



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:47 am BST

PDB ID : 6S4N
Title : LXRbeta ligand binding domain in complex with small molecule inhibitors
Authors : Sandmark, J.; Jansson, A.
Deposited on : 2019-06-28
Resolution : 1.90 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 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 : 2.11
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) : 2.11

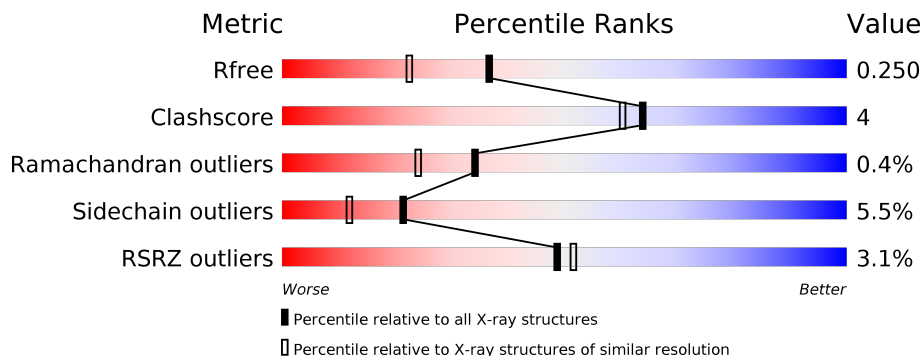
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	245	<p>2% 80% 13% . . .</p>
1	B	245	<p>4% 78% 15% . 5%</p>
1	C	245	<p>5% 78% 13% . 9%</p>
1	D	245	<p>% 84% 10% . .</p>

2 Entry composition [i](#)

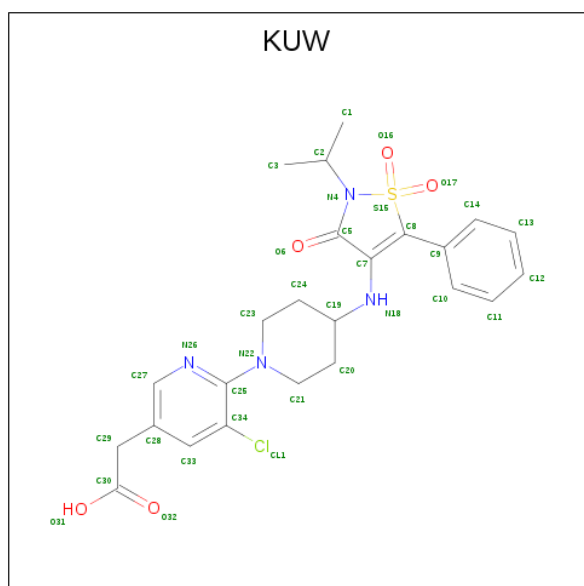
There are 4 unique types of molecules in this entry. The entry contains 8422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	235	Total 1931	C 1234	N 341	O 349	S 7	44	2	0
1	A	236	Total 1929	C 1233	N 339	O 350	S 7	33	2	0
1	B	233	Total 1922	C 1233	N 336	O 346	S 7	20	4	0
1	C	224	Total 1845	C 1182	N 322	O 334	S 7	11	4	0

- Molecule 2 is 2-[5-chloranyl-6-[4-[[1,1,3-tris(oxidanylidene)-5-phenyl-2-propan-2-yl-1,2-thiazol-4-yl]amino]piperidin-1-yl]pyridin-3-yl]ethanoic acid (three-letter code: KUW) (formula: C₂₄H₂₇ClN₄O₅S) (labeled as "Ligand of Interest" by author).



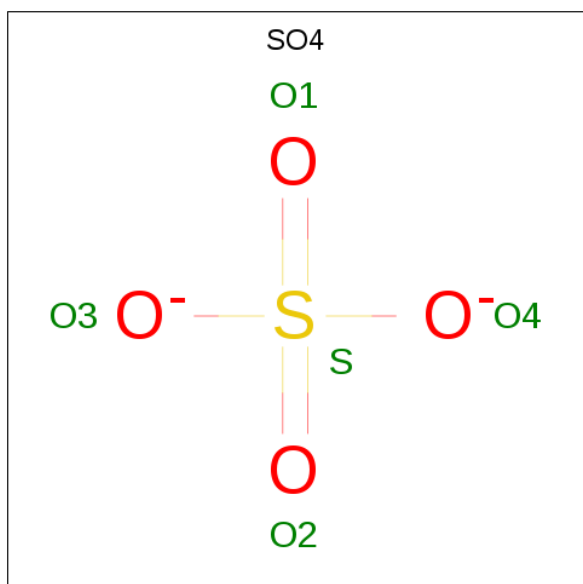
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	D	1	Total 35	C 24	Cl 1	N 4	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	D	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	135	Total	O	0	0
			135	135		
4	A	159	Total	O	0	0
			159	159		

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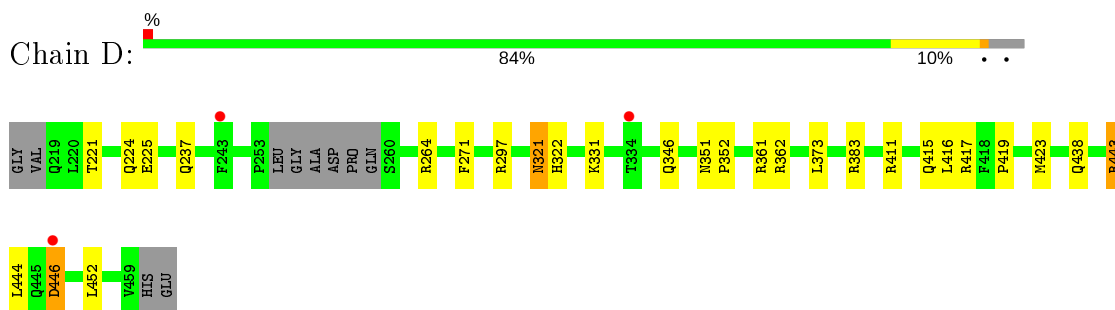
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	105	Total 105	O 105	0	0
4	C	146	Total 146	O 146	0	0

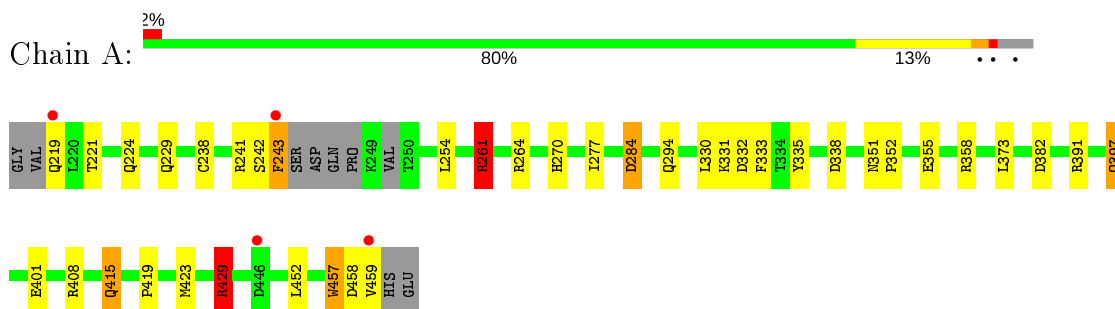
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

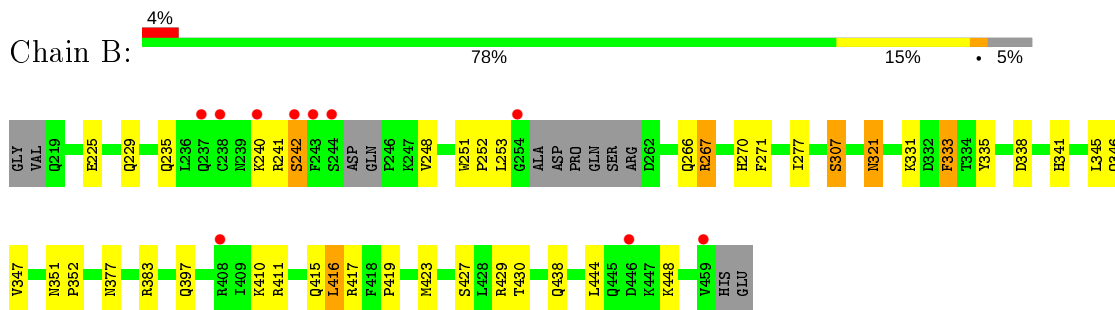
- Molecule 1: Oxysterols receptor LXR-beta



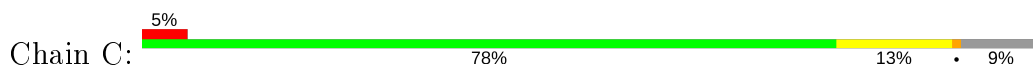
- Molecule 1: Oxysterols receptor LXR-beta

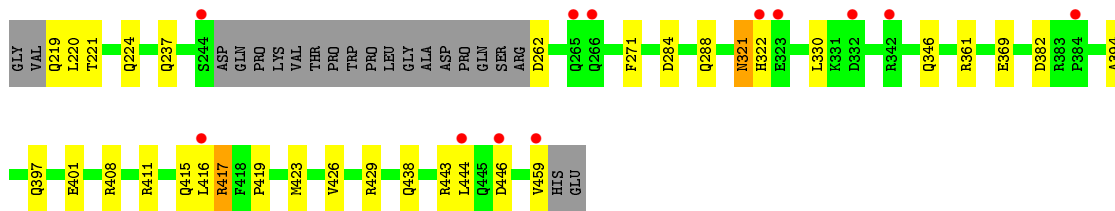


- Molecule 1: Oxysterols receptor LXR-beta



- Molecule 1: Oxysterols receptor LXR-beta





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.43Å 109.40Å 88.98Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	54.72 – 1.90 54.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (54.72-1.90) 92.3 (54.70-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0135 2015/10/01	Depositor
R, R_{free}	0.215 , 0.245 0.219 , 0.250	Depositor DCC
R_{free} test set	3875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8422	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.43 % 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 1.5522e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KUW, SO4

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	0.63	3/1972 (0.2%)	0.96	10/2665 (0.4%)
1	B	0.58	1/1971 (0.1%)	0.83	8/2663 (0.3%)
1	C	0.84	3/1889 (0.2%)	0.98	7/2550 (0.3%)
1	D	0.78	4/1974 (0.2%)	0.83	9/2668 (0.3%)
All	All	0.71	11/7806 (0.1%)	0.90	34/10546 (0.3%)

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	D	1	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	446	ASP	CB-CG	24.43	2.03	1.51
1	D	411	ARG	CD-NE	21.10	1.82	1.46
1	C	408	ARG	CD-NE	-14.32	1.22	1.46
1	D	443	ARG	CG-CD	-10.76	1.25	1.51
1	A	264	ARG	CD-NE	-10.70	1.28	1.46
1	A	358	ARG	CD-NE	-9.15	1.30	1.46
1	B	252	PRO	C-N	-8.96	1.13	1.34
1	D	297	ARG	CG-CD	8.00	1.72	1.51
1	D	264	ARG	CB-CG	-6.58	1.34	1.52
1	C	415	GLN	CB-CG	6.20	1.69	1.52
1	A	355	GLU	CB-CG	5.35	1.62	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	ASP	CB-CG-OD1	18.12	134.61	118.30
1	C	446	ASP	CB-CG-OD2	-17.89	102.20	118.30
1	A	264	ARG	CD-NE-CZ	15.82	145.74	123.60
1	A	358	ARG	CD-NE-CZ	15.68	145.55	123.60
1	C	446	ASP	CA-CB-CG	-13.11	84.55	113.40
1	A	261	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	C	417	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	D	417	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	D	417	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	A	264	ARG	CG-CD-NE	8.24	129.09	111.80
1	A	333	PHE	CB-CG-CD1	6.75	125.52	120.80
1	B	253	LEU	O-C-N	6.61	134.43	123.20
1	A	333	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	D	297	ARG	CG-CD-NE	6.04	124.48	111.80
1	D	383	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	417	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	382	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	457	TRP	N-CA-C	-5.79	95.37	111.00
1	A	261	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	362	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	B	253	LEU	CA-C-N	-5.75	104.71	116.20
1	B	333	PHE	CB-CG-CD1	5.72	124.80	120.80
1	A	429	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	338	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	383	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	267	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	C	411	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	237	GLN	CG-CD-OE1	-5.51	110.57	121.60
1	C	415	GLN	CA-CB-CG	-5.44	101.42	113.40
1	D	411	ARG	CG-CD-NE	-5.35	100.56	111.80
1	D	297	ARG	CB-CG-CD	-5.21	98.07	111.60
1	B	345	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	267	ARG	CG-CD-NE	5.02	122.35	111.80
1	D	264	ARG	CA-CB-CG	5.01	124.42	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	331	LYS	CA

There are no planarity outliers.

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	1929	0	1961	17	0
1	B	1922	0	1958	30	0
1	C	1845	0	1889	19	0
1	D	1931	0	1966	7	0
2	A	35	0	0	0	0
2	B	70	0	0	5	0
2	C	35	0	0	0	0
2	D	105	0	0	1	0
3	A	5	0	0	0	0
4	A	159	0	0	3	0
4	B	105	0	0	2	0
4	C	146	0	0	1	0
4	D	135	0	0	0	0
All	All	8422	0	7774	65	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 (65) 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:D:346:GLN:H	1:D:438:GLN:HE22	1.20	0.90
1:B:346:GLN:H	1:B:438:GLN:HE22	1.24	0.85
1:C:346:GLN:H	1:C:438:GLN:HE22	1.25	0.80
1:A:270:HIS:HE2	1:A:335:TYR:HH	1.36	0.73
1:A:261:ARG:HH11	1:A:261:ARG:HG2	1.54	0.71
1:B:225:GLU:HB3	2:B:502:KUW:CL1	2.28	0.71
1:B:341[B]:HIS:CE1	1:B:347:VAL:HG22	2.27	0.69
1:B:341[B]:HIS:HE1	1:B:347:VAL:HG22	1.58	0.69
1:B:427:SER:HA	1:C:382:ASP:OD2	1.95	0.66
1:A:397:GLN:NE2	4:A:602:HOH:O	2.30	0.65
1:B:416:LEU:HD12	1:C:397:GLN:HE21	1.63	0.63
2:B:502:KUW:C21	2:B:502:KUW:CL1	2.89	0.58
1:C:221:THR:H	1:C:224:GLN:HE21	1.50	0.58
1:A:229:GLN:NE2	4:A:605:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:SER:HB3	1:B:277:ILE:HG23	1.88	0.56
1:B:411:ARG:HD2	1:B:417:ARG:HD2	1.87	0.56
1:B:430:THR:OG1	1:C:429:ARG:NH1	2.34	0.55
1:A:221:THR:H	1:A:224:GLN:HE21	1.53	0.55
1:A:238:CYS:SG	1:A:284:ASP:HB3	2.47	0.55
1:B:229:GLN:HE22	2:B:502:KUW:C19	2.23	0.51
1:C:346:GLN:N	1:C:438:GLN:HE22	2.03	0.50
1:B:346:GLN:N	1:B:438:GLN:HE22	2.02	0.50
1:B:397[A]:GLN:HE21	1:C:416:LEU:HD13	1.76	0.50
1:B:270:HIS:NE2	1:B:335:TYR:OH	2.38	0.49
1:B:242:SER:HB3	1:B:277:ILE:CG2	2.43	0.49
1:C:443:ARG:HD2	4:C:649:HOH:O	2.13	0.48
1:B:321:ASN:C	1:B:321:ASN:HD22	2.17	0.48
1:D:321:ASN:C	1:D:321:ASN:HD22	2.17	0.48
1:B:225:GLU:CB	2:B:502:KUW:CL1	2.99	0.47
1:C:322:HIS:HB2	1:C:361:ARG:CD	2.44	0.47
1:B:429:ARG:HG2	1:C:426:VAL:HG13	1.97	0.47
1:C:321:ASN:C	1:C:321:ASN:HD22	2.18	0.47
1:A:429:ARG:HA	1:A:429:ARG:HD3	1.77	0.46
1:B:415:GLN:NE2	1:C:219:GLN:HE21	2.13	0.46
1:B:251:TRP:CZ2	1:B:267:ARG:HD3	2.49	0.46
1:D:322:HIS:HB2	1:D:361:ARG:CD	2.46	0.46
1:A:242:SER:O	1:A:243:PHE:CD1	2.69	0.46
1:D:346:GLN:N	1:D:438:GLN:HE22	2.00	0.45
1:C:284:ASP:O	1:C:288[A]:GLN:HG2	2.17	0.44
1:A:408:ARG:HG3	4:A:704:HOH:O	2.16	0.44
1:D:419:PRO:O	1:D:423:MET:HG2	2.18	0.44
1:B:307:SER:OG	1:B:377:ASN:OD1	2.29	0.44
1:A:391:ARG:HG3	1:C:394:ALA:HB2	1.99	0.43
1:A:242:SER:HB2	1:A:277:ILE:HG23	2.01	0.43
1:B:248:VAL:HG21	1:B:333:PHE:HE2	1.83	0.43
1:B:347:VAL:HG23	4:B:657:HOH:O	2.18	0.43
1:B:416:LEU:HD12	1:C:397:GLN:NE2	2.30	0.43
2:D:501:KUW:C21	2:D:501:KUW:CL1	3.03	0.43
1:A:419:PRO:O	1:A:423:MET:HG2	2.18	0.43
1:B:410:LYS:HG2	1:B:411:ARG:HG3	2.00	0.43
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.34	0.43
1:B:419:PRO:O	1:B:423:MET:HG2	2.20	0.42
1:A:351:ASN:HB2	1:A:352:PRO:HD3	2.02	0.41
1:B:229:GLN:NE2	2:B:502:KUW:C19	2.83	0.41
1:B:351:ASN:HB2	1:B:352:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:HD11	1:C:401:GLU:HG3	2.02	0.41
1:B:266:GLN:NE2	4:B:604:HOH:O	2.53	0.41
1:C:369:GLU:OE1	1:C:417:ARG:NH2	2.51	0.41
1:B:429:ARG:HD3	1:B:429:ARG:HA	1.95	0.40
1:C:419:PRO:O	1:C:423:MET:HG2	2.21	0.40
1:D:351:ASN:HB2	1:D:352:PRO:HD3	2.03	0.40
1:A:415:GLN:HA	1:A:415:GLN:HE21	1.87	0.40
1:A:294:GLN:HG2	1:C:397:GLN:NE2	2.36	0.40
1:D:221:THR:H	1:D:224:GLN:HE21	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/245 (96%)	230 (98%)	1 (0%)	3 (1%)	12	4
1	B	231/245 (94%)	228 (99%)	3 (1%)	0	100	100
1	C	224/245 (91%)	221 (99%)	3 (1%)	0	100	100
1	D	233/245 (95%)	230 (99%)	2 (1%)	1 (0%)	34	24
All	All	922/980 (94%)	909 (99%)	9 (1%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	446	ASP
1	A	331	LYS
1	A	332	ASP
1	A	458	ASP

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	211/217 (97%)	196 (93%)	15 (7%)	14	6
1	B	211/217 (97%)	200 (95%)	11 (5%)	23	14
1	C	203/217 (94%)	195 (96%)	8 (4%)	32	23
1	D	212/217 (98%)	201 (95%)	11 (5%)	23	14
All	All	837/868 (96%)	792 (95%)	45 (5%)	21	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	225	GLU
1	D	271	PHE
1	D	321	ASN
1	D	331	LYS
1	D	373	LEU
1	D	415	GLN
1	D	416	LEU
1	D	443	ARG
1	D	444	LEU
1	D	446	ASP
1	D	452	LEU
1	A	219	GLN
1	A	241	ARG
1	A	243	PHE
1	A	254	LEU
1	A	261	ARG
1	A	284	ASP
1	A	330	LEU
1	A	338	ASP
1	A	373	LEU
1	A	397	GLN
1	A	401	GLU
1	A	415	GLN
1	A	429	ARG

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	459	VAL
1	B	235	GLN
1	B	240	LYS
1	B	241	ARG
1	B	242	SER
1	B	271	PHE
1	B	307	SER
1	B	321	ASN
1	B	331	LYS
1	B	416	LEU
1	B	444	LEU
1	B	448	LYS
1	C	220	LEU
1	C	237	GLN
1	C	262	ASP
1	C	271	PHE
1	C	321	ASN
1	C	330	LEU
1	C	444	LEU
1	C	459	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	224	GLN
1	D	229	GLN
1	D	300	GLN
1	D	321	ASN
1	D	438	GLN
1	A	219	GLN
1	A	224	GLN
1	A	229	GLN
1	A	294	GLN
1	A	300	GLN
1	A	346	GLN
1	A	396	GLN
1	A	415	GLN
1	B	224	GLN
1	B	229	GLN
1	B	266	GLN
1	B	294	GLN

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Mol	Chain	Res	Type
1	B	300	GLN
1	B	321	ASN
1	B	396	GLN
1	B	415	GLN
1	B	438	GLN
1	C	224	GLN
1	C	294	GLN
1	C	300	GLN
1	C	321	ASN
1	C	322	HIS
1	C	396	GLN
1	C	438	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	KUW	D	502	-	32,38,38	0.97	3 (9%)	38,56,56	2.24	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KUW	B	502	-	32,38,38	1.60	4 (12%)	38,56,56	2.28	14 (36%)
2	KUW	D	503	-	32,38,38	0.99	1 (3%)	38,56,56	2.06	15 (39%)
2	KUW	C	501	-	32,38,38	1.04	2 (6%)	38,56,56	1.89	13 (34%)
3	SO4	A	502	-	4,4,4	0.20	0	6,6,6	0.21	0
2	KUW	D	501	-	32,38,38	0.95	1 (3%)	38,56,56	1.93	13 (34%)
2	KUW	A	501	-	32,38,38	1.02	2 (6%)	38,56,56	2.07	11 (28%)
2	KUW	B	501	-	32,38,38	1.00	1 (3%)	38,56,56	2.05	15 (39%)

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	KUW	D	502	-	-	6/18/54/54	0/4/4/4
2	KUW	B	502	-	-	3/18/54/54	0/4/4/4
2	KUW	D	503	-	-	6/18/54/54	0/4/4/4
2	KUW	C	501	-	-	2/18/54/54	0/4/4/4
2	KUW	D	501	-	-	5/18/54/54	0/4/4/4
2	KUW	A	501	-	-	4/18/54/54	0/4/4/4
2	KUW	B	501	-	-	3/18/54/54	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	KUW	O17-S15	-5.01	1.39	1.43
2	B	502	KUW	O16-S15	-4.83	1.39	1.43
2	B	502	KUW	C7-C8	-3.41	1.34	1.39
2	B	501	KUW	C7-N18	3.10	1.41	1.33
2	D	503	KUW	C7-N18	3.08	1.41	1.33
2	C	501	KUW	C7-N18	3.00	1.40	1.33
2	A	501	KUW	C7-N18	2.99	1.40	1.33
2	D	501	KUW	C7-N18	2.93	1.40	1.33
2	D	502	KUW	C7-N18	2.61	1.39	1.33
2	D	502	KUW	C7-C8	-2.23	1.36	1.39
2	D	502	KUW	C23-N22	2.10	1.50	1.46
2	B	502	KUW	C7-N18	2.08	1.38	1.33
2	C	501	KUW	C21-N22	2.04	1.49	1.46
2	A	501	KUW	C23-N22	2.03	1.49	1.46

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	KUW	O16-S15-C8	-6.80	101.79	112.43
2	D	502	KUW	O16-S15-C8	-6.35	102.49	112.43
2	B	502	KUW	O16-S15-O17	4.88	123.84	116.15
2	D	502	KUW	C24-C19-N18	4.65	120.18	110.56
2	A	501	KUW	O16-S15-O17	4.54	123.30	116.15
2	D	502	KUW	O16-S15-N4	-4.46	106.96	111.30
2	D	503	KUW	O16-S15-O17	4.43	123.14	116.15
2	A	501	KUW	O16-S15-N4	-4.34	107.08	111.30
2	D	503	KUW	O16-S15-N4	-4.33	107.09	111.30
2	A	501	KUW	O6-C5-C7	-4.29	119.37	129.12
2	B	501	KUW	O16-S15-O17	4.28	122.90	116.15
2	B	502	KUW	C25-C34-CL1	4.25	125.10	121.43
2	D	503	KUW	O16-S15-C8	-4.23	105.80	112.43
2	B	501	KUW	O16-S15-N4	-4.21	107.21	111.30
2	D	501	KUW	O16-S15-N4	-4.09	107.32	111.30
2	D	503	KUW	O6-C5-C7	-4.02	119.97	129.12
2	D	501	KUW	O6-C5-C7	-3.99	120.04	129.12
2	A	501	KUW	O17-S15-C8	-3.97	106.22	112.43
2	A	501	KUW	O16-S15-C8	-3.95	106.24	112.43
2	B	502	KUW	C20-C19-N18	-3.94	102.41	110.56
2	D	502	KUW	C23-C24-C19	-3.91	103.65	110.50
2	D	502	KUW	C23-N22-C21	3.81	119.93	111.52
2	D	501	KUW	O16-S15-O17	3.79	122.13	116.15
2	C	501	KUW	O6-C5-C7	-3.75	120.59	129.12
2	B	501	KUW	O17-S15-C8	-3.74	106.57	112.43
2	C	501	KUW	O17-S15-C8	-3.72	106.61	112.43
2	B	501	KUW	O6-C5-C7	-3.70	120.70	129.12
2	D	501	KUW	C23-N22-C21	3.69	119.66	111.52
2	D	501	KUW	O17-S15-C8	-3.52	106.92	112.43
2	B	501	KUW	C23-N22-C21	3.50	119.24	111.52
2	D	502	KUW	O6-C5-C7	-3.50	121.16	129.12
2	D	502	KUW	O16-S15-O17	3.47	121.63	116.15
2	C	501	KUW	C23-N22-C21	3.45	119.13	111.52
2	B	502	KUW	C34-C25-N26	-3.39	117.45	122.91
2	D	502	KUW	O6-C5-N4	-3.38	120.88	124.76
2	C	501	KUW	O17-S15-N4	-3.33	108.06	111.30
2	B	501	KUW	O17-S15-N4	-3.20	108.19	111.30
2	A	501	KUW	C33-C28-C27	3.15	119.75	116.71
2	B	502	KUW	C21-C20-C19	3.15	116.02	110.50
2	D	502	KUW	C19-N18-C7	3.13	137.94	125.32
2	B	502	KUW	O16-S15-N4	-3.10	108.29	111.30
2	C	501	KUW	C25-C34-CL1	3.09	124.10	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	KUW	C23-N22-C21	3.05	118.24	111.52
2	B	501	KUW	C33-C28-C27	3.05	119.65	116.71
2	C	501	KUW	C33-C28-C27	2.97	119.58	116.71
2	C	501	KUW	O16-S15-O17	2.97	120.83	116.15
2	D	501	KUW	C33-C28-C27	2.96	119.57	116.71
2	D	501	KUW	C25-C34-CL1	2.91	123.94	121.43
2	D	503	KUW	O17-S15-C8	-2.86	107.95	112.43
2	C	501	KUW	O6-C5-N4	-2.85	121.49	124.76
2	B	502	KUW	C19-N18-C7	2.84	136.78	125.32
2	B	502	KUW	O6-C5-N4	-2.80	121.54	124.76
2	B	501	KUW	C25-C34-CL1	2.80	123.85	121.43
2	C	501	KUW	C34-C25-N26	-2.77	118.44	122.91
2	B	502	KUW	O6-C5-C7	-2.70	122.97	129.12
2	A	501	KUW	C28-C27-N26	-2.67	119.75	123.95
2	B	502	KUW	C33-C34-CL1	-2.66	114.20	118.49
2	A	501	KUW	C27-N26-C25	2.61	123.48	115.17
2	B	502	KUW	C27-N26-C25	2.57	123.35	115.17
2	D	503	KUW	C21-C20-C19	2.56	115.00	110.50
2	B	501	KUW	O6-C5-N4	-2.55	121.83	124.76
2	D	503	KUW	C33-C28-C27	2.54	119.17	116.71
2	D	503	KUW	C23-N22-C25	-2.54	110.20	119.05
2	B	501	KUW	C34-C33-C28	-2.54	118.72	120.46
2	D	502	KUW	C34-C25-N26	-2.51	118.87	122.91
2	C	501	KUW	C27-N26-C25	2.50	123.12	115.17
2	D	503	KUW	C27-N26-C25	2.50	123.11	115.17
2	D	501	KUW	C28-C27-N26	-2.49	120.04	123.95
2	A	501	KUW	C34-C25-N26	-2.47	118.94	122.91
2	D	503	KUW	C20-C19-N18	-2.46	105.48	110.56
2	B	501	KUW	C14-C9-C8	-2.43	117.86	120.55
2	D	501	KUW	C27-N26-C25	2.41	122.83	115.17
2	D	503	KUW	O6-C5-N4	-2.37	122.04	124.76
2	D	503	KUW	C28-C27-N26	-2.37	120.23	123.95
2	C	501	KUW	C28-C27-N26	-2.35	120.25	123.95
2	B	501	KUW	C27-N26-C25	2.32	122.56	115.17
2	D	503	KUW	C34-C25-N26	-2.31	119.19	122.91
2	D	501	KUW	C34-C25-N26	-2.30	119.20	122.91
2	C	501	KUW	C34-C33-C28	-2.29	118.90	120.46
2	D	502	KUW	C27-N26-C25	2.28	122.43	115.17
2	D	503	KUW	C23-N22-C21	2.28	116.54	111.52
2	B	501	KUW	C34-C25-N26	-2.20	119.36	122.91
2	B	501	KUW	O16-S15-C8	-2.18	109.02	112.43
2	D	501	KUW	O6-C5-N4	-2.16	122.27	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	KUW	O16-S15-C8	-2.14	109.08	112.43
2	B	502	KUW	C23-N22-C21	2.09	116.14	111.52
2	B	501	KUW	C28-C27-N26	-2.08	120.67	123.95
2	B	502	KUW	C24-C19-N18	-2.08	106.25	110.56
2	A	501	KUW	C34-C33-C28	-2.07	119.05	120.46
2	D	502	KUW	C21-C20-C19	-2.06	106.89	110.50
2	C	501	KUW	O16-S15-N4	-2.05	109.31	111.30
2	D	503	KUW	C14-C9-C8	-2.02	118.32	120.55
2	D	501	KUW	O17-S15-N4	-2.01	109.34	111.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	502	KUW	C8-C7-N18-C19
2	D	502	KUW	C24-C19-N18-C7
2	B	502	KUW	C3-C2-N4-C5
2	D	503	KUW	C8-C7-N18-C19
2	D	502	KUW	N26-C25-N22-C21
2	D	501	KUW	N26-C25-N22-C23
2	D	502	KUW	C34-C25-N22-C21
2	D	501	KUW	C34-C25-N22-C23
2	A	501	KUW	C3-C2-N4-C5
2	D	503	KUW	N26-C25-N22-C21
2	D	503	KUW	C5-C7-N18-C19
2	D	503	KUW	C1-C2-N4-S15
2	C	501	KUW	C3-C2-N4-S15
2	D	501	KUW	C3-C2-N4-S15
2	A	501	KUW	C3-C2-N4-S15
2	B	501	KUW	C3-C2-N4-S15
2	D	502	KUW	C3-C2-N4-C5
2	C	501	KUW	C3-C2-N4-C5
2	B	501	KUW	C3-C2-N4-C5
2	D	503	KUW	N26-C25-N22-C23
2	D	503	KUW	C1-C2-N4-C5
2	D	501	KUW	C3-C2-N4-C5
2	D	501	KUW	C7-C8-C9-C10
2	A	501	KUW	C7-C8-C9-C10
2	A	501	KUW	C7-C8-C9-C14
2	B	501	KUW	C7-C8-C9-C10
2	D	502	KUW	C5-C7-N18-C19
2	B	502	KUW	C5-C7-N18-C19

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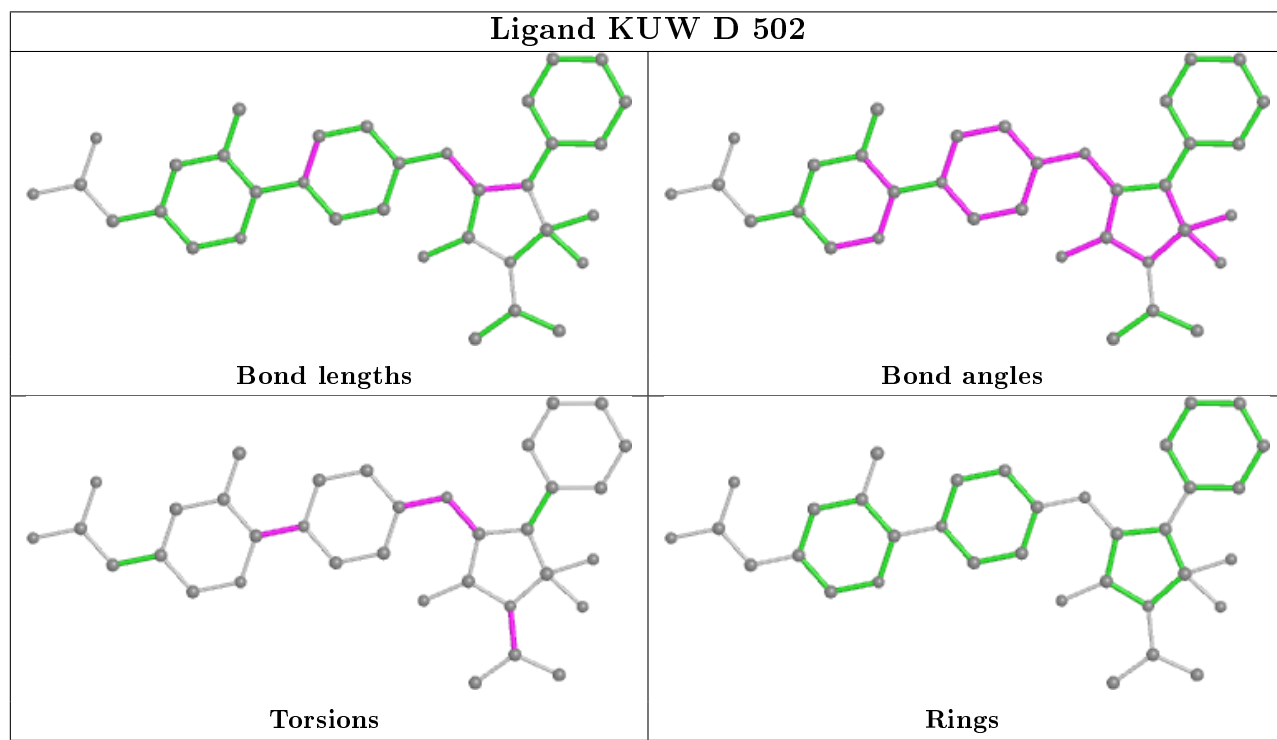
Mol	Chain	Res	Type	Atoms
2	B	502	KUW	C8-C7-N18-C19

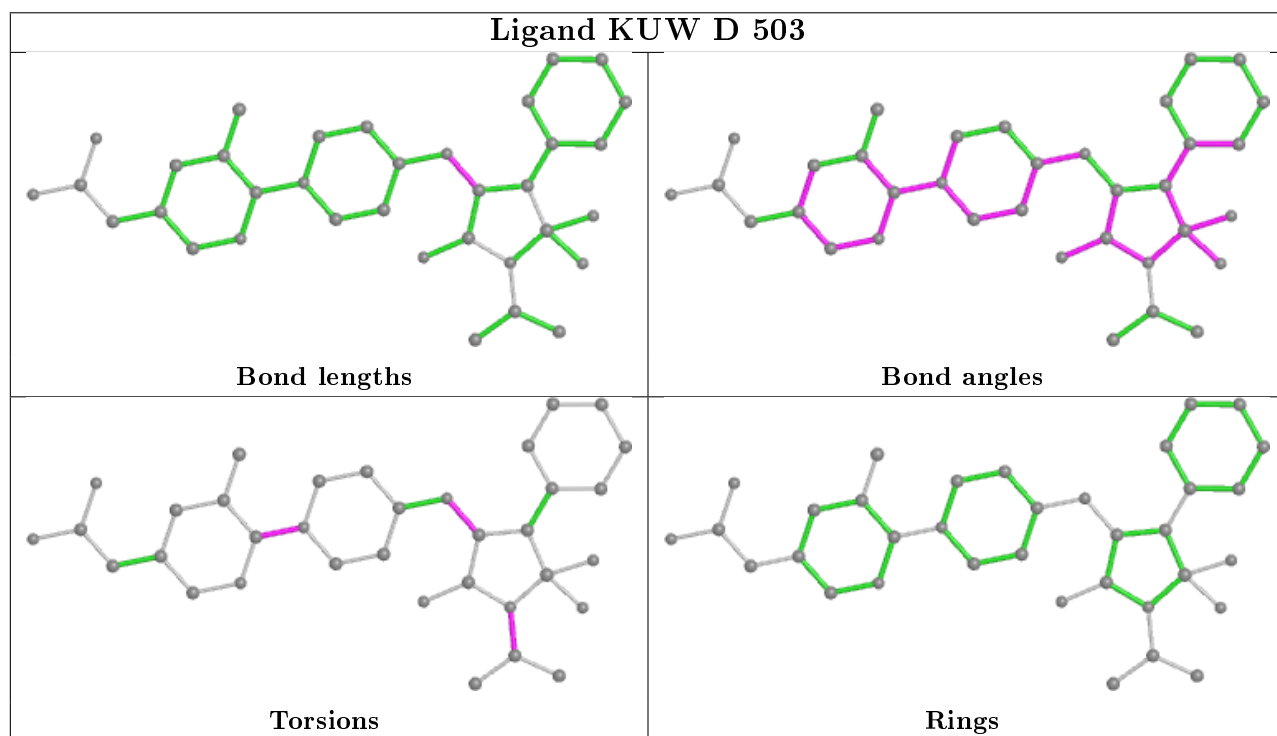
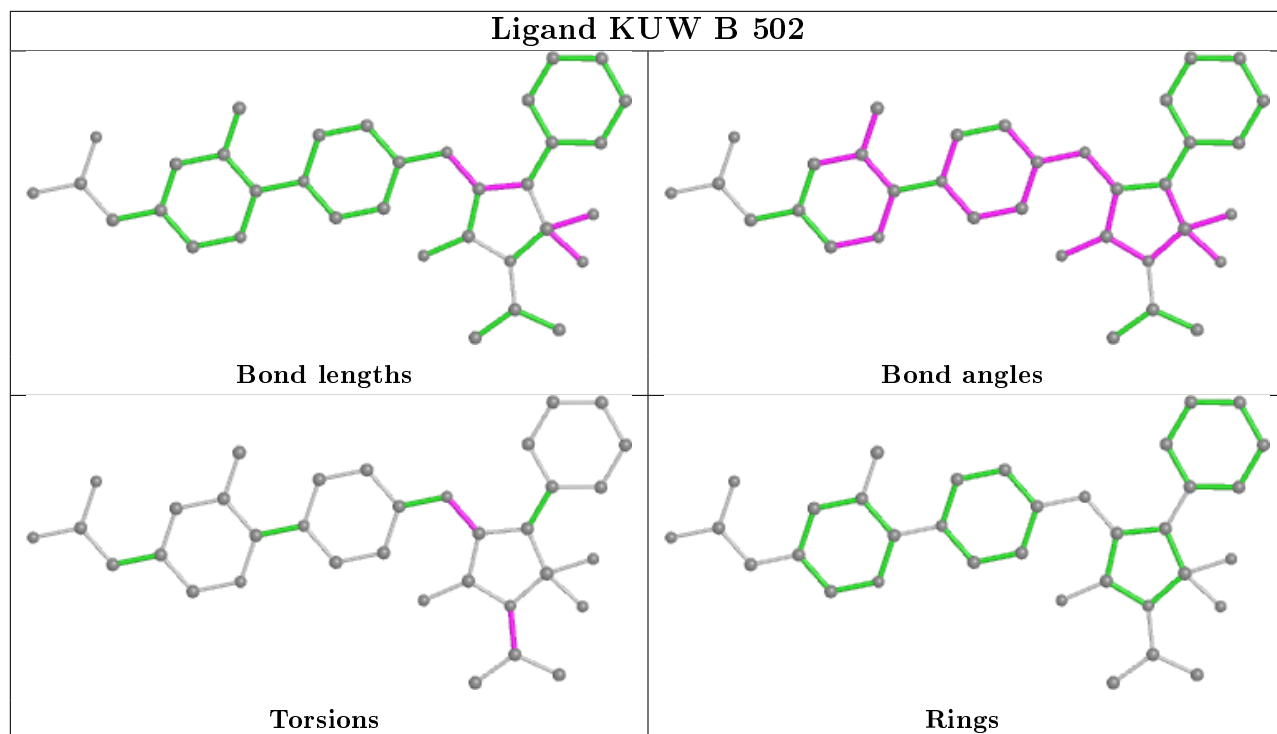
There are no ring outliers.

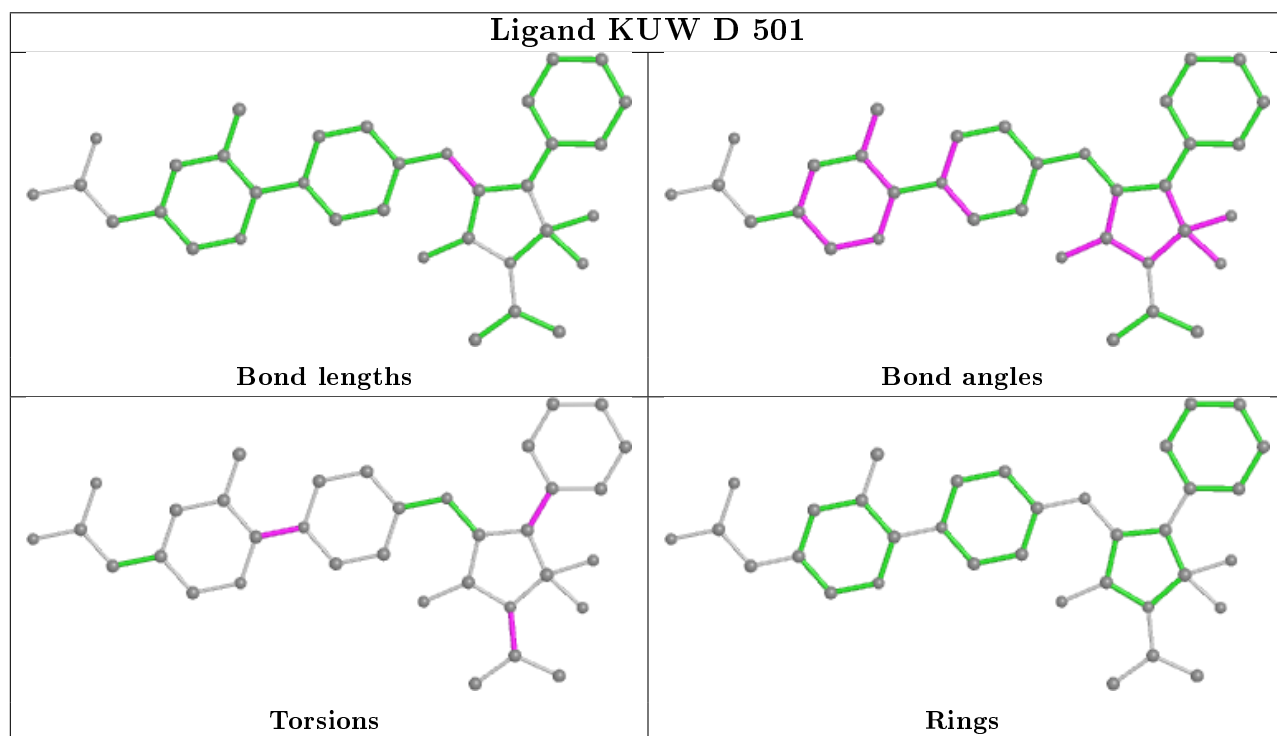
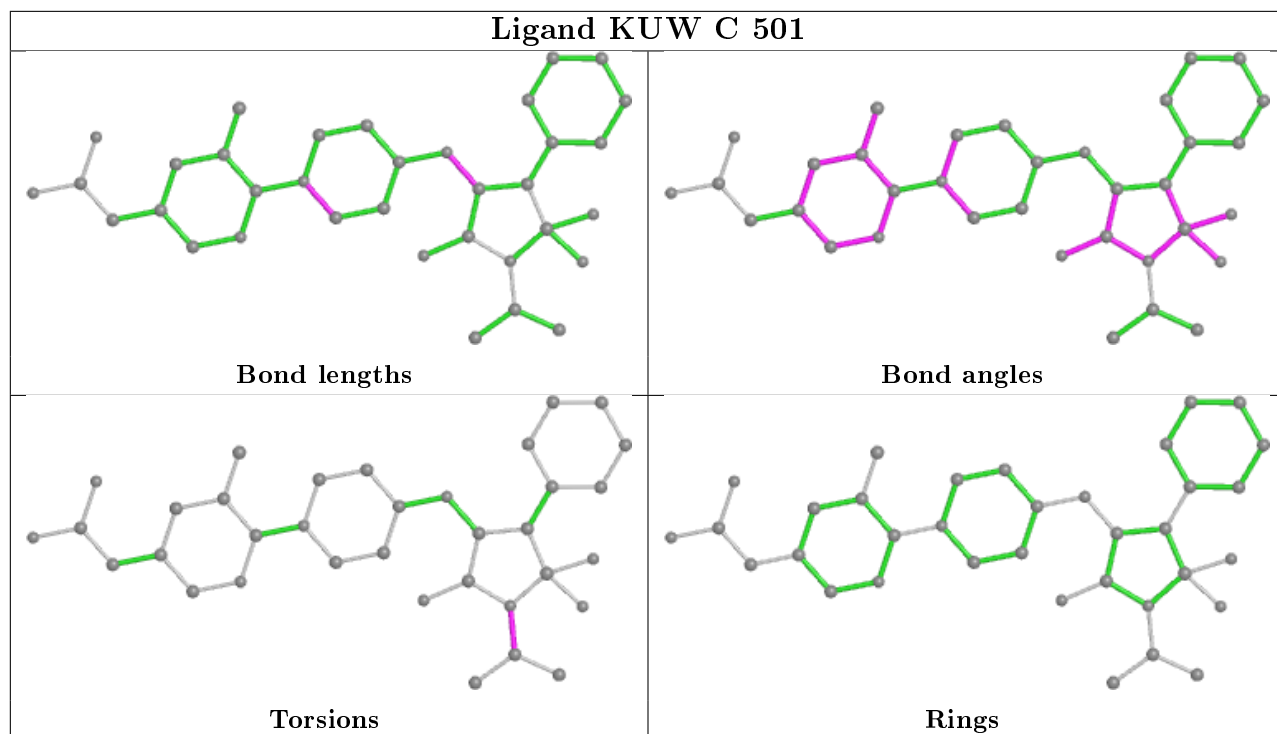
2 monomers are involved in 6 short contacts:

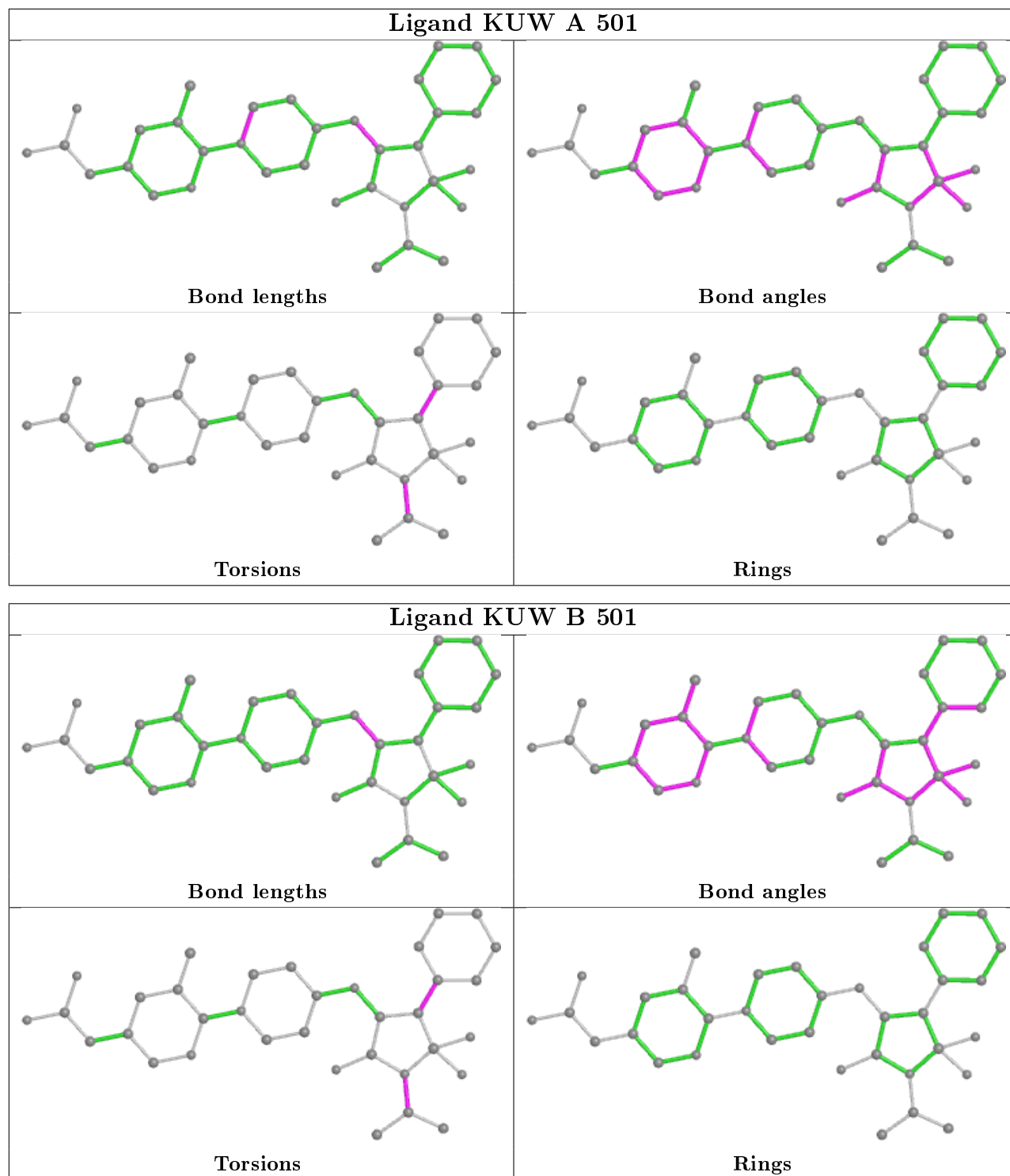
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	KUW	5	0
2	D	501	KUW	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	252:PRO	C	253:LEU	N	1.13

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	236/245 (96%)	0.19	4 (1%) 70 72	13, 22, 39, 64	8 (3%)
1	B	233/245 (95%)	0.34	10 (4%) 35 38	15, 24, 47, 75	5 (2%)
1	C	224/245 (91%)	0.31	12 (5%) 25 29	13, 23, 44, 58	3 (1%)
1	D	235/245 (95%)	0.12	3 (1%) 77 79	13, 22, 39, 51	10 (4%)
All	All	928/980 (94%)	0.24	29 (3%) 49 51	13, 23, 43, 75	26 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	VAL	4.5
1	B	244	SER	4.5
1	C	444	LEU	3.9
1	C	244	SER	3.8
1	B	459	VAL	3.7
1	B	243	PHE	3.7
1	A	446	ASP	3.7
1	A	459	VAL	3.5
1	B	254	GLY	3.2
1	C	416	LEU	3.1
1	D	243	PHE	2.9
1	B	238	CYS	2.9
1	B	446	ASP	2.9
1	C	446	ASP	2.8
1	C	323	GLU	2.6
1	D	446	ASP	2.6
1	B	237	GLN	2.5
1	B	408	ARG	2.5
1	C	322	HIS	2.4
1	C	332	ASP	2.4
1	A	243	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	265	GLN	2.3
1	C	342	ARG	2.3
1	C	384	PRO	2.3
1	D	334[A]	THR	2.2
1	B	242	SER	2.2
1	C	266	GLN	2.2
1	A	219	GLN	2.1
1	B	240	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

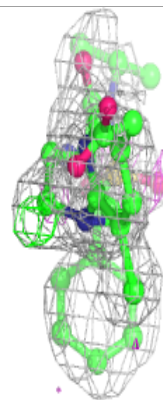
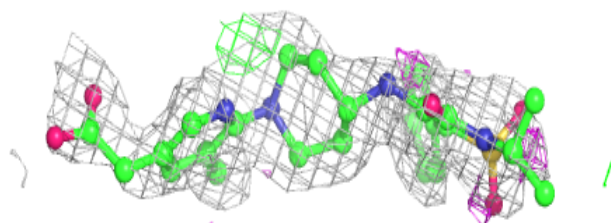
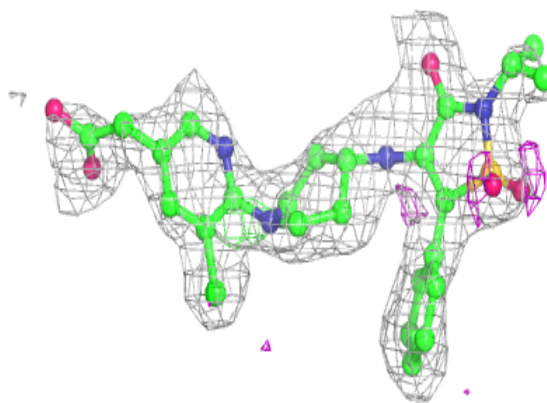
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KUW	D	503	35/35	0.79	0.24	44,51,55,57	0
2	KUW	B	502	35/35	0.87	0.18	31,37,65,73	0
2	KUW	D	502	35/35	0.88	0.18	30,37,58,60	0
2	KUW	C	501	35/35	0.96	0.10	18,19,26,28	0
2	KUW	A	501	35/35	0.96	0.10	16,18,26,27	0
2	KUW	B	501	35/35	0.96	0.11	17,18,26,27	0
3	SO4	A	502	5/5	0.97	0.18	26,27,29,31	0
2	KUW	D	501	35/35	0.97	0.10	15,16,22,23	0

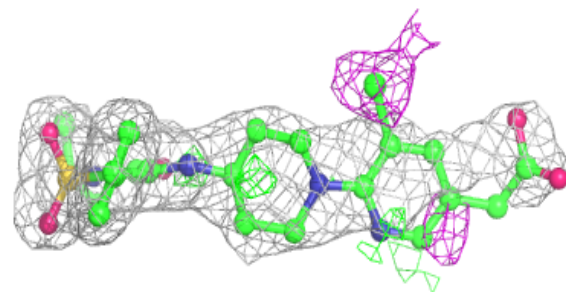
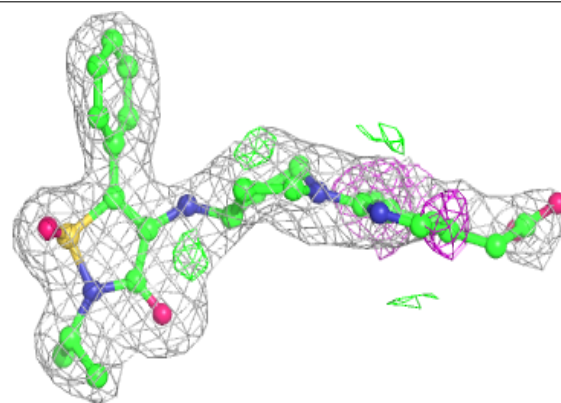
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K UW D 503:

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

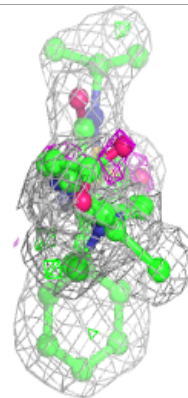
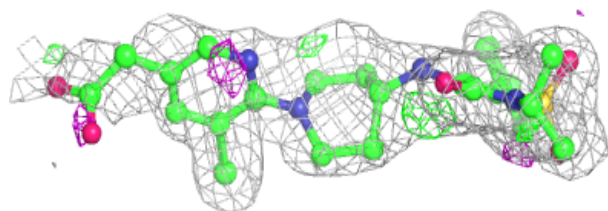
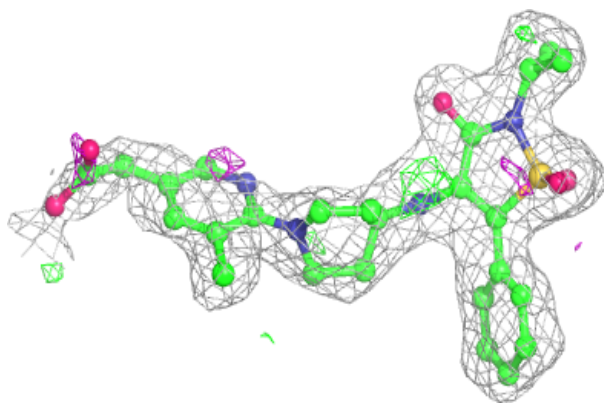
**Electron density around K UW B 502:**

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

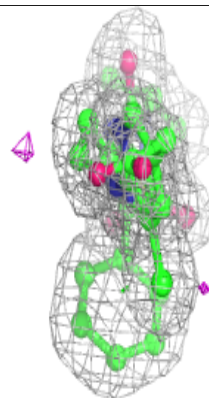
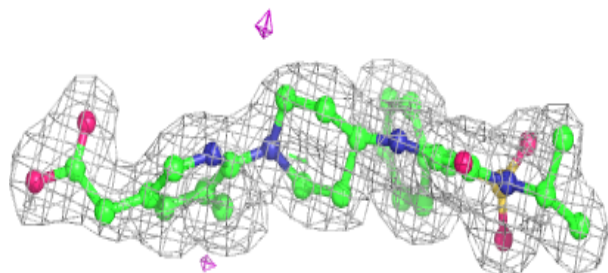
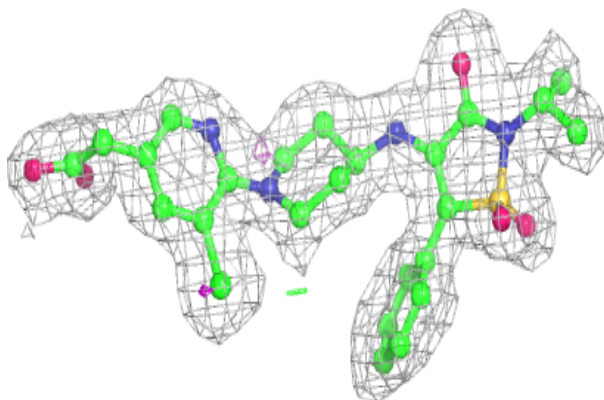


Electron density around K UW D 502:

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

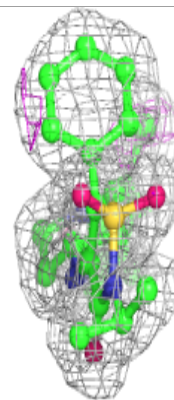
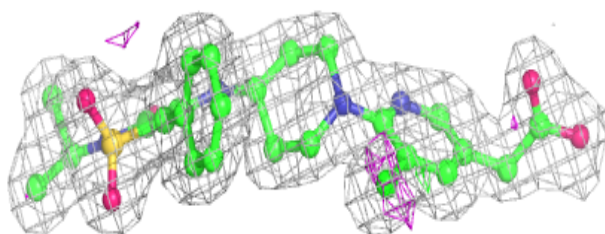
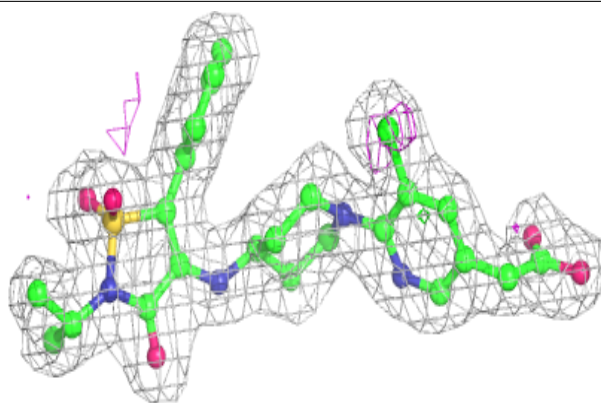
**Electron density around K UW C 501:**

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

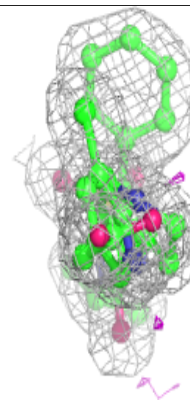
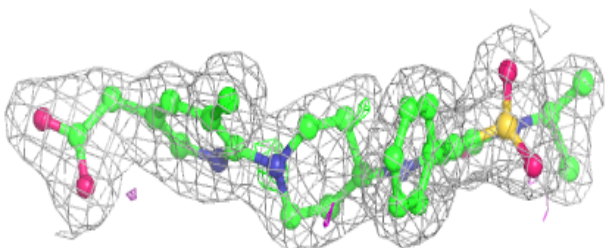
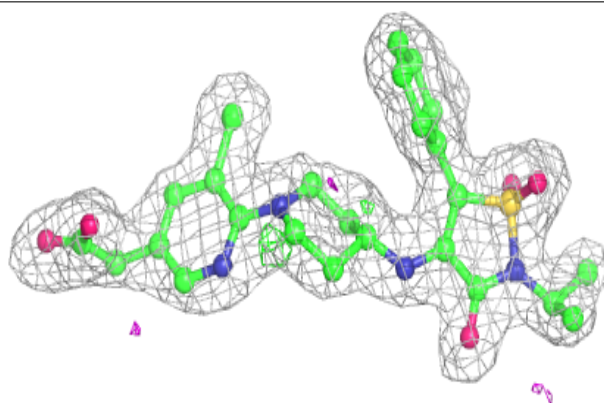


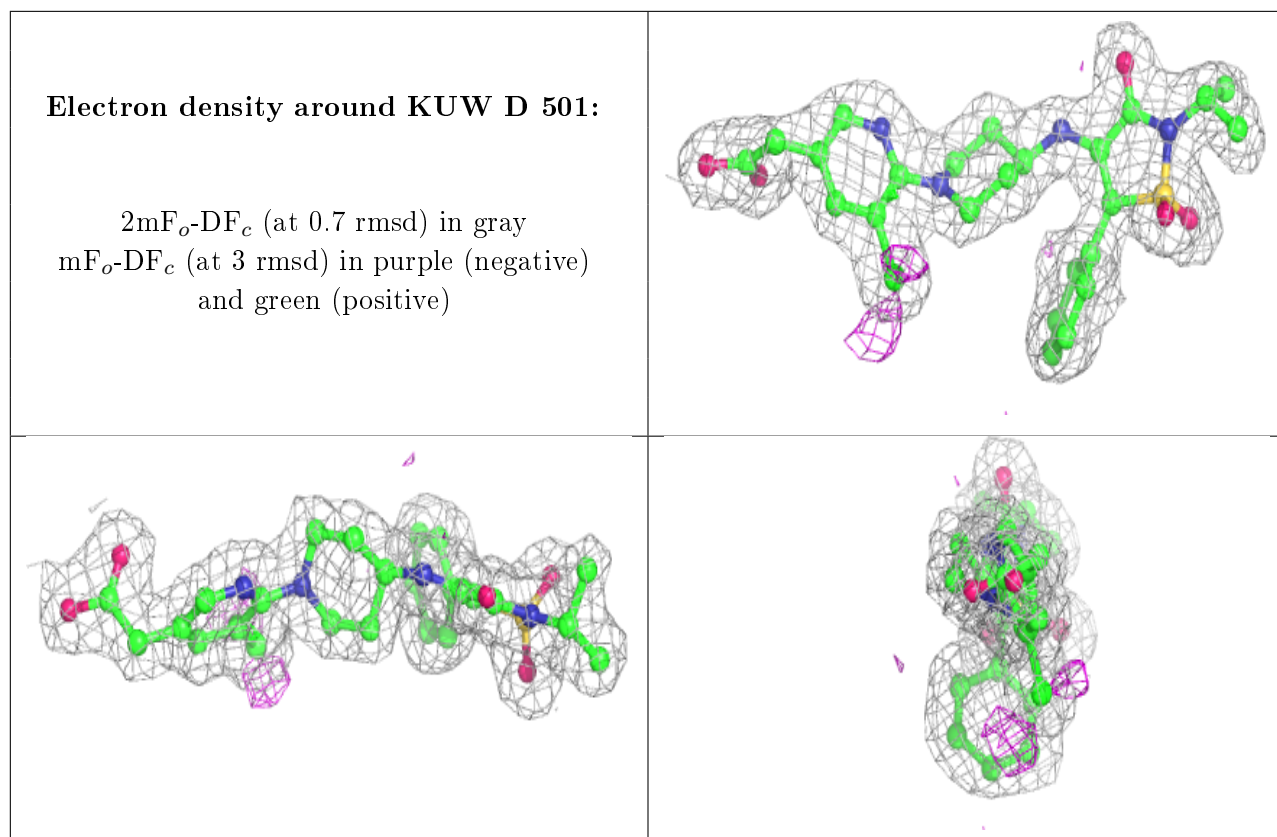
Electron density around K UW A 501:

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

**Electron density around K UW B 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.