



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 05:00 AM UTC

PDB ID : 5IE5 / pdb_00005ie5
Title : Crystal structure of a lactonase double mutant in complex with substrate a
Authors : Zheng, Y.Y.; Xu, Z.X.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2016-02-25
Resolution : 2.39 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

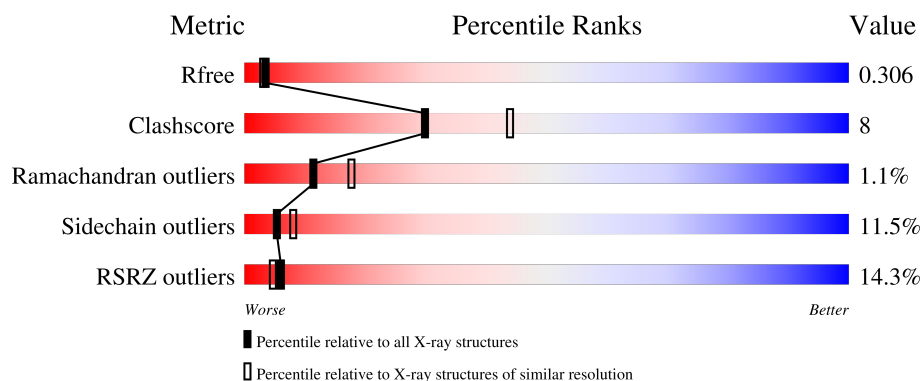
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	264	2% 82% 15% ••
1	B	264	3% 82% 16% •
1	C	264	32% 37% 20% 5% 38%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5648 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.

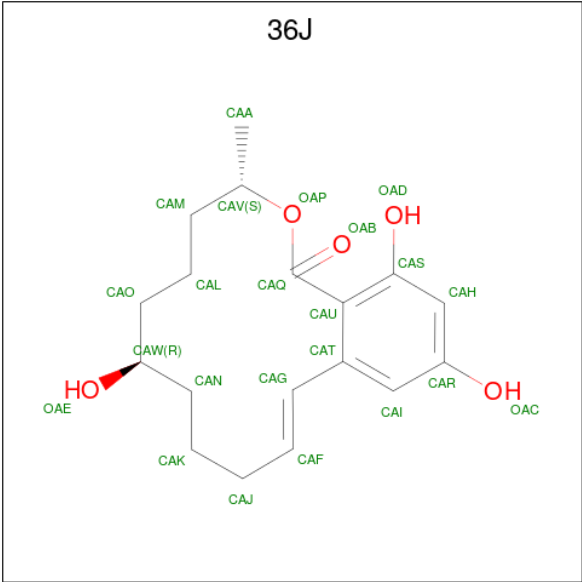
- Molecule 1 is a protein called Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2023	C 1283	N 343	O 386	S 11	0	0	0
1	B	264	Total 2023	C 1283	N 343	O 386	S 11	0	0	0
1	C	164	Total 1255	C 806	N 207	O 235	S 7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	SER	engineered mutation	UNP Q8NKB0
A	153	HIS	VAL	engineered mutation	UNP Q8NKB0
B	102	ALA	SER	engineered mutation	UNP Q8NKB0
B	153	HIS	VAL	engineered mutation	UNP Q8NKB0
C	102	ALA	SER	engineered mutation	UNP Q8NKB0
C	153	HIS	VAL	engineered mutation	UNP Q8NKB0

- Molecule 2 is (3S,7R,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (CCD ID: 36J) (formula: C₁₈H₂₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		

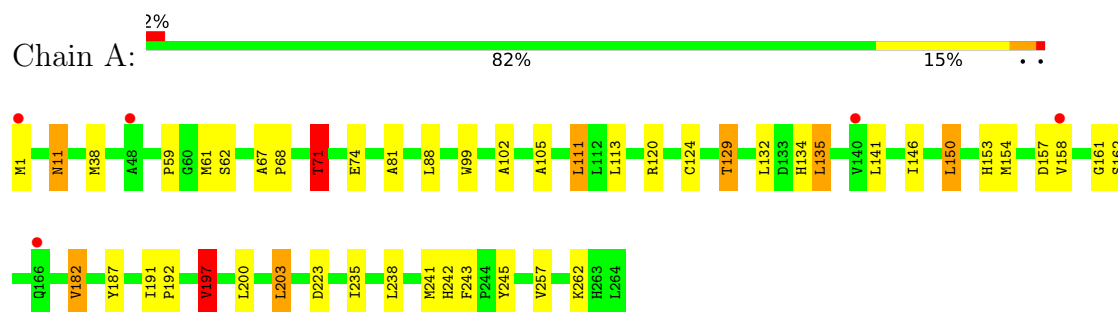
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	114	Total	O	0	0
			114	114		
3	C	71	Total	O	0	0
			71	71		

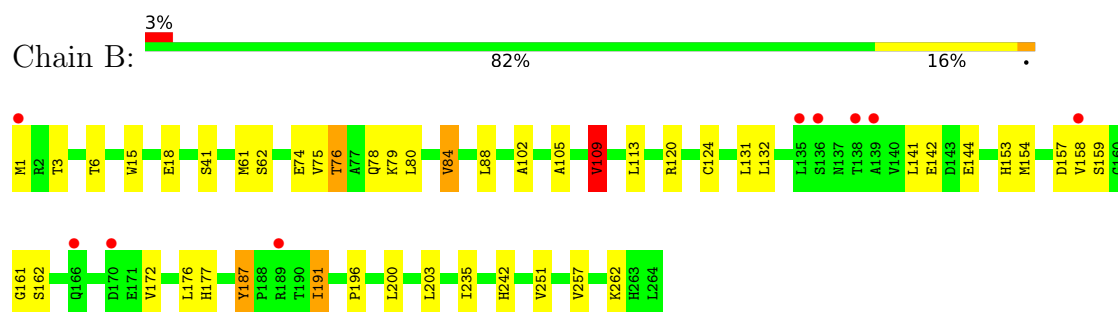
3 Residue-property plots [i](#)

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.

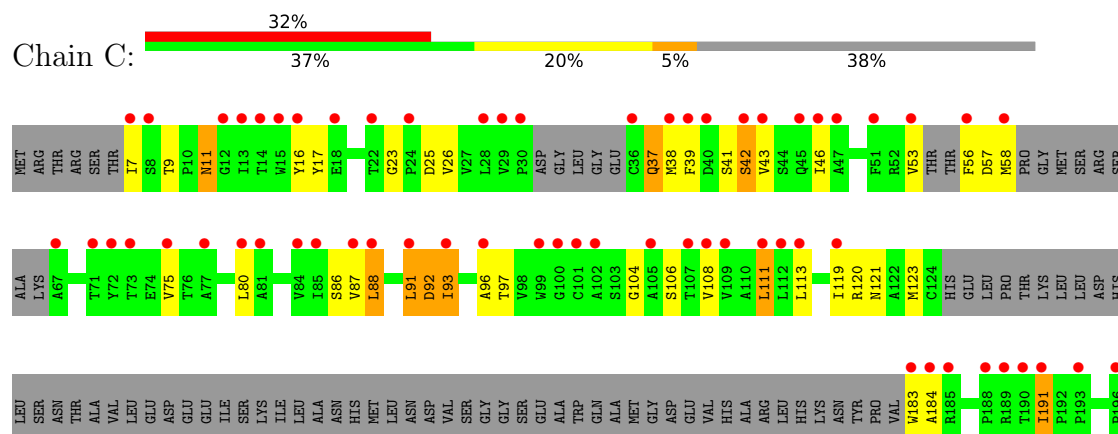
• Molecule 1: Zearalenone hydrolase

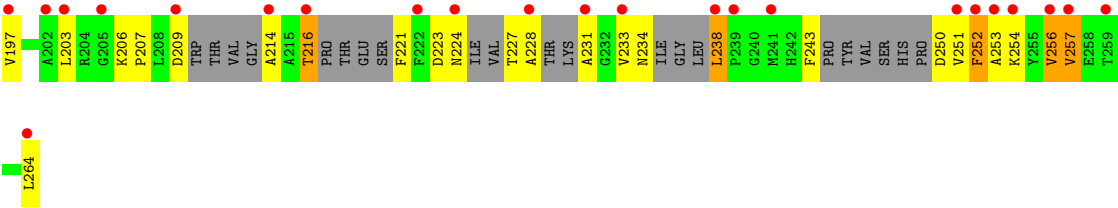


• Molecule 1: Zearalenone hydrolase



• Molecule 1: Zearalenone hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.16Å 86.16Å 471.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.39 25.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.39) 99.5 (25.00-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.214 , 0.270 0.265 , 0.306	Depositor DCC
R_{free} test set	2064 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: 36J

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	0.73	0/2075	0.97	2/2834 (0.1%)
1	B	0.76	0/2075	0.99	1/2834 (0.0%)
1	C	0.64	0/1279	0.90	2/1734 (0.1%)
All	All	0.72	0/5429	0.96	5/7402 (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	2
1	B	0	1
1	C	0	5
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	23	GLY	CA-C-N	6.25	126.27	119.90
1	C	23	GLY	C-N-CA	6.25	126.27	119.90
1	B	109	VAL	N-CA-CB	5.72	119.16	110.58
1	A	71	THR	N-CA-CB	-5.63	101.66	110.44
1	A	192	PRO	N-CA-C	5.47	117.38	110.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	197	VAL	Mainchain
1	B	120	ARG	Sidechain
1	C	214	ALA	Peptide
1	C	223	ASP	Peptide
1	C	238	LEU	Peptide
1	C	250	ASP	Peptide
1	C	91	LEU	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	2023	0	1989	33	0
1	B	2023	0	1989	18	0
1	C	1255	0	1222	33	0
2	A	23	0	22	8	0
2	B	23	0	22	5	0
3	A	116	0	0	1	1
3	B	114	0	0	0	1
3	C	71	0	0	1	0
All	All	5648	0	5244	90	1

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 8.

All (90) 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:38:MET:CE	1:A:245:TYR:HE2	1.75	1.00
1:C:88:LEU:O	1:C:92:ASP:O	1.88	0.92
1:C:209:ASP:OD1	1:C:234:ASN:ND2	2.13	0.82
1:A:67:ALA:HB1	1:A:71:THR:HG21	1.62	0.80
1:A:38:MET:CE	1:A:245:TYR:CE2	2.65	0.76
1:B:76:THR:HG22	1:B:79:LYS:H	1.51	0.76
1:B:109:VAL:HG22	1:B:196:PRO:HG2	1.70	0.74
1:B:242:HIS:CD2	2:B:301:36J:H5	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:PHE:O	1:C:224:ASN:HB2	1.92	0.69
1:A:38:MET:HE2	1:A:245:TYR:HE2	1.56	0.68
1:A:38:MET:HE3	1:A:245:TYR:HE2	1.56	0.67
1:A:38:MET:HE3	1:A:245:TYR:CE2	2.31	0.65
1:A:158:VAL:HG21	2:A:300:36J:H2	1.81	0.61
1:C:227:THR:O	1:C:231:ALA:HB3	2.03	0.59
1:C:26:VAL:O	1:C:53:VAL:C	2.46	0.58
2:A:300:36J:OAB	2:A:300:36J:OAD	2.16	0.57
1:A:129:THR:HG21	1:A:223:ASP:OD1	2.05	0.56
2:B:301:36J:H15	2:B:301:36J:OAP	2.06	0.56
1:C:216:THR:C	3:C:308:HOH:O	2.48	0.56
1:A:102:ALA:HB1	2:A:300:36J:CAQ	2.36	0.56
1:A:81:ALA:HB1	1:A:111:LEU:HD13	1.88	0.55
2:B:301:36J:OAD	2:B:301:36J:OAB	2.21	0.54
1:C:16:TYR:O	1:C:56:PHE:HA	2.08	0.54
1:C:38:MET:HE1	1:C:243:PHE:CD1	2.43	0.54
1:C:97:THR:OG1	1:C:121:ASN:ND2	2.41	0.54
1:A:129:THR:HG23	3:A:476:HOH:O	2.09	0.53
1:C:9:THR:OG1	1:C:11:ASN:ND2	2.42	0.52
1:C:228:ALA:HB1	1:C:233:VAL:HB	1.92	0.51
1:C:92:ASP:O	1:C:93:ILE:HB	2.11	0.51
1:A:59:PRO:CB	1:A:71:THR:HG23	2.40	0.51
1:A:105:ALA:HB1	1:A:124:CYS:HB2	1.93	0.51
1:A:197:VAL:HG22	1:A:203:LEU:HD21	1.93	0.50
1:C:120:ARG:HG2	1:C:121:ASN:HD22	1.76	0.50
1:A:146:ILE:HG23	1:A:150:LEU:HD22	1.94	0.50
1:B:102:ALA:HB1	2:B:301:36J:CAQ	2.42	0.50
1:A:59:PRO:HB2	1:A:71:THR:HG23	1.92	0.49
1:C:253:ALA:O	1:C:257:VAL:HG13	2.12	0.49
1:A:38:MET:HE1	1:A:243:PHE:CD1	2.48	0.49
1:A:11:ASN:H	1:A:11:ASN:ND2	2.09	0.49
1:B:105:ALA:HB1	1:B:124:CYS:HB2	1.95	0.49
1:C:96:ALA:O	1:C:119:ILE:HA	2.13	0.49
1:C:252:PHE:C	1:C:252:PHE:CD1	2.91	0.48
1:A:242:HIS:CD2	2:A:300:36J:H3	2.48	0.48
1:A:146:ILE:CG2	1:A:150:LEU:HD22	2.43	0.48
1:B:187:TYR:CD2	1:B:191:ILE:HD13	2.49	0.48
1:A:154:MET:HE1	2:A:300:36J:H5	1.97	0.47
1:A:134:HIS:CE1	1:A:135:LEU:HD13	2.50	0.47
1:C:39:PHE:O	1:C:43:VAL:N	2.44	0.47
1:A:38:MET:HE1	1:A:243:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG23	1:C:7:ILE:O	2.14	0.46
1:C:97:THR:CG2	1:C:123:MET:CE	2.94	0.46
1:A:61:MET:SD	1:A:182:VAL:HG22	2.56	0.45
2:A:300:36J:OAP	2:A:300:36J:H15	2.16	0.45
1:C:42:SER:O	1:C:46:ILE:HB	2.17	0.45
1:A:61:MET:O	1:A:62:SER:C	2.57	0.45
1:C:91:LEU:HB2	1:C:93:ILE:HD12	1.98	0.45
1:B:76:THR:HG23	1:B:78:GLN:OE1	2.16	0.45
1:C:75:VAL:HG12	1:C:191:ILE:HD11	1.98	0.45
1:B:153:HIS:ND1	1:B:157:ASP:OD2	2.47	0.44
1:A:68:PRO:O	1:A:71:THR:HB	2.18	0.44
1:B:154:MET:O	1:B:159:SER:HB3	2.17	0.44
1:C:197:VAL:HG22	1:C:197:VAL:O	2.17	0.44
1:B:102:ALA:HB2	1:B:242:HIS:CE1	2.53	0.44
1:C:17:TYR:HA	1:C:56:PHE:HA	1.99	0.44
1:A:102:ALA:HB2	1:A:242:HIS:NE2	2.33	0.43
1:A:153:HIS:ND1	1:A:157:ASP:OD2	2.42	0.43
1:B:102:ALA:HB2	1:B:242:HIS:NE2	2.33	0.43
1:C:7:ILE:O	1:C:7:ILE:CG2	2.66	0.43
1:A:134:HIS:ND1	1:A:135:LEU:HD13	2.33	0.43
1:C:104:GLY:O	1:C:108:VAL:HG13	2.19	0.43
1:C:58:MET:HE3	1:C:80:LEU:HD22	2.02	0.42
1:C:121:ASN:HA	1:C:207:PRO:HB2	2.00	0.42
1:B:144:GLU:OE2	1:B:177:HIS:CE1	2.72	0.42
1:C:252:PHE:O	1:C:256:VAL:HG23	2.19	0.42
1:B:80:LEU:O	1:B:84:VAL:HG13	2.19	0.42
1:B:75:VAL:HG21	1:B:187:TYR:CE1	2.55	0.42
1:B:158:VAL:O	1:B:158:VAL:HG22	2.19	0.41
2:B:301:36J:OAP	2:B:301:36J:CAG	2.67	0.41
1:C:183:TRP:O	1:C:184:ALA:C	2.62	0.41
2:A:300:36J:OAP	2:A:300:36J:CAG	2.68	0.41
1:C:25:ASP:O	1:C:120:ARG:NH2	2.53	0.41
1:B:61:MET:O	1:B:62:SER:C	2.61	0.41
1:C:108:VAL:HA	1:C:111:LEU:HB2	2.03	0.41
1:B:6:THR:HA	1:B:15:TRP:O	2.21	0.41
1:C:38:MET:HE1	1:C:243:PHE:HD1	1.83	0.41
1:A:81:ALA:CB	1:A:111:LEU:HD13	2.51	0.40
1:A:99:TRP:CD1	1:A:99:TRP:C	2.96	0.40
1:A:157:ASP:O	1:A:241:MET:HE1	2.22	0.40
1:A:154:MET:HE1	2:A:300:36J:H1	2.03	0.40
1:B:3:THR:O	1:B:18:GLU:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:491:HOH:O	3:B:482:HOH:O[6_555]	2.09	0.11

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	262/264 (99%)	251 (96%)	9 (3%)	2 (1%)	16	25
1	B	262/264 (99%)	253 (97%)	7 (3%)	2 (1%)	16	25
1	C	142/264 (54%)	131 (92%)	8 (6%)	3 (2%)	5	7
All	All	666/792 (84%)	635 (95%)	24 (4%)	7 (1%)	11	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	ASP
1	C	37	GLN
1	C	93	ILE
1	B	187	TYR
1	A	161	GLY
1	A	187	TYR
1	B	161	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	220/220 (100%)	198 (90%)	22 (10%)	7	11
1	B	220/220 (100%)	198 (90%)	22 (10%)	7	11
1	C	134/220 (61%)	112 (84%)	22 (16%)	2	3
All	All	574/660 (87%)	508 (88%)	66 (12%)	5	8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ASN
1	A	71	THR
1	A	74	GLU
1	A	88	LEU
1	A	111	LEU
1	A	113	LEU
1	A	129	THR
1	A	132	LEU
1	A	135	LEU
1	A	141	LEU
1	A	150	LEU
1	A	162	SER
1	A	182	VAL
1	A	191	ILE
1	A	197	VAL
1	A	200	LEU
1	A	203	LEU
1	A	235	ILE
1	A	238	LEU
1	A	257	VAL
1	A	262	LYS
1	B	1	MET
1	B	41	SER
1	B	74	GLU
1	B	76	THR
1	B	84	VAL
1	B	88	LEU
1	B	109	VAL
1	B	113	LEU
1	B	131	LEU
1	B	132	LEU
1	B	141	LEU
1	B	142	GLU

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Mol	Chain	Res	Type
1	B	162	SER
1	B	172	VAL
1	B	176	LEU
1	B	191	ILE
1	B	200	LEU
1	B	203	LEU
1	B	235	ILE
1	B	251	VAL
1	B	257	VAL
1	B	262	LYS
1	C	11	ASN
1	C	37	GLN
1	C	41	SER
1	C	42	SER
1	C	57	ASP
1	C	86	SER
1	C	87	VAL
1	C	88	LEU
1	C	106	SER
1	C	111	LEU
1	C	113	LEU
1	C	191	ILE
1	C	203	LEU
1	C	206	LYS
1	C	216	THR
1	C	238	LEU
1	C	251	VAL
1	C	252	PHE
1	C	254	LYS
1	C	256	VAL
1	C	257	VAL
1	C	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	95	HIS
1	A	263	HIS
1	B	121	ASN
1	B	137	ASN
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	177	HIS
1	B	261	GLN
1	C	11	ASN
1	C	37	GLN
1	C	121	ASN
1	C	263	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	36J	B	301	-	24,24,24	1.57	4 (16%)	32,32,32	1.32	7 (21%)
2	36J	A	300	-	24,24,24	1.53	3 (12%)	32,32,32	1.53	7 (21%)

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	36J	B	301	-	-	7/22/22/22	0/2/2/2
2	36J	A	300	-	-	8/22/22/22	1/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	36J	CAT-CAG	-4.59	1.39	1.47
2	A	300	36J	CAT-CAG	-4.51	1.39	1.47
2	B	301	36J	CAU-CAQ	-4.35	1.40	1.50
2	A	300	36J	CAU-CAQ	-4.31	1.40	1.50
2	B	301	36J	CAG-CAF	2.81	1.40	1.31
2	A	300	36J	CAG-CAF	2.76	1.40	1.31
2	B	301	36J	CAJ-CAF	-2.00	1.39	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	36J	OAP-CAV-CAA	3.26	115.26	107.96
2	A	300	36J	OAD-CAS-CAU	-3.13	115.35	121.14
2	A	300	36J	CAV-OAP-CAQ	3.09	123.42	117.67
2	A	300	36J	CAK-CAN-CAW	-2.87	106.76	114.68
2	B	301	36J	OAD-CAS-CAU	-2.85	115.87	121.14
2	A	300	36J	CAT-CAG-CAF	-2.66	119.94	125.55
2	B	301	36J	CAN-CAK-CAJ	-2.34	109.41	114.47
2	A	300	36J	CAS-CAH-CAR	-2.28	117.57	119.67
2	B	301	36J	CAA-CAV-CAM	-2.20	108.22	113.90
2	B	301	36J	CAV-OAP-CAQ	2.18	121.72	117.67
2	A	300	36J	CAN-CAK-CAJ	-2.13	109.86	114.47
2	B	301	36J	CAK-CAN-CAW	-2.11	108.86	114.68
2	B	301	36J	OAP-CAV-CAA	2.09	112.65	107.96
2	B	301	36J	CAJ-CAF-CAG	-2.07	120.88	125.48

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	36J	CAL-CAM-CAV-CAA
2	A	300	36J	CAA-CAV-OAP-CAQ
2	A	300	36J	CAU-CAQ-OAP-CAV
2	B	301	36J	CAA-CAV-OAP-CAQ
2	A	300	36J	OAB-CAQ-OAP-CAV
2	A	300	36J	CAL-CAM-CAV-OAP

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Mol	Chain	Res	Type	Atoms
2	A	300	36J	CAF-CAJ-CAK-CAN
2	B	301	36J	CAM-CAV-OAP-CAQ
2	B	301	36J	CAL-CAO-CAW-CAN
2	B	301	36J	CAM-CAL-CAO-CAW
2	A	300	36J	CAG-CAF-CAJ-CAK
2	A	300	36J	CAJ-CAK-CAN-CAW
2	B	301	36J	CAL-CAO-CAW-OAE
2	B	301	36J	CAJ-CAK-CAN-CAW
2	B	301	36J	CAL-CAM-CAV-CAA

All (1) ring outliers are listed below:

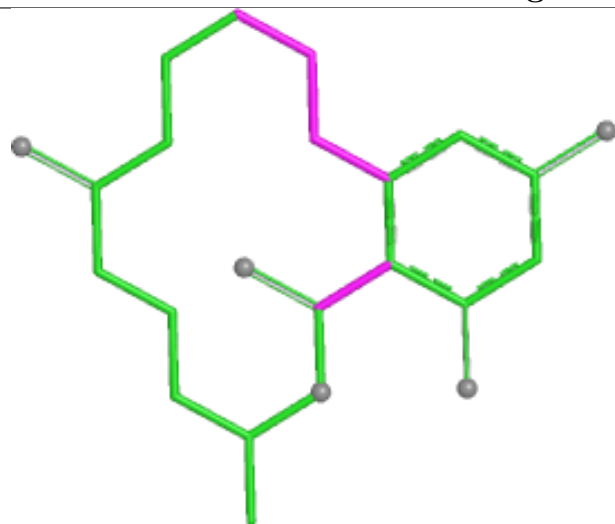
Mol	Chain	Res	Type	Atoms
2	A	300	36J	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C

2 monomers are involved in 13 short contacts:

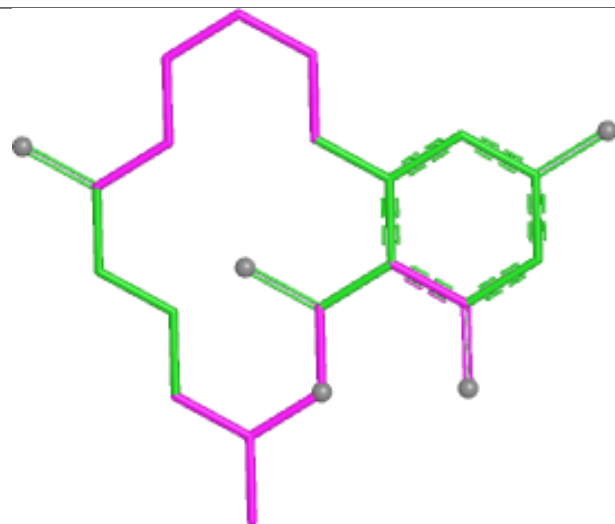
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	36J	5	0
2	A	300	36J	8	0

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.

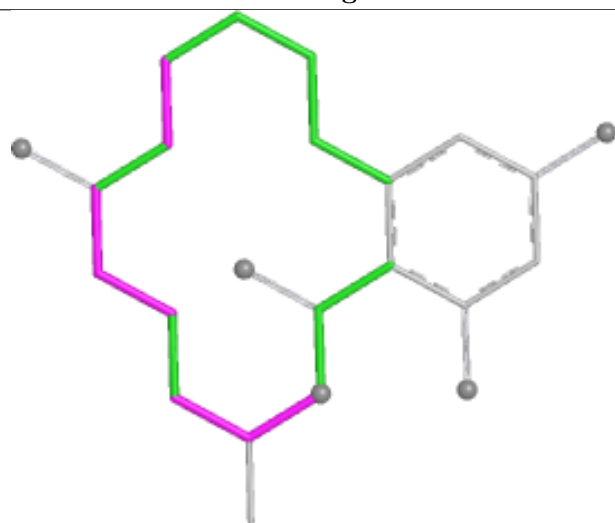
Ligand 36J B 301



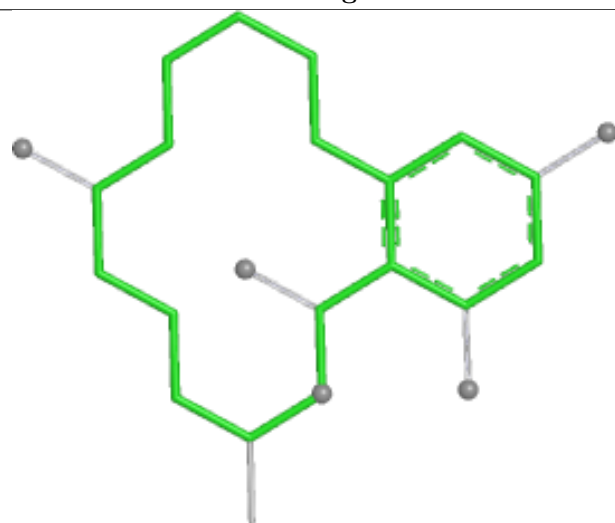
Bond lengths



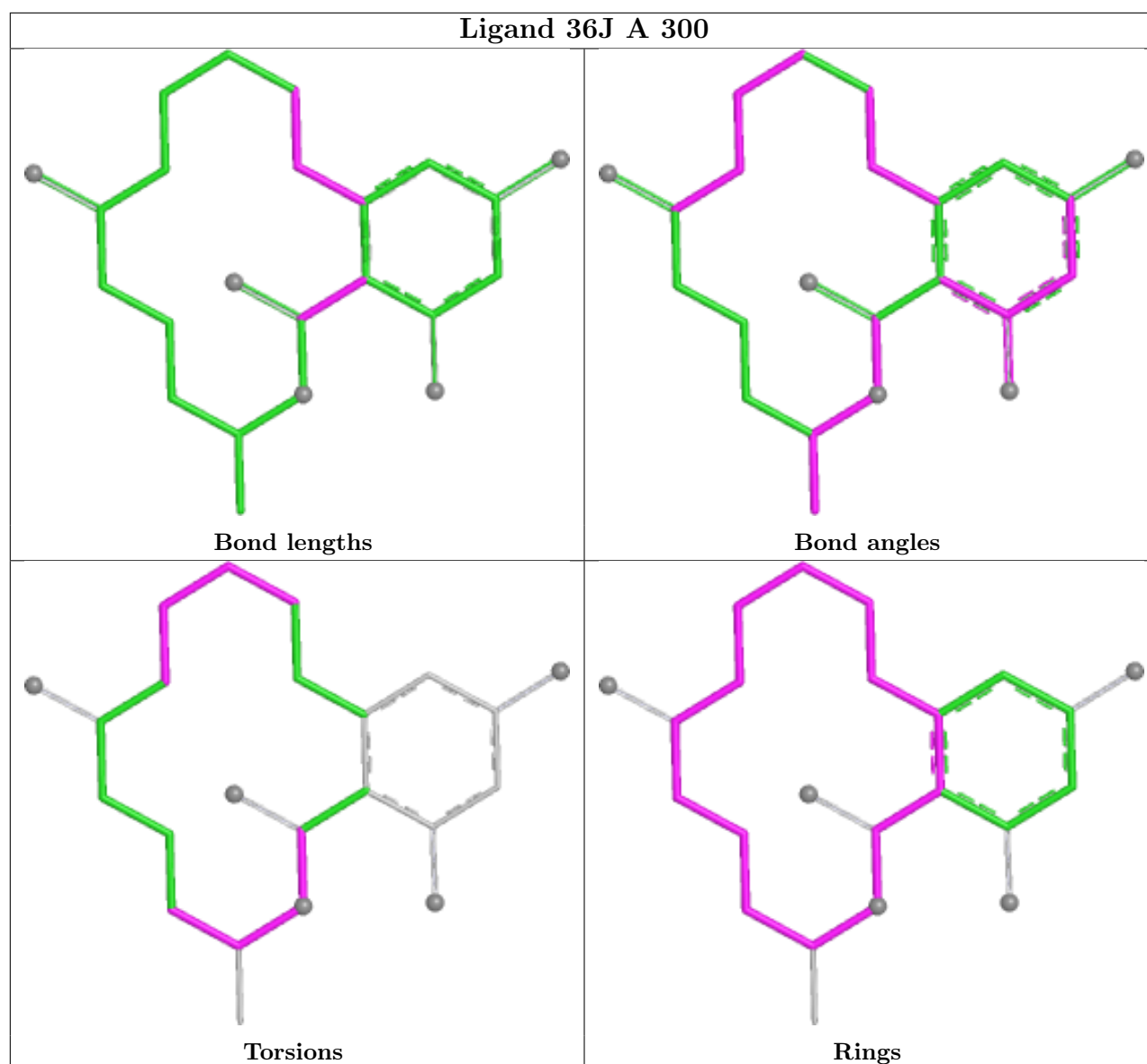
Bond angles



Torsions



Rings



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	264/264 (100%)	0.31	5 (1%) 66 62	16, 25, 47, 62	0
1	B	264/264 (100%)	0.32	9 (3%) 48 44	18, 26, 44, 75	0
1	C	164/264 (62%)	2.22	85 (51%) 0 0	30, 45, 59, 63	0
All	All	692/792 (87%)	0.77	99 (14%) 6 5	16, 28, 55, 75	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	5.7
1	C	251	VAL	5.1
1	C	43	VAL	4.7
1	C	112	LEU	4.3
1	C	80	LEU	4.2
1	C	39	PHE	4.2
1	A	48	ALA	4.1
1	C	53	VAL	4.0
1	C	108	VAL	4.0
1	C	30	PRO	3.9
1	C	238	LEU	3.9
1	C	87	VAL	3.8
1	C	264	LEU	3.8
1	C	228	ALA	3.8
1	C	254	LYS	3.7
1	C	72	TYR	3.7
1	C	216	THR	3.6
1	C	99	TRP	3.6
1	C	191	ILE	3.5
1	C	56	PHE	3.5
1	C	47	ALA	3.5
1	C	88	LEU	3.5
1	C	77	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	239	PRO	3.3
1	C	111	LEU	3.3
1	C	113	LEU	3.2
1	A	158	VAL	3.1
1	C	12	GLY	3.1
1	C	46	ILE	3.1
1	C	81	ALA	3.1
1	B	135	LEU	3.0
1	C	36	CYS	3.0
1	C	209	ASP	3.0
1	C	51	PHE	2.9
1	C	224	ASN	2.9
1	C	252	PHE	2.9
1	C	14	THR	2.9
1	C	233	VAL	2.9
1	B	136	SER	2.8
1	C	105	ALA	2.8
1	C	231	ALA	2.8
1	A	140	VAL	2.8
1	C	109	VAL	2.8
1	C	257	VAL	2.8
1	C	183	TRP	2.8
1	C	58	MET	2.8
1	C	241	MET	2.8
1	C	222	PHE	2.8
1	C	85	ILE	2.7
1	C	18	GLU	2.7
1	C	102	ALA	2.7
1	C	15	TRP	2.7
1	C	7	ILE	2.7
1	C	256	VAL	2.7
1	C	107	THR	2.7
1	C	71	THR	2.6
1	C	73	THR	2.6
1	C	24	PRO	2.6
1	B	158	VAL	2.6
1	B	1	MET	2.6
1	C	45	GLN	2.6
1	C	29	VAL	2.6
1	C	75	VAL	2.6
1	C	185	ARG	2.5
1	C	214	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	67	ALA	2.5
1	C	8	SER	2.5
1	C	16	TYR	2.5
1	C	193	PRO	2.5
1	C	100	GLY	2.5
1	B	138	THR	2.4
1	C	38	MET	2.4
1	C	189	ARG	2.4
1	C	202	ALA	2.4
1	C	22	THR	2.4
1	C	253	ALA	2.4
1	C	93	ILE	2.4
1	C	91	LEU	2.4
1	C	184	ALA	2.4
1	C	84	VAL	2.4
1	C	259	THR	2.3
1	C	40	ASP	2.3
1	C	203	LEU	2.3
1	C	119	ILE	2.3
1	C	188	PRO	2.2
1	C	13	ILE	2.2
1	A	166	GLN	2.2
1	B	189	ARG	2.2
1	A	1	MET	2.2
1	C	101	CYS	2.1
1	C	42	SER	2.1
1	C	96	ALA	2.1
1	C	205	GLY	2.1
1	B	139	ALA	2.1
1	C	197	VAL	2.1
1	C	190	THR	2.1
1	B	166	GLN	2.1
1	B	170	ASP	2.1
1	C	196	PRO	2.1

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

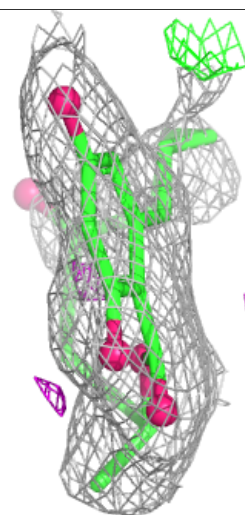
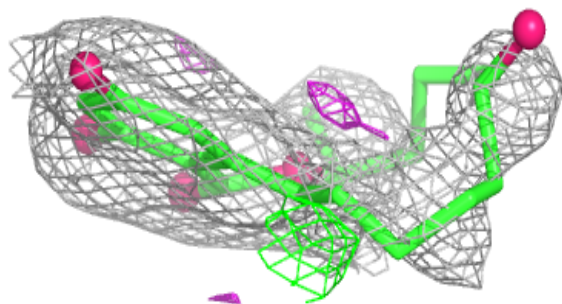
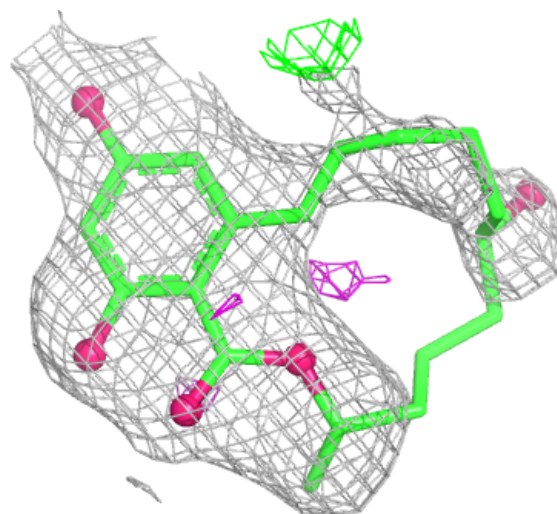
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	36J	B	301	23/23	0.87	0.20	39,55,91,94	0
2	36J	A	300	23/23	0.90	0.20	41,64,100,103	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.

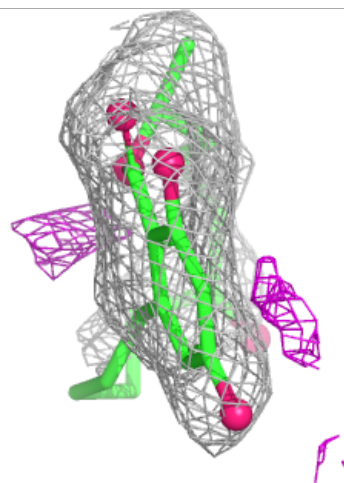
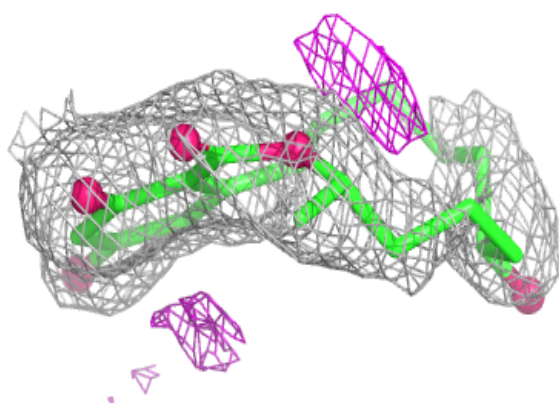
Electron density around 36J B 301:

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



Electron density around 36J A 300:

$2mF_o-DF_c$ (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.