



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2023 – 07:51 AM EDT

PDB ID : 8EWV
Title : DNA-encoded library (DEL)-enabled discovery of proximity inducing small molecules
Authors : Schreiber, S.L.; Shu, W.; Ma, X.; Michaud, G.; Bonazzi, S.; Berst, F.
Deposited on : 2022-10-24
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

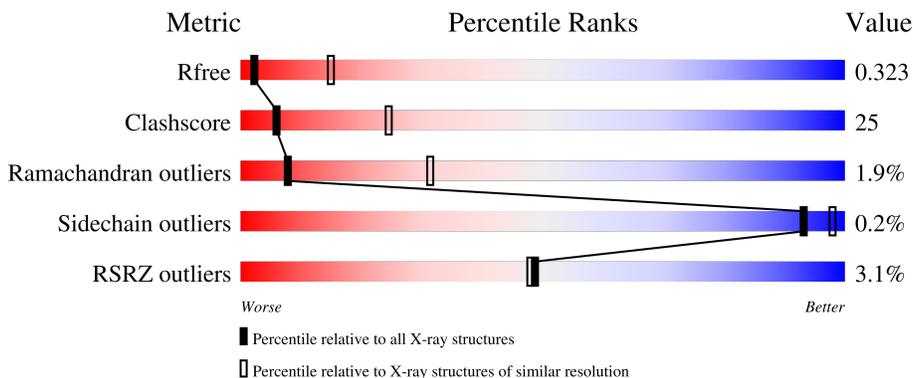
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	118	 3% 50% 32% 14%
1	E	118	 2% 49% 35% 14%
1	I	118	 13% 41% 41% 14%
1	M	118	 % 43% 38% 14%
1	Q	118	 5% 43% 40% 14%

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Mol	Chain	Length	Quality of chain
1	U	118	
2	B	96	
2	F	96	
2	J	96	
2	N	96	
2	R	96	
2	V	96	
3	C	162	
3	G	162	
3	K	162	
3	O	162	
3	S	162	
3	W	162	
4	D	127	
4	H	127	
4	L	127	
4	P	127	
4	T	127	
4	X	127	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22123 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	102	805	509	135	157	4	0	0	0
1	E	102	805	509	135	157	4	0	0	0
1	I	102	798	504	135	155	4	0	0	0
1	M	102	805	509	135	157	4	0	0	0
1	Q	102	805	509	135	157	4	0	0	0
1	U	102	805	509	135	157	4	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	90	706	455	113	132	6	0	0	0
2	F	90	709	456	114	133	6	0	0	0
2	J	90	698	449	112	131	6	0	0	0
2	N	90	705	455	113	131	6	0	0	0
2	R	90	706	455	113	132	6	0	0	0
2	V	90	705	455	113	131	6	0	0	0

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	146	Total	C	N	O	S	0	0	0
			1189	757	218	212	2			
3	G	146	Total	C	N	O	S	0	0	0
			1189	757	218	212	2			
3	K	146	Total	C	N	O	S	0	0	0
			1193	759	219	213	2			
3	O	146	Total	C	N	O	S	0	0	0
			1189	757	218	212	2			
3	S	146	Total	C	N	O	S	0	0	0
			1189	757	218	212	2			
3	W	146	Total	C	N	O	S	0	0	0
			1189	757	218	212	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	PRO	-	expression tag	UNP P40337
G	52	GLY	-	expression tag	UNP P40337
G	53	PRO	-	expression tag	UNP P40337
K	52	GLY	-	expression tag	UNP P40337
K	53	PRO	-	expression tag	UNP P40337
O	52	GLY	-	expression tag	UNP P40337
O	53	PRO	-	expression tag	UNP P40337
S	52	GLY	-	expression tag	UNP P40337
S	53	PRO	-	expression tag	UNP P40337
W	52	GLY	-	expression tag	UNP P40337
W	53	PRO	-	expression tag	UNP P40337

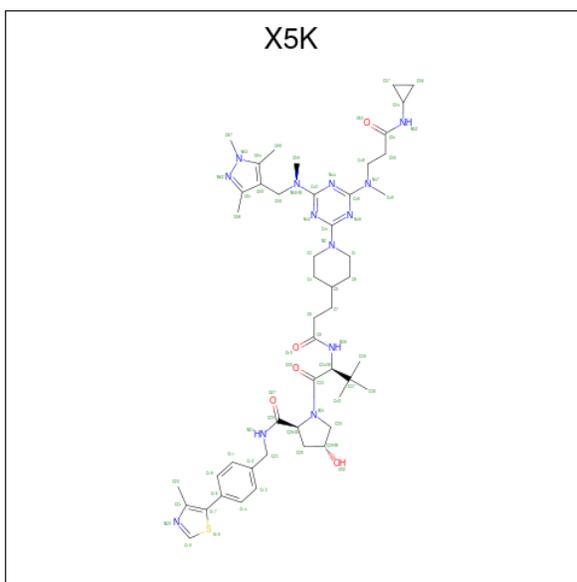
- Molecule 4 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	109	Total	C	N	O	S	0	0	0
			922	602	147	167	6			
4	H	109	Total	C	N	O	S	0	0	0
			922	602	147	167	6			
4	L	109	Total	C	N	O	S	0	0	0
			922	602	147	167	6			
4	P	109	Total	C	N	O	S	0	0	0
			922	602	147	167	6			
4	T	109	Total	C	N	O	S	0	0	0
			921	602	147	166	6			
4	X	109	Total	C	N	O	S	0	0	0
			922	602	147	167	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	42	SER	-	expression tag	UNP O60885
D	43	MET	-	expression tag	UNP O60885
H	42	SER	-	expression tag	UNP O60885
H	43	MET	-	expression tag	UNP O60885
L	42	SER	-	expression tag	UNP O60885
L	43	MET	-	expression tag	UNP O60885
P	42	SER	-	expression tag	UNP O60885
P	43	MET	-	expression tag	UNP O60885
T	42	SER	-	expression tag	UNP O60885
T	43	MET	-	expression tag	UNP O60885
X	42	SER	-	expression tag	UNP O60885
X	43	MET	-	expression tag	UNP O60885

- Molecule 5 is N-{3-[1-(4-{[3-(cyclopropylamino)-3-oxopropyl](methyl)amino}-6-{methyl[(1,3,5-trimethyl-1H-pyrazol-4-yl)methyl]amino}-1,3,5-triazin-2-yl)piperidin-4-yl]propanoyl}-3-methyl-L-valyl-(4R)-4-hydroxy-N-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-L-proline amide (three-letter code: X5K) (formula: C₄₈H₆₉N₁₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			S	
5	C	1	Total	67	48	13	5	1	0	0
5	G	1	Total	67	48	13	5	1	0	0
5	K	1	Total	67	48	13	5	1	0	0

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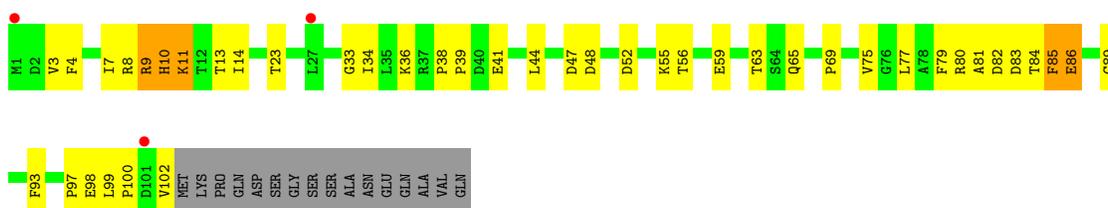
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	S	0	0
			67	48	13	5	1		
5	S	1	Total	C	N	O	S	0	0
			67	48	13	5	1		
5	W	1	Total	C	N	O	S	0	0
			67	48	13	5	1		

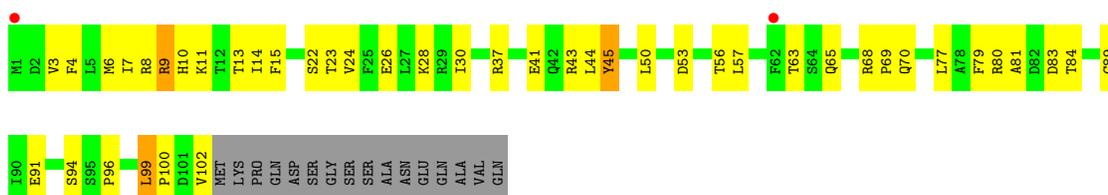
3 Residue-property plots [i](#)

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.

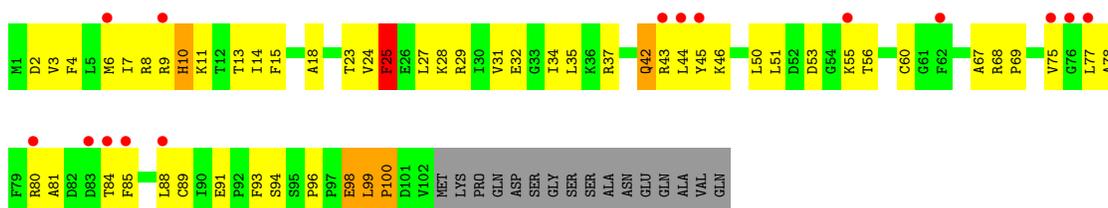
- Molecule 1: Elongin-B



- Molecule 1: Elongin-B



- Molecule 1: Elongin-B

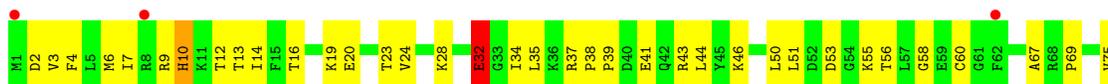


- Molecule 1: Elongin-B

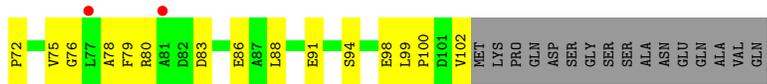




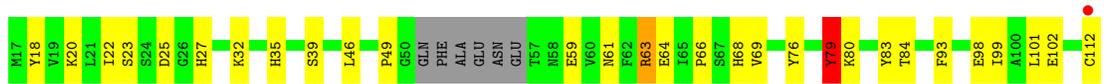
● Molecule 1: Elongin-B



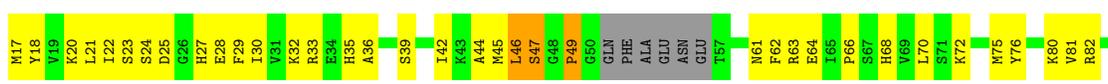
● Molecule 1: Elongin-B



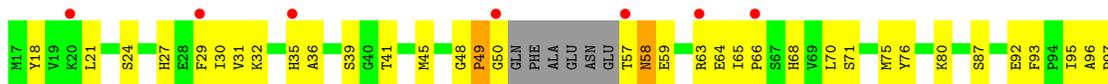
● Molecule 2: Elongin-C



● Molecule 2: Elongin-C



● Molecule 2: Elongin-C

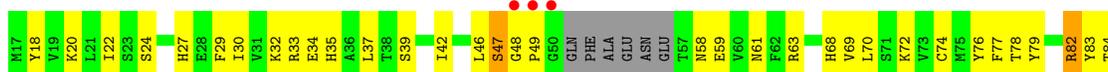




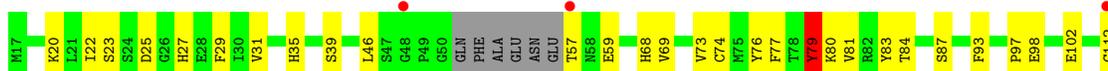
• Molecule 2: Elongin-C



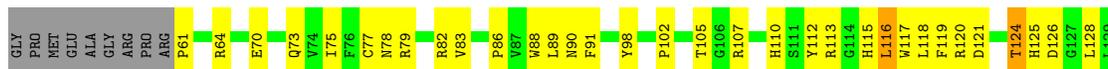
• Molecule 2: Elongin-C



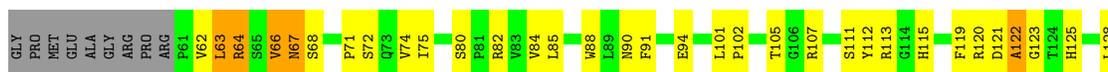
• Molecule 2: Elongin-C



• Molecule 3: von Hippel-Lindau disease tumor suppressor



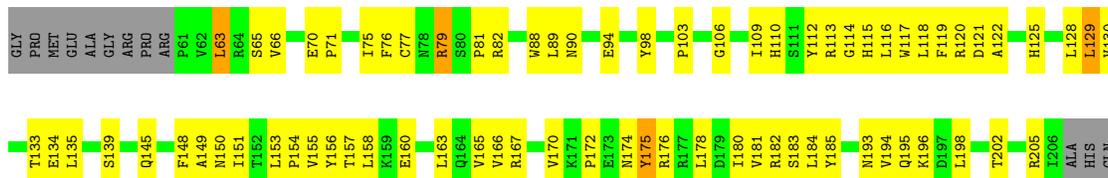
• Molecule 3: von Hippel-Lindau disease tumor suppressor





ALA
HIS
GLN
ARG
MET
GLY
ASP

• Molecule 3: von Hippel-Lindau disease tumor suppressor



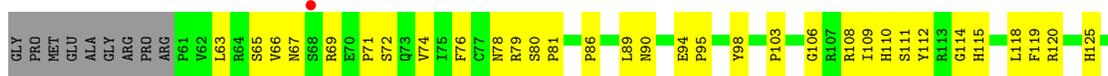
ARG
MET
GLY
ASP

• Molecule 3: von Hippel-Lindau disease tumor suppressor



ALA
HIS
GLN
ARG
MET
GLY
ASP

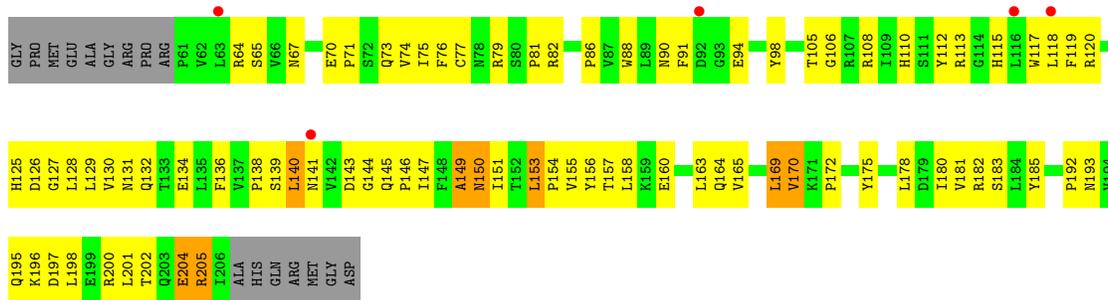
• Molecule 3: von Hippel-Lindau disease tumor suppressor



R200
L201
T202
Q203
E204
R205
T206
ALA
HIS
GLN
ARG
MET
GLY
ASP

• Molecule 3: von Hippel-Lindau disease tumor suppressor

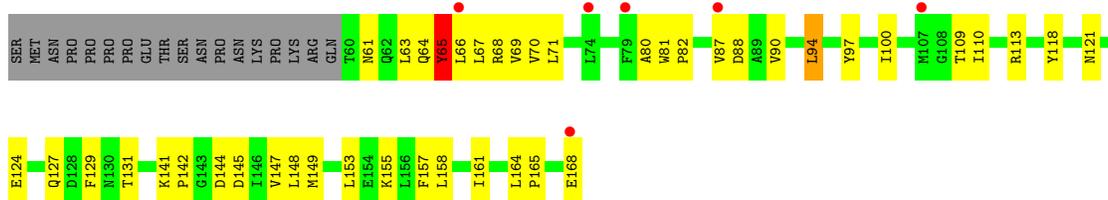




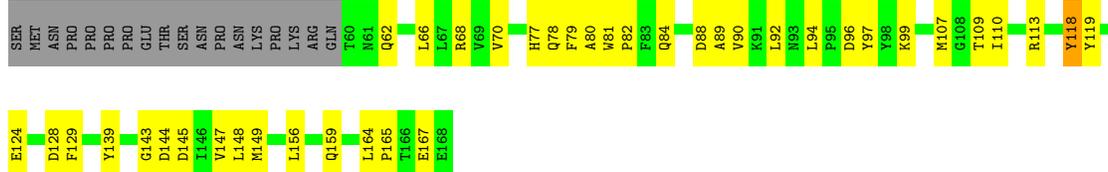
• Molecule 4: Bromodomain-containing protein 4



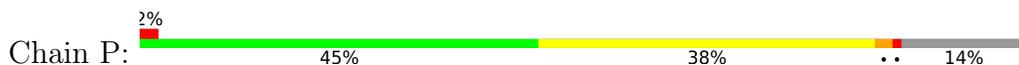
• Molecule 4: Bromodomain-containing protein 4



• Molecule 4: Bromodomain-containing protein 4

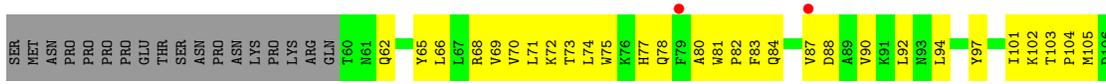


• Molecule 4: Bromodomain-containing protein 4

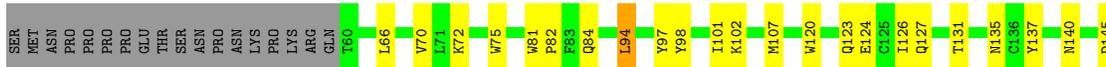




• Molecule 4: Bromodomain-containing protein 4



• Molecule 4: Bromodomain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.48Å 164.05Å 256.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 3.40 49.01 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.01-3.40) 100.0 (49.01-3.40)	Depositor EDS
R_{merge}	0.77	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874+SVN, PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.280 , 0.324 0.280 , 0.323	Depositor DCC
R_{free} test set	3227 reflections (4.98%)	wwPDB-VI
Wilson B-factor (Å ²)	67.0	Xtrriage
Anisotropy	0.568	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22123	wwPDB-VI
Average B, all atoms (Å ²)	90.0	wwPDB-VI

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1020e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: X5K

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	0.33	0/821	0.80	0/1111
1	E	0.38	0/821	0.89	5/1111 (0.5%)
1	I	0.56	2/814 (0.2%)	1.19	5/1102 (0.5%)
1	M	0.38	0/819	0.84	4/1105 (0.4%)
1	Q	0.40	0/821	0.86	2/1111 (0.2%)
1	U	0.35	0/821	0.92	4/1111 (0.4%)
2	B	0.49	0/721	0.97	4/973 (0.4%)
2	F	0.36	0/724	0.70	0/977
2	J	0.41	0/713	0.72	0/964
2	N	0.40	0/720	0.86	3/973 (0.3%)
2	R	0.38	0/721	0.78	1/973 (0.1%)
2	V	0.59	3/720 (0.4%)	0.96	3/972 (0.3%)
3	C	0.37	0/1220	0.87	3/1665 (0.2%)
3	G	0.59	3/1220 (0.2%)	0.84	1/1665 (0.1%)
3	K	0.37	0/1224	0.81	4/1670 (0.2%)
3	O	0.36	0/1220	0.81	2/1665 (0.1%)
3	S	0.41	0/1220	0.90	3/1665 (0.2%)
3	W	0.51	2/1220 (0.2%)	0.95	8/1665 (0.5%)
4	D	0.32	0/946	0.68	1/1283 (0.1%)
4	H	0.38	0/946	0.74	2/1283 (0.2%)
4	L	0.31	0/946	0.70	1/1283 (0.1%)
4	P	0.37	0/946	0.84	4/1283 (0.3%)
4	T	0.38	0/945	0.70	1/1283 (0.1%)
4	X	0.38	0/946	0.64	1/1283 (0.1%)
All	All	0.42	10/22235 (0.0%)	0.84	62/30176 (0.2%)

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	I	0	2
1	M	0	3
1	Q	0	1
1	U	0	2
2	B	0	2
2	F	0	1
2	J	0	2
2	N	0	1
2	R	0	2
2	V	0	2
3	C	0	2
3	S	0	2
3	W	0	2
4	H	0	1
4	P	0	1
4	X	0	1
All	All	0	29

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	150	ASN	CG-ND2	8.67	1.54	1.32
2	V	79	TYR	CG-CD2	8.35	1.50	1.39
1	I	42	GLN	CB-CG	8.16	1.74	1.52
3	W	150	ASN	CB-CG	6.86	1.66	1.51
3	G	67	ASN	CG-ND2	6.48	1.49	1.32

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	25	PHE	CB-CG-CD2	-22.51	105.05	120.80
2	V	79	TYR	CB-CG-CD2	-16.88	110.87	121.00
2	B	79	TYR	CB-CG-CD2	-16.21	111.28	121.00
1	I	25	PHE	CB-CG-CD1	14.43	130.90	120.80
1	U	4	PHE	CB-CG-CD2	-11.69	112.61	120.80

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	9	ARG	Peptide
2	B	63	ARG	Sidechain
2	B	79	TYR	Sidechain
3	C	124	THR	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	805	0	802	41	0
1	E	805	0	802	51	0
1	I	798	0	789	55	0
1	M	805	0	800	46	0
1	Q	805	0	802	51	0
1	U	805	0	802	54	0
2	B	706	0	704	34	0
2	F	709	0	708	55	0
2	J	698	0	681	49	0
2	N	705	0	704	22	0
2	R	706	0	704	50	0
2	V	705	0	701	29	0
3	C	1189	0	1190	76	0
3	G	1189	0	1190	75	0
3	K	1193	0	1196	83	0
3	O	1189	0	1190	90	0
3	S	1189	0	1190	80	0
3	W	1189	0	1190	81	1
4	D	922	0	917	29	0
4	H	922	0	917	42	0
4	L	922	0	917	29	1
4	P	922	0	917	42	0
4	T	921	0	917	34	0
4	X	922	0	917	27	0
5	C	67	0	0	3	0
5	G	67	0	0	0	0
5	K	67	0	0	2	0
5	O	67	0	0	2	0
5	S	67	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	W	67	0	0	0	0
All	All	22123	0	21647	1095	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 25.

The worst 5 of 1095 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:I:42:GLN:CG	1:I:42:GLN:CB	1.74	1.61
3:W:120:ARG:HD3	3:W:126:ASP:HA	1.23	1.12
1:Q:41:GLU:HB2	1:Q:80:ARG:HB3	1.32	1.10
3:S:90:ASN:HD21	4:T:78:GLN:HB2	1.18	1.09
3:K:63:LEU:HD13	3:K:202:THR:HG22	1.31	1.08

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)
4:L:124:GLU:OE2	3:W:182:ARG:NH1[2_355]	2.07	0.13

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	100/118 (85%)	80 (80%)	15 (15%)	5 (5%)	2	14
1	E	100/118 (85%)	76 (76%)	21 (21%)	3 (3%)	4	23
1	I	100/118 (85%)	83 (83%)	13 (13%)	4 (4%)	3	18
1	M	96/118 (81%)	84 (88%)	7 (7%)	5 (5%)	2	13
1	Q	100/118 (85%)	81 (81%)	16 (16%)	3 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	100/118 (85%)	79 (79%)	20 (20%)	1 (1%)	15	46
2	B	86/96 (90%)	78 (91%)	7 (8%)	1 (1%)	13	41
2	F	86/96 (90%)	76 (88%)	8 (9%)	2 (2%)	6	28
2	J	86/96 (90%)	77 (90%)	7 (8%)	2 (2%)	6	28
2	N	86/96 (90%)	76 (88%)	9 (10%)	1 (1%)	13	41
2	R	86/96 (90%)	75 (87%)	7 (8%)	4 (5%)	2	15
2	V	86/96 (90%)	77 (90%)	9 (10%)	0	100	100
3	C	144/162 (89%)	119 (83%)	21 (15%)	4 (3%)	5	24
3	G	144/162 (89%)	133 (92%)	10 (7%)	1 (1%)	22	55
3	K	144/162 (89%)	128 (89%)	14 (10%)	2 (1%)	11	37
3	O	144/162 (89%)	124 (86%)	16 (11%)	4 (3%)	5	24
3	S	144/162 (89%)	120 (83%)	21 (15%)	3 (2%)	7	30
3	W	144/162 (89%)	121 (84%)	21 (15%)	2 (1%)	11	37
4	D	107/127 (84%)	99 (92%)	8 (8%)	0	100	100
4	H	107/127 (84%)	100 (94%)	7 (6%)	0	100	100
4	L	107/127 (84%)	97 (91%)	10 (9%)	0	100	100
4	P	107/127 (84%)	97 (91%)	8 (8%)	2 (2%)	8	31
4	T	107/127 (84%)	100 (94%)	5 (5%)	2 (2%)	8	31
4	X	107/127 (84%)	97 (91%)	10 (9%)	0	100	100
All	All	2618/3018 (87%)	2277 (87%)	290 (11%)	51 (2%)	8	31

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	85	PHE
3	C	175	TYR
3	C	193	ASN
1	E	79	PHE

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	90/103 (87%)	90 (100%)	0	100	100
1	E	90/103 (87%)	90 (100%)	0	100	100
1	I	88/103 (85%)	87 (99%)	1 (1%)	73	86
1	M	90/103 (87%)	90 (100%)	0	100	100
1	Q	90/103 (87%)	90 (100%)	0	100	100
1	U	90/103 (87%)	90 (100%)	0	100	100
2	B	79/85 (93%)	79 (100%)	0	100	100
2	F	80/85 (94%)	80 (100%)	0	100	100
2	J	76/85 (89%)	76 (100%)	0	100	100
2	N	79/85 (93%)	79 (100%)	0	100	100
2	R	79/85 (93%)	79 (100%)	0	100	100
2	V	78/85 (92%)	78 (100%)	0	100	100
3	C	135/148 (91%)	135 (100%)	0	100	100
3	G	135/148 (91%)	133 (98%)	2 (2%)	65	82
3	K	136/148 (92%)	136 (100%)	0	100	100
3	O	135/148 (91%)	135 (100%)	0	100	100
3	S	135/148 (91%)	134 (99%)	1 (1%)	84	92
3	W	135/148 (91%)	135 (100%)	0	100	100
4	D	102/120 (85%)	102 (100%)	0	100	100
4	H	102/120 (85%)	102 (100%)	0	100	100
4	L	102/120 (85%)	102 (100%)	0	100	100
4	P	102/120 (85%)	102 (100%)	0	100	100
4	T	102/120 (85%)	102 (100%)	0	100	100
4	X	102/120 (85%)	102 (100%)	0	100	100
All	All	2432/2736 (89%)	2428 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	64	ARG
3	G	182	ARG
1	I	68	ARG

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Mol	Chain	Res	Type
3	S	200	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	132	GLN
3	S	96	GLN
2	V	35	HIS
3	K	145	GLN
2	J	35	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	X5K	K	501	-	67,73,73	0.38	1 (1%)	87,106,106	0.73	3 (3%)
5	X5K	C	501	-	67,73,73	0.41	1 (1%)	87,106,106	0.72	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	X5K	S	501	-	67,73,73	0.37	1 (1%)	87,106,106	0.72	3 (3%)
5	X5K	O	501	-	67,73,73	0.43	1 (1%)	87,106,106	0.71	2 (2%)
5	X5K	G	501	-	67,73,73	0.41	1 (1%)	87,106,106	0.71	4 (4%)
5	X5K	W	501	-	67,73,73	0.39	1 (1%)	87,106,106	0.62	1 (1%)

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	X5K	K	501	-	-	15/59/85/85	0/7/7/7
5	X5K	C	501	-	-	21/59/85/85	0/7/7/7
5	X5K	S	501	-	-	15/59/85/85	0/7/7/7
5	X5K	O	501	-	-	18/59/85/85	0/7/7/7
5	X5K	G	501	-	-	16/59/85/85	0/7/7/7
5	X5K	W	501	-	-	16/59/85/85	0/7/7/7

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	501	X5K	C64-N63	-2.50	1.33	1.37
5	C	501	X5K	C64-N63	-2.50	1.33	1.37
5	G	501	X5K	C64-N63	-2.38	1.33	1.37
5	W	501	X5K	C64-N63	-2.36	1.33	1.37
5	K	501	X5K	C64-N63	-2.25	1.34	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	501	X5K	C58-C60-C61	3.27	131.01	127.05
5	S	501	X5K	C59-N55-C58	-3.17	106.43	114.84
5	C	501	X5K	C58-C60-C61	2.91	130.57	127.05
5	K	501	X5K	C59-N55-C58	-2.77	107.47	114.84
5	C	501	X5K	C7-C5-C4	2.66	118.46	112.11

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

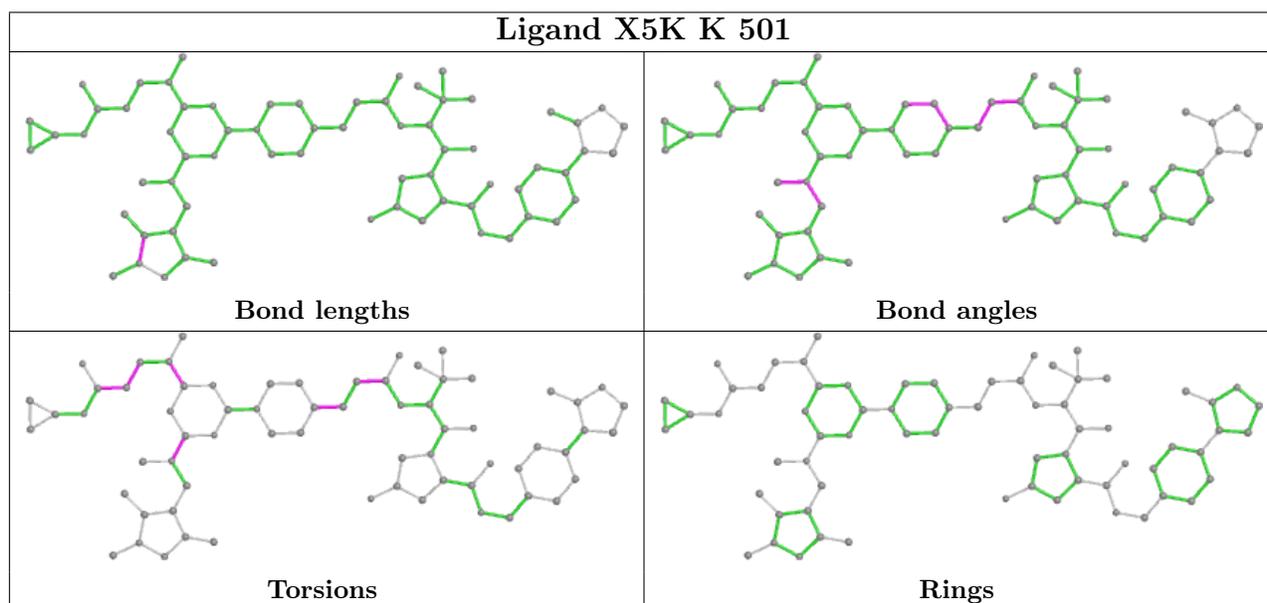
Mol	Chain	Res	Type	Atoms
5	C	501	X5K	N42-C43-N55-C58
5	C	501	X5K	N42-C43-N55-C59
5	C	501	X5K	N44-C43-N55-C58
5	C	501	X5K	N44-C43-N55-C59
5	C	501	X5K	N44-C45-N47-C48

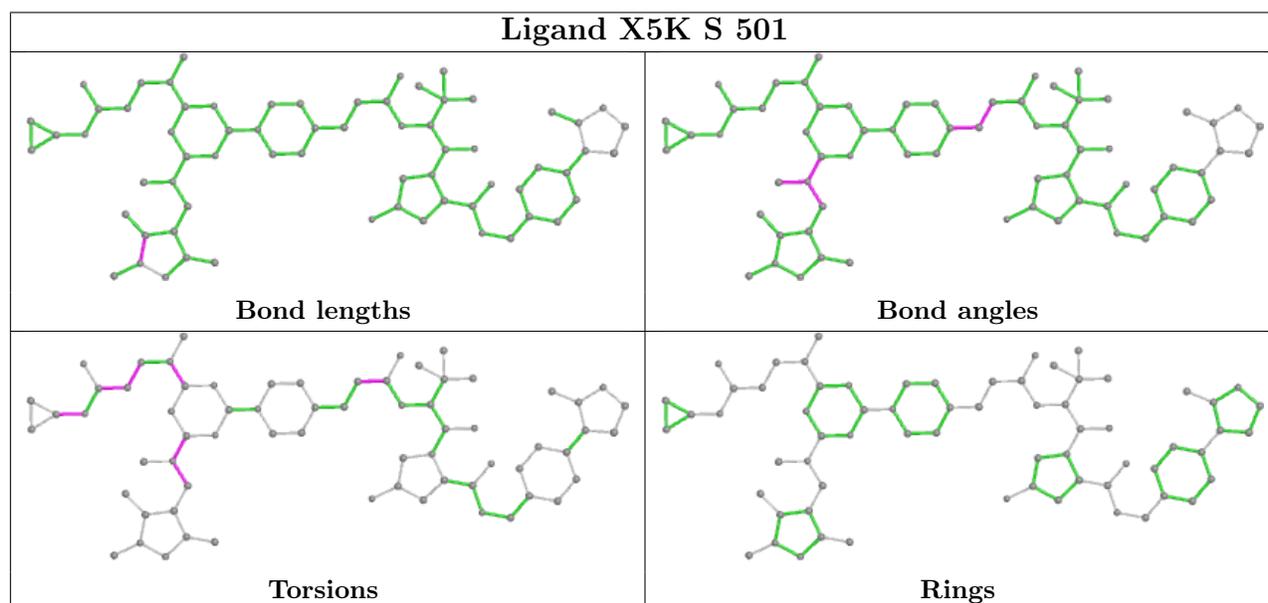
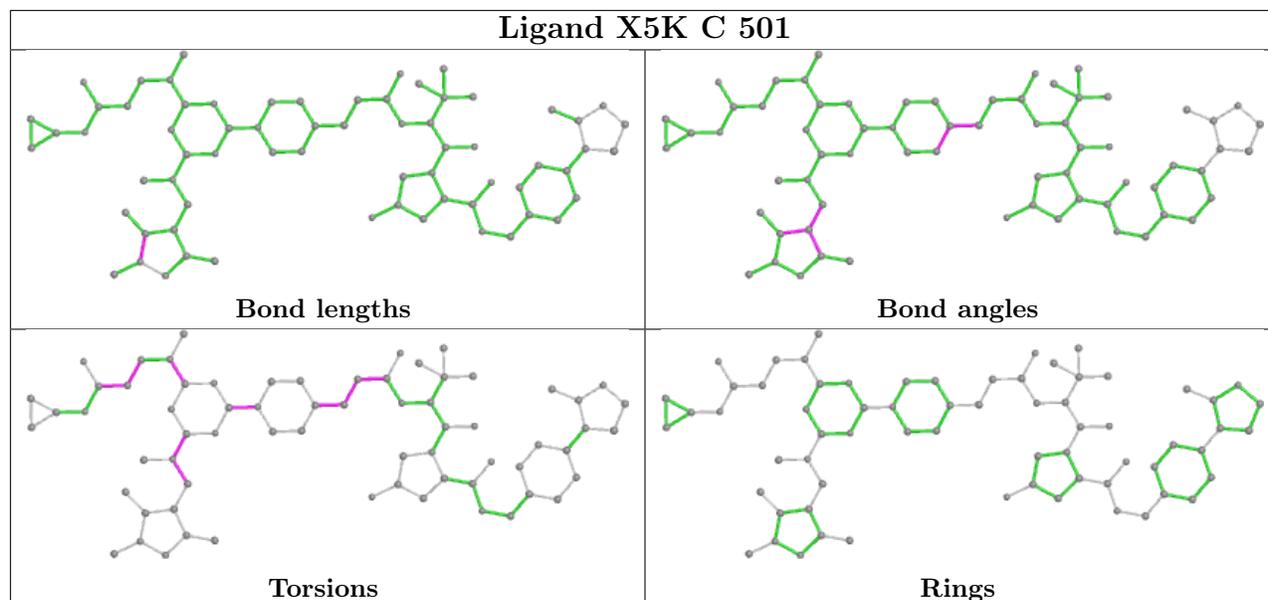
There are no ring outliers.

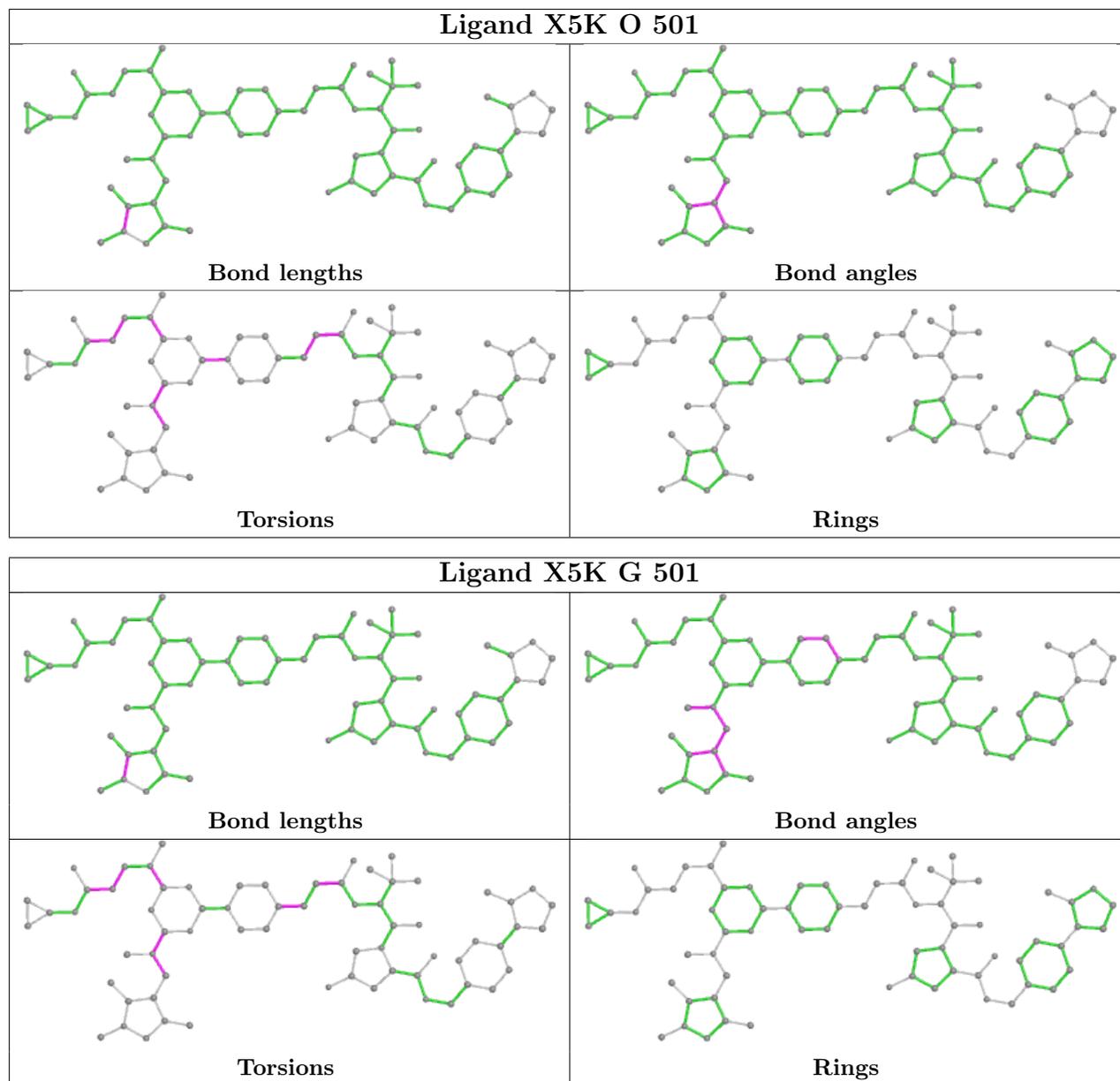
4 monomers are involved in 9 short contacts:

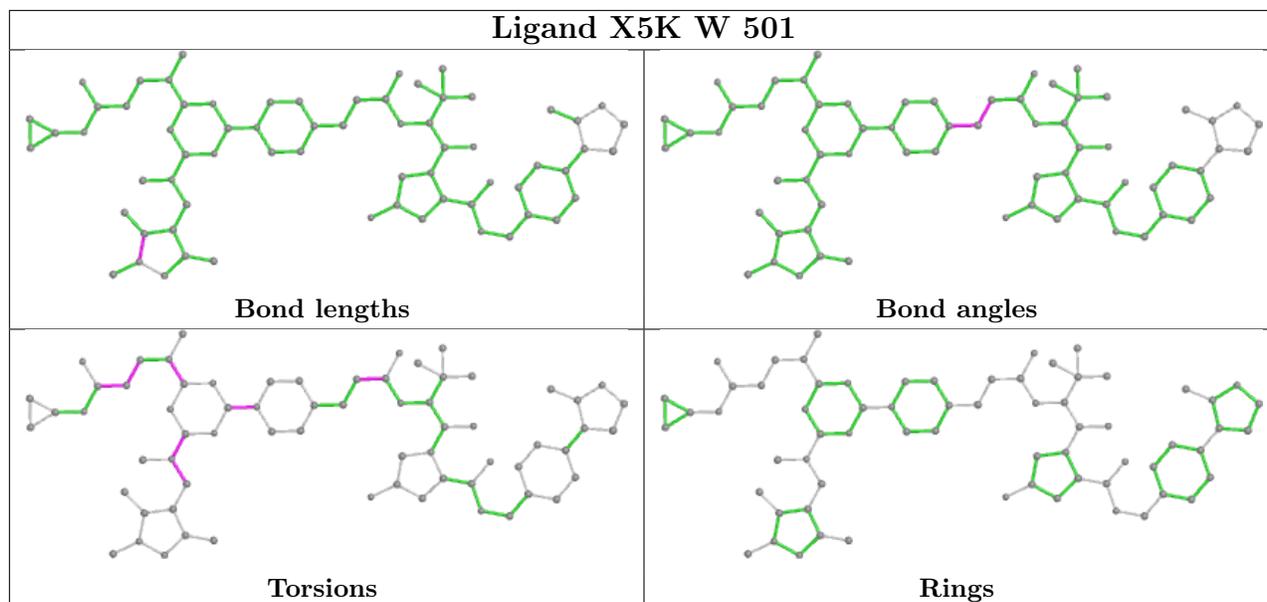
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	501	X5K	2	0
5	C	501	X5K	3	0
5	S	501	X5K	2	0
5	O	501	X5K	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	75:VAL	C	76:GLY	N	3.90
1	M	77:LEU	C	78:ALA	N	3.54

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	102/118 (86%)	0.19	3 (2%) 51 50	60, 106, 137, 165	0
1	E	102/118 (86%)	0.24	2 (1%) 65 64	59, 104, 145, 170	0
1	I	102/118 (86%)	0.98	15 (14%) 2 3	95, 141, 191, 210	0
1	M	102/118 (86%)	0.34	1 (0%) 82 81	67, 115, 155, 199	0
1	Q	102/118 (86%)	0.46	6 (5%) 22 23	66, 101, 150, 168	0
1	U	102/118 (86%)	0.29	4 (3%) 39 38	54, 94, 157, 169	0
2	B	90/96 (93%)	0.24	1 (1%) 80 79	37, 66, 106, 120	0
2	F	90/96 (93%)	0.21	0 100 100	29, 61, 96, 141	0
2	J	90/96 (93%)	0.59	8 (8%) 9 11	72, 108, 156, 184	0
2	N	90/96 (93%)	0.29	4 (4%) 34 34	55, 81, 128, 185	0
2	R	90/96 (93%)	0.20	3 (3%) 46 45	34, 59, 100, 171	0
2	V	90/96 (93%)	0.20	3 (3%) 46 45	34, 58, 112, 167	0
3	C	146/162 (90%)	0.17	1 (0%) 87 87	39, 72, 121, 160	0
3	G	146/162 (90%)	0.08	0 100 100	29, 63, 112, 173	0
3	K	146/162 (90%)	-0.00	0 100 100	38, 79, 136, 165	0
3	O	146/162 (90%)	0.11	1 (0%) 87 87	34, 74, 129, 160	0
3	S	146/162 (90%)	0.18	2 (1%) 75 74	37, 75, 117, 193	0
3	W	146/162 (90%)	0.23	5 (3%) 45 44	44, 83, 142, 198	0
4	D	109/127 (85%)	0.60	10 (9%) 9 10	40, 127, 176, 204	0
4	H	109/127 (85%)	0.38	6 (5%) 25 25	31, 77, 124, 151	0
4	L	109/127 (85%)	0.23	0 100 100	28, 60, 108, 138	0
4	P	109/127 (85%)	0.27	2 (1%) 68 67	39, 71, 122, 172	0
4	T	109/127 (85%)	0.34	3 (2%) 53 51	68, 109, 156, 174	0
4	X	109/127 (85%)	0.23	2 (1%) 68 67	85, 125, 163, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2682/3018 (88%)	0.28	82 (3%) 49 48	28, 86, 154, 210	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	76	GLY	13.3
2	J	112	CYS	7.6
1	I	45	TYR	6.8
1	I	77	LEU	6.0
1	I	55	LYS	5.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

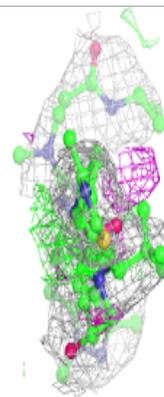
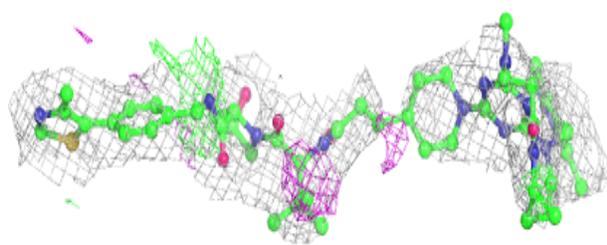
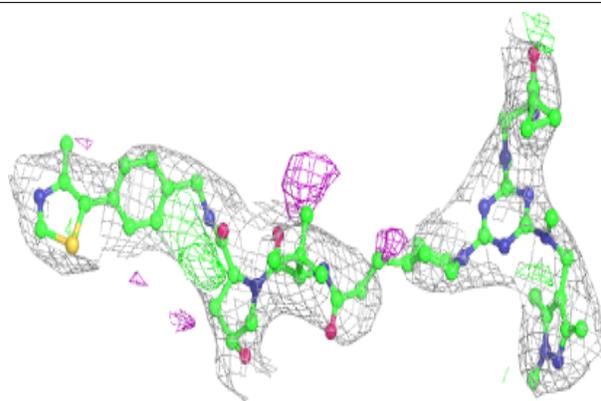
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	X5K	C	501	67/67	0.89	0.34	33,59,87,100	0
5	X5K	W	501	67/67	0.89	0.36	57,84,108,109	0
5	X5K	S	501	67/67	0.90	0.34	42,73,92,99	0
5	X5K	G	501	67/67	0.90	0.36	29,53,73,96	0
5	X5K	K	501	67/67	0.91	0.32	38,58,81,103	0
5	X5K	O	501	67/67	0.91	0.30	47,65,87,101	0

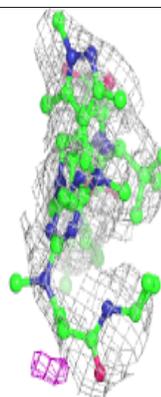
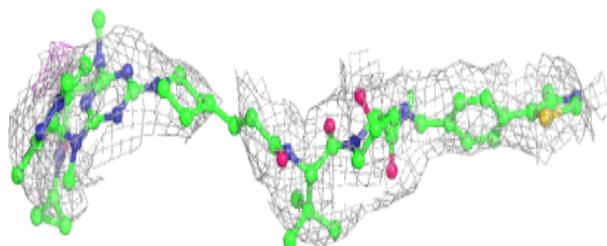
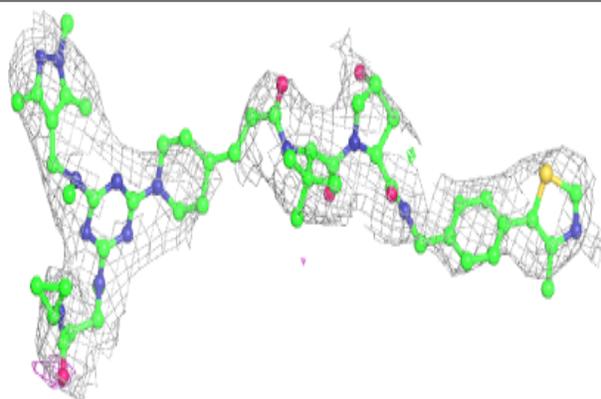
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X5K C 501:

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

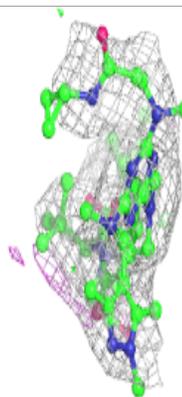
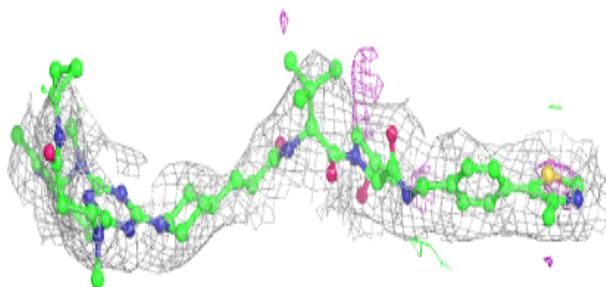
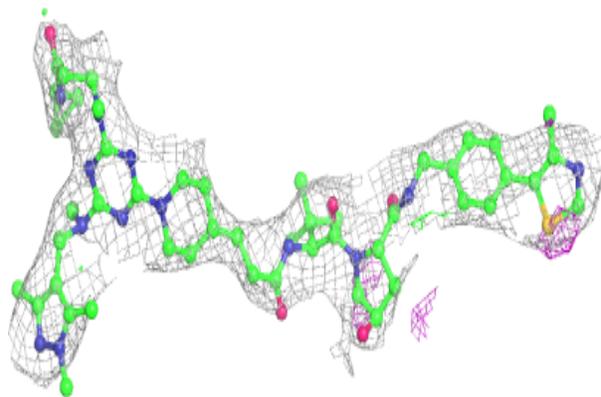
**Electron density around X5K W 501:**

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

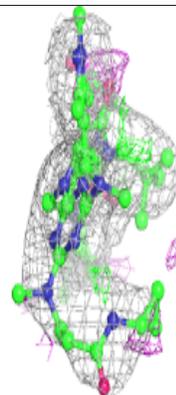
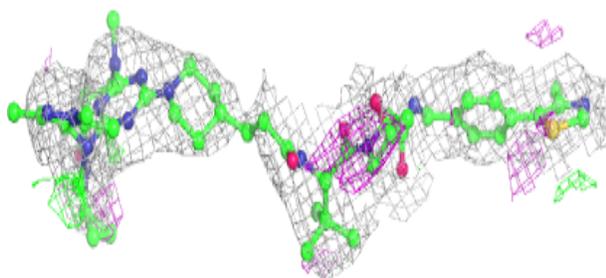
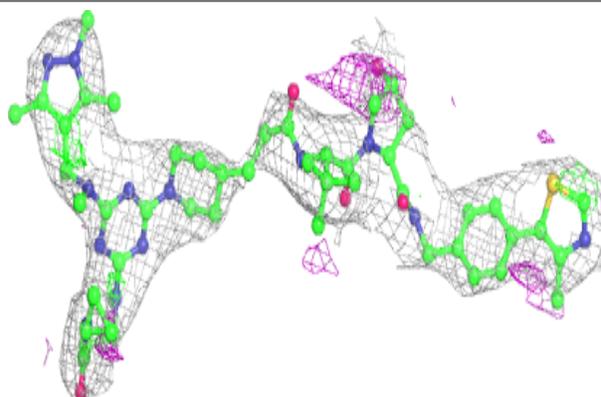


Electron density around X5K S 501:

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

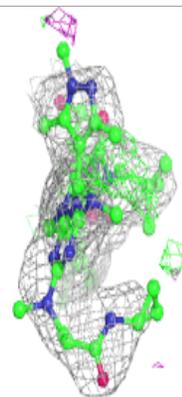
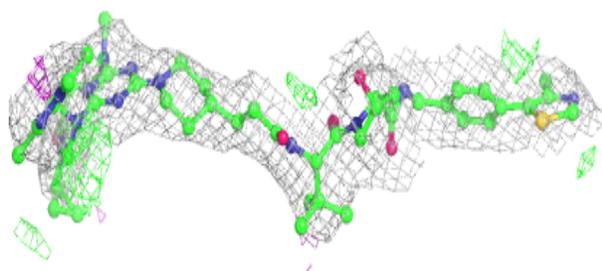
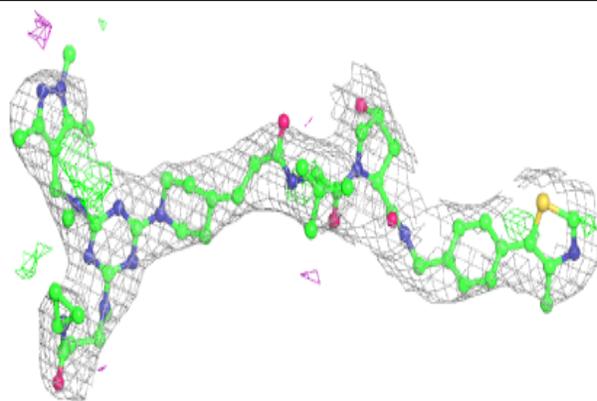
**Electron density around X5K G 501:**

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

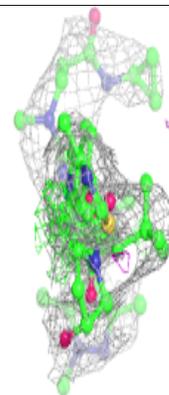
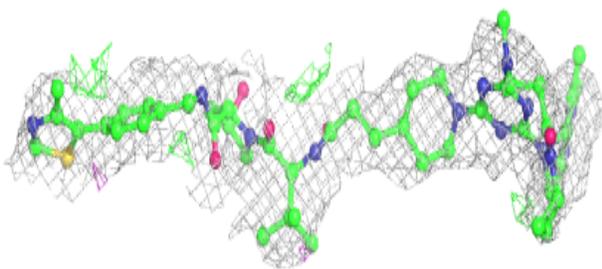
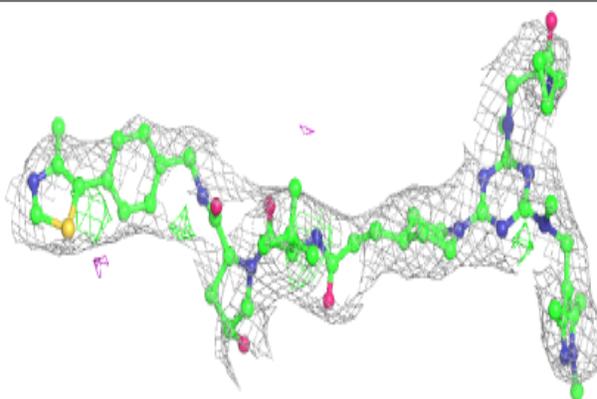


Electron density around X5K K 501:

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

**Electron density around X5K O 501:**

$2mF_o-DF_c$ (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.