



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2023 – 05:30 PM EST

PDB ID : 7FT2
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z235449082
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.04 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 : 2.32.1
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) : 2.32.1

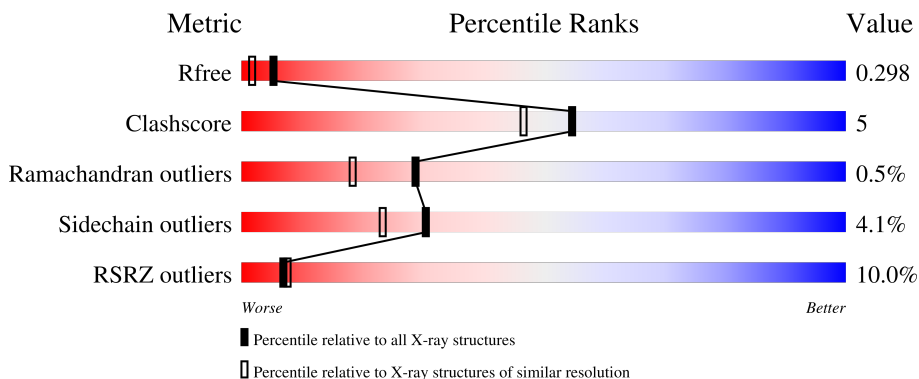
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	195	
1	B	195	
1	C	195	
1	D	195	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLY	C	304	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6447 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 Syntenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1481	935	262	275	9	0	1	0
1	B	193	1495	943	264	279	9	0	1	0
1	C	193	1506	949	268	280	9	0	2	0
1	D	191	1489	939	263	278	9	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

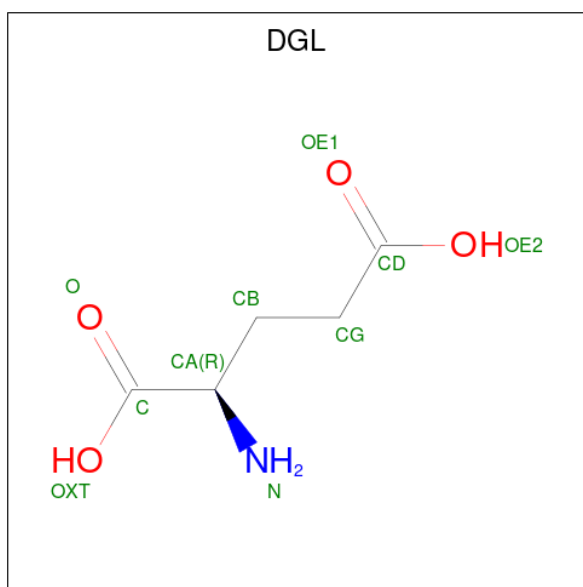
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag	UNP O00560
D	105	MET	-	expression tag	UNP O00560

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



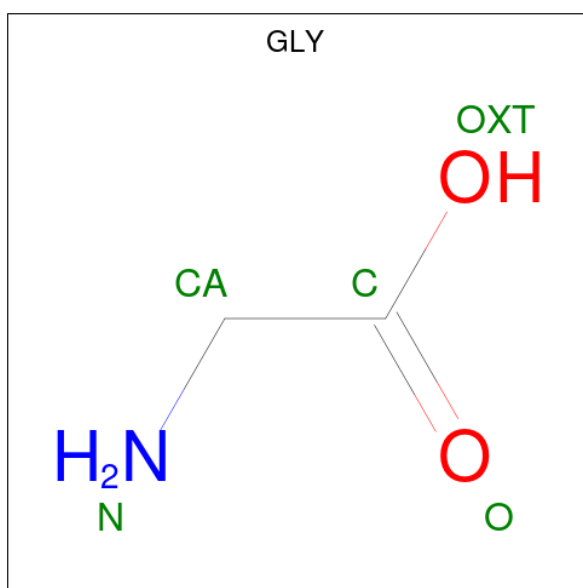
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
3	B	1	Total	10	5	1	4	0	0
3	D	1	Total	10	5	1	4	0	0

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



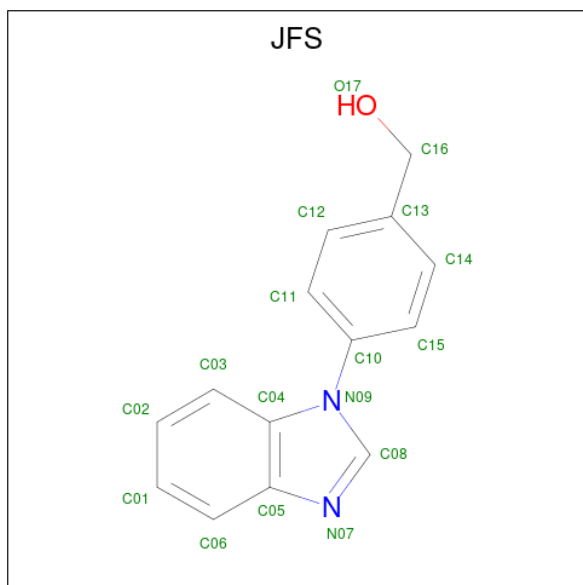
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
4	B	1	Total	5	2	1	2	0	0
4	C	1	Total	5	2	1	2	0	0

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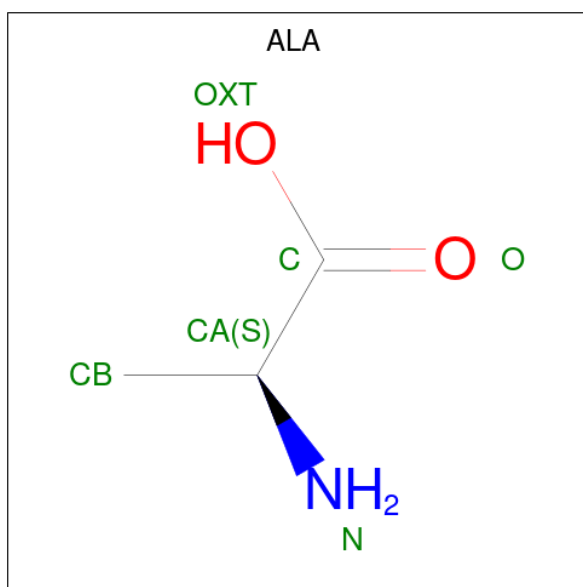
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	D	1	5	2	1	2	0	0

- Molecule 5 is [4-(1H-benzimidazol-1-yl)phenyl]methanol (three-letter code: JFS) (formula: C₁₄H₁₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	17	14	2	1	0	0
5	D	1	17	14	2	1	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	6	3	1	2	0	0

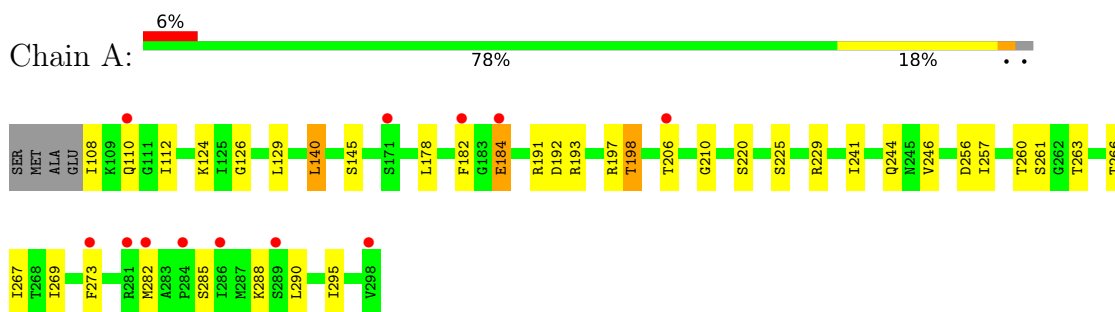
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total	O	0	0
			56	56		
7	B	109	Total	O	0	1
			109	109		
7	C	94	Total	O	0	0
			94	94		
7	D	110	Total	O	0	0
			110	110		

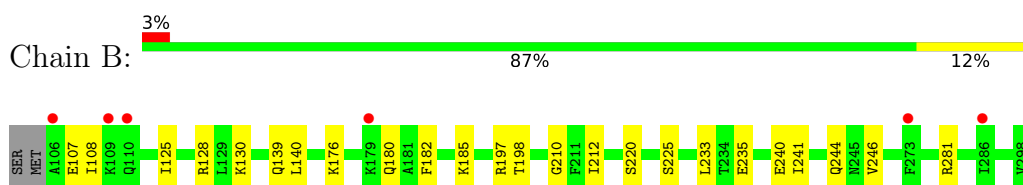
3 Residue-property plots [i](#)

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.

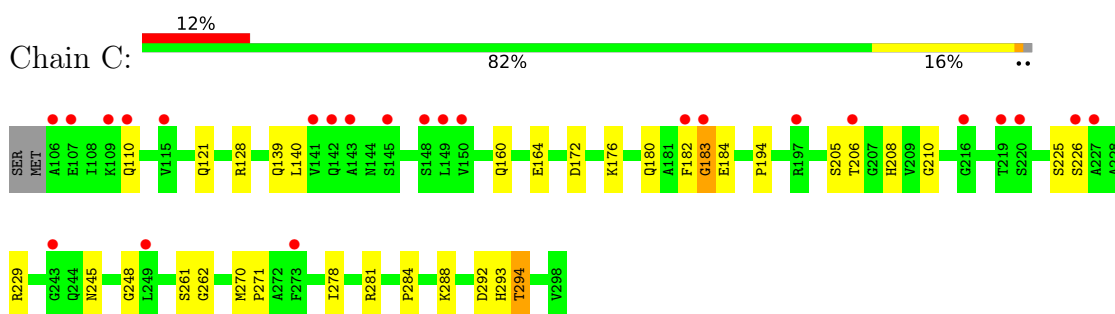
- Molecule 1: Syntenin-1



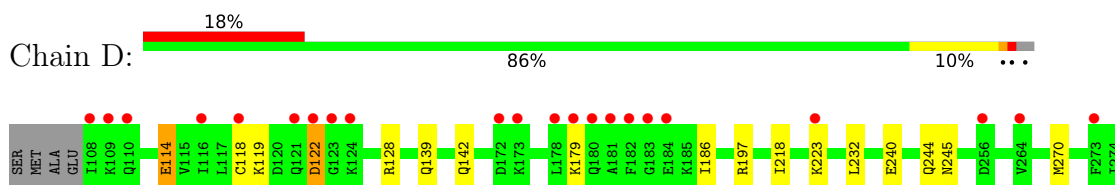
- Molecule 1: Syntenin-1

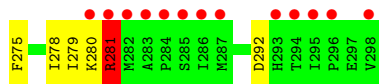


- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.58Å 49.92Å 117.52Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	117.15 – 2.04 117.15 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (117.15-2.04) 99.7 (117.15-2.04)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.268 , 0.322 0.254 , 0.298	Depositor DCC
R_{free} test set	2877 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6447	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0586e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGL, JFS, EDO

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	0.76	0/1502	0.98	1/2019 (0.0%)
1	B	0.80	0/1516	0.98	2/2038 (0.1%)
1	C	0.80	0/1527	0.92	0/2052
1	D	0.78	0/1510	0.92	0/2030
All	All	0.79	0/6055	0.95	3/8139 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	198	THR	CA-CB-OG1	-5.36	97.75	109.00
1	B	235	GLU	CB-CA-C	5.32	121.04	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLN	Peptide

5.2 Too-close contacts [i](#)

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	1481	0	1530	18	0
1	B	1495	0	1541	12	0
1	C	1506	0	1553	23	0
1	D	1489	0	1533	14	0
2	A	8	0	12	1	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	B	10	0	7	0	0
3	D	10	0	7	0	0
4	B	5	0	2	0	0
4	C	5	0	2	0	0
4	D	5	0	2	1	0
5	C	17	0	0	0	0
5	D	17	0	0	0	0
6	D	6	0	4	0	0
7	A	56	0	0	0	0
7	B	109	0	0	0	0
7	C	94	0	0	2	0
7	D	110	0	0	5	0
All	All	6447	0	6229	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 5.

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:C:128:ARG:NH1	1:C:281:ARG:O	2.22	0.72
1:D:128:ARG:NH1	7:D:404:HOH:O	2.25	0.70
1:C:183:GLY:O	1:C:184:GLU:OE1	2.10	0.69
1:D:280:LYS:O	1:D:281:ARG:HB2	1.94	0.66
1:A:112:ILE:HD11	1:A:191:ARG:NH2	2.12	0.65
1:C:248:GLY:O	1:C:288:LYS:HE2	1.99	0.62
1:C:128:ARG:NE	1:C:139:GLN:OE1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:NH2	7:D:401:HOH:O	2.12	0.59
1:A:197:ARG:HD3	1:C:194:PRO:O	2.02	0.58
1:D:128:ARG:HD3	1:D:139:GLN:OE1	2.03	0.57
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.86	0.57
1:A:256:ASP:O	1:A:260:THR:HG23	2.03	0.57
1:C:206:THR:HG1	1:C:208:HIS:HD1	1.52	0.56
1:D:197:ARG:NH1	7:D:405:HOH:O	2.31	0.56
1:C:245:ASN:O	1:C:293:HIS:HD2	1.90	0.55
1:D:119:LYS:HE3	1:D:186:ILE:HD11	1.90	0.54
1:C:281:ARG:O	1:C:281:ARG:HG2	2.07	0.54
1:C:226:SER:HA	1:C:229:ARG:NH2	2.23	0.53
1:C:292:ASP:OD1	1:C:294:THR:OG1	2.26	0.53
1:A:244:GLN:NE2	1:A:257:ILE:HD13	2.23	0.53
1:C:210:GLY:HA3	1:C:225:SER:HB2	1.90	0.53
1:D:128:ARG:NH1	1:D:139:GLN:OE1	2.41	0.53
1:C:184:GLU:HA	7:C:403:HOH:O	2.10	0.51
1:B:240:GLU:HA	1:B:244:GLN:O	2.11	0.51
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.93	0.50
1:B:128:ARG:NH2	1:B:281:ARG:O	2.45	0.50
1:D:218:ILE:HD13	1:D:232:LEU:HD21	1.94	0.48
1:A:267:ILE:HG22	1:A:269:ILE:HG23	1.95	0.48
1:D:270:MET:SD	1:D:278:ILE:HD12	2.54	0.48
1:A:210:GLY:HA3	1:A:225:SER:CB	2.44	0.47
1:A:241:ILE:HD12	1:A:246:VAL:HG11	1.96	0.47
1:B:176:LYS:O	1:B:180:GLN:HG3	2.13	0.47
1:A:140:LEU:HD22	1:B:182:PHE:HE1	1.80	0.47
1:A:140:LEU:HD12	1:A:282:MET:SD	2.55	0.46
1:C:160:GLN:HA	1:C:164:GLU:O	2.15	0.45
1:C:176:LYS:HE2	1:C:180:GLN:HE22	1.81	0.45
1:C:210:GLY:HA3	1:C:225:SER:CB	2.46	0.45
1:A:124:LYS:HE2	1:B:185:LYS:HB3	1.98	0.45
1:C:172:ASP:OD1	1:C:281:ARG:NH1	2.49	0.45
1:C:261:SER:OG	1:C:262:GLY:N	2.48	0.45
1:C:176:LYS:HE2	1:C:180:GLN:NE2	2.31	0.45
1:D:240:GLU:HA	1:D:244:GLN:O	2.17	0.45
1:B:210:GLY:HA3	1:B:225:SER:HB2	1.99	0.44
1:C:182:PHE:O	1:C:183:GLY:O	2.36	0.44
1:B:212:ILE:HD12	1:B:220:SER:OG	2.19	0.43
1:C:229:ARG:NH2	7:C:401:HOH:O	2.50	0.43
1:A:192:ASP:O	1:A:193:ARG:C	2.57	0.43
1:D:114:GLU:OE2	7:D:402:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PHE:O	1:D:279:ILE:HG12	2.18	0.43
1:D:245:ASN:HB3	1:D:292:ASP:O	2.19	0.42
1:C:245:ASN:O	1:C:293:HIS:CD2	2.71	0.42
1:B:130:LYS:HE2	1:B:281:ARG:HD3	2.00	0.42
1:B:241:ILE:HD12	1:B:246:VAL:HG11	2.01	0.42
1:A:129:LEU:HD11	1:A:178:LEU:HD11	2.02	0.41
1:A:126:GLY:HA3	1:A:145:SER:HB2	2.03	0.41
1:A:206:THR:O	1:A:206:THR:HG22	2.21	0.41
1:D:122:ASP:OD1	1:D:122:ASP:N	2.54	0.41
1:C:270:MET:O	1:C:271:PRO:C	2.59	0.41
1:C:270:MET:SD	1:C:278:ILE:HD12	2.61	0.41
1:A:198:THR:HG23	1:A:266:THR:HG23	2.02	0.41
1:B:107:GLU:H	1:B:107:GLU:CD	2.25	0.40
4:D:306:GLY:N	7:D:418:HOH:O	2.54	0.40
1:A:273[B]:PHE:CE2	2:A:301:EDO:H22	2.57	0.40
1:B:197:ARG:NH2	1:B:233:LEU:HD12	2.36	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	190/195 (97%)	177 (93%)	11 (6%)	2 (1%)	14	5
1	B	192/195 (98%)	188 (98%)	4 (2%)	0	100	100
1	C	193/195 (99%)	185 (96%)	7 (4%)	1 (0%)	29	18
1	D	191/195 (98%)	183 (96%)	7 (4%)	1 (0%)	29	18
All	All	766/780 (98%)	733 (96%)	29 (4%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	A	184	GLU
1	C	183	GLY
1	D	281	ARG

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	166/168 (99%)	156 (94%)	10 (6%)	19	11
1	B	167/168 (99%)	163 (98%)	4 (2%)	49	42
1	C	168/168 (100%)	162 (96%)	6 (4%)	35	28
1	D	167/168 (99%)	160 (96%)	7 (4%)	30	22
All	All	668/672 (99%)	641 (96%)	27 (4%)	30	24

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

Mol	Chain	Res	Type
1	A	108	ILE
1	A	140	LEU
1	A	184	GLU
1	A	198	THR
1	A	220	SER
1	A	261	SER
1	A	263	THR
1	A	285	SER
1	A	288	LYS
1	A	295	ILE
1	B	108	ILE
1	B	125	ILE
1	B	139	GLN
1	B	140	LEU
1	C	110	GLN
1	C	121	GLN
1	C	140	LEU
1	C	205	SER

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Mol	Chain	Res	Type
1	C	284	PRO
1	C	294	THR
1	D	114	GLU
1	D	118	CYS
1	D	122	ASP
1	D	142	GLN
1	D	179	LYS
1	D	223	LYS
1	D	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	180	GLN
1	A	208	HIS
1	A	244	GLN
1	B	110	GLN
1	B	180	GLN
1	C	110	GLN
1	C	134	ASN
1	C	142	GLN
1	C	180	GLN
1	C	293	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 monosaccharides in this entry.

5.6 Ligand geometry i

16 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
6	ALA	D	304	-	5,5,5	0.97	0	6,6,6	1.03	1 (16%)
2	EDO	D	302	-	3,3,3	0.23	0	2,2,2	0.11	0
2	EDO	A	301	-	3,3,3	0.15	0	2,2,2	0.23	0
2	EDO	B	302	-	3,3,3	0.15	0	2,2,2	0.38	0
3	DGL	B	303	-	8,9,9	0.96	0	10,11,11	1.45	2 (20%)
2	EDO	C	303	-	3,3,3	0.19	0	2,2,2	0.15	0
4	GLY	B	304	-	4,4,4	0.98	0	3,4,4	1.39	0
5	JFS	D	301	-	19,19,19	1.64	4 (21%)	21,26,26	1.36	2 (9%)
5	JFS	C	301	-	19,19,19	1.74	3 (15%)	21,26,26	0.83	0
2	EDO	A	302	-	3,3,3	0.34	0	2,2,2	0.44	0
3	DGL	D	305	-	8,9,9	1.13	0	10,11,11	1.02	0
4	GLY	D	306	-	4,4,4	1.17	1 (25%)	3,4,4	1.30	0
2	EDO	B	301	-	3,3,3	0.16	0	2,2,2	0.20	0
2	EDO	C	302	-	3,3,3	0.08	0	2,2,2	0.14	0
4	GLY	C	304	-	4,4,4	0.85	0	3,4,4	1.78	2 (66%)
2	EDO	D	303	-	3,3,3	0.13	0	2,2,2	0.32	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
6	ALA	D	304	-	-	2/4/4/4	-
2	EDO	D	302	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
3	DGL	B	303	-	-	2/9/9/9	-
2	EDO	C	303	-	-	0/1/1/1	-
4	GLY	B	304	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JFS	D	301	-	-	2/6/6/6	0/3/3/3
5	JFS	C	301	-	-	0/6/6/6	0/3/3/3
2	EDO	A	302	-	-	1/1/1/1	-
3	DGL	D	305	-	-	3/9/9/9	-
4	GLY	D	306	-	-	0/2/2/2	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-
4	GLY	C	304	-	-	2/2/2/2	-
2	EDO	D	303	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	JFS	C10-N09	4.89	1.51	1.44
5	C	301	JFS	C10-N09	4.88	1.51	1.44
5	D	301	JFS	C08-N09	-2.53	1.34	1.36
5	C	301	JFS	C02-C03	2.48	1.42	1.36
5	C	301	JFS	C01-C06	2.38	1.42	1.36
4	D	306	GLY	OXT-C	-2.22	1.23	1.30
5	D	301	JFS	C01-C06	2.10	1.41	1.36
5	D	301	JFS	C14-C15	2.05	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	JFS	C11-C10-N09	3.86	124.06	119.41
5	D	301	JFS	C15-C10-N09	-3.39	115.33	119.41
3	B	303	DGL	OXT-C-O	-2.79	117.76	124.09
3	B	303	DGL	OXT-C-CA	2.32	121.27	113.38
4	C	304	GLY	OXT-C-CA	2.22	122.29	113.45
6	D	304	ALA	OXT-C-O	-2.03	119.48	124.09
4	C	304	GLY	OXT-C-O	-2.00	118.31	123.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	304	GLY	O-C-CA-N
4	C	304	GLY	OXT-C-CA-N
5	D	301	JFS	C11-C10-N09-C04

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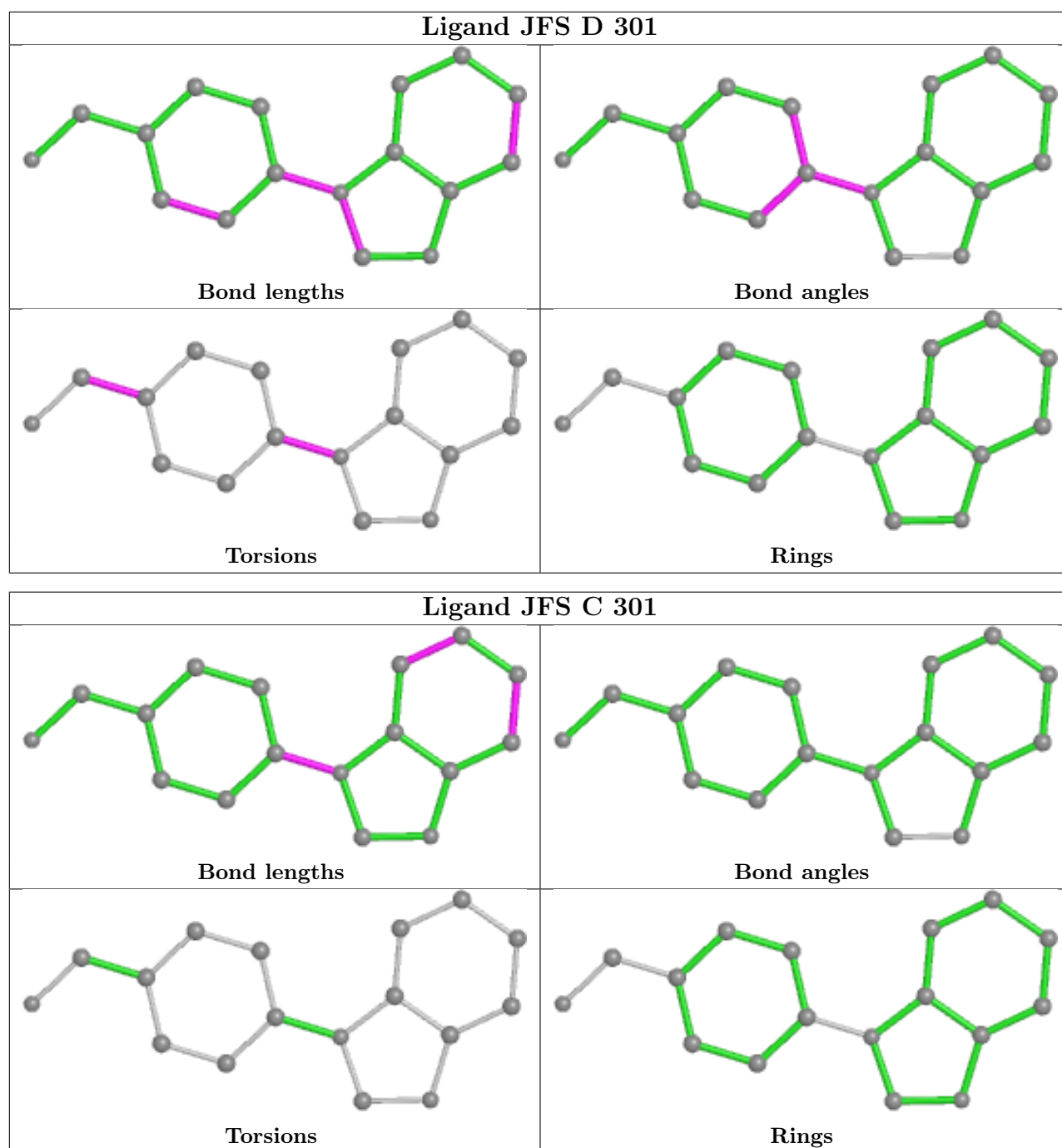
Mol	Chain	Res	Type	Atoms
4	B	304	GLY	O-C-CA-N
4	B	304	GLY	OXT-C-CA-N
2	A	302	EDO	O1-C1-C2-O2
3	D	305	DGL	OXT-C-CA-CB
3	D	305	DGL	O-C-CA-CB
3	B	303	DGL	CA-CB-CG-CD
6	D	304	ALA	OXT-C-CA-N
6	D	304	ALA	O-C-CA-N
3	D	305	DGL	N-CA-CB-CG
5	D	301	JFS	C14-C13-C16-O17
3	B	303	DGL	OE1-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EDO	1	0
4	D	306	GLY	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, 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	191/195 (97%)	0.48	12 (6%) 20 21	29, 44, 75, 106	10 (5%)
1	B	193/195 (98%)	0.06	6 (3%) 49 53	24, 35, 54, 67	4 (2%)
1	C	193/195 (98%)	0.62	24 (12%) 4 3	21, 34, 58, 83	43 (22%)
1	D	191/195 (97%)	0.61	35 (18%) 1 1	22, 34, 54, 69	35 (18%)
All	All	768/780 (98%)	0.44	77 (10%) 7 7	21, 37, 63, 106	92 (11%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	VAL	6.9
1	D	283	ALA	5.8
1	A	182	PHE	5.5
1	C	106	ALA	5.5
1	D	286	ILE	5.3
1	C	110	GLN	5.2
1	C	143	ALA	5.1
1	C	145	SER	5.0
1	D	282	MET	5.0
1	D	287	MET	4.9
1	A	284	PRO	4.8
1	D	178	LEU	4.7
1	A	110	GLN	4.6
1	A	298	VAL	4.5
1	D	273[A]	PHE	4.5
1	D	284	PRO	4.4
1	C	142	GLN	4.4
1	A	289	SER	4.4
1	D	181	ALA	4.2
1	A	282	MET	4.1
1	D	295	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	107	GLU	4.0
1	D	293	HIS	4.0
1	D	294	THR	3.9
1	C	115	VAL	3.9
1	C	183	GLY	3.9
1	D	121	GLN	3.9
1	D	298	VAL	3.9
1	A	184	GLU	3.7
1	B	286	ILE	3.7
1	B	106	ALA	3.7
1	D	184	GLU	3.6
1	B	273[A]	PHE	3.6
1	C	273[A]	PHE	3.6
1	C	249	LEU	3.5
1	A	273[A]	PHE	3.5
1	D	223	LYS	3.5
1	D	182	PHE	3.5
1	C	182	PHE	3.5
1	D	183	GLY	3.4
1	D	124	LYS	3.4
1	D	118	CYS	3.4
1	A	281	ARG	3.3
1	C	150	VAL	3.3
1	D	285	SER	3.2
1	C	206	THR	3.1
1	D	108	ILE	3.1
1	D	109	LYS	3.0
1	D	296	PRO	3.0
1	C	149	LEU	3.0
1	C	197[A]	ARG	2.9
1	B	109	LYS	2.9
1	D	180	GLN	2.9
1	D	281	ARG	2.8
1	D	110	GLN	2.7
1	C	227	ALA	2.7
1	D	123	GLY	2.7
1	B	110	GLN	2.7
1	C	109	LYS	2.6
1	C	220	SER	2.6
1	C	216	GLY	2.6
1	B	179	LYS	2.5
1	D	172	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	116	ILE	2.5
1	D	122	ASP	2.4
1	D	173	LYS	2.4
1	C	226	SER	2.4
1	D	179	LYS	2.3
1	A	171	SER	2.3
1	C	219	THR	2.2
1	A	206	THR	2.1
1	C	148	SER	2.1
1	D	264	VAL	2.1
1	D	280	LYS	2.1
1	D	256[A]	ASP	2.1
1	A	286	ILE	2.0
1	C	243	GLY	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.

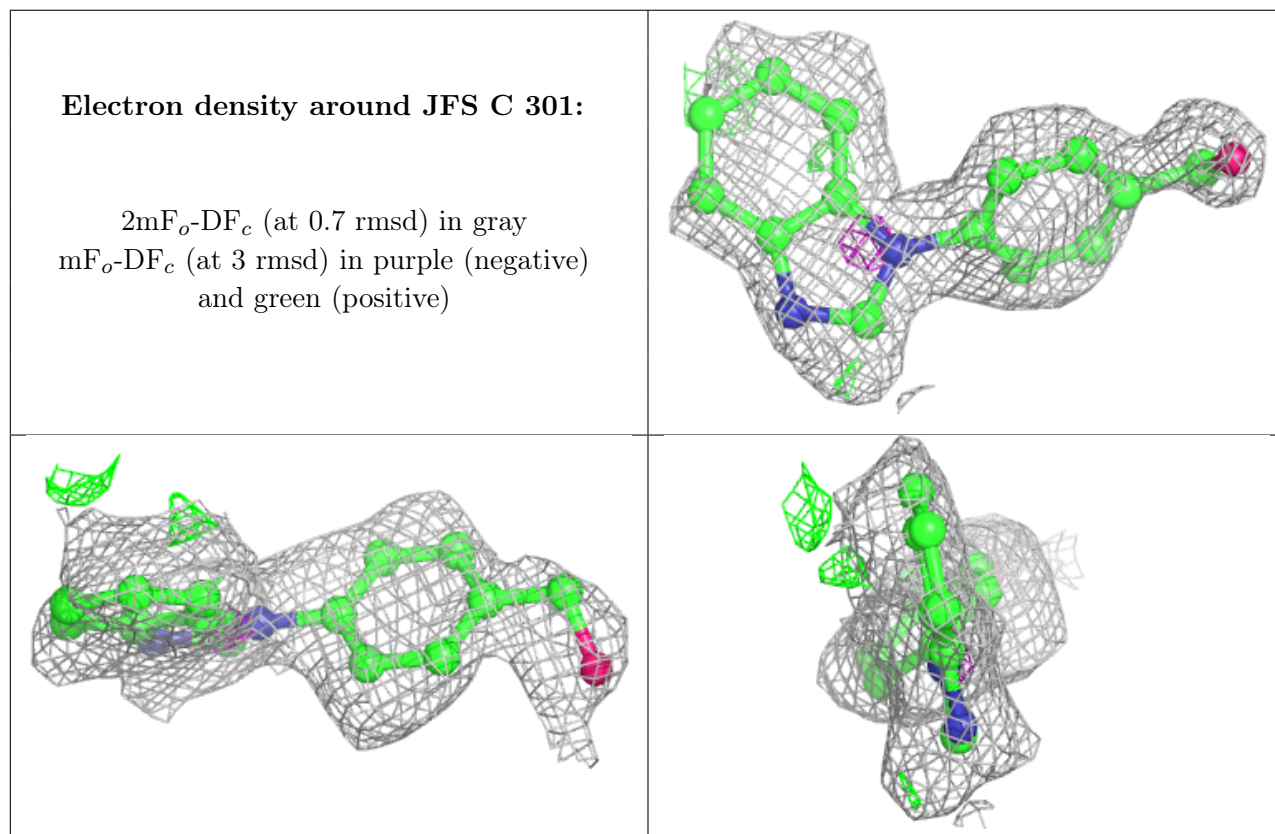
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLY	B	304	5/5	0.27	0.23	54,57,59,60	0
5	JFS	C	301	17/17	0.72	0.22	51,51,52,52	17
2	EDO	A	302	4/4	0.78	0.21	46,53,54,54	0
4	GLY	C	304	5/5	0.79	0.30	49,55,56,59	0
3	DGL	D	305	10/10	0.80	0.26	44,57,64,65	0
5	JFS	D	301	17/17	0.80	0.23	35,36,39,39	17
6	ALA	D	304	6/6	0.86	0.21	46,53,58,63	0
2	EDO	D	302	4/4	0.87	0.14	29,31,32,33	0
3	DGL	B	303	10/10	0.87	0.23	45,63,68,71	0

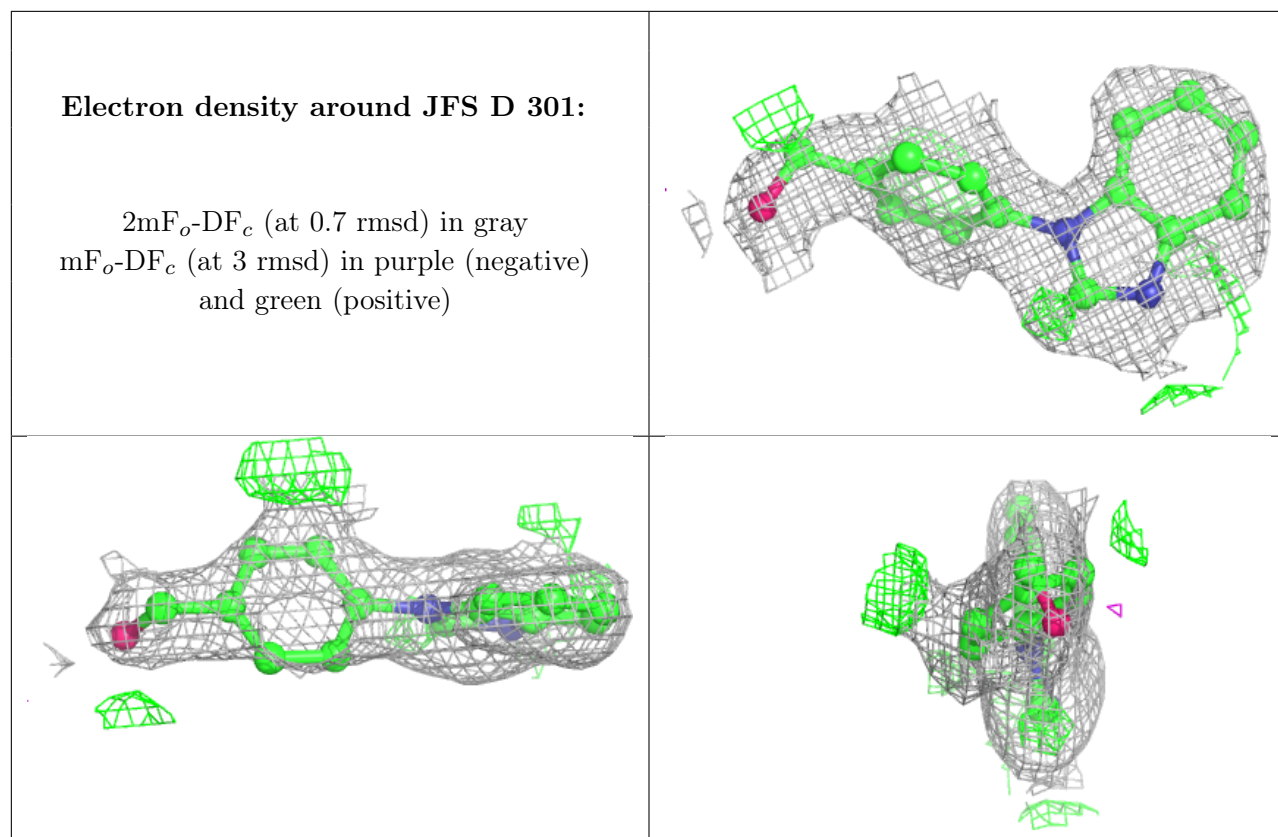
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GLY	D	306	5/5	0.90	0.32	60,64,72,78	0
2	EDO	A	301	4/4	0.91	0.13	37,37,38,39	0
2	EDO	C	302	4/4	0.92	0.12	36,36,36,37	0
2	EDO	B	302	4/4	0.93	0.18	29,30,31,33	0
2	EDO	C	303	4/4	0.94	0.19	29,29,30,31	0
2	EDO	B	301	4/4	0.94	0.14	36,43,45,45	0
2	EDO	D	303	4/4	0.95	0.14	32,37,37,38	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.