



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 8PC2 / pdb_00008pc2
Title : SelDeg51 in complex with FKBP51FK1 domain and pVHL:EloB:EloC
Authors : Meyners, C.; Walz, M.; Geiger, T.M.; Hausch, F.
Deposited on : 2023-06-09
Resolution : 2.80 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

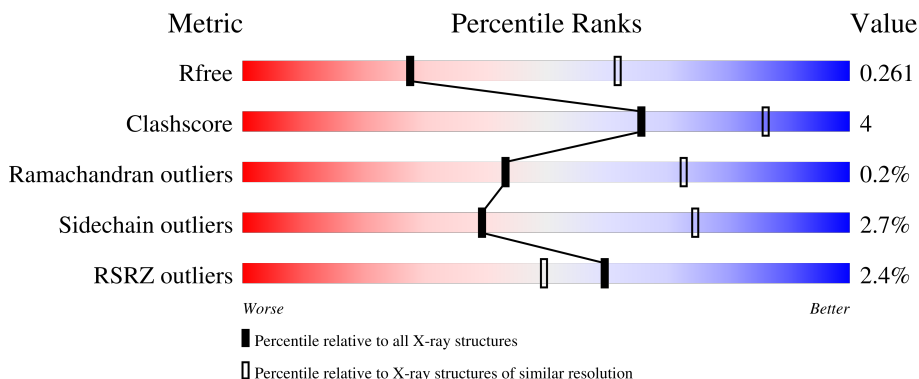
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



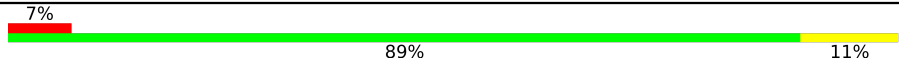


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	162	 80% 9% 8%
1	B	162	 82% 9% 8%
2	C	97	 76% 13% 10%
2	E	97	 74% 14% 10%
3	D	104	 87% 13%

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Mol	Chain	Length	Quality of chain
3	F	104	 7% 89% 11%
4	G	128	 2% 82% 12% 6%
4	H	128	 5% 81% 11% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14339 atoms, of which 7115 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 von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	149	2393	761	1198	220	212	2	38	0	0
1	A	149	2385	761	1188	217	217	2	37	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLY	-	expression tag	UNP P40337
B	53	SER	-	expression tag	UNP P40337
A	52	GLY	-	expression tag	UNP P40337
A	53	SER	-	expression tag	UNP P40337

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	C	87	1359	438	679	109	127	6	29	0	0
2	E	87	1368	441	685	108	129	5	28	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	D	104	1590	506	794	132	153	5	26	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	F	104	1550	496	769	130	151	4	30	0	0

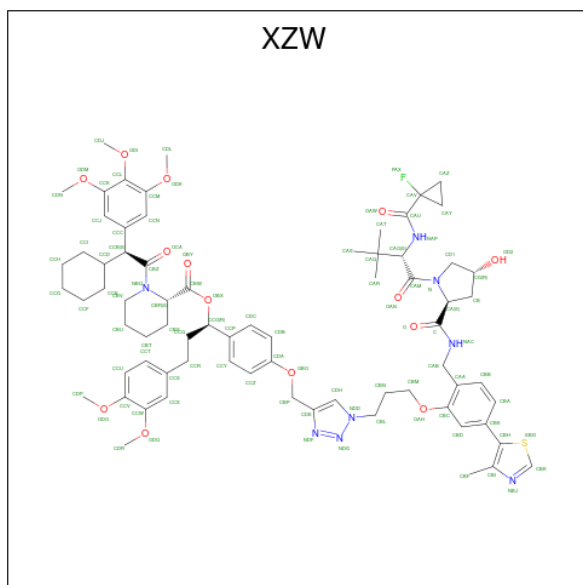
- Molecule 4 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	G	120	1721	561	850	143	165	2	38	0	0
4	H	118	1585	527	770	130	157	1	47	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	GLY	-	expression tag	UNP Q13451
G	14	ALA	-	expression tag	UNP Q13451
G	15	PRO	-	expression tag	UNP Q13451
G	19	THR	ALA	engineered mutation	UNP Q13451
G	103	ALA	CYS	engineered mutation	UNP Q13451
G	107	ILE	CYS	engineered mutation	UNP Q13451
H	13	GLY	-	expression tag	UNP Q13451
H	14	ALA	-	expression tag	UNP Q13451
H	15	PRO	-	expression tag	UNP Q13451
H	19	THR	ALA	engineered mutation	UNP Q13451
H	103	ALA	CYS	engineered mutation	UNP Q13451
H	107	ILE	CYS	engineered mutation	UNP Q13451

- Molecule 5 is [(1 {R})-3-(3,4-dimethoxyphenyl)-1-[4-[[1-[3-[2-[[[(2 {S}),4 {R})-1-[(2 {S})-2-[(1-fluoranyl)cyclopropyl]carbonylamino]-3,3-dimethyl-butanoyl]-4-oxidanyl-pyrrolidin-2-yl]carbonylamino]methyl]-5-(4-methyl-1,3-thiazol-5-yl)phenoxy]propyl]-1,2,3-triazol-4-yl]methoxy]phenyl]propyl] (2 {S})-1-[(2 {S})-2-cyclohexyl-2-(3,4,5-trimethoxyphenyl)ethanoyl]piperidine-2-carboxylate (CCD ID: XZW) (formula: C₇₂H₉₁FN₈O₁₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	F	H	N	O			S
5	B	1	Total	C	F	H	N	O	S	1	0
			187	72	1	91	8	14	1		
5	A	1	Total	C	F	H	N	O	S	1	0
			187	72	1	91	8	14	1		

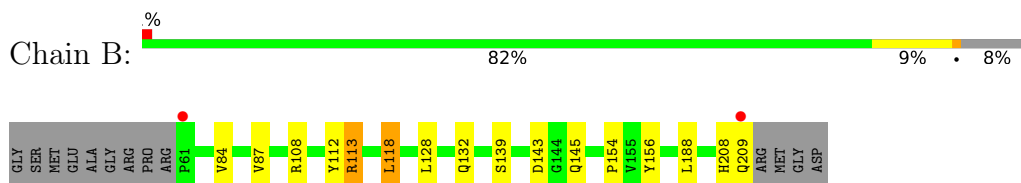
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	7	Total 7 7	0	0
6	G	3	Total 3 3	0	0
6	A	3	Total 3 3	0	0
6	E	1	Total 1 1	0	0

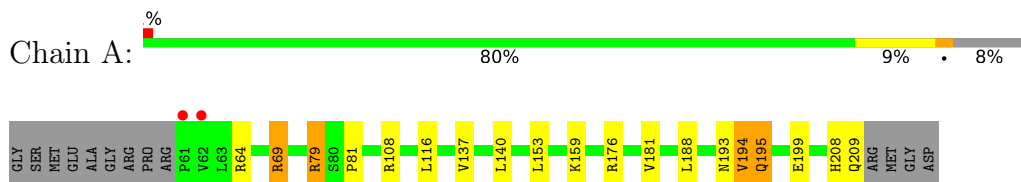
3 Residue-property plots [i](#)

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.

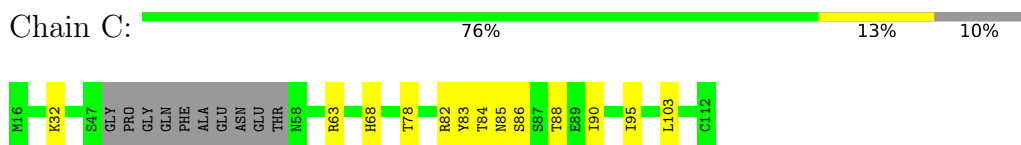
- Molecule 1: von Hippel-Lindau disease tumor suppressor



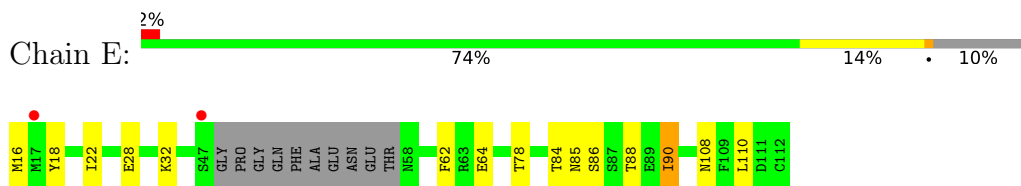
- Molecule 1: von Hippel-Lindau disease tumor suppressor



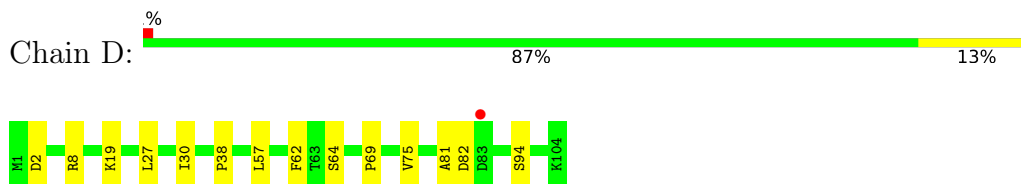
- Molecule 2: Elongin-C



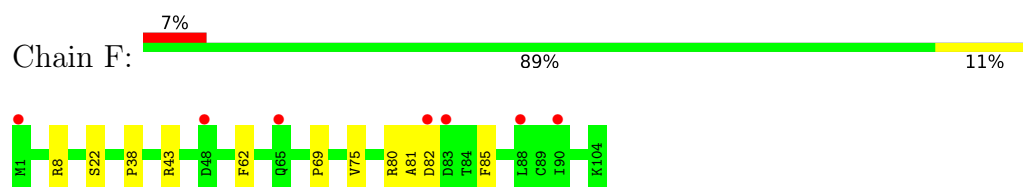
- Molecule 2: Elongin-C



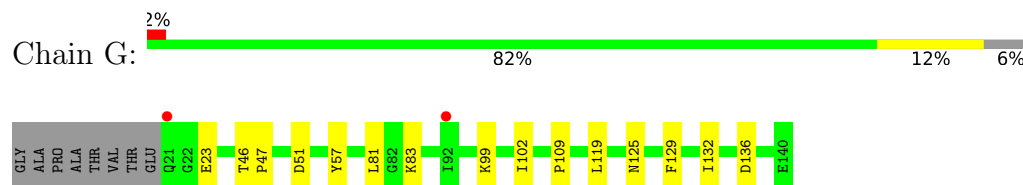
- Molecule 3: Elongin-B



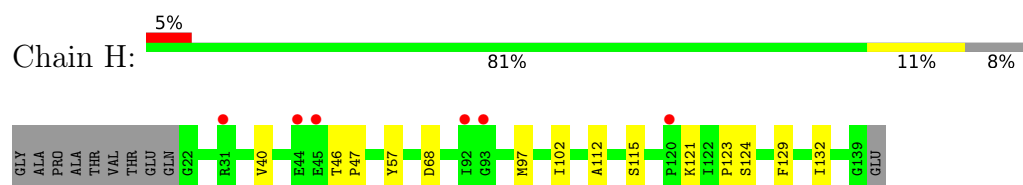
- Molecule 3: Elongin-B



- Molecule 4: Peptidyl-prolyl cis-trans isomerase FKBP5



- Molecule 4: Peptidyl-prolyl cis-trans isomerase FKBP5



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.65Å 68.42Å 159.26Å 90.00° 114.45° 90.00°	Depositor
Resolution (Å)	48.74 – 2.80 48.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.74-2.80) 98.3 (48.74-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.210 , 0.261 0.210 , 0.261	Depositor DCC
R_{free} test set	1674 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.7	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	0.93	EDS
Total number of atoms	14339	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XZW

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	0.59	0/1229	1.08	0/1682
1	B	0.62	0/1227	1.09	0/1678
2	C	0.60	0/694	1.03	1/939 (0.1%)
2	E	0.58	0/697	1.06	1/942 (0.1%)
3	D	0.61	0/812	1.06	2/1100 (0.2%)
3	F	0.58	0/797	1.06	1/1084 (0.1%)
4	G	0.58	0/890	1.08	3/1206 (0.2%)
4	H	0.54	0/834	0.98	0/1141
All	All	0.59	0/7180	1.06	8/9772 (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	4
1	B	0	2
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	10

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	83	LYS	CB-CA-C	6.58	121.67	111.02
3	F	38	PRO	N-CA-C	6.46	117.49	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	64	GLU	CB-CG-CD	6.40	123.47	112.60
3	D	38	PRO	N-CA-C	5.90	116.90	110.58
2	C	32	LYS	CB-CA-C	5.77	118.08	110.06
3	D	19	LYS	CB-CA-C	5.65	119.17	109.51
4	G	23	GLU	CB-CG-CD	5.43	121.83	112.60
4	G	51	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	176	ARG	Sidechain
1	A	69	ARG	Sidechain
1	A	79	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	113	ARG	Sidechain
2	C	82	ARG	Sidechain
3	D	8	ARG	Sidechain
2	E	16	MET	Peptide
3	F	8	ARG	Sidechain

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	1197	1188	1172	9	0
1	B	1195	1198	1180	8	0
2	C	680	679	664	8	0
2	E	683	685	672	7	0
3	D	796	794	779	6	0
3	F	781	769	746	6	0
4	G	871	850	813	8	0
4	H	815	770	715	6	0
5	A	96	91	0	0	0
5	B	96	91	0	2	0
6	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	0	0	0
6	E	1	0	0	0	0
6	G	3	0	0	0	0
All	All	7224	7115	6741	53	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 4.

All (53) 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)
2:E:86:SER:HB2	2:E:90:ILE:HD11	1.69	0.73
2:C:78:THR:HG22	3:D:69:PRO:HB3	1.80	0.62
2:E:84:THR:O	2:E:85:ASN:HB2	2.00	0.62
1:B:87:VAL:HB	1:B:118:LEU:HD12	1.83	0.61
2:C:86:SER:HB2	2:C:90:ILE:HD11	1.82	0.61
1:A:159:LYS:HE3	2:E:108:ASN:OD1	2.01	0.61
2:C:83:TYR:HB3	2:C:90:ILE:HD12	1.81	0.60
3:D:2:ASP:O	3:D:64:SER:HB3	2.07	0.55
2:E:78:THR:HG22	3:F:69:PRO:HB3	1.91	0.53
4:H:57:TYR:OH	4:H:68:ASP:OD2	2.19	0.52
2:C:68:HIS:ND1	3:D:94:SER:OG	2.38	0.52
1:B:113:ARG:HH21	1:B:113:ARG:HG2	1.74	0.52
1:B:143:ASP:HA	4:G:119:LEU:HD13	1.91	0.51
1:A:116:LEU:HD13	1:A:137:VAL:HG22	1.94	0.50
1:B:112:TYR:CZ	5:B:301:XZW:CAZ	2.96	0.49
3:D:62:PHE:CZ	3:D:75:VAL:HG22	2.49	0.48
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.76	0.48
2:C:95:ILE:HD13	2:C:103:LEU:HD23	1.95	0.48
1:A:193:ASN:O	1:A:194:VAL:HG23	2.14	0.47
3:D:27:LEU:HD22	3:D:57:LEU:HD21	1.97	0.47
3:F:62:PHE:CZ	3:F:75:VAL:HG22	2.49	0.47
4:H:129:PHE:C	4:H:129:PHE:CD1	2.93	0.47
1:A:208:HIS:O	1:A:209:GLN:C	2.58	0.47
4:G:129:PHE:CD1	4:G:129:PHE:C	2.94	0.46
1:B:208:HIS:O	1:B:209:GLN:C	2.59	0.46
4:G:46:THR:HB	4:G:47:PRO:HD2	1.96	0.46
2:C:84:THR:O	2:C:85:ASN:HB2	2.16	0.46
2:E:22:ILE:HG12	2:E:28:GLU:HG2	1.98	0.45
1:B:209:GLN:HB3	4:H:123:PRO:HB3	1.98	0.45
2:C:63:ARG:HG2	2:C:63:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:115:SER:O	4:H:124:SER:OG	2.18	0.44
1:B:84:VAL:HG22	1:B:128:LEU:CD1	2.48	0.43
5:B:301:XZW:NDG	5:B:301:XZW:CBM	2.81	0.43
1:A:193:ASN:O	1:A:194:VAL:CB	2.66	0.43
4:G:102:ILE:HA	4:G:132:ILE:O	2.18	0.43
3:F:43:ARG:NH1	3:F:85:PHE:HB2	2.34	0.43
3:F:43:ARG:HH11	3:F:85:PHE:HB2	1.84	0.43
2:E:62:PHE:CE2	2:E:110:LEU:HD21	2.54	0.42
4:H:102:ILE:HA	4:H:132:ILE:O	2.20	0.42
1:B:154:PRO:HG2	1:B:156:TYR:CE1	2.54	0.42
4:G:99:LYS:HE3	4:G:136:ASP:HA	2.02	0.42
4:G:47:PRO:HB2	4:G:81:LEU:HD22	2.01	0.42
2:E:18:TYR:CE1	2:E:32:LYS:HG3	2.54	0.42
3:D:81:ALA:O	3:D:82:ASP:C	2.62	0.42
4:G:109:PRO:HG3	4:G:125:ASN:C	2.45	0.42
1:A:193:ASN:O	1:A:194:VAL:HB	2.19	0.41
3:F:81:ALA:O	3:F:82:ASP:C	2.62	0.41
1:A:195:GLN:O	1:A:199:GLU:HG3	2.20	0.41
4:H:47:PRO:HD3	4:H:97:MET:O	2.19	0.41
3:F:43:ARG:HH11	3:F:85:PHE:CB	2.33	0.41
4:G:57:TYR:CD1	4:G:57:TYR:C	2.99	0.41
1:A:81:PRO:HD2	1:A:153:LEU:HG	2.02	0.41
2:C:63:ARG:HH11	2:C:63:ARG:CG	2.35	0.41

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	147/162 (91%)	140 (95%)	6 (4%)	1 (1%)	18 47
1	B	147/162 (91%)	142 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	83/97 (86%)	79 (95%)	4 (5%)	0	100	100
2	E	83/97 (86%)	80 (96%)	3 (4%)	0	100	100
3	D	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
3	F	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
4	G	118/128 (92%)	114 (97%)	4 (3%)	0	100	100
4	H	116/128 (91%)	113 (97%)	2 (2%)	1 (1%)	14	41
All	All	898/982 (91%)	862 (96%)	34 (4%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	VAL
4	H	112	ALA

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	134/148 (90%)	128 (96%)	6 (4%)	24	58
1	B	133/148 (90%)	128 (96%)	5 (4%)	29	64
2	C	75/86 (87%)	74 (99%)	1 (1%)	61	86
2	E	76/86 (88%)	74 (97%)	2 (3%)	40	75
3	D	85/92 (92%)	84 (99%)	1 (1%)	63	87
3	F	81/92 (88%)	79 (98%)	2 (2%)	42	76
4	G	83/105 (79%)	83 (100%)	0	100	100
4	H	72/105 (69%)	69 (96%)	3 (4%)	26	61
All	All	739/862 (86%)	719 (97%)	20 (3%)	39	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	LEU
1	B	132	GLN
1	B	139	SER
1	B	145	GLN
1	B	188	LEU
2	C	88	THR
3	D	30	ILE
1	A	69	ARG
1	A	79	ARG
1	A	140	LEU
1	A	181	VAL
1	A	188	LEU
1	A	195	GLN
2	E	88	THR
2	E	90	ILE
3	F	22	SER
3	F	80	ARG
4	H	40	VAL
4	H	46	THR
4	H	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	132	GLN
1	B	209	GLN
4	G	104	HIS
4	G	125	ASN
1	A	209	GLN

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
5	XZW	A	301	-	103,105,105	1.91	17 (16%)	141,150,150	2.35	41 (29%)
5	XZW	B	301	-	103,105,105	2.62	17 (16%)	141,150,150	2.63	43 (30%)

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
5	XZW	A	301	-	-	8/90/127/127	0/10/10/10
5	XZW	B	301	-	-	14/90/127/127	0/10/10/10

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	XZW	NDD-NDG	-12.84	1.14	1.34
5	B	301	XZW	CCC-CCB	-8.92	1.39	1.52
5	A	301	XZW	CCP-CCO	-8.72	1.36	1.51
5	B	301	XZW	FAX-CAV	-8.46	1.28	1.42
5	B	301	XZW	NDF-NDG	7.53	1.44	1.32
5	B	301	XZW	CCP-CCO	-7.09	1.39	1.51
5	B	301	XZW	CCB-CBZ	6.52	1.60	1.52
5	B	301	XZW	CBR-CBW	-6.22	1.41	1.52
5	B	301	XZW	CA-C	-6.09	1.38	1.52
5	A	301	XZW	CBE-CBH	-5.73	1.36	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	XZW	NDD-NDG	-5.34	1.26	1.34
5	B	301	XZW	CBE-CBH	-5.18	1.37	1.48
5	A	301	XZW	CA-C	-4.91	1.41	1.52
5	A	301	XZW	CCC-CCB	-4.30	1.46	1.52
5	A	301	XZW	CBR-CBW	-3.88	1.45	1.52
5	B	301	XZW	CDH-CDE	-3.60	1.30	1.36
5	A	301	XZW	CCB-CBZ	3.52	1.56	1.52
5	A	301	XZW	NDF-NDG	-3.39	1.26	1.32
5	B	301	XZW	CBR-NBQ	3.12	1.51	1.47
5	B	301	XZW	CCH-CCI	2.98	1.60	1.53
5	B	301	XZW	CDE-NDF	-2.97	1.31	1.36
5	B	301	XZW	CCR-CCS	-2.94	1.43	1.51
5	B	301	XZW	CBS-CBR	-2.86	1.46	1.53
5	A	301	XZW	CDH-CDE	-2.83	1.32	1.36
5	A	301	XZW	FAX-CAV	2.75	1.46	1.42
5	A	301	XZW	OBX-CBW	2.75	1.40	1.34
5	A	301	XZW	CCR-CCS	-2.74	1.44	1.51
5	A	301	XZW	CBV-NBQ	2.39	1.51	1.47
5	B	301	XZW	CBF-CBI	2.35	1.54	1.49
5	B	301	XZW	CAY-CAV	2.28	1.51	1.48
5	A	301	XZW	CD1-N	2.21	1.50	1.47
5	A	301	XZW	CDE-NDF	-2.14	1.32	1.36
5	A	301	XZW	CB-CA	2.07	1.57	1.53
5	A	301	XZW	CBB-CAA	2.02	1.42	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	XZW	CBK-SBG-CBH	12.09	95.29	88.96
5	A	301	XZW	CBK-SBG-CBH	11.26	94.85	88.96
5	A	301	XZW	SBG-CBK-NBJ	-10.30	107.23	116.08
5	B	301	XZW	CBL-NDD-CDH	-10.16	109.86	128.83
5	B	301	XZW	CBL-NDD-NDG	9.89	140.65	120.78
5	B	301	XZW	SBG-CBK-NBJ	-9.69	107.75	116.08
5	B	301	XZW	ODQ-CCW-CCV	5.84	123.33	115.40
5	B	301	XZW	CBP-CDE-NDF	5.62	130.80	121.49
5	B	301	XZW	CDE-NDF-NDG	-5.49	103.08	109.01
5	B	301	XZW	CBI-CBH-SBG	-5.39	106.34	109.64
5	A	301	XZW	CBI-CBH-SBG	-5.36	106.35	109.64
5	A	301	XZW	CBL-NDD-NDG	5.18	131.18	120.78
5	B	301	XZW	CCE-CCD-CCB	-5.18	104.75	111.81
5	A	301	XZW	OBX-CCO-CCQ	5.12	117.06	105.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	XZW	NDD-NDG-NDF	5.09	111.60	107.02
5	A	301	XZW	CBL-NDD-CDH	-4.84	119.79	128.83
5	B	301	XZW	CBP-CDE-CDH	-4.71	122.09	130.22
5	A	301	XZW	CBK-NBJ-CBI	4.46	115.72	110.71
5	B	301	XZW	NDD-NDG-NDF	4.45	111.02	107.02
5	A	301	XZW	OBX-CCO-CCP	-4.37	102.88	109.71
5	B	301	XZW	CBM-OAH-CBC	-4.32	107.27	117.69
5	A	301	XZW	OAW-CAU-NAP	4.29	131.34	122.71
5	A	301	XZW	CBS-CBR-NBQ	-4.06	105.12	110.55
5	A	301	XZW	CBP-CDE-CDH	-3.91	123.48	130.22
5	B	301	XZW	CBK-NBJ-CBI	3.81	115.00	110.71
5	B	301	XZW	CCI-CCD-CCB	3.79	116.97	111.81
5	A	301	XZW	CCC-CCB-CBZ	3.76	115.37	108.58
5	A	301	XZW	CD1-N-CA	-3.75	106.86	111.83
5	B	301	XZW	ODQ-CCW-CCX	-3.71	117.68	124.08
5	A	301	XZW	CCH-CCI-CCD	3.70	118.50	111.89
5	A	301	XZW	CAQ-CAO-CAM	-3.69	108.31	113.23
5	A	301	XZW	CBP-CDE-NDF	3.42	127.16	121.49
5	A	301	XZW	CBD-CBC-CAA	3.42	124.03	120.49
5	B	301	XZW	CBE-CBD-CBC	3.39	124.14	119.60
5	B	301	XZW	CBE-CBH-SBG	3.36	125.01	118.77
5	B	301	XZW	CBA-CBE-CBD	-3.27	115.46	119.25
5	B	301	XZW	CCI-CCD-CCE	-3.23	103.90	109.43
5	A	301	XZW	CCO-OBX-CBW	3.18	122.21	116.65
5	A	301	XZW	CAO-CAM-N	-3.12	114.73	118.46
5	A	301	XZW	OBX-CBW-CBR	3.11	117.25	110.80
5	B	301	XZW	ODO-CCV-CCW	3.10	119.61	115.40
5	B	301	XZW	OBX-CCO-CCP	-3.08	104.89	109.71
5	A	301	XZW	ODI-CCL-CCM	-3.07	115.73	120.12
5	A	301	XZW	ODI-CCL-CCK	3.03	124.47	120.12
5	A	301	XZW	CDE-NDF-NDG	-3.02	105.75	109.01
5	A	301	XZW	CAY-CAZ-CAV	-2.95	58.00	60.42
5	A	301	XZW	CG-CB-CA	-2.88	100.38	103.75
5	B	301	XZW	CDE-CDH-NDD	2.86	109.33	105.33
5	B	301	XZW	CAT-CAQ-CAO	2.82	115.48	109.71
5	A	301	XZW	CAB-NAC-C	2.78	126.11	122.29
5	A	301	XZW	CBB-CAA-CBC	-2.74	114.64	118.37
5	A	301	XZW	CBP-OBO-CDA	-2.71	112.78	117.63
5	B	301	XZW	OBX-CBW-CBR	2.57	116.13	110.80
5	A	301	XZW	CCF-CCE-CCD	-2.54	107.35	111.89
5	B	301	XZW	CAZ-CAV-CAU	-2.54	111.01	116.20
5	B	301	XZW	CBU-CBV-NBQ	-2.54	106.73	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	XZW	CDR-ODQ-CCW	2.48	121.15	117.51
5	B	301	XZW	CAM-CAO-NAP	2.45	110.37	107.40
5	A	301	XZW	CB-CA-N	2.44	106.08	103.17
5	B	301	XZW	OAW-CAU-NAP	2.44	127.61	122.71
5	B	301	XZW	CAS-CAQ-CAO	-2.41	104.77	109.71
5	A	301	XZW	CBT-CBS-CBR	-2.39	105.43	110.97
5	A	301	XZW	CBT-CBU-CBV	2.38	115.60	111.19
5	B	301	XZW	CDN-ODM-CCK	-2.38	114.03	117.51
5	A	301	XZW	OAN-CAM-N	2.37	125.65	121.38
5	B	301	XZW	ODO-CCV-CCU	-2.33	120.38	124.30
5	B	301	XZW	OCA-CBZ-NBQ	-2.32	117.21	121.38
5	A	301	XZW	CBS-CBR-CBW	2.29	116.64	110.61
5	A	301	XZW	OBY-CBW-CBR	-2.27	119.45	124.46
5	B	301	XZW	CAQ-CAO-CAM	-2.27	110.21	113.23
5	A	301	XZW	CAY-CAV-CAZ	2.25	61.80	59.50
5	B	301	XZW	CBB-CAA-CBC	-2.25	115.30	118.37
5	B	301	XZW	CAA-CAB-NAC	-2.22	108.67	113.15
5	B	301	XZW	CCN-CCC-CCB	2.21	123.62	120.33
5	A	301	XZW	ODK-CCM-CCN	2.18	127.84	124.08
5	B	301	XZW	CBS-CBR-NBQ	2.18	113.47	110.55
5	A	301	XZW	CBE-CBH-SBG	2.17	122.81	118.77
5	B	301	XZW	CCG-CCF-CCE	-2.14	107.02	111.42
5	B	301	XZW	CCB-CBZ-NBQ	2.13	121.89	118.28
5	B	301	XZW	CBA-CBB-CAA	2.12	124.16	121.39
5	A	301	XZW	ODK-CCM-CCL	-2.08	111.58	115.14
5	A	301	XZW	CCZ-CDA-CDB	-2.07	117.15	120.16
5	B	301	XZW	CCG-CCH-CCI	2.03	115.60	111.42
5	B	301	XZW	CB-CA-N	2.02	105.57	103.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	XZW	NDD-CBL-CBN-CBM
5	B	301	XZW	CBZ-CCB-CCD-CCE
5	B	301	XZW	CCC-CCB-CCD-CCE
5	B	301	XZW	CCC-CCB-CCD-CCI
5	B	301	XZW	CCX-CCW-ODQ-CDR
5	B	301	XZW	CCV-CCW-ODQ-CDR
5	A	301	XZW	CCL-CCK-ODM-CDN
5	A	301	XZW	CCJ-CCK-ODM-CDN
5	A	301	XZW	CCM-CCL-ODI-CDJ

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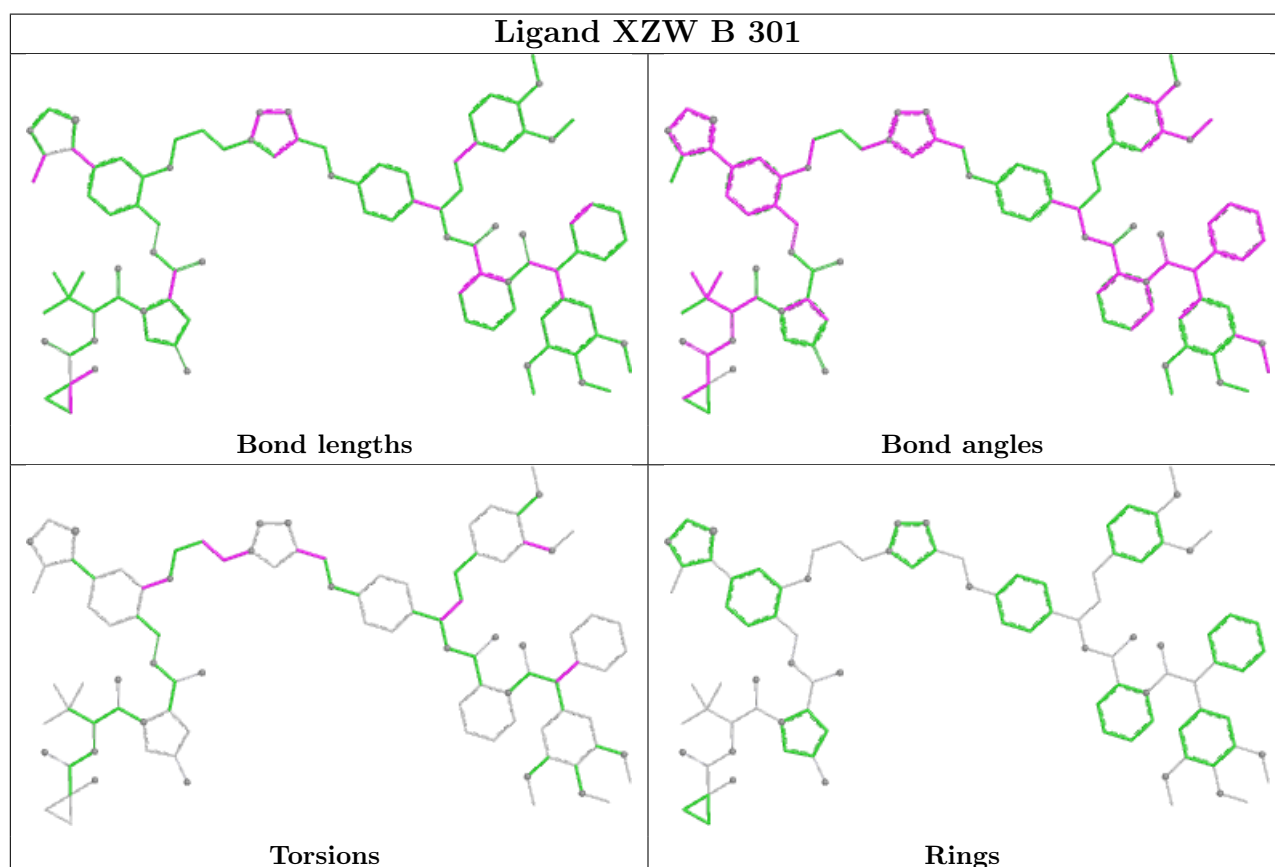
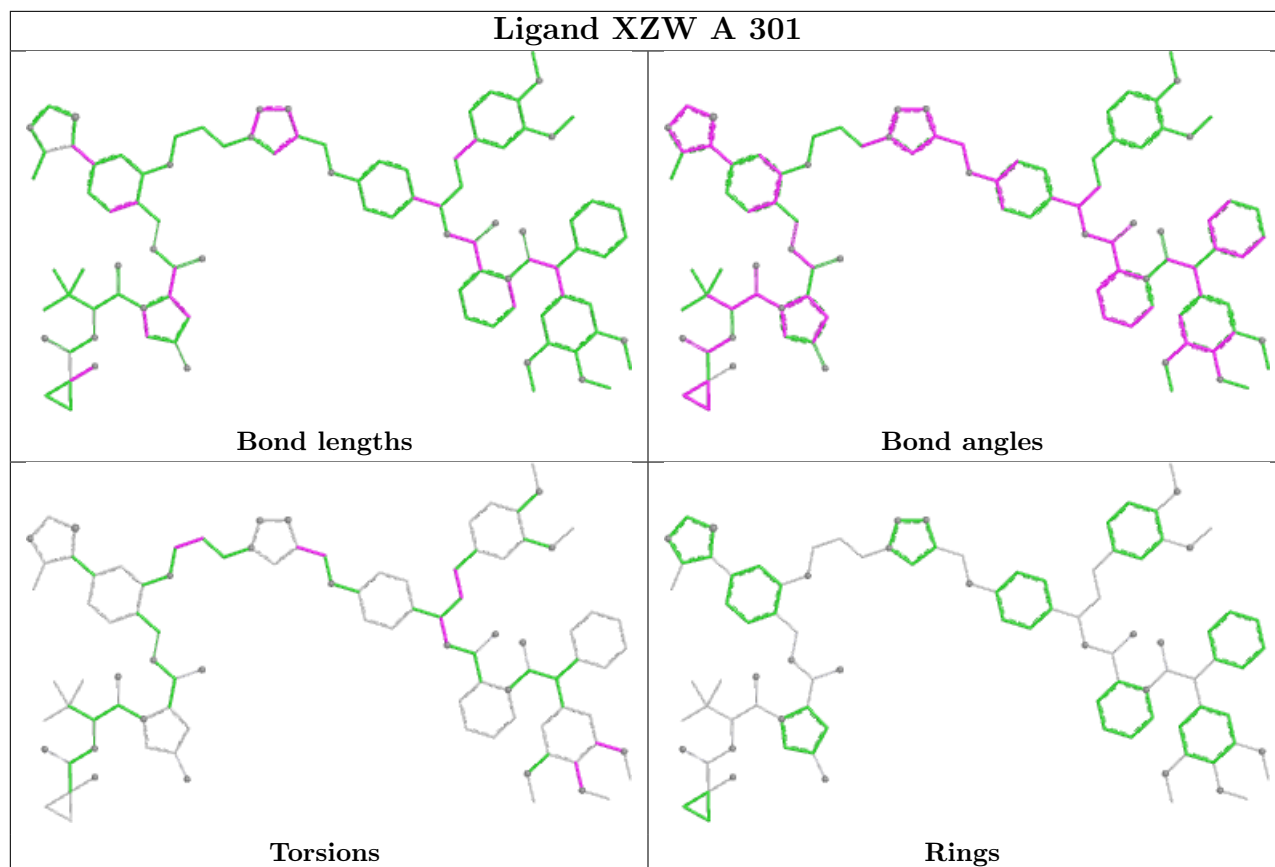
Mol	Chain	Res	Type	Atoms
5	A	301	XZW	OAH-CBM-CBN-CBL
5	B	301	XZW	OBO-CBP-CDE-CDH
5	B	301	XZW	OBO-CBP-CDE-NDF
5	A	301	XZW	CCK-CCL-ODI-CDJ
5	B	301	XZW	CBN-CBL-NDD-CDH
5	B	301	XZW	CBN-CBL-NDD-NDG
5	A	301	XZW	CCO-CCQ-CCR-CCS
5	B	301	XZW	CBD-CBC-OAH-CBM
5	B	301	XZW	CAA-CBC-OAH-CBM
5	A	301	XZW	CCQ-CCO-OBX-CBW
5	A	301	XZW	OBO-CBP-CDE-NDF
5	B	301	XZW	CBZ-CCB-CCD-CCI
5	B	301	XZW	CCP-CCO-CCQ-CCR

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	XZW	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 [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	149/162 (91%)	-0.27	2 (1%) 75 66	50, 71, 101, 120	0
1	B	149/162 (91%)	-0.46	2 (1%) 75 66	46, 62, 103, 138	0
2	C	87/97 (89%)	-0.35	0 100 100	51, 66, 100, 108	0
2	E	87/97 (89%)	-0.26	2 (2%) 61 51	55, 75, 98, 113	0
3	D	104/104 (100%)	-0.29	1 (0%) 79 72	52, 71, 96, 116	0
3	F	104/104 (100%)	-0.11	7 (6%) 24 17	61, 84, 111, 133	0
4	G	120/128 (93%)	-0.25	2 (1%) 69 60	49, 76, 99, 115	0
4	H	118/128 (92%)	0.57	6 (5%) 33 25	80, 117, 146, 163	0
All	All	918/982 (93%)	-0.18	22 (2%) 59 49	46, 75, 124, 163	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	21	GLN	4.8
4	H	45	GLU	4.3
4	H	120	PRO	4.0
2	E	47	SER	3.7
1	B	209	GLN	3.5
4	H	44	GLU	3.2
1	A	61	PRO	3.1
4	H	93	GLY	3.1
4	G	92	ILE	2.7
3	F	88	LEU	2.5
4	H	31	ARG	2.5
3	F	82	ASP	2.4
3	F	90	ILE	2.4
3	F	83	ASP	2.4
3	F	1	MET	2.4
1	B	61	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	83	ASP	2.4
3	F	48	ASP	2.3
2	E	17	MET	2.3
3	F	65	GLN	2.2
4	H	92	ILE	2.1
1	A	62	VAL	2.1

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 [i](#)

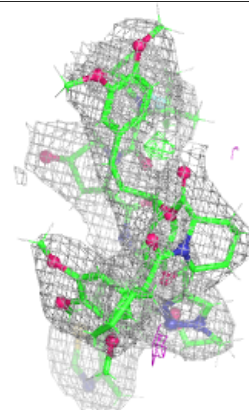
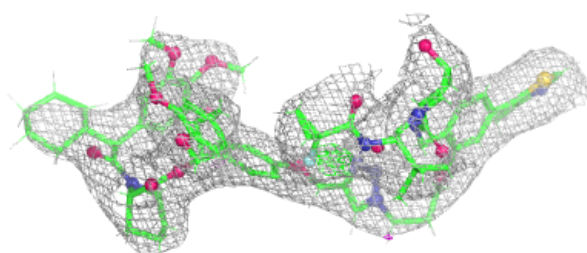
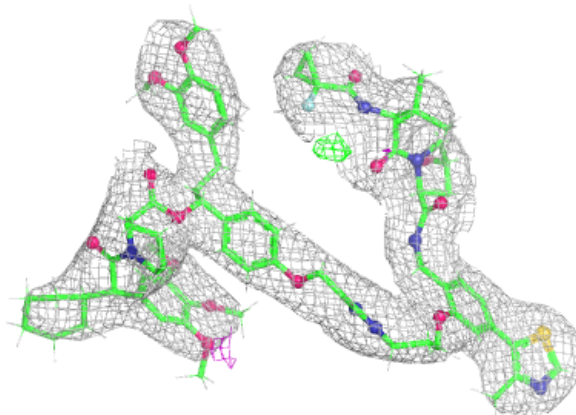
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	XZW	A	301	96/96	0.95	0.08	30,77,102,108	1
5	XZW	B	301	96/96	0.96	0.07	30,66,75,90	1

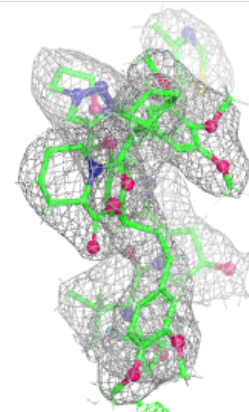
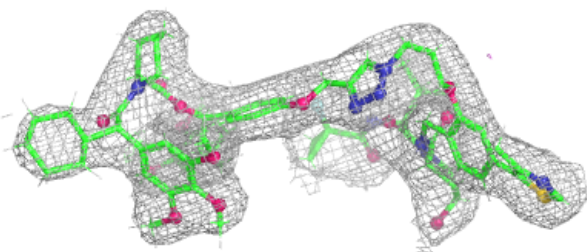
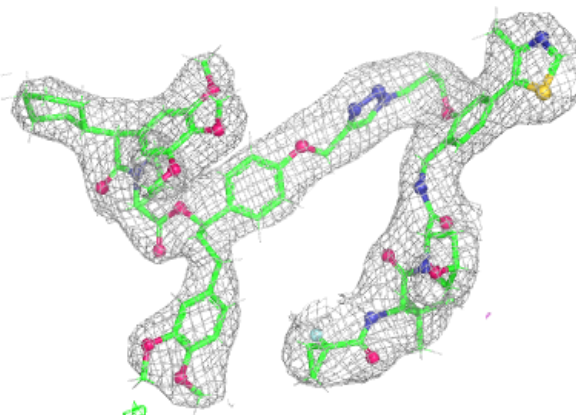
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XZW 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 XZW 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.