



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:13 PM UTC

PDB ID : 7XRI / pdb_00007xri
Title : Feruloyl esterase mutant -S106A
Authors : Hwang, J.S.; Lee, J.H.; Do, H.; Lee, C.W.
Deposited on : 2022-05-10
Resolution : 2.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

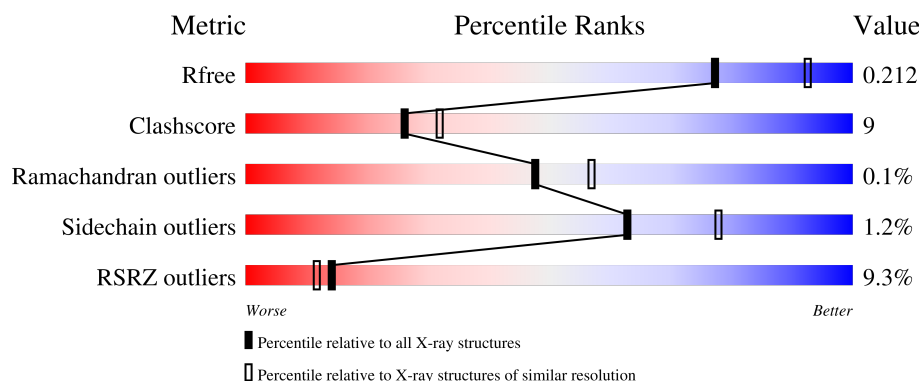
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	258	2% 83% 16% .
1	B	258	% 86% 13% .
1	C	258	2% 80% 16% ..
1	D	258	32% 71% 22% 5%

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
2	ZYC	A	301	-	-	X	-
2	ZYC	B	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8372 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 Cinnamoyl esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1988	1256	338	387	7			
1	B	256	Total	C	N	O	S	0	0	0
			1994	1262	338	387	7			
1	C	256	Total	C	N	O	S	0	0	0
			1988	1256	338	387	7			
1	D	244	Total	C	N	O	S	0	0	0
			1898	1202	324	367	5			

There are 48 discrepancies between the modelled and reference sequences:

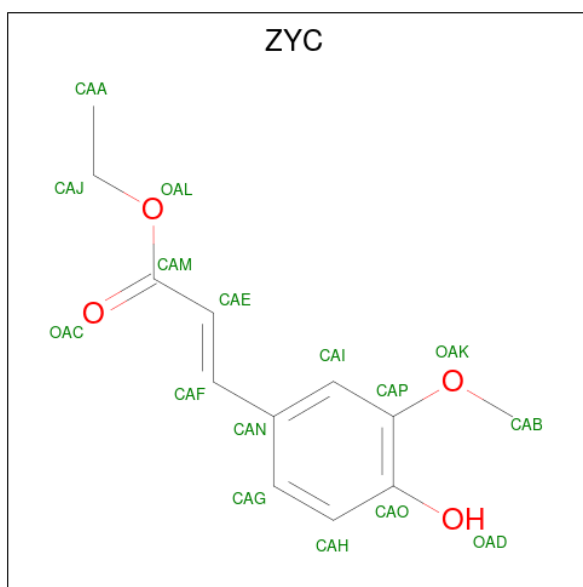
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A060IN49
A	-9	THR	-	expression tag	UNP A0A060IN49
A	-8	THR	-	expression tag	UNP A0A060IN49
A	-7	GLU	-	expression tag	UNP A0A060IN49
A	-6	ASN	-	expression tag	UNP A0A060IN49
A	-5	LEU	-	expression tag	UNP A0A060IN49
A	-4	TYR	-	expression tag	UNP A0A060IN49
A	-3	PHE	-	expression tag	UNP A0A060IN49
A	-2	GLN	-	expression tag	UNP A0A060IN49
A	-1	GLY	-	expression tag	UNP A0A060IN49
A	0	SER	-	expression tag	UNP A0A060IN49
A	106	ALA	SER	engineered mutation	UNP A0A060IN49
B	-10	GLY	-	expression tag	UNP A0A060IN49
B	-9	THR	-	expression tag	UNP A0A060IN49
B	-8	THR	-	expression tag	UNP A0A060IN49
B	-7	GLU	-	expression tag	UNP A0A060IN49
B	-6	ASN	-	expression tag	UNP A0A060IN49
B	-5	LEU	-	expression tag	UNP A0A060IN49
B	-4	TYR	-	expression tag	UNP A0A060IN49
B	-3	PHE	-	expression tag	UNP A0A060IN49
B	-2	GLN	-	expression tag	UNP A0A060IN49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A060IN49
B	0	SER	-	expression tag	UNP A0A060IN49
B	106	ALA	SER	engineered mutation	UNP A0A060IN49
C	-10	GLY	-	expression tag	UNP A0A060IN49
C	-9	THR	-	expression tag	UNP A0A060IN49
C	-8	THR	-	expression tag	UNP A0A060IN49
C	-7	GLU	-	expression tag	UNP A0A060IN49
C	-6	ASN	-	expression tag	UNP A0A060IN49
C	-5	LEU	-	expression tag	UNP A0A060IN49
C	-4	TYR	-	expression tag	UNP A0A060IN49
C	-3	PHE	-	expression tag	UNP A0A060IN49
C	-2	GLN	-	expression tag	UNP A0A060IN49
C	-1	GLY	-	expression tag	UNP A0A060IN49
C	0	SER	-	expression tag	UNP A0A060IN49
C	106	ALA	SER	engineered mutation	UNP A0A060IN49
D	-10	GLY	-	expression tag	UNP A0A060IN49
D	-9	THR	-	expression tag	UNP A0A060IN49
D	-8	THR	-	expression tag	UNP A0A060IN49
D	-7	GLU	-	expression tag	UNP A0A060IN49
D	-6	ASN	-	expression tag	UNP A0A060IN49
D	-5	LEU	-	expression tag	UNP A0A060IN49
D	-4	TYR	-	expression tag	UNP A0A060IN49
D	-3	PHE	-	expression tag	UNP A0A060IN49
D	-2	GLN	-	expression tag	UNP A0A060IN49
D	-1	GLY	-	expression tag	UNP A0A060IN49
D	0	SER	-	expression tag	UNP A0A060IN49
D	106	ALA	SER	engineered mutation	UNP A0A060IN49

- Molecule 2 is ethyl (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate (CCD ID: ZYC) (formula: C₁₂H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	D	1	Total	C	O	0	0
			16	12	4		

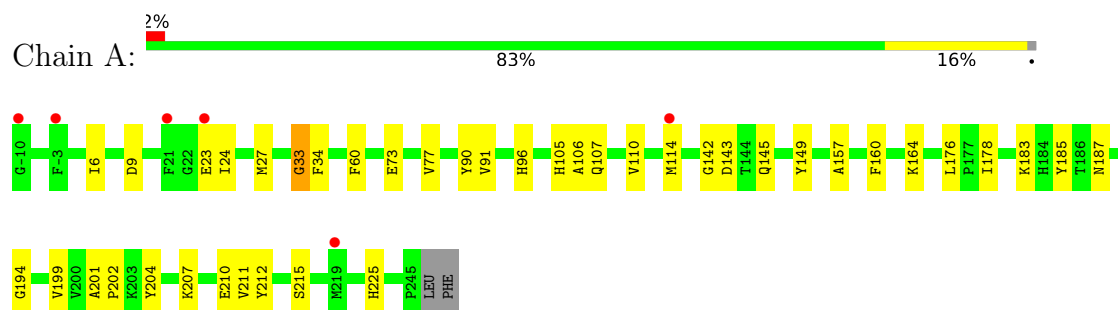
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total	O	0	0
			137	137		
3	B	131	Total	O	0	0
			131	131		
3	C	110	Total	O	0	0
			110	110		
3	D	62	Total	O	0	0
			62	62		

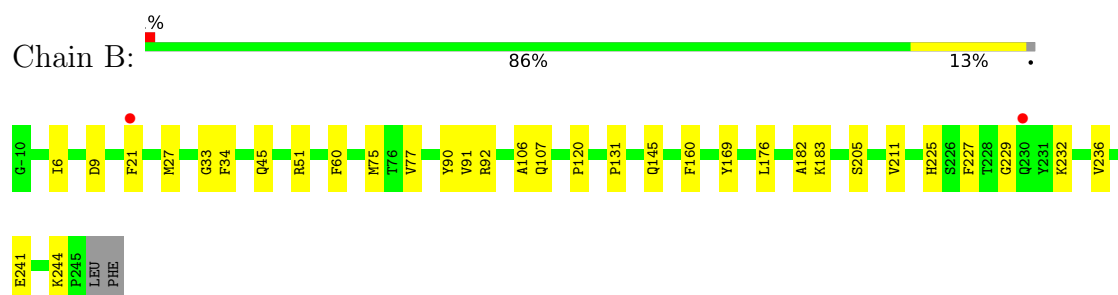
3 Residue-property plots [i](#)

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.

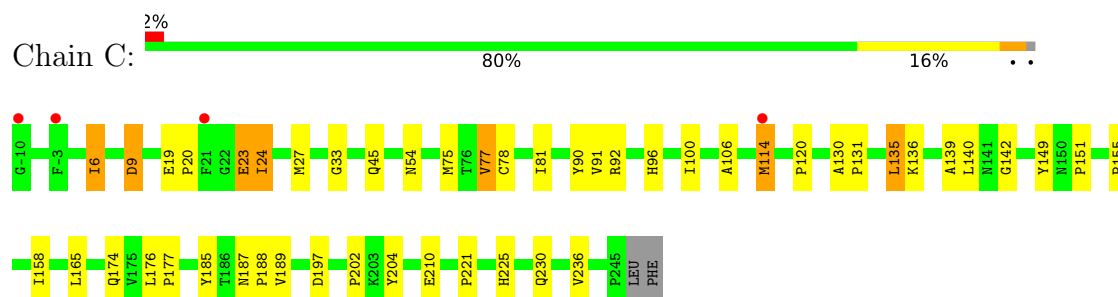
• Molecule 1: Cinnamoyl esterase



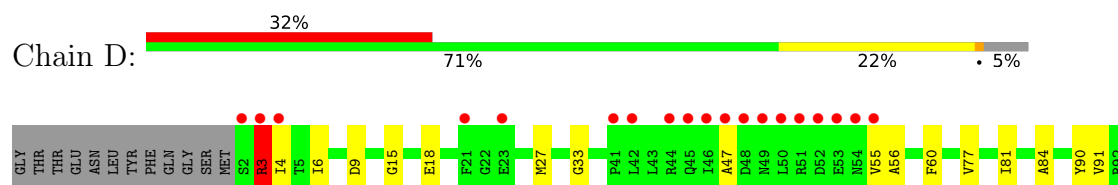
• Molecule 1: Cinnamoyl esterase

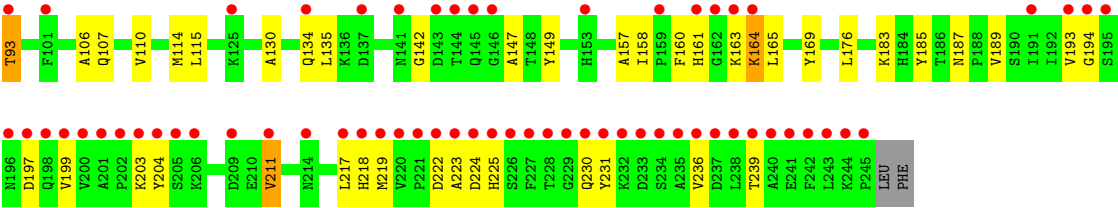


• Molecule 1: Cinnamoyl esterase



• Molecule 1: Cinnamoyl esterase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.38Å 153.39Å 91.25Å 90.00° 127.40° 90.00°	Depositor
Resolution (Å)	45.85 – 2.19 45.85 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.85-2.19) 98.4 (45.85-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.18Å)	Xtriage
Refinement program	REFMAC 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.186 , 0.214 (Not available) , 0.212	Depositor DCC
R_{free} test set	3603 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: ZYC

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	1.19	1/2031 (0.0%)	1.40	5/2759 (0.2%)
1	B	1.18	1/2038 (0.0%)	1.39	4/2768 (0.1%)
1	C	1.38	11/2031 (0.5%)	1.48	8/2759 (0.3%)
1	D	1.09	0/1940	1.48	9/2637 (0.3%)
All	All	1.21	13/8040 (0.2%)	1.44	26/10923 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	ALA	C-O	-9.26	1.19	1.23
1	C	120	PRO	C-O	-7.96	1.14	1.24
1	C	151	PRO	C-O	-6.59	1.15	1.24
1	C	221	PRO	C-O	-6.35	1.16	1.23
1	C	204	TYR	C-O	-6.09	1.17	1.24
1	C	202	PRO	C-O	-5.85	1.16	1.24
1	C	135	LEU	C-O	-5.78	1.17	1.24
1	C	136	LYS	C-O	-5.65	1.17	1.24
1	B	120	PRO	C-O	-5.43	1.17	1.24
1	C	155	PRO	C-O	-5.17	1.17	1.23
1	C	131	PRO	C-O	-5.12	1.17	1.23
1	C	106	ALA	C-O	-5.11	1.17	1.24
1	A	105	HIS	CE1-NE2	5.03	1.37	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	ASP	CB-CA-C	-7.11	101.29	111.95
1	B	182	ALA	CA-C-N	6.92	130.25	120.28
1	B	182	ALA	C-N-CA	6.92	130.25	120.28
1	D	199	VAL	N-CA-C	-6.22	104.44	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	GLU	CB-CG-CD	6.12	123.01	112.60
1	D	165	LEU	CA-C-N	6.07	125.75	119.92
1	D	165	LEU	C-N-CA	6.07	125.75	119.92
1	C	210	GLU	O-C-N	5.95	128.20	122.07
1	C	78	CYS	O-C-N	5.77	128.25	122.08
1	A	194	GLY	CA-C-N	5.71	128.72	120.38
1	A	194	GLY	C-N-CA	5.71	128.72	120.38
1	D	33	GLY	CA-C-N	5.53	130.05	121.26
1	D	33	GLY	C-N-CA	5.53	130.05	121.26
1	C	114	MET	O-C-N	5.52	128.05	122.09
1	B	229	GLY	CA-C-N	5.31	127.65	120.38
1	B	229	GLY	C-N-CA	5.31	127.65	120.38
1	C	77	VAL	CA-C-N	5.30	128.16	120.79
1	C	77	VAL	C-N-CA	5.30	128.16	120.79
1	D	161	HIS	O-C-N	-5.21	116.10	122.55
1	A	33	GLY	CA-C-N	5.20	128.72	121.02
1	A	33	GLY	C-N-CA	5.20	128.72	121.02
1	D	93	THR	CA-CB-OG1	-5.19	101.81	109.60
1	D	219	MET	CA-C-O	-5.17	116.42	122.37
1	A	204	TYR	CB-CA-C	5.11	118.90	110.88
1	C	6	ILE	CA-C-O	-5.11	116.57	121.63
1	D	164	LYS	O-C-N	5.04	129.12	123.27

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	1988	0	1931	44	0
1	B	1994	0	1938	38	0
1	C	1988	0	1931	24	0
1	D	1898	0	1845	43	0
2	A	16	0	13	23	0
2	B	16	0	13	23	0
2	C	16	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	13	2	0
3	A	137	0	0	2	0
3	B	131	0	0	1	0
3	C	110	0	0	0	0
3	D	62	0	0	0	0
All	All	8372	0	7697	147	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 9.

All (147) 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:B:107:GLN:H	2:B:301:ZYC:CAA	1.42	1.30
1:B:107:GLN:N	2:B:301:ZYC:HAAB	1.48	1.25
1:A:107:GLN:H	2:A:301:ZYC:CAA	1.51	1.21
1:A:107:GLN:N	2:A:301:ZYC:HAAB	1.56	1.20
1:A:33:GLY:HA2	2:A:301:ZYC:HAA	1.49	0.95
1:B:33:GLY:HA2	2:B:301:ZYC:HAA	1.48	0.93
1:B:107:GLN:CB	2:B:301:ZYC:HAAA	1.98	0.92
1:B:33:GLY:CA	2:B:301:ZYC:HAA	2.00	0.92
1:A:107:GLN:H	2:A:301:ZYC:HAAB	0.73	0.89
1:D:110:VAL:HG12	1:D:114:MET:HE2	1.55	0.88
1:B:34:PHE:N	2:B:301:ZYC:HAJ	1.89	0.87
1:A:34:PHE:H	2:A:301:ZYC:CAA	1.88	0.86
1:A:107:GLN:CB	2:A:301:ZYC:HAAA	2.06	0.85
1:B:107:GLN:N	2:B:301:ZYC:CAA	2.19	0.85
1:A:114:MET:HE1	1:A:176:LEU:HG	1.60	0.84
1:B:34:PHE:H	2:B:301:ZYC:CAA	1.91	0.83
1:A:33:GLY:CA	2:A:301:ZYC:HAA	2.08	0.82
1:A:107:GLN:HB2	2:A:301:ZYC:HAAA	1.63	0.81
1:B:34:PHE:H	2:B:301:ZYC:CAJ	1.95	0.79
1:B:107:GLN:HB2	2:B:301:ZYC:HAAA	1.67	0.76
1:A:107:GLN:CB	2:A:301:ZYC:CAA	2.64	0.76
1:B:107:GLN:H	2:B:301:ZYC:HAAB	0.63	0.76
1:C:45:GLN:HG2	1:C:236:VAL:HG21	1.66	0.76
1:D:110:VAL:CG1	1:D:114:MET:HE2	2.18	0.73
1:B:34:PHE:H	2:B:301:ZYC:HAJ	1.46	0.71
1:A:34:PHE:H	2:A:301:ZYC:CAJ	2.03	0.70
1:B:107:GLN:HB3	2:B:301:ZYC:HAAA	1.73	0.69
1:B:107:GLN:CB	2:B:301:ZYC:CAA	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLN:N	2:A:301:ZYC:CAA	2.32	0.68
1:A:34:PHE:H	2:A:301:ZYC:HAJ	1.60	0.67
1:A:34:PHE:N	2:A:301:ZYC:HAJ	2.09	0.66
1:D:3:ARG:HG2	1:D:3:ARG:HH21	1.61	0.66
1:B:45:GLN:HG2	1:B:236:VAL:HG21	1.76	0.66
1:C:6:ILE:HD11	1:C:90:TYR:CG	2.31	0.66
1:D:77:VAL:HG11	1:D:176:LEU:HD21	1.77	0.66
1:B:51:ARG:NH1	3:B:401:HOH:O	2.27	0.65
1:D:157:ALA:HB1	1:D:164:LYS:CG	2.28	0.64
1:C:27:MET:HG2	1:C:91:VAL:HG13	1.80	0.64
1:D:4:ILE:HG12	1:D:15:GLY:C	2.26	0.61
1:A:107:GLN:HB3	2:A:301:ZYC:HAAA	1.83	0.61
1:D:81:ILE:HD11	1:D:114:MET:HE3	1.84	0.60
1:A:183:LYS:HB3	1:A:211:VAL:HG13	1.85	0.59
1:D:197:ASP:HB2	1:D:225:HIS:N	2.18	0.59
1:D:106:ALA:HA	1:D:130:ALA:O	2.03	0.58
1:D:193:VAL:HG12	1:D:217:LEU:HD21	1.84	0.58
1:A:77:VAL:HG11	1:A:176:LEU:HD21	1.84	0.58
1:D:157:ALA:HB1	1:D:164:LYS:HG2	1.86	0.58
1:A:145:GLN:HE21	1:A:160:PHE:HZ	1.52	0.57
1:B:183:LYS:HG3	1:B:211:VAL:HG13	1.85	0.57
1:A:107:GLN:HB3	2:A:301:ZYC:CAA	2.33	0.57
1:A:207:LYS:NZ	1:A:210:GLU:OE2	2.20	0.56
1:B:34:PHE:N	2:B:301:ZYC:CAJ	2.60	0.56
1:D:107:GLN:N	2:D:301:ZYC:OAC	2.37	0.56
1:D:183:LYS:HB3	1:D:211:VAL:HG13	1.87	0.56
1:D:4:ILE:HG12	1:D:15:GLY:O	2.06	0.55
1:C:142:GLY:HA2	1:C:149:TYR:CE1	2.41	0.55
1:C:27:MET:HG2	1:C:91:VAL:CG1	2.36	0.55
1:A:34:PHE:H	2:A:301:ZYC:HAAA	1.71	0.55
1:A:114:MET:SD	1:A:178:ILE:HA	2.47	0.55
1:B:106:ALA:CB	2:B:301:ZYC:HAAB	2.36	0.54
1:C:77:VAL:HG11	1:C:176:LEU:HD21	1.89	0.54
1:B:34:PHE:H	2:B:301:ZYC:HAAA	1.73	0.54
1:B:107:GLN:CA	2:B:301:ZYC:CAA	2.86	0.54
1:A:9:ASP:O	1:B:9:ASP:O	2.26	0.53
1:C:20:PRO:HG3	1:C:54:ASN:HA	1.90	0.53
1:D:3:ARG:HH21	1:D:3:ARG:CG	2.21	0.53
1:A:157:ALA:HB1	1:A:164:LYS:HG2	1.91	0.53
1:D:197:ASP:HB3	1:D:225:HIS:HB2	1.90	0.53
1:C:9:ASP:O	1:D:9:ASP:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ILE:HD11	1:C:114:MET:SD	2.50	0.52
1:B:33:GLY:CA	2:B:301:ZYC:CAA	2.83	0.52
1:C:33:GLY:HA3	2:C:301:ZYC:HAAB	1.92	0.52
1:B:107:GLN:HB3	2:B:301:ZYC:CAA	2.36	0.52
1:B:92:ARG:NE	1:B:92:ARG:HA	2.25	0.51
1:D:160:PHE:O	1:D:163:LYS:HG2	2.11	0.50
1:A:207:LYS:HE3	3:A:516:HOH:O	2.10	0.50
1:B:169:TYR:C	1:B:169:TYR:CD1	2.90	0.49
1:A:6:ILE:HD12	1:A:60:PHE:CZ	2.46	0.49
1:D:84:ALA:HB1	1:D:115:LEU:HD22	1.93	0.49
1:D:142:GLY:HA2	1:D:149:TYR:CE1	2.47	0.49
1:A:6:ILE:HD11	1:A:90:TYR:CG	2.48	0.48
1:B:33:GLY:HA3	2:B:301:ZYC:HAA	1.88	0.48
1:D:194:GLY:CA	1:D:223:ALA:HB3	2.44	0.48
1:B:6:ILE:HD11	1:B:90:TYR:CG	2.48	0.48
1:A:107:GLN:CA	2:A:301:ZYC:CAA	2.91	0.48
1:C:185:TYR:HE2	1:C:189:VAL:HG22	1.78	0.48
1:C:197:ASP:OD1	1:C:225:HIS:HB2	2.14	0.47
1:D:27:MET:HG2	1:D:91:VAL:CG1	2.44	0.47
1:D:147:ALA:HB1	1:D:158:ILE:HD12	1.95	0.47
1:D:134:GLN:HB2	1:D:204:TYR:CE2	2.50	0.47
1:D:197:ASP:HB2	1:D:224:ASP:HA	1.97	0.47
1:A:225:HIS:HE2	2:A:301:ZYC:CAM	2.28	0.47
1:C:158:ILE:HD11	1:C:165:LEU:HD23	1.97	0.47
1:D:185:TYR:CZ	1:D:187:ASN:HB2	2.49	0.47
1:B:77:VAL:HG11	1:B:176:LEU:HD21	1.97	0.46
1:D:90:TYR:O	1:D:93:THR:HG22	2.15	0.46
1:D:197:ASP:CB	1:D:225:HIS:N	2.79	0.46
1:C:24:ILE:HD13	1:C:96:HIS:O	2.16	0.46
1:D:106:ALA:HB1	2:D:301:ZYC:OAC	2.16	0.46
1:A:201:ALA:HB1	1:A:202:PRO:HD2	1.98	0.46
1:B:131:PRO:HD2	1:B:205:SER:OG	2.16	0.46
1:D:18:GLU:HG3	1:D:47:ALA:HB1	1.97	0.46
1:A:183:LYS:HB3	1:A:211:VAL:CG1	2.45	0.45
1:C:92:ARG:HA	1:C:100:ILE:HD11	1.99	0.45
1:D:222:ASP:O	1:D:231:TYR:CZ	2.70	0.45
1:B:33:GLY:HA3	2:B:301:ZYC:CAJ	2.46	0.45
1:B:27:MET:HG2	1:B:91:VAL:HG13	1.98	0.45
1:B:227:PHE:O	1:B:232:LYS:HB2	2.17	0.45
1:C:75:MET:HE3	1:C:75:MET:HB3	1.86	0.44
1:C:139:ALA:HA	1:C:149:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:CB	2:A:301:ZYC:HAAB	2.47	0.44
1:A:142:GLY:HA2	1:A:149:TYR:CE2	2.53	0.44
1:C:114:MET:HE1	1:C:176:LEU:HG	1.99	0.44
1:C:185:TYR:CE2	1:C:189:VAL:HG22	2.53	0.44
1:D:194:GLY:HA3	1:D:223:ALA:HB3	2.00	0.43
1:A:185:TYR:CZ	1:A:187:ASN:HB2	2.54	0.43
1:A:110:VAL:CG1	1:A:114:MET:HE2	2.49	0.43
1:B:145:GLN:HE21	1:B:160:PHE:HZ	1.66	0.43
1:D:6:ILE:HG12	1:D:60:PHE:CE2	2.54	0.43
1:C:135:LEU:C	1:C:135:LEU:HD12	2.44	0.43
1:D:3:ARG:CG	1:D:3:ARG:NH2	2.79	0.43
1:B:241:GLU:HA	1:B:244:LYS:HD3	2.01	0.43
1:D:197:ASP:HB3	1:D:225:HIS:CB	2.49	0.42
1:D:169:TYR:CD1	1:D:169:TYR:C	2.96	0.42
1:D:236:VAL:O	1:D:239:THR:N	2.53	0.42
1:A:24:ILE:HA	1:A:96:HIS:O	2.19	0.42
1:A:212:TYR:HB2	1:A:215:SER:HB3	2.01	0.42
1:A:143:ASP:HB3	3:A:435:HOH:O	2.19	0.42
1:B:225:HIS:HE2	2:B:301:ZYC:CAM	2.32	0.42
1:A:33:GLY:CA	2:A:301:ZYC:CAA	2.92	0.42
1:C:6:ILE:HD11	1:C:90:TYR:CD1	2.55	0.42
1:D:135:LEU:HD12	1:D:135:LEU:C	2.45	0.42
1:B:75:MET:HE3	1:B:75:MET:HB3	1.77	0.42
1:A:27:MET:HG2	1:A:91:VAL:HG13	2.01	0.41
1:B:6:ILE:HD12	1:B:60:PHE:CZ	2.55	0.41
1:A:34:PHE:N	2:A:301:ZYC:CAA	2.70	0.41
1:D:217:LEU:HD22	1:D:218:HIS:N	2.35	0.41
1:A:34:PHE:N	2:A:301:ZYC:CAJ	2.73	0.41
1:C:187:ASN:HB3	1:C:188:PRO:CD	2.50	0.41
1:D:185:TYR:HE2	1:D:189:VAL:HG22	1.86	0.41
1:A:199:VAL:HG11	2:A:301:ZYC:HAE	2.02	0.41
1:C:176:LEU:HA	1:C:177:PRO:HD3	1.95	0.40
1:D:4:ILE:HG13	1:D:60:PHE:CZ	2.56	0.40
1:D:55:VAL:HG12	1:D:56:ALA:O	2.21	0.40
1:A:73:GLU:CD	1:A:164:LYS:HD2	2.46	0.40
1:C:140:LEU:HD23	1:C:174:GLN:HG2	2.03	0.40
1:D:114:MET:HE1	1:D:176:LEU:HD21	2.04	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	254/258 (98%)	245 (96%)	9 (4%)	0	100	100
1	B	254/258 (98%)	246 (97%)	8 (3%)	0	100	100
1	C	254/258 (98%)	245 (96%)	9 (4%)	0	100	100
1	D	242/258 (94%)	226 (93%)	15 (6%)	1 (0%)	30	34
All	All	1004/1032 (97%)	962 (96%)	41 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	ARG

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	212/215 (99%)	211 (100%)	1 (0%)	81	90
1	B	213/215 (99%)	212 (100%)	1 (0%)	81	90
1	C	212/215 (99%)	208 (98%)	4 (2%)	50	66
1	D	202/215 (94%)	198 (98%)	4 (2%)	48	64
All	All	839/860 (98%)	829 (99%)	10 (1%)	63	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	B	21	PHE
1	C	19	GLU
1	C	23	GLU
1	C	24	ILE
1	C	230	GLN
1	D	3	ARG
1	D	203	LYS
1	D	211	VAL
1	D	230	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	B	45	GLN
1	B	49	ASN
1	B	141	ASN
1	B	145	GLN
1	C	49	ASN
1	C	96	HIS
1	C	161	HIS
1	C	184	HIS
1	C	214	ASN
1	D	54	ASN
1	D	141	ASN
1	D	153	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZYC	A	301	-	16,16,16	1.16	1 (6%)	20,20,20	1.32	2 (10%)
2	ZYC	B	301	-	16,16,16	1.27	1 (6%)	20,20,20	1.45	2 (10%)
2	ZYC	C	301	-	16,16,16	0.98	1 (6%)	20,20,20	1.01	2 (10%)
2	ZYC	D	301	-	16,16,16	0.79	0	20,20,20	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZYC	A	301	-	-	3/10/10/10	0/1/1/1
2	ZYC	B	301	-	-	3/10/10/10	0/1/1/1
2	ZYC	C	301	-	-	4/10/10/10	0/1/1/1
2	ZYC	D	301	-	-	5/10/10/10	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ZYC	OAL-CAM	-3.74	1.25	1.34
2	A	301	ZYC	OAL-CAM	-3.65	1.26	1.34
2	C	301	ZYC	OAC-CAM	-2.26	1.17	1.21

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ZYC	OAL-CAJ-CAA	-4.33	92.86	108.40
2	B	301	ZYC	OAL-CAJ-CAA	-3.97	94.16	108.40
2	C	301	ZYC	OAL-CAJ-CAA	3.26	120.10	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ZYC	CAJ-OAL-CAM	-2.87	110.70	116.38
2	A	301	ZYC	CAJ-OAL-CAM	-2.45	111.53	116.38
2	C	301	ZYC	CAJ-OAL-CAM	2.07	120.48	116.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZYC	CAM-CAE-CAF-CAN
2	D	301	ZYC	CAM-CAE-CAF-CAN
2	D	301	ZYC	OAC-CAM-OAL-CAJ
2	D	301	ZYC	CAE-CAM-OAL-CAJ
2	C	301	ZYC	CAA-CAJ-OAL-CAM
2	C	301	ZYC	CAM-CAE-CAF-CAN
2	C	301	ZYC	CAO-CAP-OAK-CAB
2	A	301	ZYC	CAE-CAF-CAN-CAG
2	A	301	ZYC	CAE-CAF-CAN-CAI
2	C	301	ZYC	CAI-CAP-OAK-CAB
2	D	301	ZYC	CAE-CAF-CAN-CAG
2	D	301	ZYC	CAE-CAF-CAN-CAI
2	B	301	ZYC	CAE-CAF-CAN-CAG
2	B	301	ZYC	CAE-CAF-CAN-CAI
2	B	301	ZYC	CAM-CAE-CAF-CAN

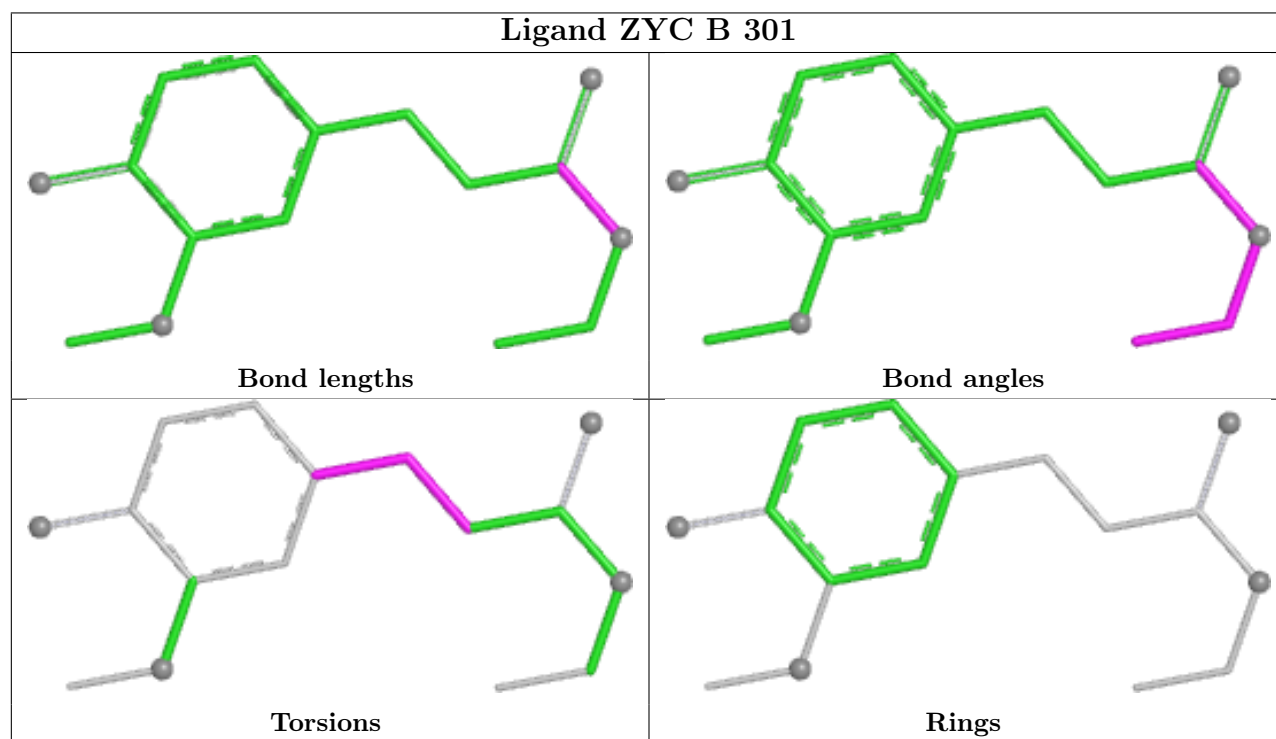
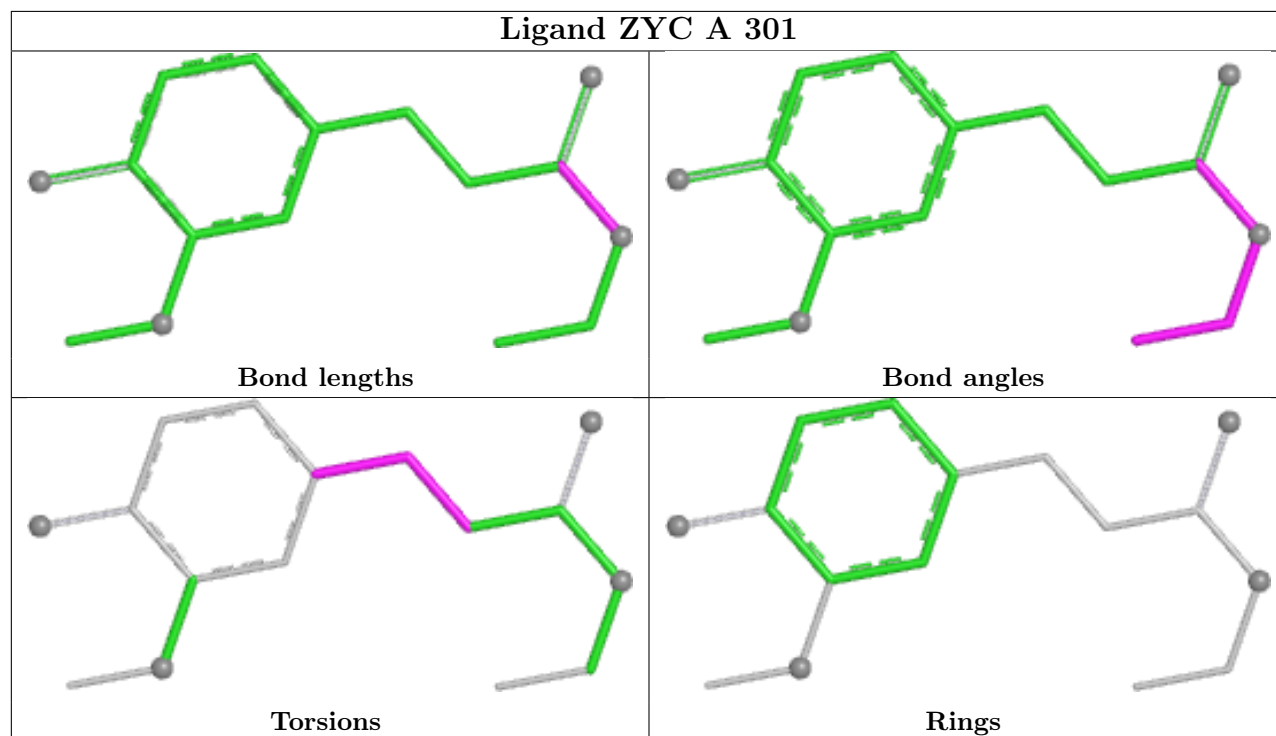
There are no ring outliers.

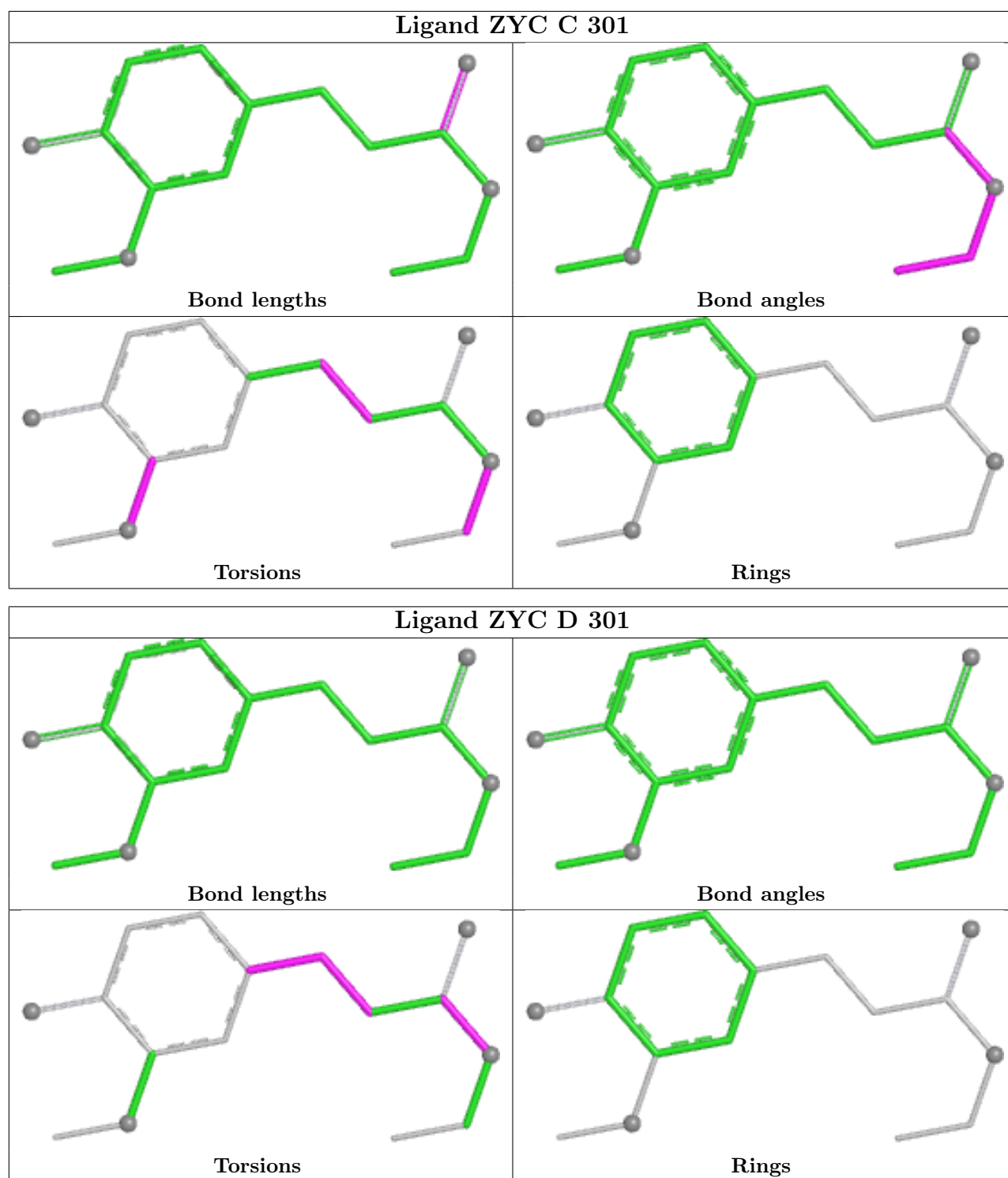
4 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ZYC	23	0
2	B	301	ZYC	23	0
2	C	301	ZYC	1	0
2	D	301	ZYC	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 ⓘ

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	256/258 (99%)	-0.18	6 (2%) 61 58	8, 16, 30, 42	0
1	B	256/258 (99%)	-0.23	2 (0%) 82 80	9, 16, 29, 50	0
1	C	256/258 (99%)	-0.10	4 (1%) 70 67	11, 19, 30, 39	0
1	D	244/258 (94%)	1.67	82 (33%) 1 0	15, 33, 72, 291	0
All	All	1012/1032 (98%)	0.27	94 (9%) 14 12	8, 19, 47, 291	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	LEU	16.1
1	D	101	PHE	11.0
1	D	50	LEU	9.8
1	D	244	LYS	9.0
1	D	125	LYS	9.0
1	D	245	PRO	8.8
1	D	240	ALA	8.3
1	D	53	GLU	8.3
1	D	21	PHE	8.0
1	D	55	VAL	7.2
1	D	49	ASN	7.0
1	D	52	ASP	6.5
1	D	199	VAL	6.5
1	D	242	PHE	6.3
1	C	21	PHE	5.6
1	D	194	GLY	5.5
1	D	231	TYR	4.8
1	D	48	ASP	4.8
1	D	4	ILE	4.8
1	D	201	ALA	4.8
1	D	202	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	197	ASP	4.5
1	A	114	MET	4.5
1	D	220	VAL	4.4
1	D	229	GLY	4.3
1	A	21	PHE	4.2
1	D	230	GLN	4.2
1	D	193	VAL	4.1
1	D	239	THR	4.0
1	B	21	PHE	4.0
1	C	114	MET	3.9
1	D	217	LEU	3.8
1	D	141	ASN	3.8
1	D	223	ALA	3.8
1	D	51	ARG	3.7
1	D	221	PRO	3.6
1	D	198	GLN	3.6
1	D	161	HIS	3.6
1	D	241	GLU	3.6
1	D	228	THR	3.5
1	D	238	LEU	3.5
1	D	153	HIS	3.5
1	D	200	VAL	3.5
1	D	196	ASN	3.5
1	D	219	MET	3.3
1	D	233	ASP	3.3
1	D	41	PRO	3.3
1	D	235	ALA	3.3
1	D	195	SER	3.2
1	A	-3	PHE	3.2
1	D	225	HIS	3.2
1	D	146	GLY	3.0
1	D	47	ALA	2.9
1	D	54	ASN	2.9
1	D	236	VAL	2.9
1	D	164	LYS	2.8
1	D	222	ASP	2.8
1	D	145	GLN	2.8
1	D	2	SER	2.7
1	D	203	LYS	2.7
1	D	214	ASN	2.7
1	D	209	ASP	2.7
1	D	204	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	234	SER	2.6
1	D	224	ASP	2.6
1	D	232	LYS	2.6
1	D	159	PRO	2.6
1	D	205	SER	2.5
1	D	206	LYS	2.5
1	D	227	PHE	2.5
1	D	163	LYS	2.5
1	D	211	VAL	2.4
1	D	143	ASP	2.4
1	D	226	SER	2.4
1	D	23	GLU	2.3
1	A	23	GLU	2.3
1	D	137	ASP	2.3
1	D	134	GLN	2.2
1	C	-3	PHE	2.2
1	D	144	THR	2.2
1	C	-10	GLY	2.2
1	B	230	GLN	2.2
1	D	218	HIS	2.2
1	D	237	ASP	2.2
1	A	219	MET	2.1
1	D	93	THR	2.1
1	D	45	GLN	2.1
1	A	-10	GLY	2.1
1	D	42	LEU	2.1
1	D	162	GLY	2.1
1	D	46	ILE	2.1
1	D	44	ARG	2.0
1	D	191	ILE	2.0
1	D	3	ARG	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](#)

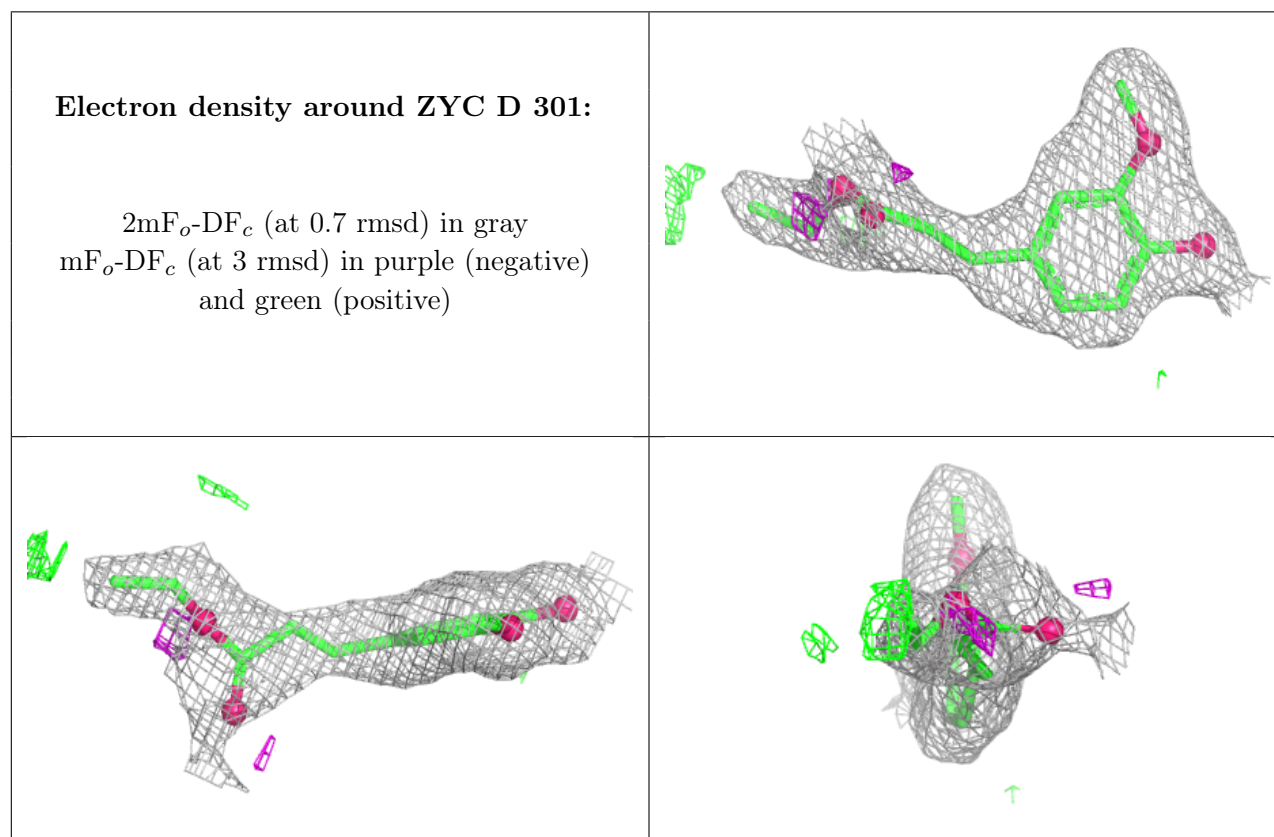
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

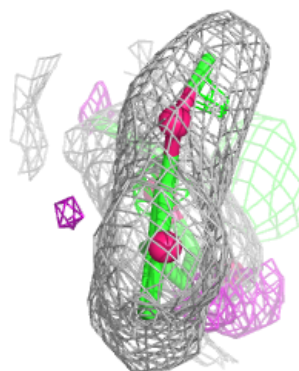
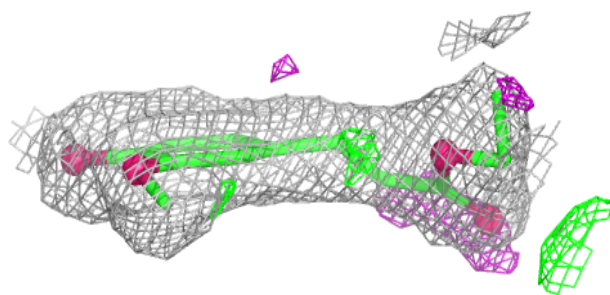
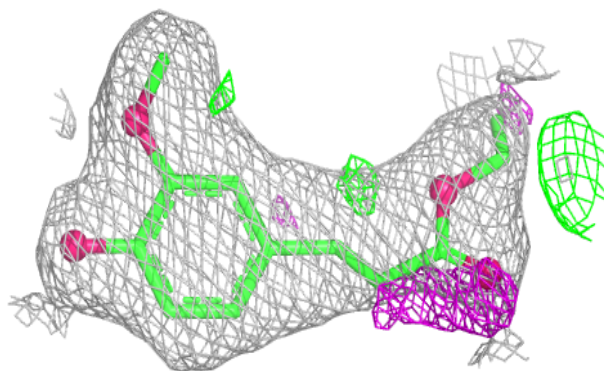
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZYC	D	301	16/16	0.85	0.15	37,46,58,71	0
2	ZYC	A	301	16/16	0.91	0.10	17,22,27,31	0
2	ZYC	C	301	16/16	0.92	0.08	16,21,25,25	0
2	ZYC	B	301	16/16	0.92	0.10	14,18,23,23	0

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.

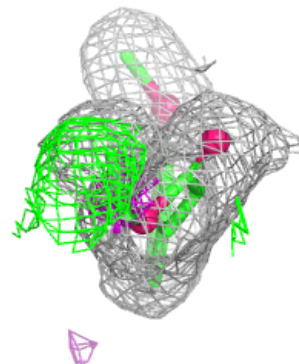
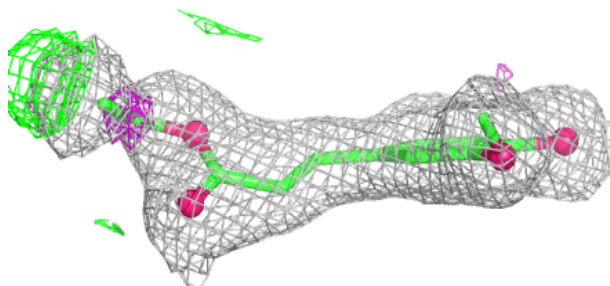
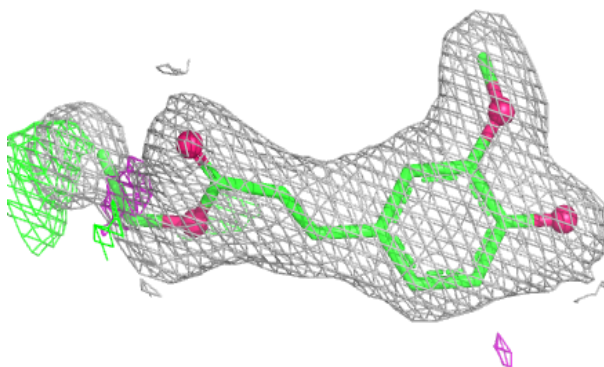


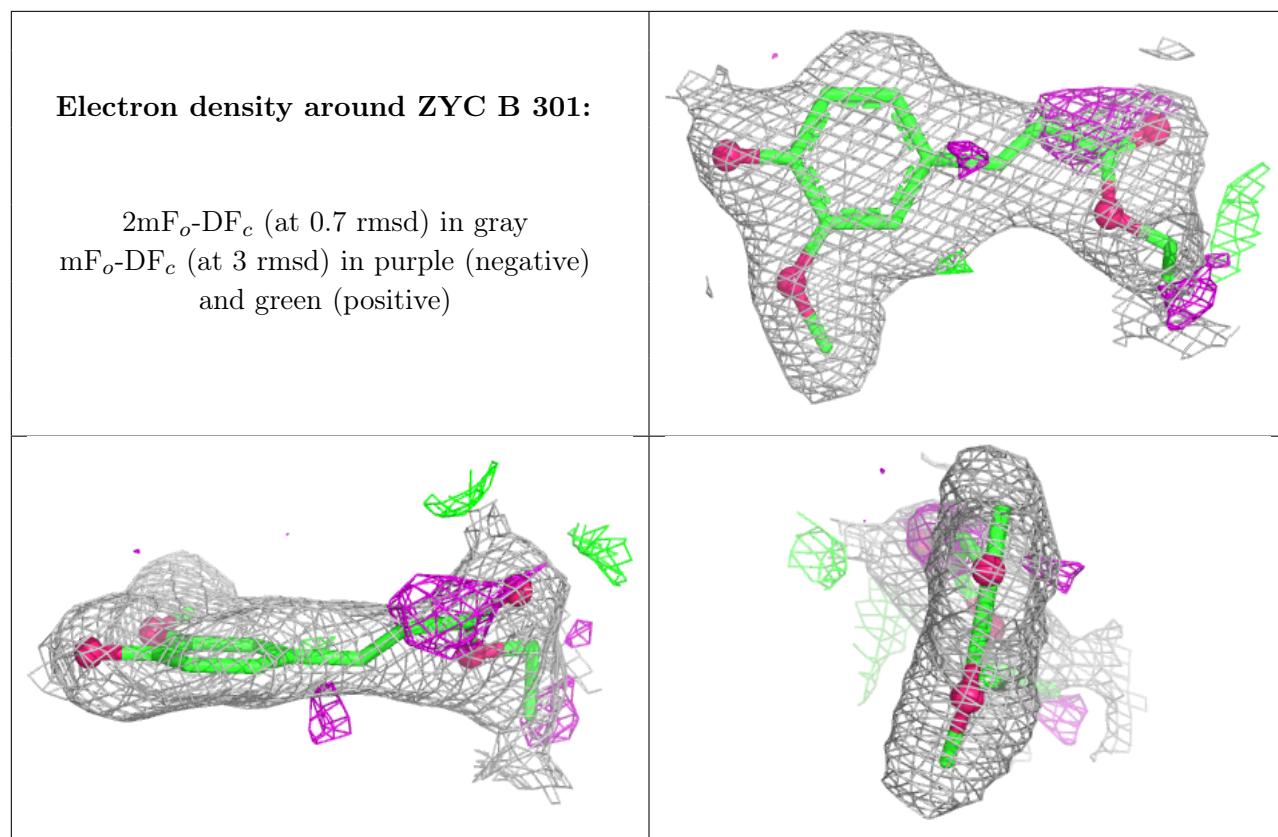
Electron density around ZYC A 301:

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

**Electron density around ZYC C 301:**

$2mF_o-DF_c$ (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.