



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 05:22 AM EDT

PDB ID : 8DQQ
Title : Crystal structure of Arabidopsis thaliana COSY in complex with scopoletin
Authors : Kim, C.Y.; Mitchell, A.J.; Gutierrez, M.; Weng, J.K.
Deposited on : 2022-07-19
Resolution : 2.33 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

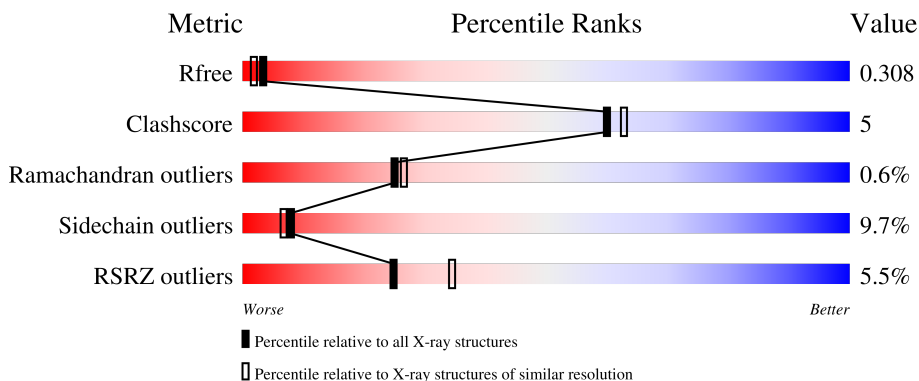
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	451	 6% 78% 16% • 5%
1	B	451	 4% 76% 18% • •

2 Entry composition [i](#)

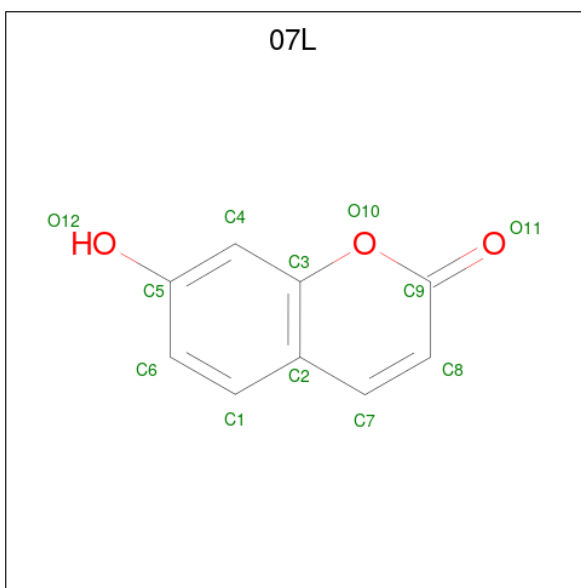
There are 5 unique types of molecules in this entry. The entry contains 6862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coumarin Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	Total 3368	C 2158	N 571	O 624	S 15	0	2	0
1	B	432	Total 3366	C 2149	N 571	O 631	S 15	0	0	0

- Molecule 2 is 7-hydroxy-2H-chromen-2-one (three-letter code: 07L) (formula: C₉H₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 12	C 9	O 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

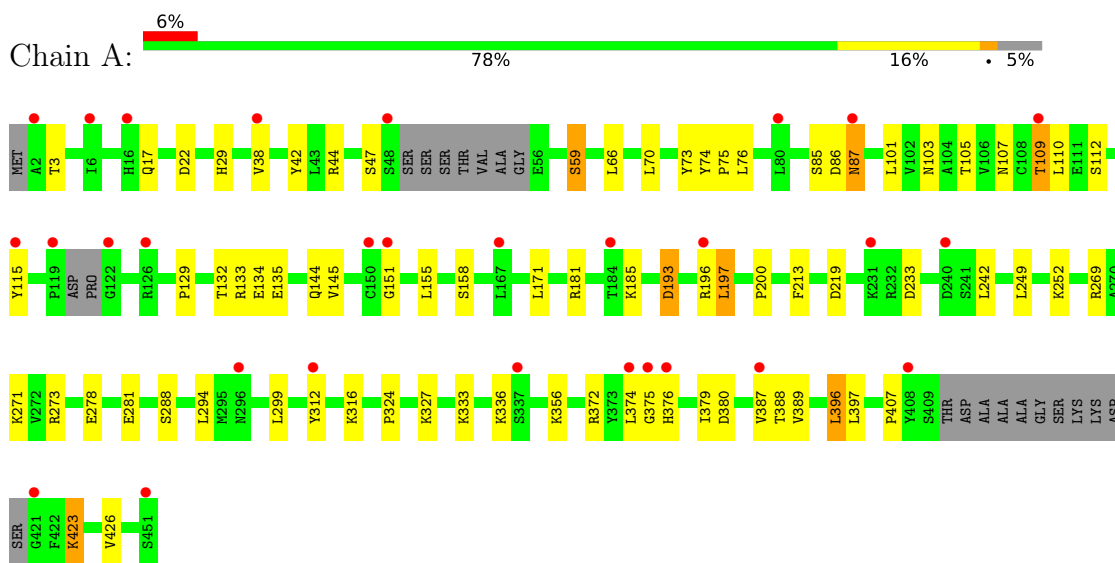
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	45	Total	O	0	0
			45	45		

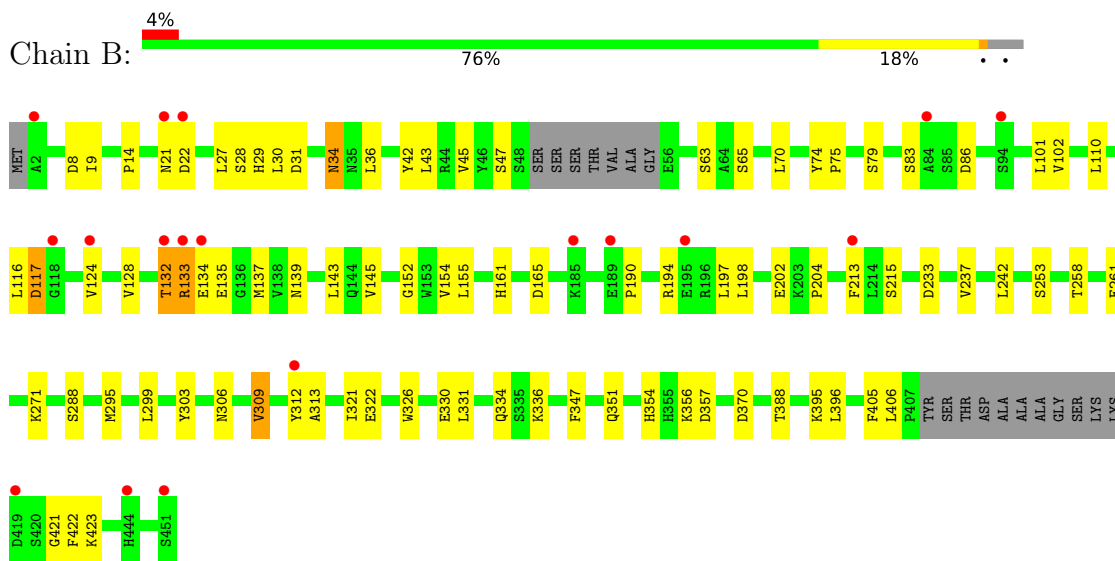
3 Residue-property plots i

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: Coumarin Synthase



• Molecule 1: Coumarin Synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.91Å 58.77Å 273.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.81 – 2.33 136.81 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.4 (136.81-2.33) 97.7 (136.81-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.253 , 0.312 0.249 , 0.308	Depositor DCC
R_{free} test set	1940 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtrriage
Anisotropy	1.271	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.037 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: 07L, ACT, CA

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	0.27	0/3452	0.51	0/4683
1	B	0.26	0/3449	0.52	0/4681
All	All	0.26	0/6901	0.51	0/9364

There are no bond length outliers.

There are no bond angle outliers.

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	3368	0	3288	27	0
1	B	3366	0	3295	35	0
2	A	12	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	4	0	3	0	0
5	A	65	0	0	4	0
5	B	45	0	0	3	0
All	All	6862	0	6592	62	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 (62) 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:144:GLN:NE2	5:A:601:HOH:O	2.16	0.77
1:A:59:SER:OG	1:A:103:ASN:OD1	2.02	0.77
1:B:295:MET:SD	5:B:639:HOH:O	2.45	0.74
1:B:133:ARG:NH1	1:B:134:GLU:OE2	2.23	0.72
1:A:423:LYS:NZ	5:A:604:HOH:O	2.28	0.66
1:B:30:LEU:HD12	1:B:198:LEU:HD13	1.77	0.64
1:B:132:THR:O	1:B:134:GLU:N	2.32	0.61
1:B:213:PHE:HB2	1:B:312:TYR:CZ	2.36	0.60
1:B:83:SER:OG	1:B:86:ASP:O	2.15	0.60
1:B:116:LEU:HD23	1:B:124:VAL:HG22	1.84	0.57
1:A:372:ARG:HA	1:A:407:PRO:HA	1.86	0.56
1:B:117:ASP:HB2	1:B:388:THR:HG21	1.87	0.55
1:A:387:VAL:HG23	1:A:388:THR:HG23	1.89	0.55
1:B:34:ASN:N	1:B:34:ASN:OD1	2.39	0.54
1:A:73:TYR:HB3	1:A:76:LEU:HD12	1.89	0.54
1:A:44:ARG:HH12	1:A:379:ILE:HG13	1.73	0.54
1:B:330:GLU:O	1:B:334:GLN:HG2	2.09	0.53
1:B:321:ILE:HG13	1:B:322:GLU:HG2	1.90	0.53
1:A:109:THR:HG22	1:A:112:SER:H	1.74	0.53
1:A:101:LEU:HD11	1:A:145:VAL:HG23	1.90	0.53
1:B:28:SER:HB3	1:B:194:ARG:HB3	1.91	0.51
1:A:87:ASN:O	1:A:87:ASN:ND2	2.45	0.50
1:A:29:HIS:CE1	1:A:200:PRO:HD3	2.47	0.50
1:B:253:SER:HB3	1:B:326:TRP:HB2	1.94	0.50
1:A:107:ASN:OD1	1:A:107:ASN:N	2.41	0.50
1:A:87:ASN:HD22	1:A:87:ASN:C	2.15	0.49
1:B:14:PRO:HG3	1:B:70:LEU:HB3	1.95	0.49
1:A:66:LEU:O	1:A:70:LEU:HG	2.13	0.48
1:A:193:ASP:HB3	1:A:197:LEU:HD22	1.96	0.48
1:A:129:PRO:HD3	1:A:144:GLN:OE1	2.14	0.48
1:B:258:THR:N	1:B:261:GLU:OE1	2.37	0.47
1:A:181:ARG:HH11	1:A:380:ASP:HB3	1.80	0.47
1:B:295:MET:HG3	1:B:299:LEU:HD13	1.97	0.47
1:B:86:ASP:OD1	1:B:86:ASP:N	2.46	0.46
1:B:313:ALA:HB1	1:B:331:LEU:HG	1.97	0.46
1:B:198:LEU:HD12	1:B:303:TYR:OH	2.16	0.46
1:B:309:VAL:HG13	5:B:622:HOH:O	2.14	0.46
1:A:74:TYR:CG	1:A:75:PRO:HD3	2.51	0.46
1:A:132:THR:HG23	1:A:134:GLU:H	1.81	0.46
1:A:324:PRO:HD2	1:A:327:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HD22	1:A:397:LEU:HG	1.98	0.45
1:A:273:ARG:HB2	5:A:614:HOH:O	2.17	0.44
1:B:152:GLY:N	5:B:609:HOH:O	2.47	0.44
1:B:165:ASP:HB3	1:B:306:ASN:HA	2.00	0.44
1:B:202:GLU:O	1:B:204:PRO:HD3	2.17	0.44
1:A:109:THR:O	1:A:110:LEU:HB2	2.18	0.43
1:B:45:VAL:HG22	1:B:154:VAL:HG22	2.00	0.43
1:B:36:LEU:HG	1:B:161:HIS:ND1	2.34	0.43
1:A:213[B]:PHE:CD2	1:A:312[B]:TYR:HB2	2.53	0.43
1:A:132:THR:HG22	1:A:135:GLU:H	1.84	0.43
1:B:27:LEU:HB3	1:B:31:ASP:HB2	2.02	0.41
1:B:134:GLU:HA	1:B:137:MET:HG3	2.01	0.41
1:B:9:ILE:HG23	1:B:102:VAL:HG22	2.02	0.41
1:B:237:VAL:O	1:B:421:GLY:HA3	2.20	0.41
1:B:347:PHE:O	1:B:351:GLN:HG2	2.21	0.41
1:B:406:LEU:O	1:B:422:PHE:HB2	2.20	0.41
1:B:354:HIS:ND1	1:B:357:ASP:OD2	2.51	0.41
1:A:269:ARG:HG2	5:A:614:HOH:O	2.20	0.41
1:B:74:TYR:CG	1:B:75:PRO:HD3	2.56	0.41
1:B:370:ASP:HA	1:B:405:PHE:HB2	2.02	0.41
1:A:374:LEU:O	1:A:376:HIS:N	2.54	0.40
1:B:101:LEU:HD11	1:B:145:VAL:HG23	2.03	0.40

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	424/451 (94%)	392 (92%)	28 (7%)	4 (1%)	17 17
1	B	426/451 (94%)	408 (96%)	17 (4%)	1 (0%)	47 55
All	All	850/902 (94%)	800 (94%)	45 (5%)	5 (1%)	25 26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLY
1	B	133	ARG
1	A	17	GLN
1	A	115	TYR
1	A	375	GLY

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	360/380 (95%)	322 (89%)	38 (11%)	6 5
1	B	364/380 (96%)	332 (91%)	32 (9%)	10 9
All	All	724/760 (95%)	654 (90%)	70 (10%)	8 7

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	22	ASP
1	A	38	VAL
1	A	42	TYR
1	A	47	SER
1	A	59	SER
1	A	85	SER
1	A	86	ASP
1	A	87	ASN
1	A	105	THR
1	A	109	THR
1	A	133	ARG
1	A	155	LEU
1	A	158	SER
1	A	171	LEU
1	A	185	LYS
1	A	193	ASP
1	A	196	ARG

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Mol	Chain	Res	Type
1	A	197	LEU
1	A	219	ASP
1	A	233	ASP
1	A	242	LEU
1	A	249	LEU
1	A	252	LYS
1	A	271	LYS
1	A	278	GLU
1	A	281	GLU
1	A	288	SER
1	A	294	LEU
1	A	299	LEU
1	A	316	LYS
1	A	333	LYS
1	A	336	LYS
1	A	356	LYS
1	A	389	VAL
1	A	396	LEU
1	A	423	LYS
1	A	426	VAL
1	B	8	ASP
1	B	21	ASN
1	B	22	ASP
1	B	29	HIS
1	B	34	ASN
1	B	42	TYR
1	B	43	LEU
1	B	47	SER
1	B	63	SER
1	B	65	SER
1	B	79	SER
1	B	110	LEU
1	B	117	ASP
1	B	128	VAL
1	B	132	THR
1	B	135	GLU
1	B	139	ASN
1	B	143	LEU
1	B	155	LEU
1	B	190	PRO
1	B	197	LEU
1	B	215	SER

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Mol	Chain	Res	Type
1	B	233	ASP
1	B	242	LEU
1	B	271	LYS
1	B	288	SER
1	B	309	VAL
1	B	336	LYS
1	B	356	LYS
1	B	395	LYS
1	B	396	LEU
1	B	423	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	B	501	-	3,3,3	1.35	0	3,3,3	1.50	0
2	07L	A	501	-	13,13,13	1.41	2 (15%)	18,18,18	1.15	2 (11%)

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	07L	A	501	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	07L	C8-C7	3.49	1.40	1.34
2	A	501	07L	C4-C3	2.80	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	07L	C7-C8-C9	-3.02	117.53	121.43
2	A	501	07L	O10-C9-C8	2.12	120.34	117.12

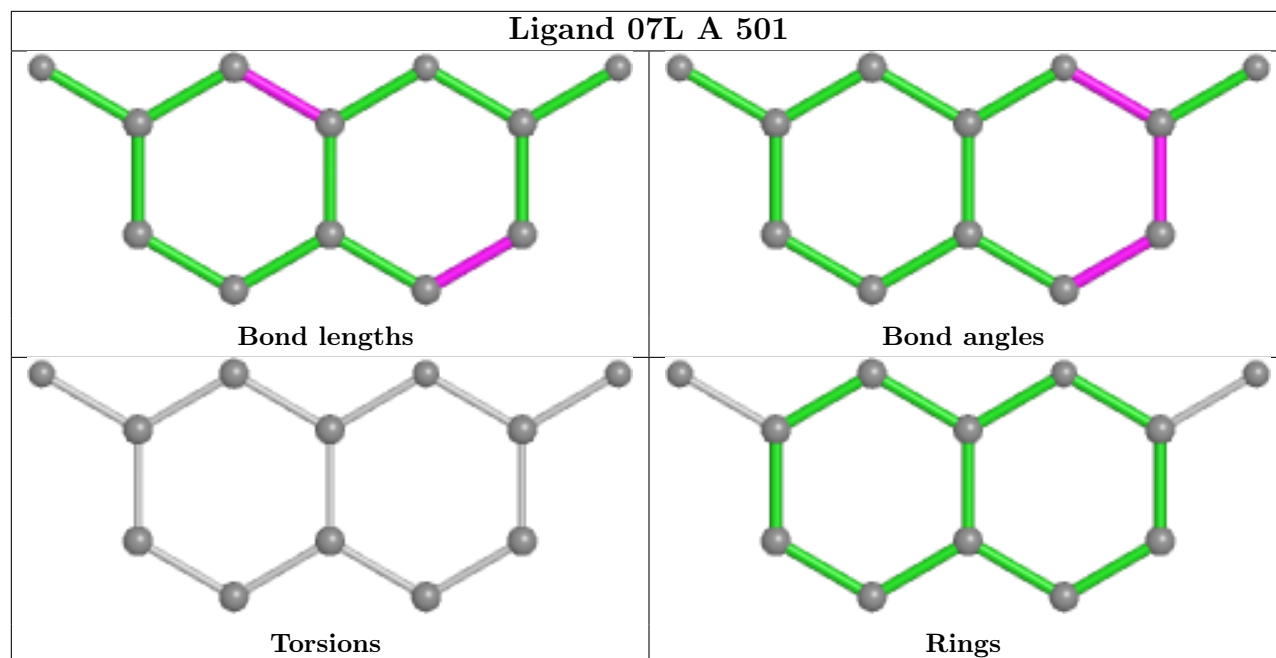
There are no chirality outliers.

There are no torsion outliers.

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 [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, 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	430/451 (95%)	0.76	29 (6%) 17 25	36, 57, 79, 92	0
1	B	432/451 (95%)	0.62	18 (4%) 36 47	41, 60, 79, 90	0
All	All	862/902 (95%)	0.69	47 (5%) 25 34	36, 58, 79, 92	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	6.9
1	A	374	LEU	4.7
1	B	84	ALA	4.6
1	A	2	ALA	4.5
1	A	375	GLY	4.4
1	A	122	GLY	3.9
1	A	126	ARG	3.8
1	B	134	GLU	3.7
1	B	2	ALA	3.6
1	B	118	GLY	3.5
1	B	312	TYR	3.4
1	B	132	THR	3.3
1	B	213	PHE	3.2
1	A	421	GLY	3.0
1	B	21	ASN	3.0
1	A	408	TYR	2.9
1	B	22	ASP	2.8
1	A	150	CYS	2.7
1	A	196	ARG	2.6
1	A	167	LEU	2.6
1	B	195	GLU	2.6
1	B	419	ASP	2.6
1	B	451	SER	2.5
1	A	119	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	16	HIS	2.4
1	A	87	ASN	2.4
1	A	240	ASP	2.4
1	A	109	THR	2.3
1	A	48	SER	2.3
1	B	444	HIS	2.3
1	A	451	SER	2.3
1	B	189	GLU	2.2
1	B	94	SER	2.2
1	B	124	VAL	2.2
1	A	376	HIS	2.2
1	A	231	LYS	2.2
1	A	38	VAL	2.2
1	A	337	SER	2.1
1	A	151	GLY	2.1
1	A	312[A]	TYR	2.1
1	A	6	ILE	2.1
1	A	184	THR	2.0
1	A	387	VAL	2.0
1	B	185	LYS	2.0
1	A	115	TYR	2.0
1	A	296	ASN	2.0
1	A	80	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 monosaccharides in this entry.

6.4 Ligands [i](#)

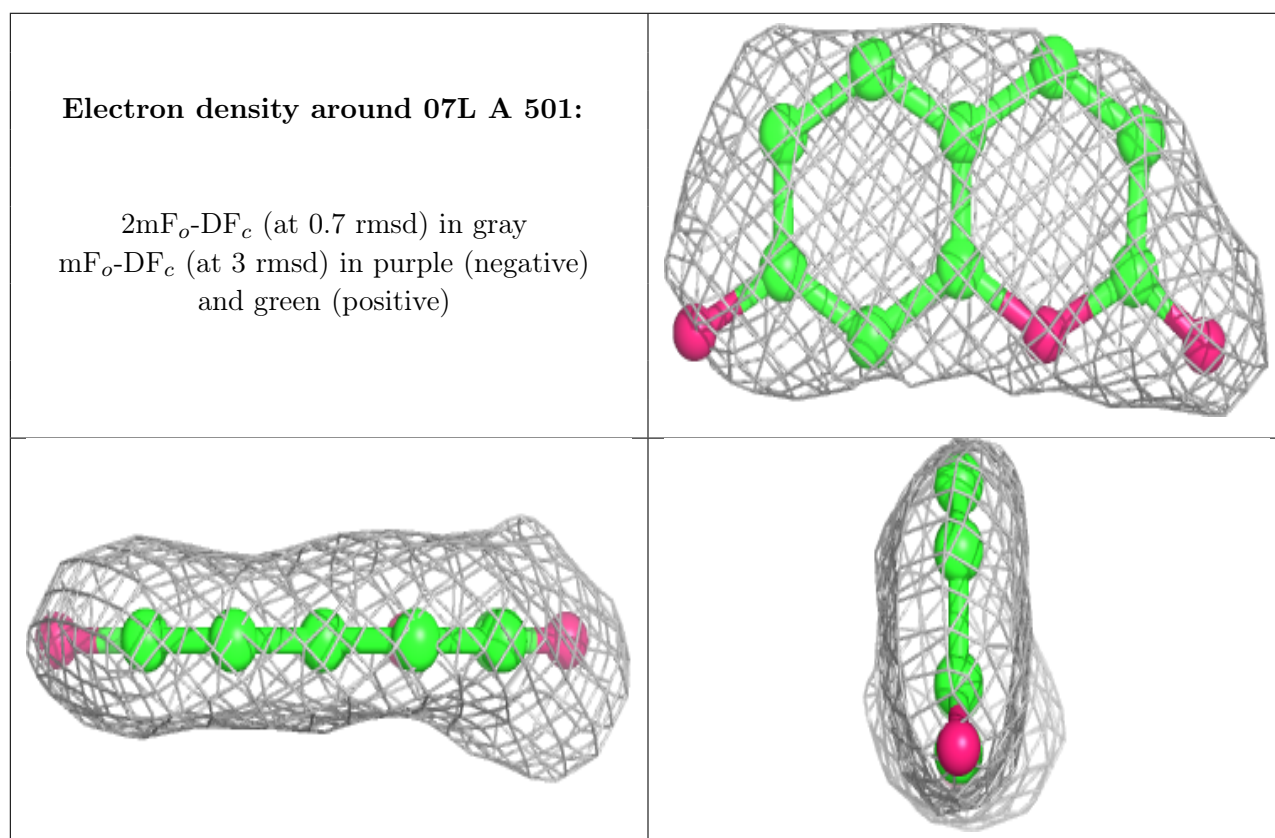
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	B	501	4/4	0.61	0.31	51,59,65,66	0
3	CA	A	502	1/1	0.75	0.23	50,50,50,50	0
3	CA	B	502	1/1	0.87	0.19	61,61,61,61	0
2	07L	A	501	12/12	0.91	0.16	48,55,57,62	12

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.