



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:51 PM UTC

PDB ID : 9ZXM / pdb\_00009zxm  
Title : DDB1 delta with compound 6  
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Deposited on : 2026-01-05  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

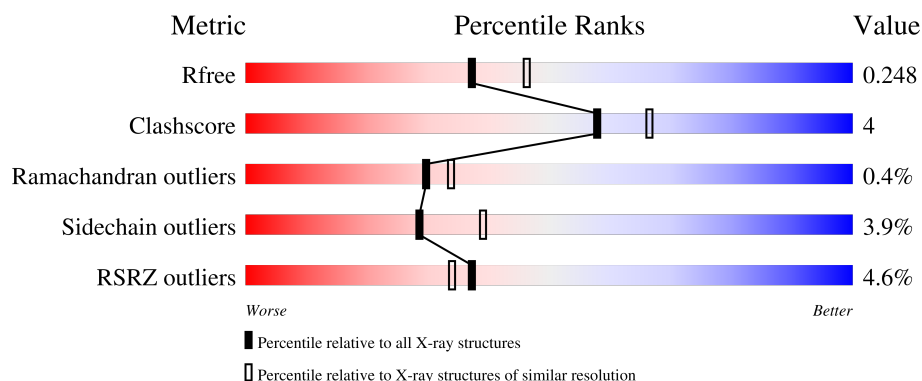
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	856	 4% 82% 11% • 6%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12813 atoms, of which 6308 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	803	Total	C	H	N	O	S	208	7	0
			12520	3977	6254	1053	1199	37			

There are 28 discrepancies between the modelled and reference sequences:

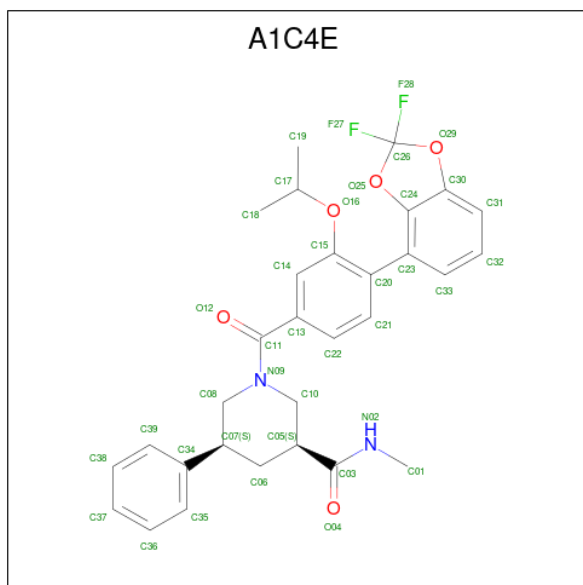
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	ASP	-	expression tag	UNP Q16531
A	-10	GLU	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	698	ILE	-	linker	UNP Q16531
A	699	GLY	-	linker	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531

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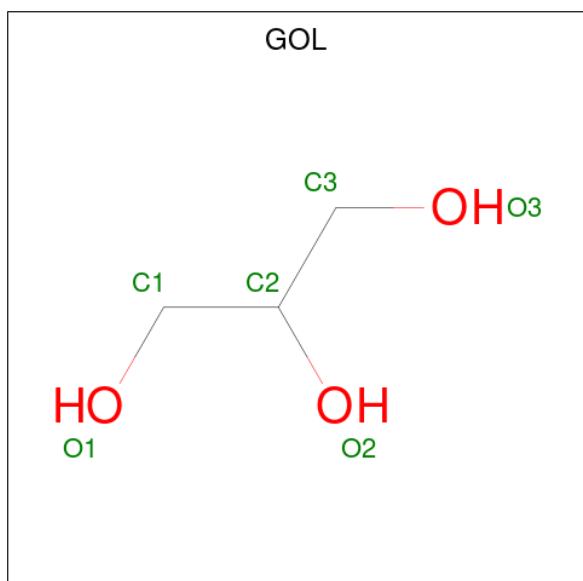
Chain	Residue	Modelled	Actual	Comment	Reference
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is (3S,5S)-1-{(4P)-4-(2,2-difluoro-2H-1,3-benzodioxol-4-yl)-3-[(propan-2-yl)oxy]benzene-1-carbonyl}-N-methyl-5-phenylpiperidine-3-carboxamide (CCD ID: A1C4E) (formula: C<sub>30</sub>H<sub>30</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			69	30	2	30	2	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total	O	0	0
			182	182		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: DNA damage-binding protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.75Å 115.92Å 120.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.11 – 2.19 33.11 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.11-2.19) 99.3 (33.11-2.19)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.191 , 0.246 0.192 , 0.248	Depositor DCC
$R_{free}$ test set	2406 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1C4E, GOL

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	0.54	0/6408	1.06	8/8674 (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	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PHE	CB-CA-C	-10.99	93.05	110.74
1	A	226	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	965	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	1041	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	824	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	778	HIS	CA-CB-CG	5.14	118.94	113.80
1	A	223	PRO	CA-C-N	5.05	126.08	120.06
1	A	223	PRO	C-N-CA	5.05	126.08	120.06

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	722	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	739	ARG	Sidechain

## 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	6266	6254	6177	56	1
2	A	39	30	0	0	0
3	A	18	24	24	0	0
4	A	182	0	0	3	0
All	All	6505	6308	6201	56	1

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 (56) 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:A:790:ASN:ND2	4:A:1301:HOH:O	2.12	0.82
1:A:118:THR:HG22	1:A:134:ARG:HH22	1.47	0.79
1:A:118:THR:CG2	1:A:134:ARG:HH22	1.98	0.76
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.68	0.74
1:A:234:GLN:HE22	1:A:257:THR:HB	1.53	0.72
1:A:290:GLN:HG3	1:A:294:THR:HG23	1.75	0.68
1:A:74:LYS:NZ	1:A:91:TYR:O	2.25	0.68
1:A:168:LYS:HE3	4:A:1335:HOH:O	1.93	0.67
1:A:257:THR:HG23	1:A:276[B]:MET:SD	2.35	0.67
1:A:989:ARG:HG2	1:A:989:ARG:HH11	1.60	0.67
1:A:954:MET:HE2	1:A:957:VAL:HG12	1.80	0.62
1:A:954:MET:HE2	1:A:957:VAL:CG1	2.30	0.61
1:A:292:ASP:OD1	1:A:294:THR:HG22	2.03	0.59
1:A:913:TYR:CZ	1:A:924:GLY:HA3	2.37	0.59
1:A:374:GLN:HE22	1:A:713:ARG:HH21	1.52	0.57
1:A:1095:GLU:OE2	1:A:1140:HIS:HE1	1.86	0.57
1:A:118:THR:HG21	1:A:165:ILE:O	2.04	0.56
1:A:1080:ARG:O	1:A:1081:LYS:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ARG:HG2	1:A:989:ARG:NH1	2.24	0.51
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.92	0.51
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.42	0.50
1:A:130:MET:HE3	1:A:176:PRO:CG	2.42	0.50
1:A:224:GLU:O	1:A:225:PRO:C	2.56	0.49
1:A:840:GLU:O	1:A:841:ALA:HB3	2.13	0.48
1:A:1027:SER:HB2	1:A:1039:LEU:HD11	1.95	0.48
1:A:1010:GLY:O	1:A:1027:SER:OG	2.31	0.47
1:A:174:GLN:N	1:A:174:GLN:OE1	2.46	0.47
1:A:290:GLN:CG	1:A:294:THR:HG23	2.45	0.47
1:A:318:ASP:O	1:A:321:VAL:HG13	2.15	0.47
1:A:743:GLN:HE22	1:A:747:GLY:C	2.23	0.46
1:A:954:MET:CE	1:A:957:VAL:HG12	2.45	0.46
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.96	0.46
1:A:118:THR:HG23	1:A:134:ARG:HH22	1.79	0.45
1:A:870:VAL:HA	1:A:883:SER:O	2.16	0.45
1:A:867:LYS:HG2	4:A:1412:HOH:O	2.17	0.45
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.32	0.45
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.52	0.44
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.88	0.44
1:A:907:ASN:ND2	1:A:931:LEU:HD11	2.32	0.44
1:A:234:GLN:NE2	1:A:257:THR:HB	2.25	0.43
1:A:246:LEU:HD12	1:A:297:LEU:HD13	2.00	0.43
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.88	0.43
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.53	0.43
1:A:883:SER:HB2	1:A:911:ALA:HB3	2.01	0.43
1:A:181:VAL:HA	1:A:189:HIS:O	2.19	0.42
1:A:989:ARG:NH1	1:A:989:ARG:CG	2.81	0.42
1:A:223:PRO:O	1:A:226:PHE:O	2.36	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.01	0.42
1:A:114:ARG:HD2	1:A:137:ASP:OD2	2.20	0.42
1:A:989:ARG:HH11	1:A:989:ARG:CG	2.31	0.41
1:A:964:ASN:ND2	1:A:978:GLN:HB3	2.36	0.41
1:A:5:TYR:HB3	1:A:1041:THR:HG23	2.02	0.41
1:A:963:ASP:O	1:A:978:GLN:HA	2.21	0.41
1:A:954:MET:CE	1:A:957:VAL:CG1	2.98	0.40
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.86	0.40
1:A:742:VAL:HG22	1:A:783:GLY:HA2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:O	1:A:291:MET:H[4_445]	1.52	0.08

## 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	800/856 (94%)	766 (96%)	31 (4%)	3 (0%)	30 34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ASP
1	A	369	ARG
1	A	1081	LYS

### 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	691/744 (93%)	664 (96%)	27 (4%)	28 39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	52	VAL
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	147	ARG
1	A	162	LEU
1	A	224	GLU
1	A	255	GLN
1	A	257	THR
1	A	297	LEU
1	A	321	VAL
1	A	340	SER
1	A	350	MET
1	A	360	VAL
1	A	744	ASP
1	A	840	GLU
1	A	888	VAL
1	A	904	ASN
1	A	965	PHE
1	A	969	GLU
1	A	988	GLU
1	A	990	GLN
1	A	991	HIS
1	A	994	GLU
1	A	1027	SER
1	A	1061	VAL
1	A	1065	VAL
1	A	1127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	163	HIS
1	A	234	GLN
1	A	290	GLN
1	A	374	GLN
1	A	877	ASN
1	A	905	HIS
1	A	907	ASN
1	A	964	ASN
1	A	1140	HIS

### 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 ⓘ

4 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	$\# Z  > 2$
2	A1C4E	A	1201	-	43,43,43	2.37	12 (27%)	59,63,63	2.64	13 (22%)
3	GOL	A	1203	-	5,5,5	0.11	0	5,5,5	0.33	0
3	GOL	A	1202	-	5,5,5	0.24	0	5,5,5	0.60	0
3	GOL	A	1204	-	5,5,5	0.13	0	5,5,5	0.18	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
2	A1C4E	A	1201	-	-	6/26/48/48	0/5/5/5
3	GOL	A	1203	-	-	2/4/4/4	-
3	GOL	A	1202	-	-	1/4/4/4	-
3	GOL	A	1204	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1C4E	C03-N02	10.46	1.48	1.33
2	A	1201	A1C4E	C05-C03	4.44	1.59	1.51
2	A	1201	A1C4E	C11-N09	4.27	1.43	1.34
2	A	1201	A1C4E	C10-N09	3.59	1.50	1.46
2	A	1201	A1C4E	F28-C26	2.99	1.37	1.33
2	A	1201	A1C4E	C06-C07	-2.92	1.49	1.53
2	A	1201	A1C4E	C13-C11	2.63	1.54	1.50
2	A	1201	A1C4E	O12-C11	-2.33	1.17	1.22
2	A	1201	A1C4E	F27-C26	2.30	1.36	1.33
2	A	1201	A1C4E	O04-C03	-2.27	1.19	1.23
2	A	1201	A1C4E	O29-C30	2.15	1.41	1.38
2	A	1201	A1C4E	C06-C05	-2.10	1.49	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1C4E	C05-C03-N02	11.23	130.38	116.18
2	A	1201	A1C4E	F28-C26-F27	9.39	113.16	105.85
2	A	1201	A1C4E	O04-C03-N02	-5.03	114.74	123.13
2	A	1201	A1C4E	F27-C26-O29	-4.76	106.78	110.10
2	A	1201	A1C4E	O04-C03-C05	-4.74	114.88	122.19
2	A	1201	A1C4E	O12-C11-N09	-4.44	115.35	122.35
2	A	1201	A1C4E	C13-C11-N09	4.31	124.05	118.66
2	A	1201	A1C4E	F28-C26-O25	-3.80	107.45	110.10
2	A	1201	A1C4E	C06-C05-C03	3.28	116.79	110.04
2	A	1201	A1C4E	F27-C26-O25	-3.27	107.82	110.10
2	A	1201	A1C4E	O29-C30-C31	3.03	130.91	124.56
2	A	1201	A1C4E	O25-C24-C23	3.02	130.11	124.28
2	A	1201	A1C4E	C01-N02-C03	2.71	126.93	122.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	A1C4E	O04-C03-N02-C01
2	A	1201	A1C4E	C05-C03-N02-C01
3	A	1203	GOL	O1-C1-C2-C3
3	A	1203	GOL	O1-C1-C2-O2
2	A	1201	A1C4E	C08-C07-C34-C35
2	A	1201	A1C4E	N02-C03-C05-C06
2	A	1201	A1C4E	O04-C03-C05-C06

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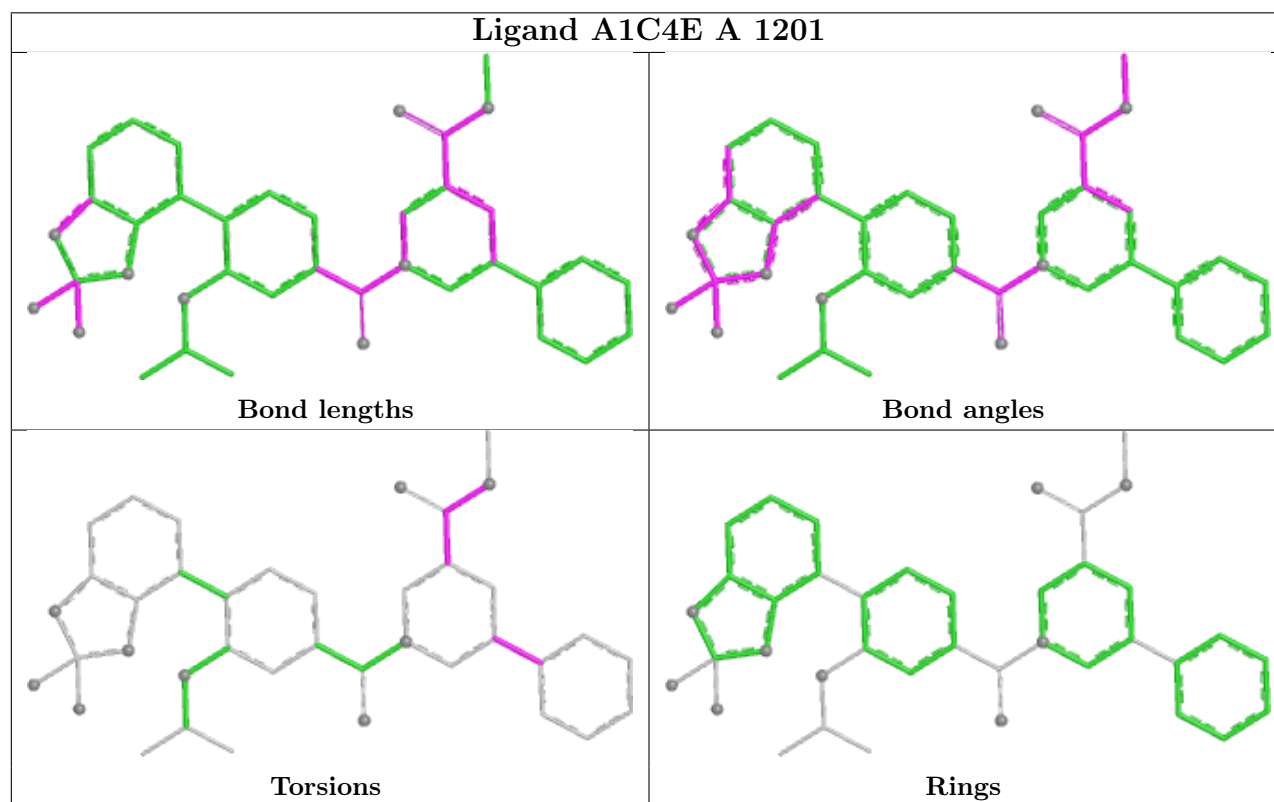
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Mol	Chain	Res	Type	Atoms
3	A	1202	GOL	O1-C1-C2-O2
2	A	1201	A1C4E	C08-C07-C34-C39

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, 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	803/856 (93%)	-0.08	37 (4%) 37 34	10, 33, 75, 119	6 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	965	PHE	9.5
1	A	1023	PRO	4.9
1	A	783	GLY	4.5
1	A	982	ALA	4.2
1	A	343	GLN	3.7
1	A	1015	GLN	3.5
1	A	949[A]	PHE	3.4
1	A	709	LYS	3.3
1	A	1	MET	3.1
1	A	782	PHE	3.0
1	A	909	ILE	2.9
1	A	341	ASN	2.8
1	A	338	VAL	2.8
1	A	393	GLY	2.8
1	A	941	ASN	2.8
1	A	951	PRO	2.8
1	A	989	ARG	2.7
1	A	906	TYR	2.6
1	A	367	LEU	2.6
1	A	344	GLY	2.5
1	A	342	GLU	2.5
1	A	370	GLN	2.5
1	A	1112	LEU	2.5
1	A	991	HIS	2.4
1	A	1079	GLU	2.4
1	A	1124	ALA	2.4
1	A	224	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1014	MET	2.4
1	A	953	TRP	2.3
1	A	1109	VAL	2.2
1	A	371	GLY	2.2
1	A	226	PHE	2.1
1	A	990	GLN	2.1
1	A	369	ARG	2.1
1	A	373	GLY	2.1
1	A	744	ASP	2.0
1	A	992	LEU	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](#)

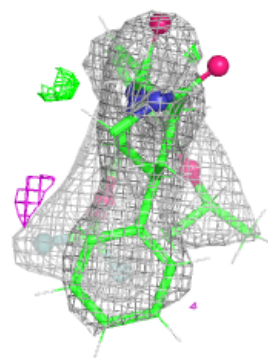
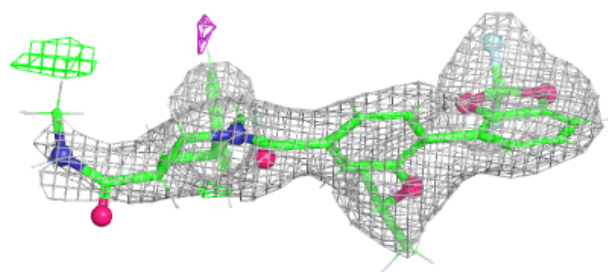
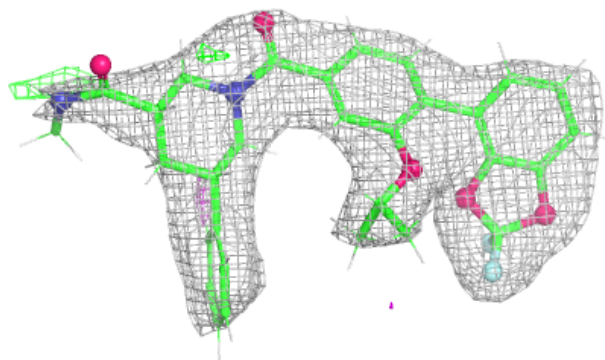
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1202	6/6	0.84	0.17	43,50,51,55	3
2	A1C4E	A	1201	39/39	0.90	0.11	42,52,77,84	0
3	GOL	A	1203	6/6	0.90	0.13	40,46,54,58	3
3	GOL	A	1204	6/6	0.90	0.11	39,45,53,57	3

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 A1C4E A 1201:**

$2mF_o-DF_c$  (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.