



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 10:15 AM EST

PDB ID : 9YDG / pdb_00009ydg
Title : Crystal structure of the human DCAF1 WDR domain in complex with OICR-41074
Authors : kimani, S.; Dong, A.; Li, Y.; Seitova, A.; Mamai, A.; Al-awar, R.; Ackloo, S.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on : 2025-09-22
Resolution : 1.54 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](#) ①) 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

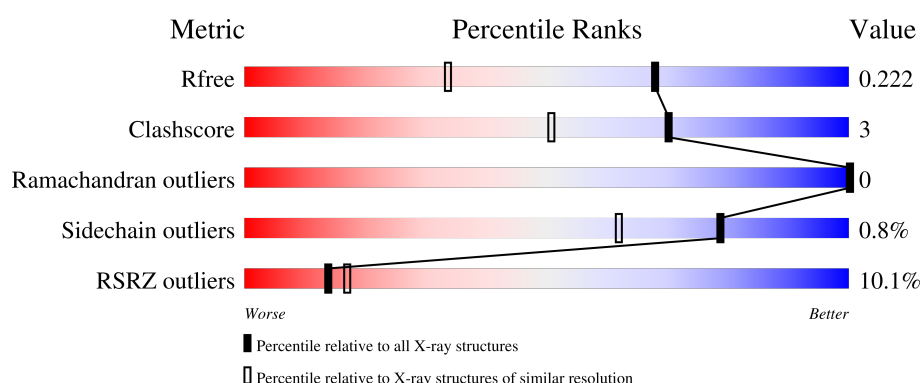
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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	315	<div> <div>12%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	B	315	<div> <div>7%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5245 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.

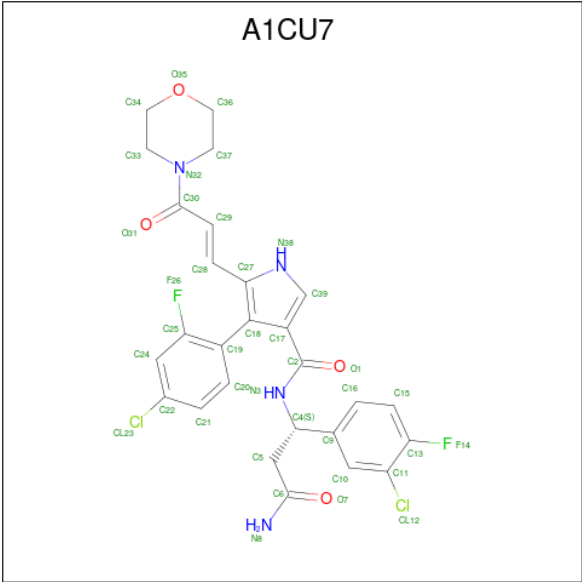
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	10	0
			2354	1491	394	452	17			
1	B	299	Total	C	N	O	S	0	10	1
			2406	1519	408	460	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	GLY	-	expression tag	UNP Q9Y4B6
A	1077	ALA	-	expression tag	UNP Q9Y4B6
A	1078	SER	-	expression tag	UNP Q9Y4B6
A	1079	ALA	-	expression tag	UNP Q9Y4B6
B	1076	GLY	-	expression tag	UNP Q9Y4B6
B	1077	ALA	-	expression tag	UNP Q9Y4B6
B	1078	SER	-	expression tag	UNP Q9Y4B6
B	1079	ALA	-	expression tag	UNP Q9Y4B6

- Molecule 2 is (4P)-N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-5-[(1E)-3-(morpholin-4-yl)-3-oxoprop-1-en-1-yl]-1H-pyrrole-3-carboxamide (CCD ID: A1CU7) (formula: C₂₇H₂₄Cl₂F₂N₄O₄) (labeled as "Ligand of Interest" by depositor).

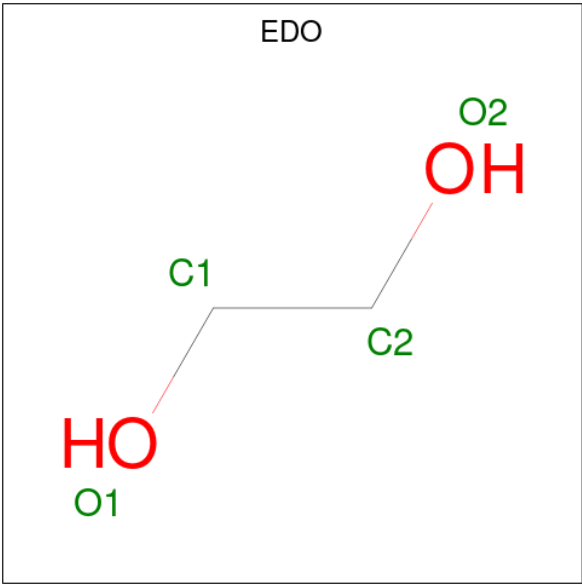


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			39	27	2	2	4	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			39	27	2	2	4	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	1
			183	183		
5	B	215	Total	O	0	3
			218	218		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.07Å 87.82Å 73.68Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	48.60 – 1.54 48.60 – 1.54	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.60-1.54) 98.2 (48.60-1.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.188 , 0.218 0.196 , 0.222	Depositor DCC
R_{free} test set	4383 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5245	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: NA, EDO, A1CU7

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	0/2414	0.91	3/3282 (0.1%)
1	B	0.55	0/2461	0.95	3/3344 (0.1%)
All	All	0.54	0/4875	0.93	6/6626 (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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1218	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	1256	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	1314	GLN	CB-CA-C	5.90	120.16	109.83
1	A	1146	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	1360	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	1260	MET	CG-SD-CE	5.21	112.36	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1352	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	2354	0	2177	10	0
1	B	2406	0	2237	21	0
2	A	39	0	0	1	0
2	B	39	0	0	0	0
3	A	2	0	0	0	0
4	B	4	0	6	0	0
5	A	183	0	0	1	0
5	B	218	0	0	3	0
All	All	5245	0	4420	31	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 (31) 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:1181:TYR:CE2	1:A:1227[A]:CYS:SG	2.31	1.22
1:A:1181:TYR:CD2	1:A:1227[A]:CYS:SG	2.57	0.93
1:B:1109:MET:HE1	1:B:1143:PRO:HG3	1.52	0.91
1:B:1098[B]:CYS:SG	1:B:1139:THR:O	2.35	0.84
1:B:1257:LYS:HE2	1:B:1260:MET:HE2	1.63	0.81
1:B:1098[B]:CYS:SG	1:B:1139:THR:C	2.72	0.72
1:B:1083:ILE:HD11	1:B:1388:GLU:HG3	1.73	0.70
1:B:1218:ASP:OD1	5:B:1501:HOH:O	2.11	0.67
1:A:1181:TYR:CZ	1:A:1227[A]:CYS:SG	2.87	0.67
1:B:1109:MET:CE	1:B:1143:PRO:HG3	2.27	0.63
1:B:1098[A]:CYS:SG	1:B:1138[A]:ILE:HG22	2.44	0.57
1:B:1109:MET:HE1	1:B:1143:PRO:CG	2.31	0.57
1:B:1335:ARG:HD3	5:B:1669:HOH:O	2.07	0.54
1:A:1141:LEU:C	1:A:1141:LEU:HD12	2.31	0.54
1:B:1260:MET:HE1	5:B:1691:HOH:O	2.11	0.49
1:A:1118:LYS:NZ	5:A:1503:HOH:O	2.46	0.49
1:B:1098[A]:CYS:SG	1:B:1141:LEU:HG	2.52	0.49
1:B:1109:MET:HG2	1:B:1119:LEU:CD2	2.43	0.48
1:B:1098[A]:CYS:SG	1:B:1138[A]:ILE:CG2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:SER:HA	1:B:1109:MET:HE2	1.97	0.46
1:B:1109:MET:HG2	1:B:1119:LEU:HD22	1.98	0.46
1:A:1273[B]:VAL:CG2	1:A:1280:TRP:HB2	2.46	0.45
1:A:1357:LEU:HD13	1:A:1366:LEU:HD11	1.99	0.44
1:A:1083:ILE:CG1	1:A:1388:GLU:HG3	2.50	0.42
1:A:1155[B]:THR:HG21	2:A:1401:A1CU7:C34	2.49	0.42
1:B:1135:ASN:OD1	1:B:1135:ASN:C	2.62	0.42
1:A:1299:VAL:HA	1:A:1309:TYR:O	2.20	0.41
1:B:1083:ILE:CD1	1:B:1388:GLU:HG3	2.46	0.41
1:B:1141:LEU:HD23	1:B:1152:THR:HG22	2.03	0.41
1:B:1210:LYS:HD3	1:B:1213:THR:OG1	2.21	0.40
1:B:1102:SER:CA	1:B:1109:MET:HE2	2.52	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	300/315 (95%)	293 (98%)	7 (2%)	0	100	100
1	B	301/315 (96%)	297 (99%)	4 (1%)	0	100	100
All	All	601/630 (95%)	590 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/276 (91%)	247 (98%)	4 (2%)	58	30
1	B	260/276 (94%)	259 (100%)	1 (0%)	89	81
All	All	511/552 (93%)	506 (99%)	5 (1%)	79	52

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1235[A]	ASP
1	A	1235[B]	ASP
1	A	1259	ASN
1	A	1357	LEU
1	B	1259	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1116	GLN
1	A	1132	ASN
1	A	1206	GLN

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
2	A1CU7	B	1401	-	41,42,42	0.81	2 (4%)	54,59,59	0.77	1 (1%)
4	EDO	B	1402	-	3,3,3	0.28	0	2,2,2	0.57	0
2	A1CU7	A	1401	-	41,42,42	0.97	2 (4%)	54,59,59	0.82	1 (1%)

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	A1CU7	B	1401	-	-	0/25/37/37	0/4/4/4
4	EDO	B	1402	-	-	0/1/1/1	-
2	A1CU7	A	1401	-	-	0/25/37/37	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	A1CU7	C19-C18	-4.01	1.45	1.50
2	A	1401	A1CU7	C27-C28	-3.83	1.42	1.46
2	B	1401	A1CU7	C19-C18	-3.12	1.46	1.50
2	B	1401	A1CU7	C27-C28	-2.71	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	A1CU7	C39-N38-C27	3.56	110.07	104.56
2	B	1401	A1CU7	C39-N38-C27	3.45	109.91	104.56

There are no chirality outliers.

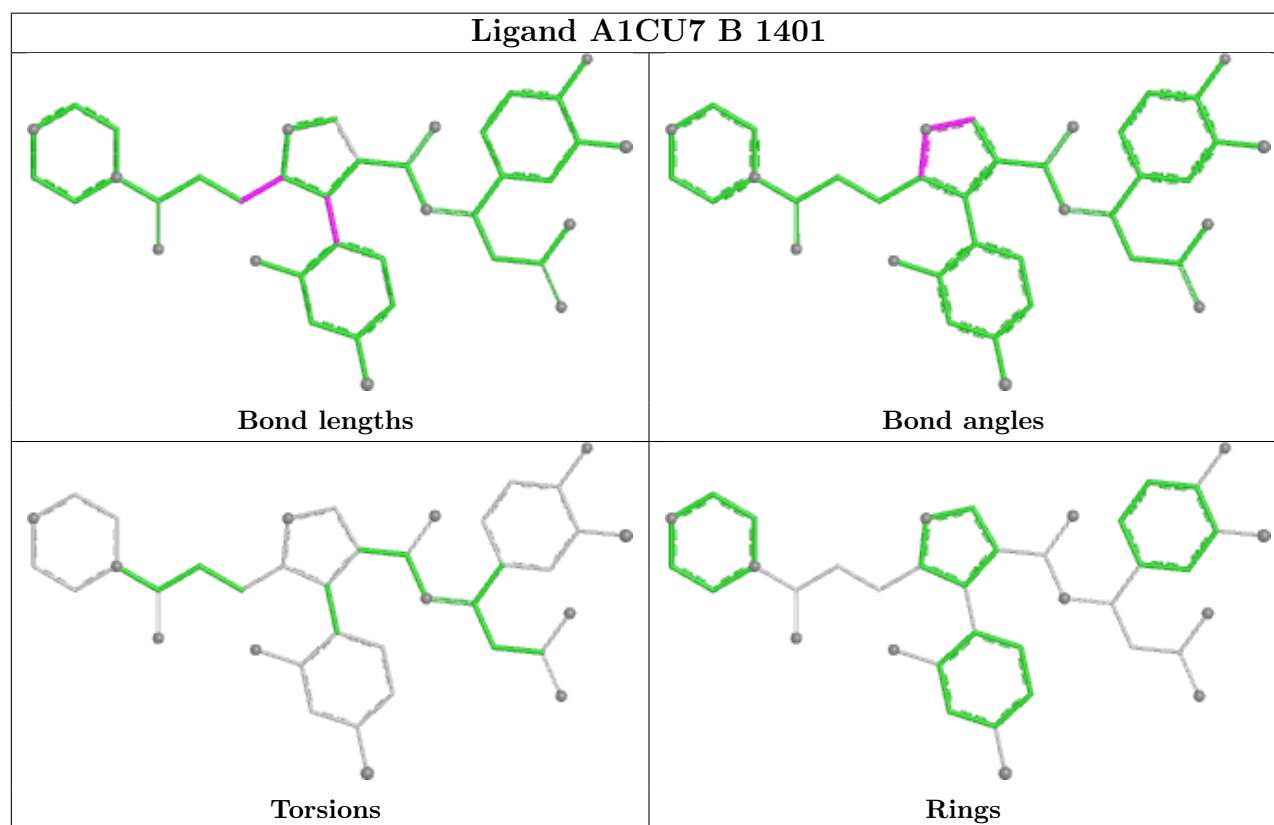
There are no torsion outliers.

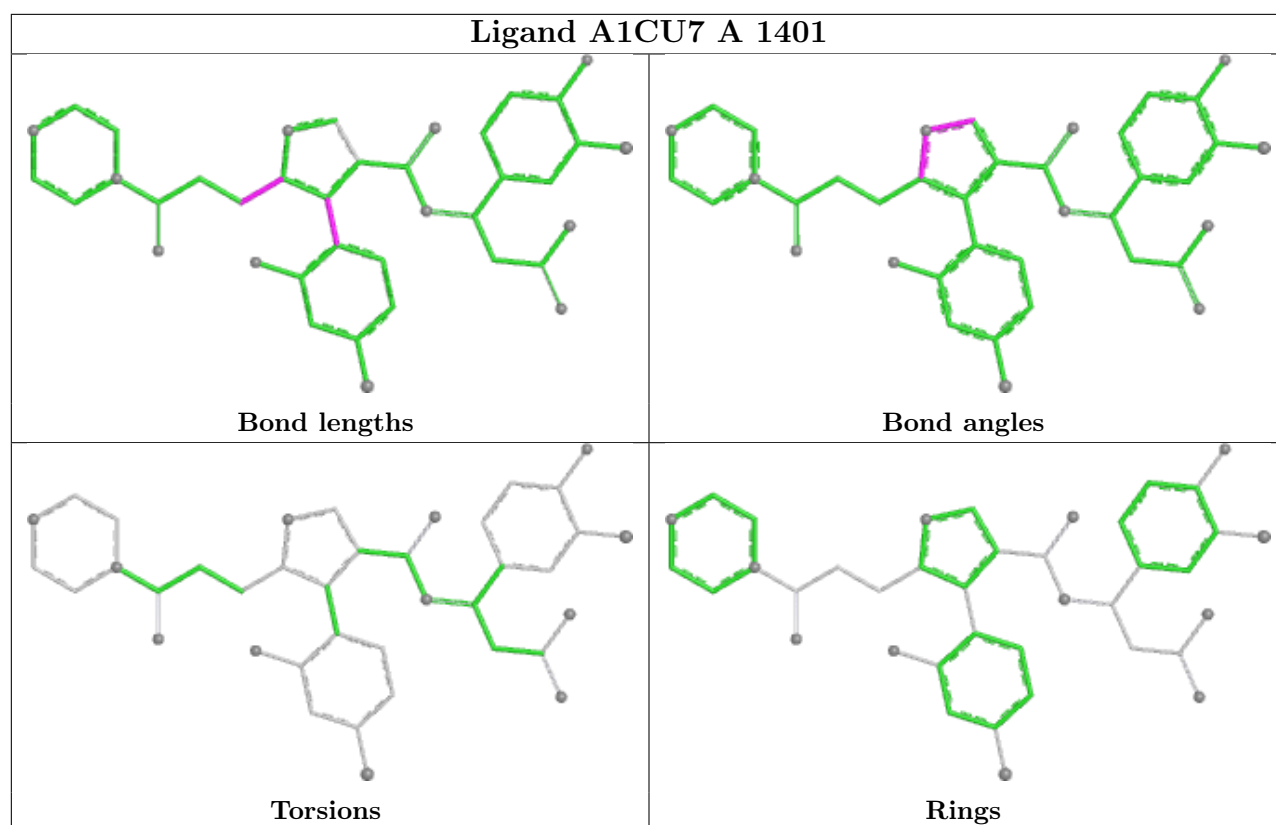
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	A1CU7	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

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	296/315 (93%)	0.67	39 (13%) 8 10	8, 23, 47, 64	10 (3%)
1	B	299/315 (94%)	0.34	21 (7%) 24 29	7, 21, 40, 61	10 (3%)
All	All	595/630 (94%)	0.51	60 (10%) 14 17	7, 22, 43, 64	20 (3%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1123	PHE	8.0
1	A	1122	VAL	6.9
1	A	1389	VAL	5.8
1	A	1079	ALA	5.2
1	A	1156	TRP	5.2
1	A	1107	PHE	5.0
1	B	1156	TRP	4.7
1	B	1107	PHE	3.9
1	B	1123	PHE	3.9
1	A	1363	ASP	3.9
1	B	1079	ALA	3.9
1	B	1169	VAL	3.8
1	A	1105	GLU	3.7
1	A	1104	ARG	3.5
1	A	1315	ALA	3.4
1	A	1361	THR	3.4
1	A	1124[A]	SER	3.3
1	A	1103	ALA	3.3
1	B	1375	MET	3.2
1	B	1316	ASP	3.2
1	A	1090	ASN	3.1
1	A	1373	GLY	3.1
1	A	1083	ILE	3.0
1	B	1363	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1364	CYS	3.0
1	B	1379	ASN	3.0
1	A	1316	ASP	3.0
1	A	1303[A]	HIS	3.0
1	B	1374	SER	3.0
1	B	1303[A]	HIS	2.9
1	A	1348	ILE	2.8
1	A	1106	ARG	2.8
1	A	1093	GLU	2.8
1	B	1390	GLY	2.6
1	A	1327	LYS	2.5
1	B	1315	ALA	2.5
1	B	1252	ILE	2.4
1	A	1365	TYR	2.4
1	A	1379	ASN	2.4
1	A	1227[A]	CYS	2.4
1	A	1289[A]	HIS	2.4
1	A	1155[A]	THR	2.4
1	B	1326	MET	2.4
1	A	1080	PHE	2.4
1	A	1177	THR	2.3
1	B	1167	LYS	2.3
1	B	1361	THR	2.3
1	A	1168	SER	2.3
1	A	1169	VAL	2.3
1	B	1365	TYR	2.2
1	B	1246	VAL	2.2
1	A	1081	ARG	2.2
1	A	1121	ASN	2.2
1	A	1135	ASN	2.2
1	A	1157[A]	SER	2.1
1	A	1282	LEU	2.1
1	A	1347	THR	2.1
1	A	1346	ALA	2.0
1	B	1092	ASP	2.0
1	B	1104	ARG	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

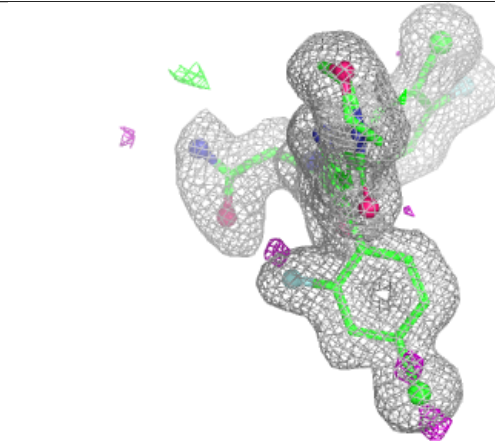
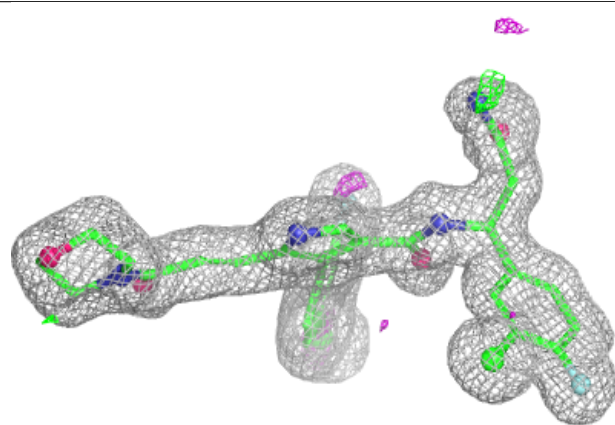
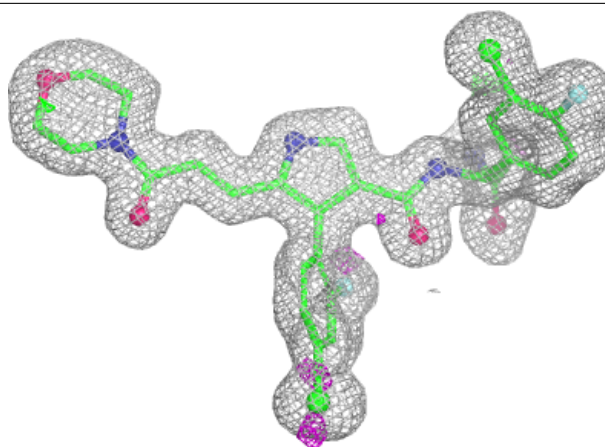
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	1402	4/4	0.88	0.13	37,41,41,42	0
3	NA	A	1403	1/1	0.89	0.09	49,49,49,49	0
2	A1CU7	A	1401	39/39	0.96	0.07	16,19,27,28	0
3	NA	A	1402	1/1	0.96	0.14	35,35,35,35	0
2	A1CU7	B	1401	39/39	0.97	0.06	14,17,26,30	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.

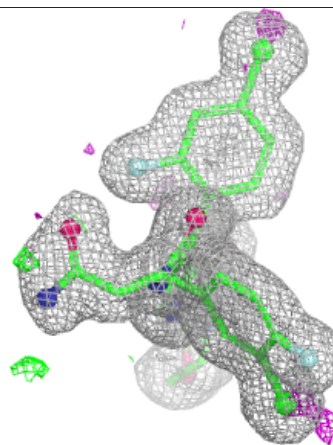
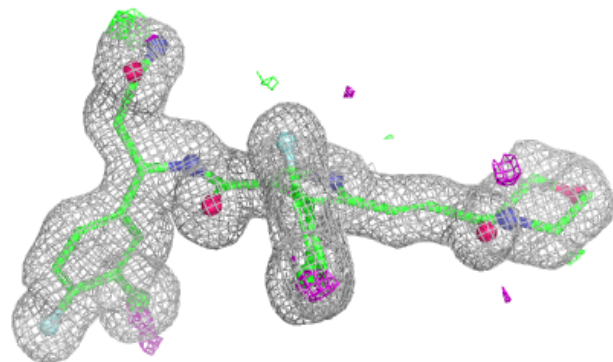
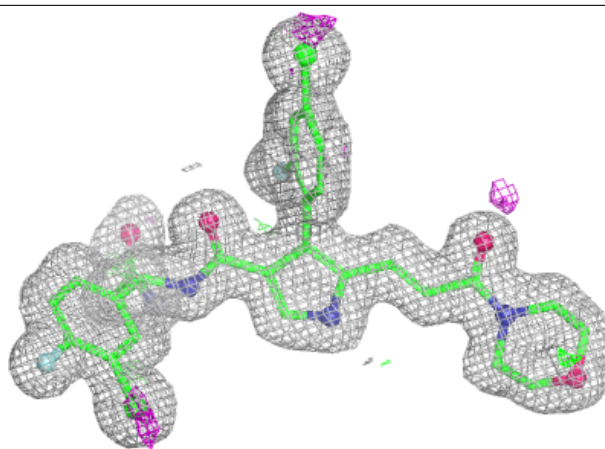
Electron density around A1CU7 A 1401:

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



Electron density around A1CU7 B 1401:

$2mF_o - DF_c$ (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.