



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:05 PM UTC

PDB ID : 9ZXN / pdb_00009zxn
Title : DDB1 delta with compound 26
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Deposited on : 2026-01-05
Resolution : 2.07 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

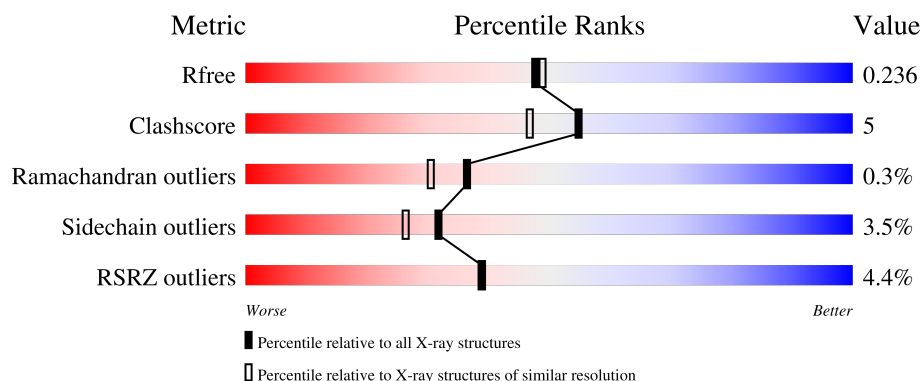
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	856	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12937 atoms, of which 6351 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	804	Total	C	H	N	O	S	231	8	0
			12588	4002	6295	1052	1199	40			

There are 28 discrepancies between the modelled and reference sequences:

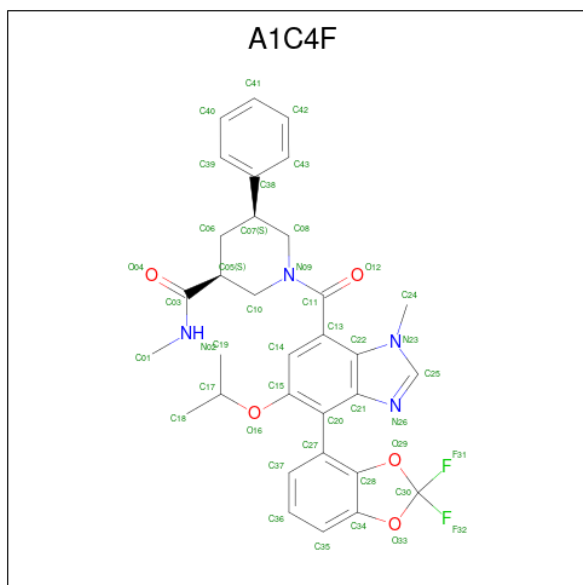
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression 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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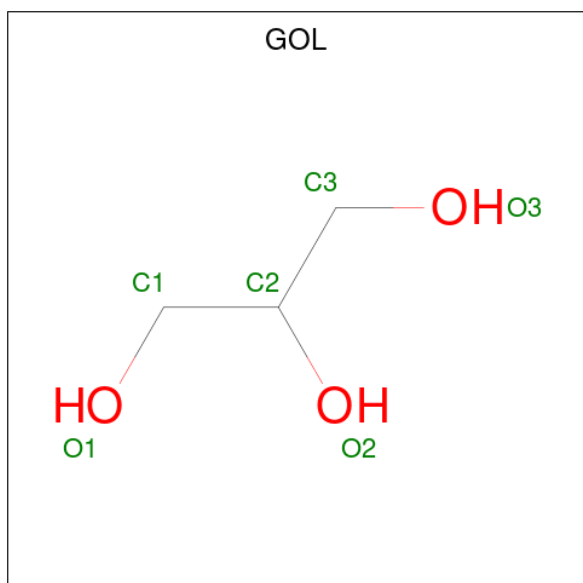
Chain	Residue	Modelled	Actual	Comment	Reference
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is (3S,5S)-1-[(4P)-4-(2,2-difluoro-2H-1,3-benzodioxol-4-yl)-1-methyl-5-[(propan-2-yl)oxy]-1H-1,3-benzimidazole-7-carbonyl]-N-methyl-5-phenylpiperidine-3-carboxamide (CCD ID: A1C4F) (formula: C₃₂H₃₂F₂N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			75	32	2	32	4	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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		

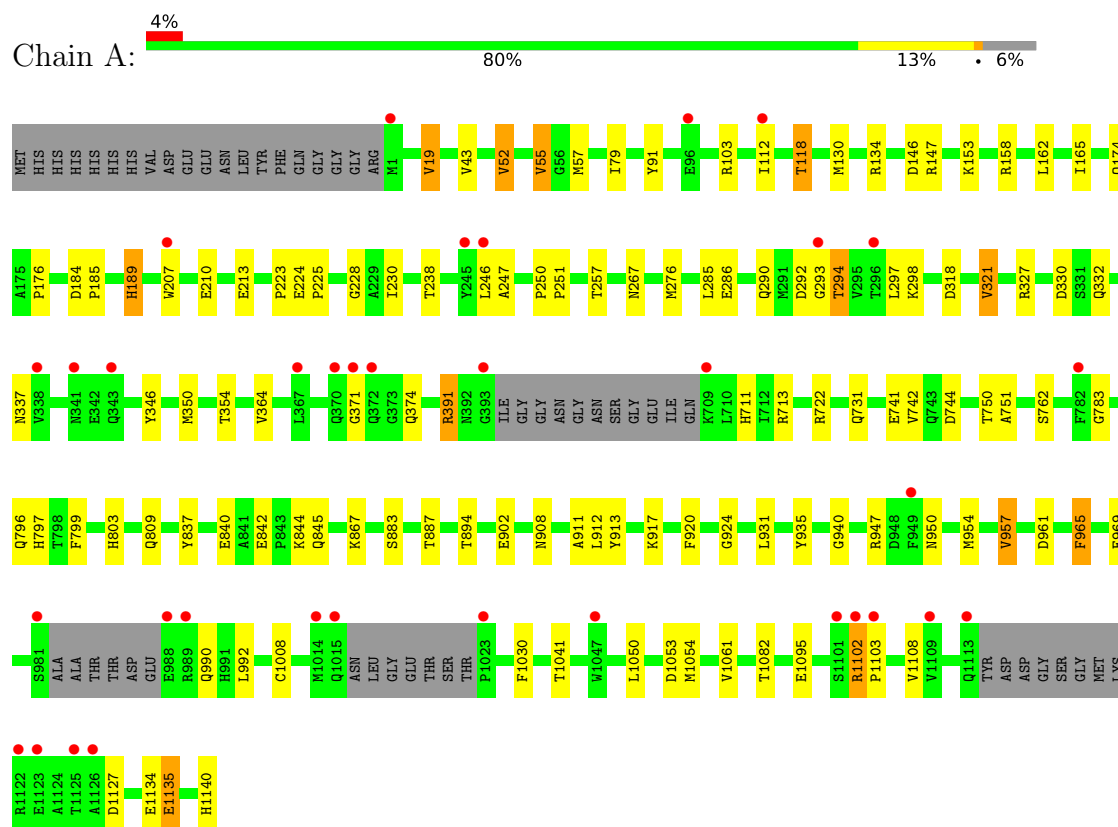
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		

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, α , β , γ	67.42Å 116.07Å 120.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.93 – 2.07 44.93 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.93-2.07) 99.9 (44.93-2.07)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.188 , 0.235 0.189 , 0.236	Depositor DCC
R_{free} test set	2852 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12937	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GOL, A1C4F

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	0.55	0/6443	1.08	18/8718 (0.2%)

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	9

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	969	GLU	N-CA-CB	-9.60	94.84	111.55
1	A	969	GLU	CB-CA-C	8.39	126.99	109.79
1	A	19	VAL	N-CA-CB	-7.94	96.54	111.62
1	A	55	VAL	N-CA-CB	-6.84	100.23	111.45
1	A	842	GLU	CB-CA-C	6.26	117.87	109.42
1	A	887	THR	CA-CB-OG1	-6.13	100.40	109.60
1	A	1030	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	146	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	330	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	1082	THR	CA-CB-OG1	-5.37	101.54	109.60
1	A	213	GLU	N-CA-CB	-5.37	101.33	109.92
1	A	894	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	799	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	965[A]	PHE	N-CA-CB	-5.28	102.30	110.65
1	A	965[B]	PHE	N-CA-CB	-5.28	102.30	110.65
1	A	354	THR	CA-CB-OG1	-5.10	101.95	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1041	THR	CA-CB-OG1	-5.08	101.97	109.60
1	A	1053	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	1102	ARG	Sidechain
1	A	158	ARG	Sidechain
1	A	223	PRO	Peptide
1	A	327	ARG	Sidechain
1	A	332	GLN	Peptide
1	A	391	ARG	Sidechain
1	A	940	GLY	Peptide
1	A	965[A]	PHE	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	6293	6295	6219	60	0
2	A	43	32	0	2	0
3	A	18	24	24	1	0
4	A	232	0	0	2	0
All	All	6586	6351	6243	61	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 5.

All (61) 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:118:THR:HG22	1:A:134:ARG:HH22	1.16	1.04
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:CG2	1:A:134:ARG:HH22	1.91	0.83
1:A:744:ASP:OD2	1:A:750:THR:HG23	1.79	0.81
1:A:1054:MET:HA	1:A:1054:MET:HE2	1.63	0.80
1:A:954[A]:MET:HE2	1:A:957:VAL:HG12	1.72	0.71
1:A:118:THR:HG22	1:A:134:ARG:NH2	1.99	0.71
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.73	0.69
1:A:374:GLN:HE22	1:A:713:ARG:NH2	1.93	0.67
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.17	0.62
1:A:293:GLY:O	1:A:294:THR:O	2.18	0.61
1:A:374:GLN:HE22	1:A:713:ARG:HH21	1.53	0.57
1:A:118:THR:HG21	1:A:165:ILE:O	2.05	0.57
1:A:230:ILE:HD11	1:A:285:LEU:HD21	1.87	0.57
3:A:1204:GOL:H11	4:A:1472:HOH:O	2.06	0.56
1:A:290:GLN:HB2	1:A:294:THR:HG23	1.88	0.56
1:A:837:TYR:HB2	1:A:840:GLU:HG3	1.88	0.56
1:A:174:GLN:N	1:A:174:GLN:OE1	2.42	0.53
1:A:950:ASN:CB	1:A:954[B]:MET:HE2	2.39	0.53
1:A:837:TYR:HB2	1:A:840:GLU:CG	2.40	0.52
1:A:292:ASP:CG	1:A:294:THR:HG22	2.35	0.51
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.92	0.51
1:A:920:PHE:CD2	2:A:1201:A1C4F:C01	2.94	0.50
1:A:742:VAL:CG2	1:A:783:GLY:HA2	2.43	0.49
1:A:731:GLN:NE2	1:A:797:HIS:NE2	2.60	0.49
1:A:742:VAL:HG22	1:A:783:GLY:HA2	1.94	0.49
1:A:337:ASN:O	1:A:346:TYR:HB3	2.14	0.48
1:A:57:MET:HE2	1:A:79:ILE:HG21	1.95	0.47
1:A:731:GLN:HA	1:A:796:GLN:OE1	2.15	0.47
1:A:913:TYR:CE1	1:A:924:GLY:HA3	2.49	0.47
1:A:954[A]:MET:HB3	1:A:954[A]:MET:HE3	1.72	0.46
1:A:290:GLN:O	1:A:292:ASP:O	2.34	0.46
1:A:391:ARG:NH1	1:A:711:HIS:ND1	2.59	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.46	0.46
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.31	0.46
1:A:207:TRP:CZ2	1:A:228:GLY:HA2	2.52	0.45
1:A:844:LYS:O	1:A:867:LYS:C	2.59	0.45
1:A:364:VAL:HG23	1:A:1008[A]:CYS:SG	2.57	0.44
1:A:225:PRO:HG2	1:A:267:ASN:CB	2.38	0.44
1:A:722:ARG:NH1	4:A:1303:HOH:O	2.40	0.44
1:A:43:VAL:HG23	1:A:52:VAL:HG21	2.00	0.44
1:A:913:TYR:CZ	1:A:924:GLY:HA3	2.52	0.44
1:A:238:THR:HG22	1:A:247:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LEU:C	1:A:931:LEU:HD12	2.43	0.43
1:A:286:GLU:O	1:A:298:LYS:N	2.45	0.43
1:A:920:PHE:HD2	2:A:1201:A1C4F:C01	2.32	0.43
1:A:224:GLU:N	1:A:225:PRO:CD	2.83	0.42
1:A:153:LYS:HA	1:A:153:LYS:HE2	2.01	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.02	0.42
1:A:961:ASP:OD1	1:A:961:ASP:C	2.63	0.42
1:A:130:MET:HE3	1:A:176:PRO:CG	2.50	0.42
1:A:1134:GLU:O	1:A:1135:GLU:C	2.61	0.41
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.88	0.41
1:A:318:ASP:O	1:A:321:VAL:HG13	2.21	0.41
1:A:184:ASP:OD1	1:A:189:HIS:NE2	2.54	0.41
1:A:908:ASN:OD1	1:A:947:ARG:NH1	2.40	0.41
1:A:1054:MET:HE1	1:A:1108:VAL:HG12	2.02	0.41
1:A:1095:GLU:OE2	1:A:1140:HIS:HE1	2.04	0.41
1:A:762:SER:O	1:A:803:HIS:HA	2.21	0.40
1:A:52:VAL:HG13	1:A:91:TYR:OH	2.22	0.40
1:A:257:THR:HB	1:A:276[B]:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	803/856 (94%)	770 (96%)	31 (4%)	2 (0%)	43 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	THR
1	A	371	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	696/744 (94%)	672 (97%)	24 (3%)	32	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	52	VAL
1	A	55	VAL
1	A	112	ILE
1	A	118	THR
1	A	147	ARG
1	A	162	LEU
1	A	189	HIS
1	A	210	GLU
1	A	246	LEU
1	A	297	LEU
1	A	321	VAL
1	A	350	MET
1	A	809	GLN
1	A	845	GLN
1	A	912	LEU
1	A	917	LYS
1	A	957	VAL
1	A	990	GLN
1	A	992	LEU
1	A	1050	LEU
1	A	1061	VAL
1	A	1127	ASP
1	A	1135	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN

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Mol	Chain	Res	Type
1	A	105	HIS
1	A	163	HIS
1	A	186	GLN
1	A	234	GLN
1	A	374	GLN
1	A	727	GLN
1	A	731	GLN
1	A	810	ASN
1	A	905	HIS
1	A	964	ASN
1	A	990	GLN
1	A	993	GLN
1	A	1140	HIS

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](#)

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	$\# Z > 2$
3	GOL	A	1204	-	5,5,5	0.13	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	1203	-	5,5,5	0.14	0	5,5,5	0.42	0
3	GOL	A	1202	-	5,5,5	0.23	0	5,5,5	0.58	0
2	A1C4F	A	1201	-	48,48,48	2.26	14 (29%)	63,72,72	2.97	21 (33%)

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	GOL	A	1204	-	-	0/4/4/4	-
3	GOL	A	1203	-	-	2/4/4/4	-
3	GOL	A	1202	-	-	1/4/4/4	-
2	A1C4F	A	1201	-	-	6/26/48/48	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1C4F	C03-N02	8.90	1.45	1.33
2	A	1201	A1C4F	C22-C21	-4.14	1.36	1.40
2	A	1201	A1C4F	C11-N09	3.95	1.43	1.34
2	A	1201	A1C4F	C10-N09	3.41	1.50	1.46
2	A	1201	A1C4F	O04-C03	-3.36	1.16	1.23
2	A	1201	A1C4F	C20-C21	3.36	1.44	1.40
2	A	1201	A1C4F	C06-C07	-3.30	1.49	1.53
2	A	1201	A1C4F	F32-C30	3.29	1.37	1.33
2	A	1201	A1C4F	C05-C03	3.24	1.57	1.51
2	A	1201	A1C4F	O29-C30	2.79	1.42	1.38
2	A	1201	A1C4F	F31-C30	2.78	1.36	1.33
2	A	1201	A1C4F	C06-C05	-2.42	1.48	1.53
2	A	1201	A1C4F	O33-C30	2.34	1.41	1.38
2	A	1201	A1C4F	C20-C15	-2.10	1.37	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1C4F	C05-C03-N02	11.72	131.00	116.18
2	A	1201	A1C4F	F32-C30-F31	9.49	113.24	105.85
2	A	1201	A1C4F	O04-C03-N02	-5.60	113.78	123.13
2	A	1201	A1C4F	F31-C30-O29	-5.55	106.23	110.10
2	A	1201	A1C4F	C21-C22-N23	5.40	106.93	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1C4F	F32-C30-O33	-5.01	106.60	110.10
2	A	1201	A1C4F	C13-C11-N09	4.87	125.81	118.24
2	A	1201	A1C4F	C27-C20-C21	-4.81	114.55	121.24
2	A	1201	A1C4F	O04-C03-C05	-4.52	115.21	122.19
2	A	1201	A1C4F	N23-C25-N26	-4.07	108.55	114.27
2	A	1201	A1C4F	C06-C05-C10	3.56	113.42	109.83
2	A	1201	A1C4F	C22-C21-N26	-3.54	107.27	110.22
2	A	1201	A1C4F	C21-N26-C25	3.25	108.56	103.45
2	A	1201	A1C4F	C13-C22-C21	-2.97	117.74	121.36
2	A	1201	A1C4F	O29-C28-C27	2.71	129.51	124.28
2	A	1201	A1C4F	C14-C15-C20	-2.64	117.99	121.69
2	A	1201	A1C4F	O33-C34-C35	2.64	130.09	124.56
2	A	1201	A1C4F	O12-C11-N09	-2.61	118.24	122.35
2	A	1201	A1C4F	C24-N23-C25	-2.22	123.13	126.89
2	A	1201	A1C4F	O12-C11-C13	-2.14	115.86	120.06
2	A	1201	A1C4F	C14-C13-C22	2.14	121.76	118.79

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	A1C4F	O04-C03-N02-C01
2	A	1201	A1C4F	C05-C03-N02-C01
3	A	1203	GOL	O1-C1-C2-C3
3	A	1203	GOL	O1-C1-C2-O2
3	A	1202	GOL	O1-C1-C2-O2
2	A	1201	A1C4F	C15-C20-C27-C37
2	A	1201	A1C4F	C08-C07-C38-C39
2	A	1201	A1C4F	C08-C07-C38-C43
2	A	1201	A1C4F	O04-C03-C05-C10

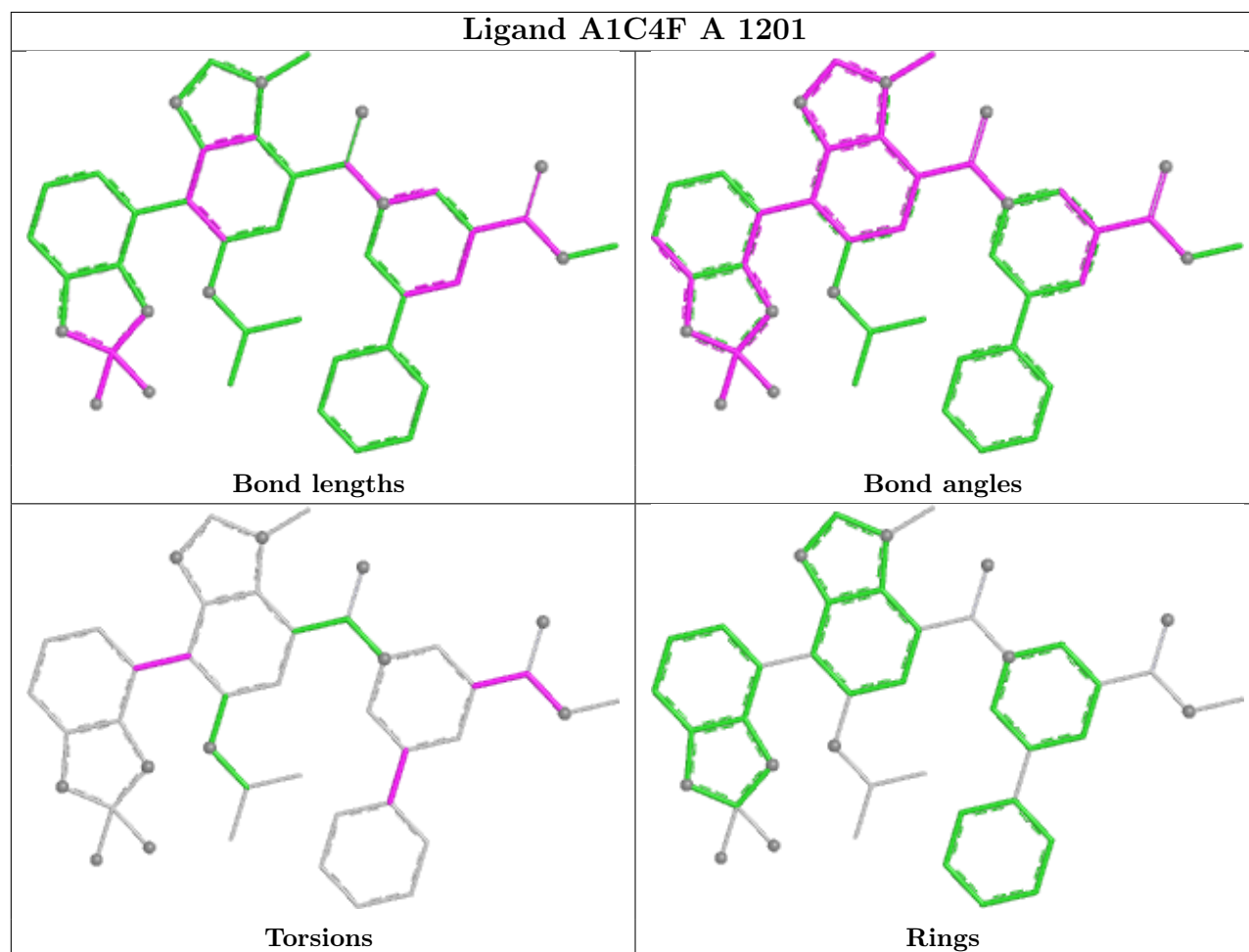
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	GOL	1	0
2	A	1201	A1C4F	2	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	803/856 (93%)	-0.17	35 (4%) 39 39	9, 33, 68, 115	5 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	4.8
1	A	988	GLU	4.6
1	A	949	PHE	4.3
1	A	1122	ARG	4.2
1	A	782	PHE	4.2
1	A	1015	GLN	3.9
1	A	989	ARG	3.7
1	A	1	MET	3.6
1	A	1113	GLN	3.4
1	A	1023	PRO	3.3
1	A	207	TRP	3.1
1	A	1014	MET	2.9
1	A	1126	ALA	2.9
1	A	370	GLN	2.8
1	A	338	VAL	2.7
1	A	981	SER	2.7
1	A	343	GLN	2.6
1	A	341	ASN	2.6
1	A	709	LYS	2.6
1	A	367	LEU	2.6
1	A	112	ILE	2.5
1	A	1123	GLU	2.4
1	A	372	GLN	2.4
1	A	1102	ARG	2.3
1	A	1109	VAL	2.3
1	A	246	LEU	2.3
1	A	245	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	296	THR	2.3
1	A	293	GLY	2.3
1	A	96	GLU	2.2
1	A	371	GLY	2.2
1	A	1047	TRP	2.1
1	A	1101	SER	2.1
1	A	1103	PRO	2.0
1	A	1125	THR	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](#)

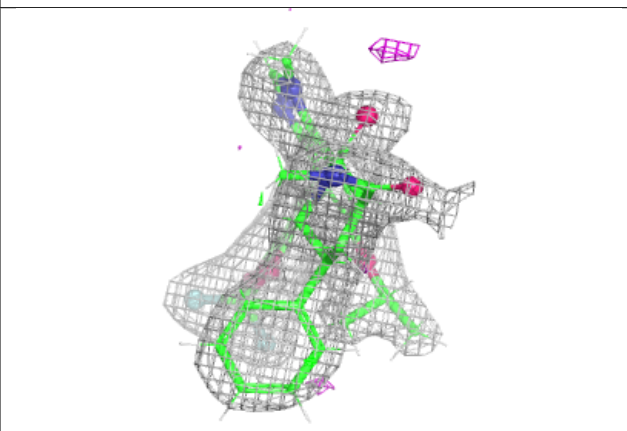
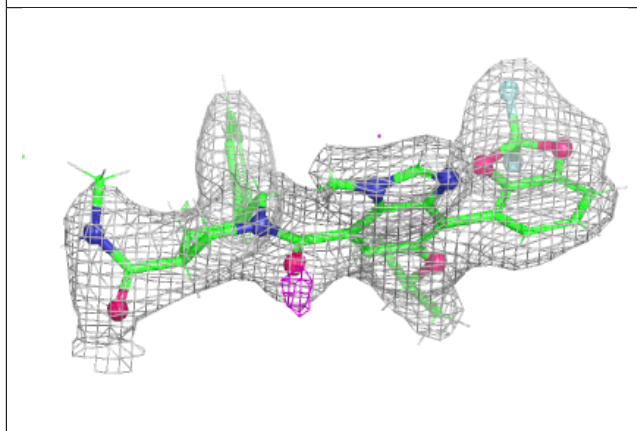
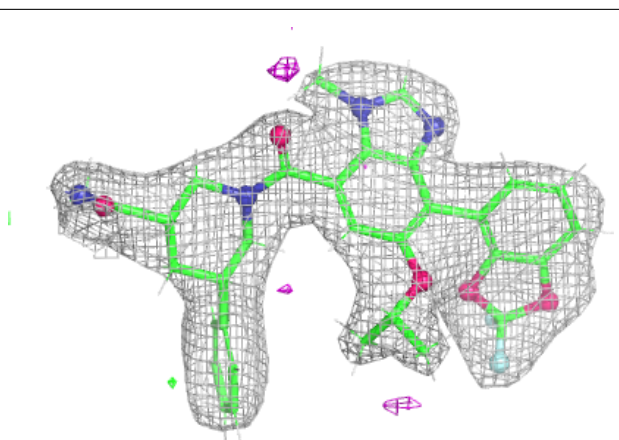
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	1202	6/6	0.89	0.14	38,51,54,55	3
3	GOL	A	1203	6/6	0.92	0.11	40,51,64,66	3
2	A1C4F	A	1201	43/43	0.93	0.10	38,47,66,69	0
3	GOL	A	1204	6/6	0.94	0.11	48,49,52,52	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 A1C4F 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.