O	CAH-CAG-CBK	-3.97	103.00	106.69
2	A	601	A1H1O	CBV-CBU-CBT	3.85	135.03	129.37
2	A	601	A1H1O	CBJ-CBI-CBQ	3.83	102.63	99.28
2	A	601	A1H1O	CAV-CBB-CBC	3.45	109.14	105.39
2	A	601	A1H1O	CBJ-CBK-CAG	3.42	101.84	99.24
2	A	601	A1H1O	CBN-CBO-CBR	-3.40	103.07	106.58
2	A	601	A1H1O	CBY-CBZ-CBR	3.23	134.12	129.37
2	A	601	A1H1O	CAU-CAT-CAS	3.21	136.10	130.88
2	A	601	A1H1O	CAV-CAU-CAT	-3.11	117.95	123.20
2	A	601	A1H1O	CBN-CBM-CBL	-3.10	117.97	123.20
2	A	601	A1H1O	CAO-CAP-CAQ	-3.04	103.86	106.69
2	A	601	A1H1O	CAW-CAX-CAY	-2.97	118.19	123.20
2	A	601	A1H1O	CBH-CAZ-CAW	2.90	108.55	105.39
2	A	601	A1H1O	OAD-PAB-OAE	2.75	113.85	105.24
2	A	601	A1H1O	CBF-CBG-CBH	-2.66	117.63	121.01
2	A	601	A1H1O	CAU-CAV-CBB	2.64	135.18	130.88
2	A	601	A1H1O	CBP-CBQ-CBI	2.64	135.18	130.88
2	A	601	A1H1O	CBU-CBT-CBN	2.64	108.26	105.39
2	A	601	A1H1O	CBD-CBC-CBB	2.33	132.80	129.37
3	B	601	BEZ	O1-C-C1	-2.30	115.31	121.45
2	A	601	A1H1O	CBE-CBD-CBC	-2.28	118.11	121.01
2	A	601	A1H1O	CBQ-CBL-CBK	-2.27	104.24	106.58
2	A	601	A1H1O	CBA-CBB-CAV	2.21	101.21	99.28
2	A	601	A1H1O	CBZ-CBU-CBT	-2.18	104.33	106.58
3	B	602	BEZ	O1-C-C1	-2.14	115.74	121.45
2	A	601	A1H1O	CBG-CBH-CAZ	2.11	132.48	129.37
2	A	601	A1H1O	CBA-CAZ-CAW	2.08	101.10	99.28

There are no chirality outliers.

All (3) torsion outliers are listed below:

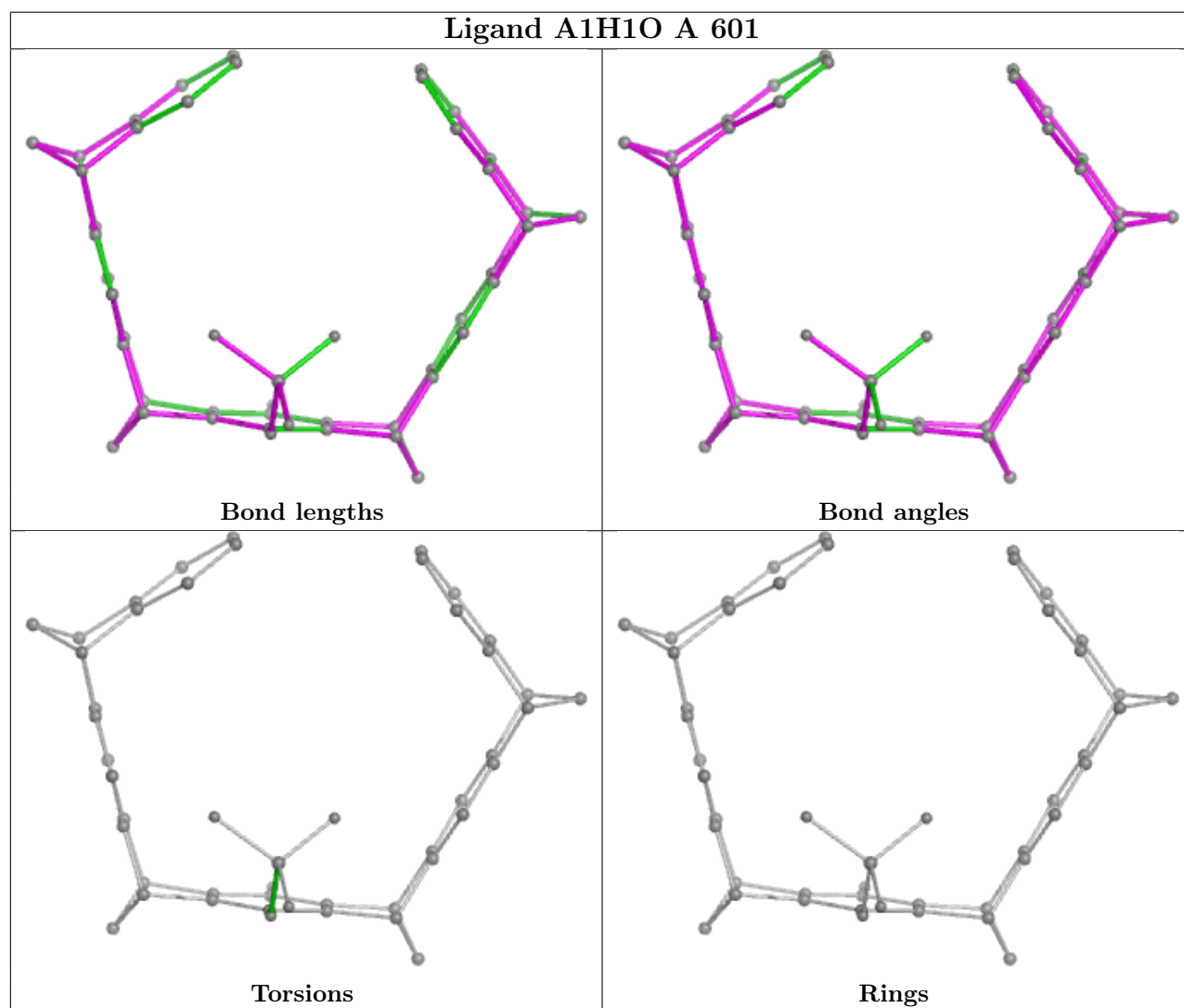
Mol	Chain	Res	Type	Atoms
3	A	602	BEZ	O2-C-C1-C6
3	B	601	BEZ	O1-C-C1-C2
3	A	602	BEZ	O1-C-C1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	BEZ	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	A	532/567 (93%)	-0.47	0 <b>100</b>   <b>100</b>	11, 16, 24, 44	0
1	B	532/567 (93%)	-0.34	2 (0%) <b>92</b>   <b>92</b>	11, 16, 29, 48	0
All	All	1064/1134 (93%)	-0.40	2 (0%) <b>95</b>   <b>94</b>	11, 16, 27, 48	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	PRO	3.0
1	B	409	SER	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.

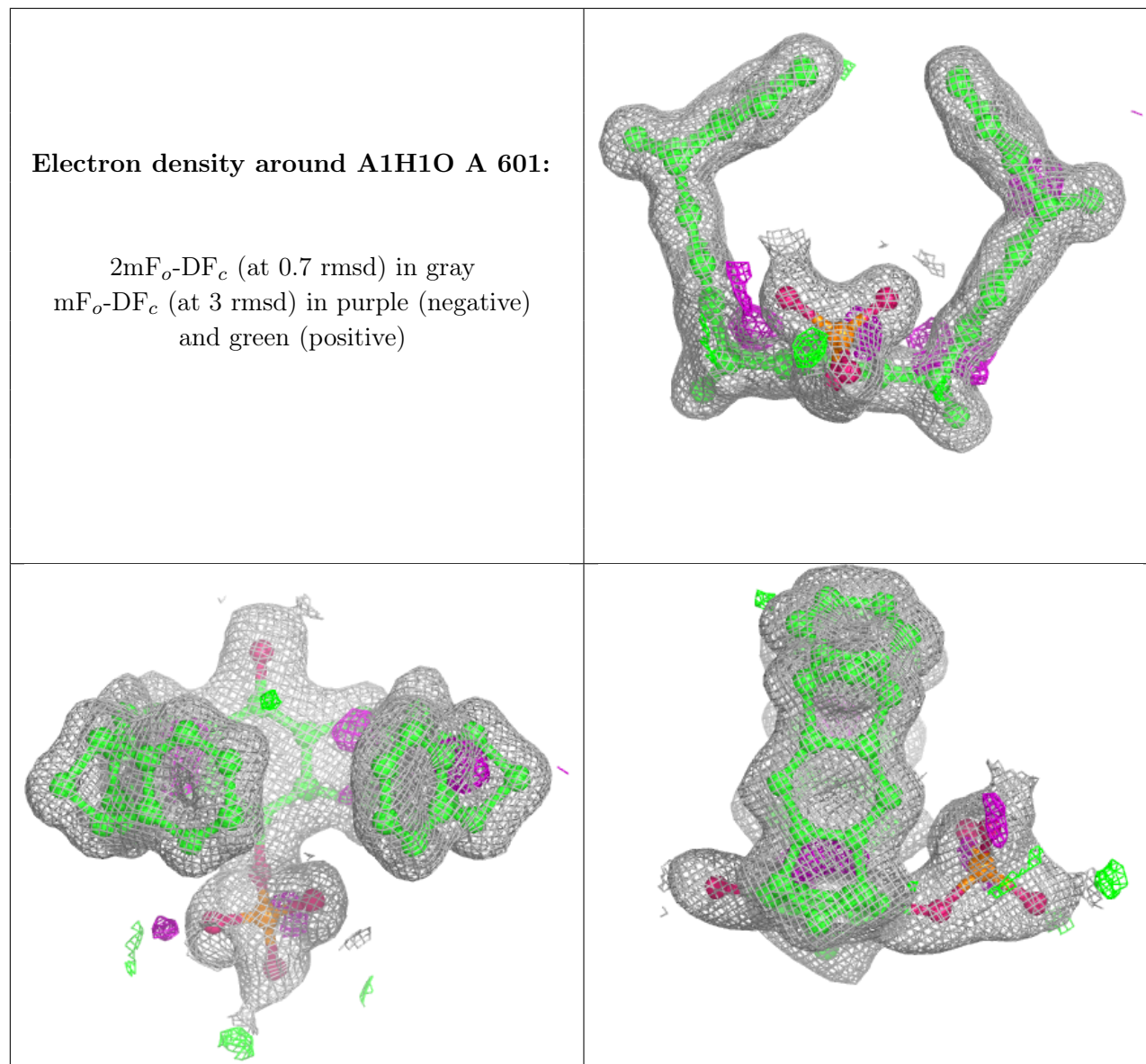
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BEZ	B	602	9/9	0.74	0.15	22,29,37,40	0
3	BEZ	A	603	9/9	0.84	0.19	21,26,34,34	0
2	A1H1O	A	601	48/48	0.93	0.10	16,20,28,35	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEZ	B	601	9/9	0.96	0.09	15,20,25,25	0
3	BEZ	A	602	9/9	0.97	0.10	14,19,24,27	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.