



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 6S4N / pdb_00006s4n
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

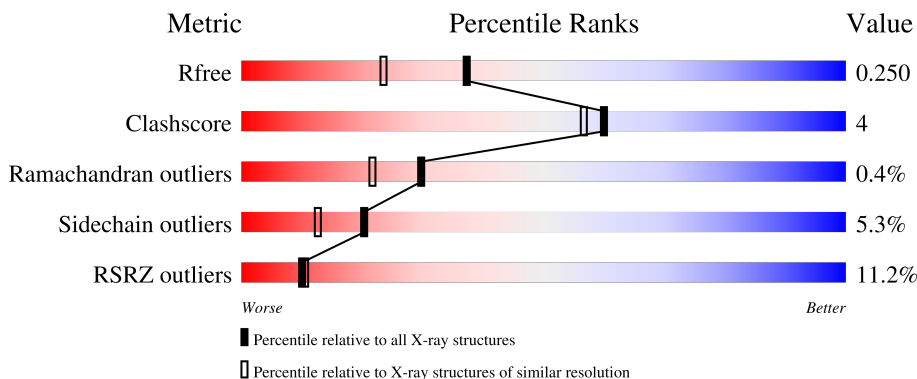
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	245	8% 81% 13% • •
1	B	245	15% 79% 15% • 5%
1	C	245	11% 78% 13% 9%
1	D	245	8% 86% 9% • •

2 Entry composition [i](#)

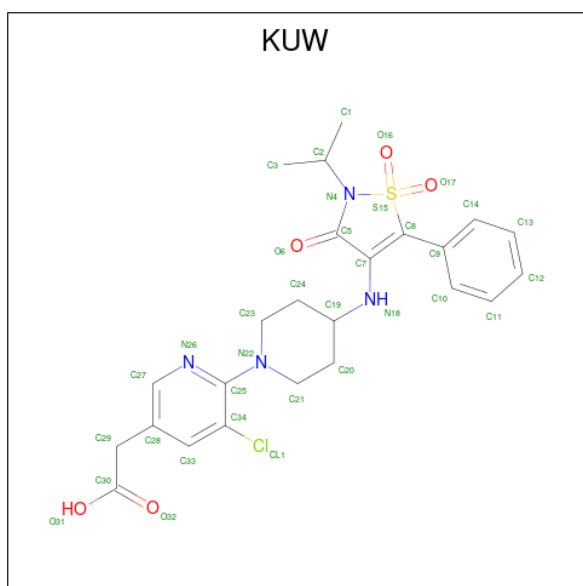
There are 4 unique types of molecules in this entry. The entry contains 8422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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 (CCD ID: KUW) (formula: C₂₄H₂₇ClN₄O₅S) (labeled as "Ligand of Interest" by depositor).



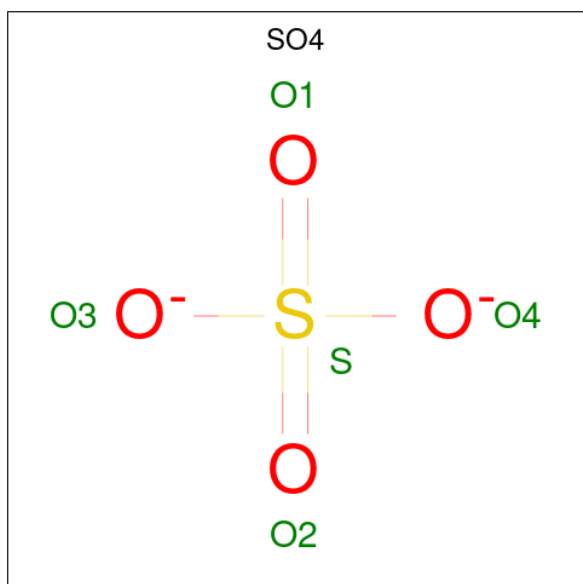
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	Cl	N	O	S	0	0
			35	24	1	4	5	1		

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

- Molecule 3 is SULFATE ION (CCD ID: 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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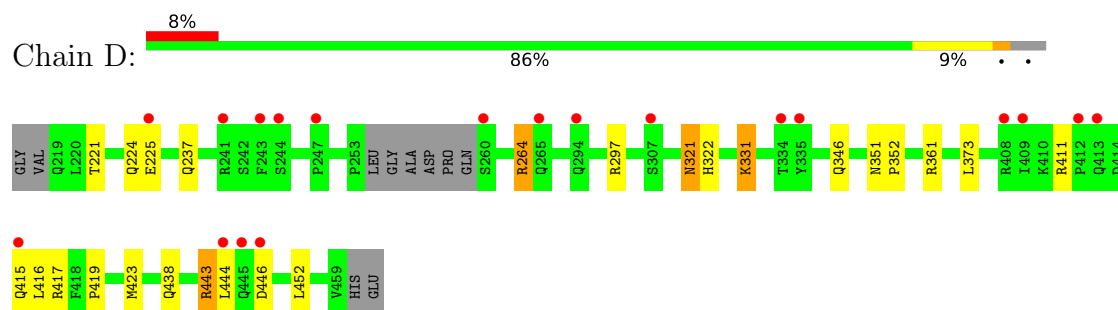
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	105	Total 105	O 105	0	0
4	C	146	Total 146	O 146	0	0

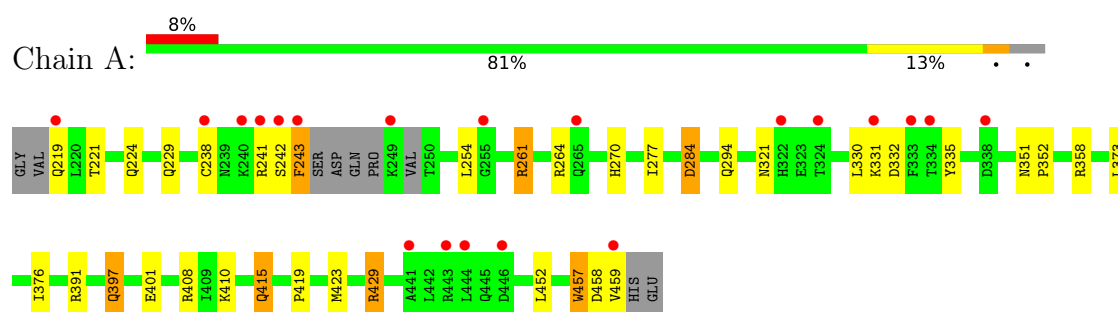
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

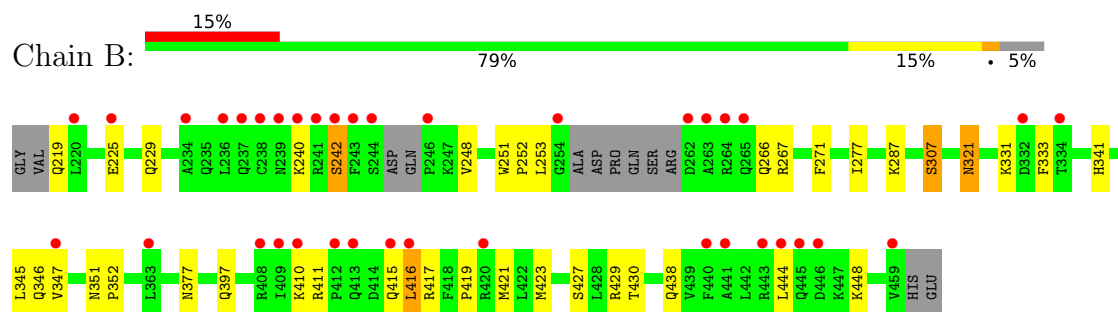
- Molecule 1: Oxysterols receptor LXR-beta



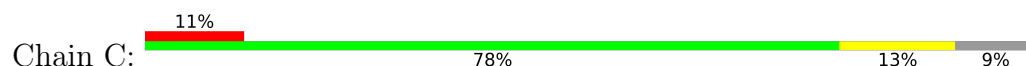
- Molecule 1: Oxysterols receptor LXR-beta

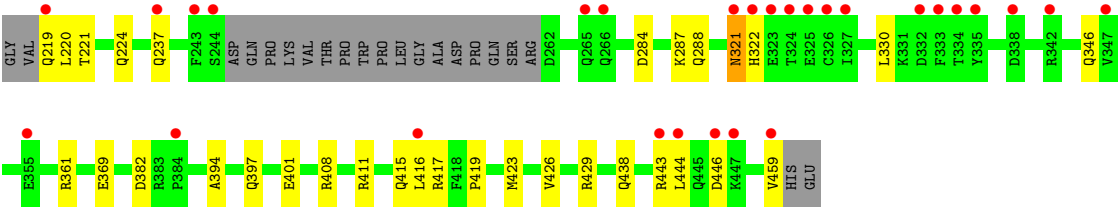


- Molecule 1: Oxysterols receptor LXR-beta



- Molecule 1: Oxysterols receptor LXR-beta





4 Data and refinement statistics

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 54.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (54.72-1.90) 92.3 (54.72-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.90Å)	Xtriage
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 (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SO4, KUW

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	0.83	2/1972 (0.1%)	1.08	6/2665 (0.2%)
1	B	0.78	1/1971 (0.1%)	1.00	4/2663 (0.2%)
1	C	0.94	3/1889 (0.2%)	1.11	4/2550 (0.2%)
1	D	0.95	4/1974 (0.2%)	1.01	9/2668 (0.3%)
All	All	0.88	10/7806 (0.1%)	1.05	23/10546 (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	D	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	411	ARG	CD-NE	25.76	1.82	1.46
1	C	446	ASP	CB-CG	20.41	2.03	1.52
1	C	408	ARG	CD-NE	-17.25	1.22	1.46
1	B	252	PRO	C-N	-14.50	1.13	1.33
1	A	264	ARG	CD-NE	-12.85	1.28	1.46
1	A	358	ARG	CD-NE	-10.97	1.30	1.46
1	D	443	ARG	CG-CD	-9.13	1.25	1.52
1	D	297	ARG	CG-CD	6.50	1.72	1.52
1	D	264	ARG	CB-CG	-5.88	1.34	1.52
1	C	415	GLN	CB-CG	5.61	1.69	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	ASP	CA-CB-CG	-28.05	84.55	112.60
1	A	264	ARG	CD-NE-CZ	15.24	145.74	124.40
1	A	358	ARG	CD-NE-CZ	15.11	145.55	124.40
1	A	457	TRP	N-CA-C	-9.94	95.37	109.69
1	B	253	LEU	O-C-N	9.68	134.43	123.01
1	A	264	ARG	CG-CD-NE	7.77	129.09	112.00
1	B	252	PRO	CA-C-N	7.12	131.61	121.42
1	B	252	PRO	C-N-CA	7.12	131.61	121.42
1	C	446	ASP	CB-CG-OD1	7.05	134.61	118.40
1	C	446	ASP	CB-CG-OD2	-7.04	102.20	118.40
1	D	237	GLN	CG-CD-NE2	7.01	126.91	116.40
1	C	415	GLN	CA-CB-CG	-6.34	101.42	114.10
1	D	417	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	D	297	ARG	CB-CG-CD	-5.75	98.07	111.30
1	D	297	ARG	CG-CD-NE	5.67	124.48	112.00
1	D	417	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	B	287	LYS	CG-CD-CE	5.39	123.70	111.30
1	A	321	ASN	CA-C-N	5.28	127.61	120.38
1	A	321	ASN	C-N-CA	5.28	127.61	120.38
1	D	331	LYS	N-CA-C	5.20	121.88	110.80
1	D	411	ARG	CG-CD-NE	-5.20	100.56	112.00
1	D	264	ARG	CA-CB-CG	5.16	124.42	114.10
1	D	237	GLN	CG-CD-OE1	-5.11	110.57	120.80

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

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	18	0
1	B	1922	0	1958	30	0
1	C	1845	0	1889	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1931	0	1966	8	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	66	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 (66) 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:CL1	2:B:502:KUW:C21	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
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:321:ASN:HD22	1:B:321:ASN:C	2.17	0.53
1:B:417:ARG:HG2	1:B:421:MET:HE3	1.91	0.53
1:D:321:ASN:C	1:D:321:ASN:HD22	2.17	0.52
1:B:229:GLN:HE22	2:B:502:KUW:C19	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ASN:C	1:C:321:ASN:HD22	2.18	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: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: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: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:CL1	2:D:501:KUW:C21	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:D:423:MET:HE1	1:A:376:ILE:HG21	2.01	0.42
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
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:D:351:ASN:HB2	1:D:352:PRO:HD3	2.03	0.40
1:C:419:PRO:O	1:C:423:MET:HG2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	9	3
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%)	30	22
All	All	922/980 (94%)	909 (99%)	9 (1%)	4 (0%)	30	22

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%)	13	7
1	B	211/217 (97%)	200 (95%)	11 (5%)	21	13
1	C	203/217 (94%)	195 (96%)	8 (4%)	28	21
1	D	212/217 (98%)	202 (95%)	10 (5%)	23	15
All	All	837/868 (96%)	793 (95%)	44 (5%)	20	12

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	225	GLU
1	D	264	ARG
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	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	373	LEU
1	A	397	GLN
1	A	401	GLU
1	A	410	LYS
1	A	415	GLN
1	A	429	ARG
1	A	452	LEU
1	A	459	VAL
1	B	219	GLN
1	B	240	LYS
1	B	242	SER
1	B	271	PHE
1	B	307	SER
1	B	321	ASN
1	B	331	LYS
1	B	345	LEU

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Mol	Chain	Res	Type
1	B	416	LEU
1	B	444	LEU
1	B	448	LYS
1	C	220	LEU
1	C	237	GLN
1	C	287	LYS
1	C	321	ASN
1	C	330	LEU
1	C	411	ARG
1	C	444	LEU
1	C	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	224	GLN
1	D	229	GLN
1	D	246	GLN
1	D	300	GLN
1	D	321	ASN
1	D	341	HIS
1	D	396	GLN
1	D	413	GLN
1	D	438	GLN
1	A	219	GLN
1	A	224	GLN
1	A	229	GLN
1	A	239	ASN
1	A	294	GLN
1	A	300	GLN
1	A	346	GLN
1	A	377	ASN
1	A	396	GLN
1	A	415	GLN
1	B	224	GLN
1	B	229	GLN
1	B	239	ASN
1	B	266	GLN
1	B	280	GLN
1	B	294	GLN
1	B	300	GLN
1	B	321	ASN

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Mol	Chain	Res	Type
1	B	346	GLN
1	B	396	GLN
1	B	415	GLN
1	B	438	GLN
1	C	224	GLN
1	C	266	GLN
1	C	300	GLN
1	C	321	ASN
1	C	322	HIS
1	C	341	HIS
1	C	377	ASN
1	C	396	GLN
1	C	397	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 oligosaccharides 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
3	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.22	0
2	KUW	D	501	-	36,38,38	1.39	4 (11%)	46,56,56	2.42	17 (36%)
2	KUW	B	501	-	36,38,38	1.43	4 (11%)	46,56,56	2.41	19 (41%)
2	KUW	D	503	-	36,38,38	1.35	4 (11%)	46,56,56	2.54	18 (39%)
2	KUW	D	502	-	36,38,38	1.41	5 (13%)	46,56,56	2.66	15 (32%)
2	KUW	A	501	-	36,38,38	1.40	5 (13%)	46,56,56	2.53	16 (34%)
2	KUW	B	502	-	36,38,38	1.80	6 (16%)	46,56,56	2.53	17 (36%)
2	KUW	C	501	-	36,38,38	1.44	4 (11%)	46,56,56	2.39	17 (36%)

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	501	-	-	6/20/54/54	0/4/4/4
2	KUW	B	501	-	-	3/20/54/54	0/4/4/4
2	KUW	D	503	-	-	8/20/54/54	0/4/4/4
2	KUW	D	502	-	-	8/20/54/54	0/4/4/4
2	KUW	A	501	-	-	4/20/54/54	0/4/4/4
2	KUW	B	502	-	-	5/20/54/54	0/4/4/4
2	KUW	C	501	-	-	4/20/54/54	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	KUW	C5-N4	-4.61	1.35	1.41
2	D	501	KUW	C5-N4	-4.59	1.35	1.41
2	C	501	KUW	C5-N4	-4.57	1.35	1.41
2	D	502	KUW	C5-N4	-4.41	1.35	1.41
2	B	502	KUW	O17-S15	-4.35	1.39	1.43
2	A	501	KUW	C5-N4	-4.22	1.35	1.41
2	B	502	KUW	O16-S15	-4.19	1.39	1.43
2	B	501	KUW	C5-N4	-4.13	1.35	1.41
2	D	503	KUW	O32-C30	3.92	1.34	1.22
2	B	501	KUW	O32-C30	3.88	1.34	1.22
2	D	502	KUW	O32-C30	3.88	1.34	1.22
2	B	502	KUW	C7-C8	-3.68	1.34	1.39
2	D	501	KUW	O32-C30	3.65	1.34	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KUW	O32-C30	3.59	1.33	1.22
2	A	501	KUW	O32-C30	3.45	1.33	1.22
2	B	502	KUW	O32-C30	3.44	1.33	1.22
2	B	502	KUW	O31-C30	-3.30	1.19	1.30
2	B	501	KUW	O31-C30	-3.23	1.20	1.30
2	D	503	KUW	C5-N4	-3.23	1.37	1.41
2	B	501	KUW	C7-N18	2.97	1.41	1.33
2	D	503	KUW	C7-N18	2.94	1.41	1.33
2	C	501	KUW	C7-N18	2.86	1.40	1.33
2	D	503	KUW	O31-C30	-2.85	1.21	1.30
2	A	501	KUW	C7-N18	2.85	1.40	1.33
2	D	502	KUW	O31-C30	-2.84	1.21	1.30
2	D	501	KUW	C7-N18	2.80	1.40	1.33
2	D	501	KUW	O31-C30	-2.79	1.21	1.30
2	A	501	KUW	O31-C30	-2.75	1.21	1.30
2	C	501	KUW	O31-C30	-2.64	1.22	1.30
2	D	502	KUW	C7-N18	2.48	1.39	1.33
2	D	502	KUW	C7-C8	-2.43	1.36	1.39
2	A	501	KUW	C34-C25	2.07	1.42	1.39

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	KUW	C7-C5-N4	9.69	118.11	106.01
2	D	503	KUW	C7-C5-N4	9.58	117.98	106.01
2	D	502	KUW	C7-C5-N4	9.55	117.94	106.01
2	C	501	KUW	C7-C5-N4	9.53	117.92	106.01
2	D	501	KUW	C7-C5-N4	9.32	117.65	106.01
2	B	501	KUW	C7-C5-N4	9.17	117.47	106.01
2	B	502	KUW	C7-C5-N4	7.58	115.48	106.01
2	B	502	KUW	O16-S15-C8	-6.59	101.79	112.41
2	D	502	KUW	O16-S15-C8	-6.15	102.49	112.41
2	B	502	KUW	C9-C8-S15	5.49	126.58	118.64
2	D	503	KUW	C9-C8-S15	5.18	126.14	118.64
2	B	502	KUW	O16-S15-O17	4.90	123.84	116.08
2	D	502	KUW	C9-C8-S15	4.83	125.64	118.64
2	D	502	KUW	C24-C19-N18	4.81	120.18	110.57
2	A	501	KUW	O16-S15-O17	4.56	123.30	116.08
2	D	502	KUW	O16-S15-N4	-4.46	106.96	111.30
2	D	503	KUW	O16-S15-O17	4.46	123.14	116.08
2	D	502	KUW	C23-C24-C19	-4.45	103.65	110.67
2	A	501	KUW	O16-S15-N4	-4.34	107.08	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	KUW	O16-S15-N4	-4.33	107.09	111.30
2	B	501	KUW	O16-S15-O17	4.31	122.90	116.08
2	A	501	KUW	O6-C5-C7	-4.29	119.37	129.08
2	B	501	KUW	O16-S15-N4	-4.21	107.21	111.30
2	D	503	KUW	O16-S15-C8	-4.10	105.80	112.41
2	D	501	KUW	O16-S15-N4	-4.09	107.32	111.30
2	B	502	KUW	C20-C19-N18	-4.08	102.41	110.57
2	D	502	KUW	O6-C5-N4	-4.03	120.88	124.84
2	D	503	KUW	O6-C5-C7	-4.02	119.97	129.08
2	D	501	KUW	O6-C5-C7	-3.99	120.04	129.08
2	A	501	KUW	O17-S15-C8	-3.84	106.22	112.41
2	A	501	KUW	O16-S15-C8	-3.83	106.24	112.41
2	B	502	KUW	C25-C34-CL1	3.82	125.10	121.50
2	D	501	KUW	O16-S15-O17	3.82	122.13	116.08
2	C	501	KUW	O6-C5-C7	-3.75	120.59	129.08
2	D	501	KUW	C1-C2-N4	-3.74	104.92	112.54
2	D	502	KUW	C23-N22-C21	3.72	119.93	111.57
2	B	501	KUW	O6-C5-C7	-3.70	120.70	129.08
2	C	501	KUW	C9-C8-S15	3.67	123.95	118.64
2	B	501	KUW	O17-S15-C8	-3.62	106.57	112.41
2	C	501	KUW	O17-S15-C8	-3.60	106.61	112.41
2	D	501	KUW	C23-N22-C21	3.60	119.66	111.57
2	A	501	KUW	C1-C2-N4	-3.57	105.26	112.54
2	B	502	KUW	C34-C25-N26	-3.56	117.45	123.00
2	D	502	KUW	O16-S15-O17	3.50	121.63	116.08
2	D	502	KUW	O6-C5-C7	-3.50	121.16	129.08
2	B	501	KUW	C23-N22-C21	3.41	119.24	111.57
2	C	501	KUW	O6-C5-N4	-3.41	121.49	124.84
2	D	501	KUW	O17-S15-C8	-3.40	106.92	112.41
2	B	502	KUW	C21-C20-C19	3.39	116.02	110.67
2	C	501	KUW	C23-N22-C21	3.36	119.13	111.57
2	B	502	KUW	O6-C5-N4	-3.35	121.54	124.84
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	D	501	KUW	C9-C8-S15	3.19	123.25	118.64
2	B	502	KUW	O16-S15-N4	-3.10	108.29	111.30
2	B	501	KUW	C9-C8-S15	3.08	123.11	118.64
2	A	501	KUW	C33-C28-C27	3.08	119.75	116.90
2	B	501	KUW	O6-C5-N4	-3.07	121.83	124.84
2	C	501	KUW	O16-S15-O17	3.00	120.83	116.08
2	B	501	KUW	C33-C28-C27	2.97	119.65	116.90
2	A	501	KUW	C23-N22-C21	2.97	118.24	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	KUW	C34-C25-N26	-2.93	118.44	123.00
2	C	501	KUW	C33-C28-C27	2.89	119.58	116.90
2	D	501	KUW	C33-C28-C27	2.88	119.57	116.90
2	A	501	KUW	C28-C27-N26	-2.85	119.75	123.99
2	D	503	KUW	O6-C5-N4	-2.85	122.04	124.84
2	D	503	KUW	O17-S15-C8	-2.76	107.95	112.41
2	C	501	KUW	C25-C34-CL1	2.76	124.10	121.50
2	B	501	KUW	C1-C2-N4	-2.75	106.93	112.54
2	D	503	KUW	C21-C20-C19	2.74	115.00	110.67
2	A	501	KUW	C9-C8-S15	2.74	122.61	118.64
2	B	502	KUW	O6-C5-C7	-2.70	122.97	129.08
2	B	501	KUW	C34-C33-C28	-2.69	118.72	120.46
2	A	501	KUW	C27-N26-C25	2.68	123.48	115.19
2	D	501	KUW	C28-C27-N26	-2.66	120.04	123.99
2	D	502	KUW	C34-C25-N26	-2.65	118.87	123.00
2	B	502	KUW	C27-N26-C25	2.64	123.35	115.19
2	D	501	KUW	O6-C5-N4	-2.61	122.27	124.84
2	A	501	KUW	C34-C25-N26	-2.61	118.94	123.00
2	B	502	KUW	C33-C34-CL1	-2.60	114.20	118.45
2	D	501	KUW	C25-C34-CL1	2.59	123.94	121.50
2	D	503	KUW	C23-N22-C25	-2.57	110.20	118.92
2	C	501	KUW	C27-N26-C25	2.56	123.12	115.19
2	D	503	KUW	C27-N26-C25	2.56	123.11	115.19
2	D	503	KUW	C20-C19-N18	-2.55	105.48	110.57
2	A	501	KUW	O31-C30-C29	2.54	123.66	113.98
2	D	503	KUW	C28-C27-N26	-2.53	120.23	123.99
2	C	501	KUW	C28-C27-N26	-2.52	120.25	123.99
2	C	501	KUW	C1-C2-N4	-2.51	107.42	112.54
2	B	501	KUW	C25-C34-CL1	2.49	123.85	121.50
2	D	501	KUW	C27-N26-C25	2.47	122.83	115.19
2	D	503	KUW	C33-C28-C27	2.45	119.17	116.90
2	D	503	KUW	C34-C25-N26	-2.44	119.19	123.00
2	D	501	KUW	C34-C25-N26	-2.44	119.20	123.00
2	C	501	KUW	C34-C33-C28	-2.42	118.90	120.46
2	D	502	KUW	C21-C20-C19	-2.39	106.89	110.67
2	B	501	KUW	C27-N26-C25	2.38	122.56	115.19
2	A	501	KUW	O6-C5-N4	-2.36	122.52	124.84
2	B	501	KUW	C14-C9-C8	-2.34	117.86	120.53
2	D	502	KUW	C27-N26-C25	2.34	122.43	115.19
2	B	501	KUW	C34-C25-N26	-2.34	119.36	123.00
2	D	502	KUW	C19-N18-C7	2.24	137.94	126.61
2	C	501	KUW	O31-C30-C29	2.24	122.51	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	KUW	O31-C30-C29	2.24	122.51	113.98
2	B	501	KUW	C28-C27-N26	-2.23	120.67	123.99
2	D	503	KUW	C23-N22-C21	2.21	116.54	111.57
2	A	501	KUW	C34-C33-C28	-2.19	119.05	120.46
2	B	502	KUW	C24-C19-N18	-2.16	106.25	110.57
2	D	503	KUW	O31-C30-C29	2.13	122.10	113.98
2	D	503	KUW	N26-C25-N22	2.13	121.53	117.01
2	B	501	KUW	O16-S15-C8	-2.10	109.02	112.41
2	D	502	KUW	C34-C33-C28	-2.10	119.10	120.46
2	B	501	KUW	C21-C20-C19	-2.09	107.36	110.67
2	B	502	KUW	C1-C2-N4	-2.09	108.29	112.54
2	D	501	KUW	O16-S15-C8	-2.06	109.08	112.41
2	C	501	KUW	O16-S15-N4	-2.05	109.31	111.30
2	B	502	KUW	C23-N22-C21	2.03	116.14	111.57
2	B	502	KUW	C19-N18-C7	2.01	136.78	126.61
2	D	501	KUW	O17-S15-N4	-2.01	109.34	111.30

There are no chirality outliers.

All (38) 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	D	503	KUW	C5-C7-N18-C19
2	B	502	KUW	C3-C2-N4-C5
2	D	501	KUW	N26-C25-N22-C23
2	D	502	KUW	N26-C25-N22-C21
2	D	502	KUW	C33-C28-C29-C30
2	D	501	KUW	C34-C25-N22-C23
2	D	502	KUW	C34-C25-N22-C21
2	A	501	KUW	C3-C2-N4-C5
2	D	503	KUW	N26-C25-N22-C21
2	B	502	KUW	C33-C28-C29-C30
2	D	503	KUW	C8-C7-N18-C19
2	D	502	KUW	C5-C7-N18-C19
2	D	502	KUW	C27-C28-C29-C30
2	B	502	KUW	C27-C28-C29-C30
2	C	501	KUW	C28-C29-C30-O31
2	C	501	KUW	C28-C29-C30-O32
2	D	502	KUW	C3-C2-N4-C5
2	B	501	KUW	C3-C2-N4-C5
2	C	501	KUW	C3-C2-N4-C5

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Mol	Chain	Res	Type	Atoms
2	D	501	KUW	C3-C2-N4-S15
2	D	503	KUW	C1-C2-N4-S15
2	A	501	KUW	C3-C2-N4-S15
2	B	501	KUW	C3-C2-N4-S15
2	C	501	KUW	C3-C2-N4-S15
2	D	503	KUW	N26-C25-N22-C23
2	D	501	KUW	C28-C29-C30-O31
2	A	501	KUW	C28-C29-C30-O31
2	A	501	KUW	C28-C29-C30-O32
2	D	501	KUW	C28-C29-C30-O32
2	D	501	KUW	C3-C2-N4-C5
2	D	503	KUW	C1-C2-N4-C5
2	D	503	KUW	C28-C29-C30-O31
2	D	503	KUW	C28-C29-C30-O32
2	B	502	KUW	C8-C7-N18-C19
2	B	502	KUW	C5-C7-N18-C19
2	B	501	KUW	N26-C25-N22-C23

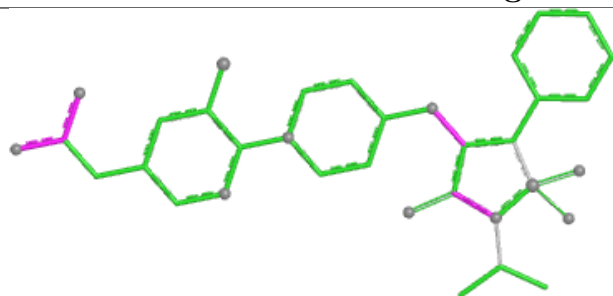
There are no ring outliers.

2 monomers are involved in 6 short contacts:

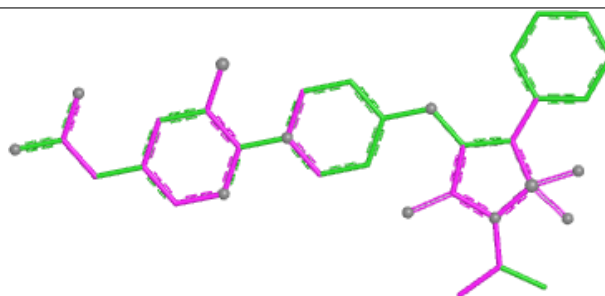
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	KUW	1	0
2	B	502	KUW	5	0

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

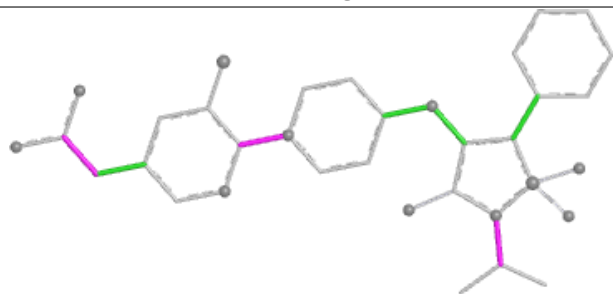
Ligand KUW D 501



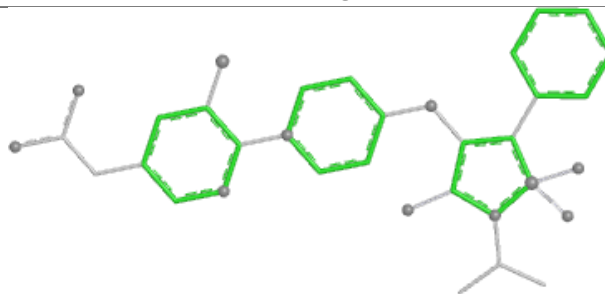
Bond lengths



Bond angles

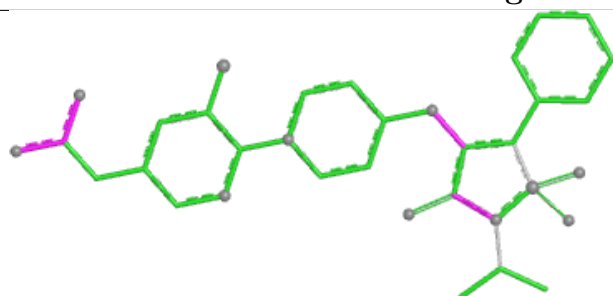


Torsions

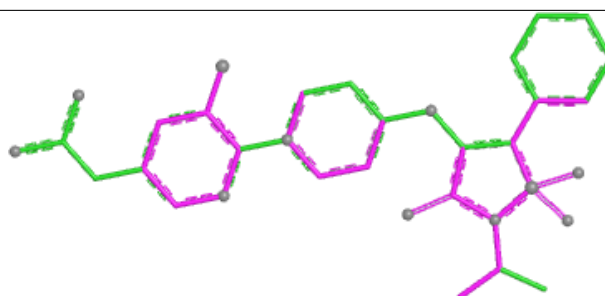


Rings

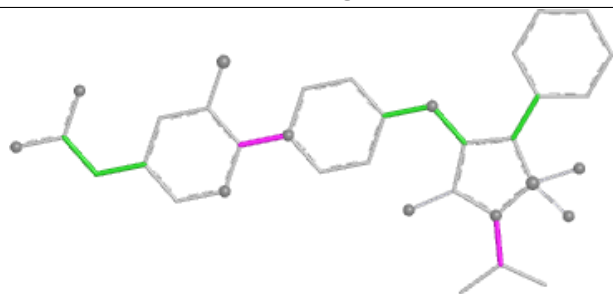
Ligand KUW B 501



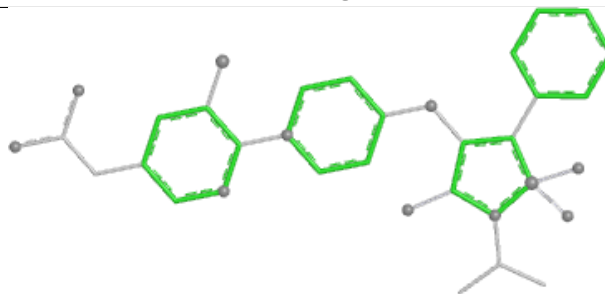
Bond lengths



Bond angles

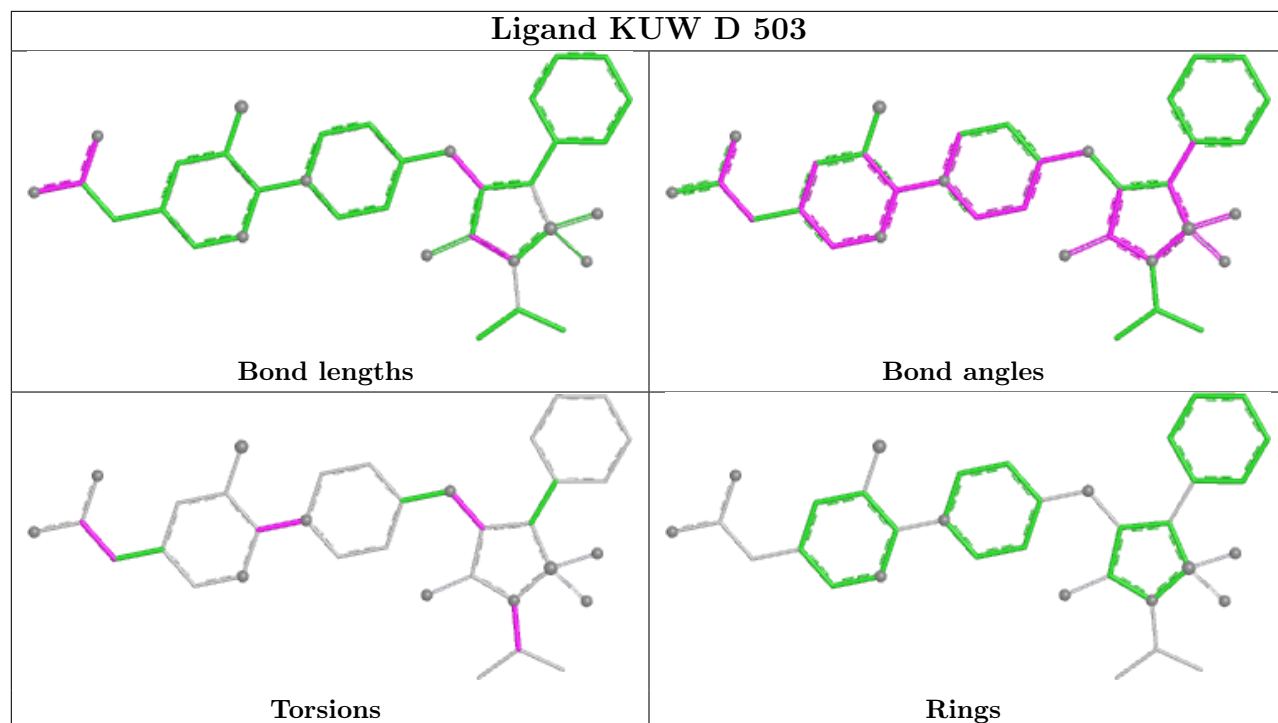


Torsions

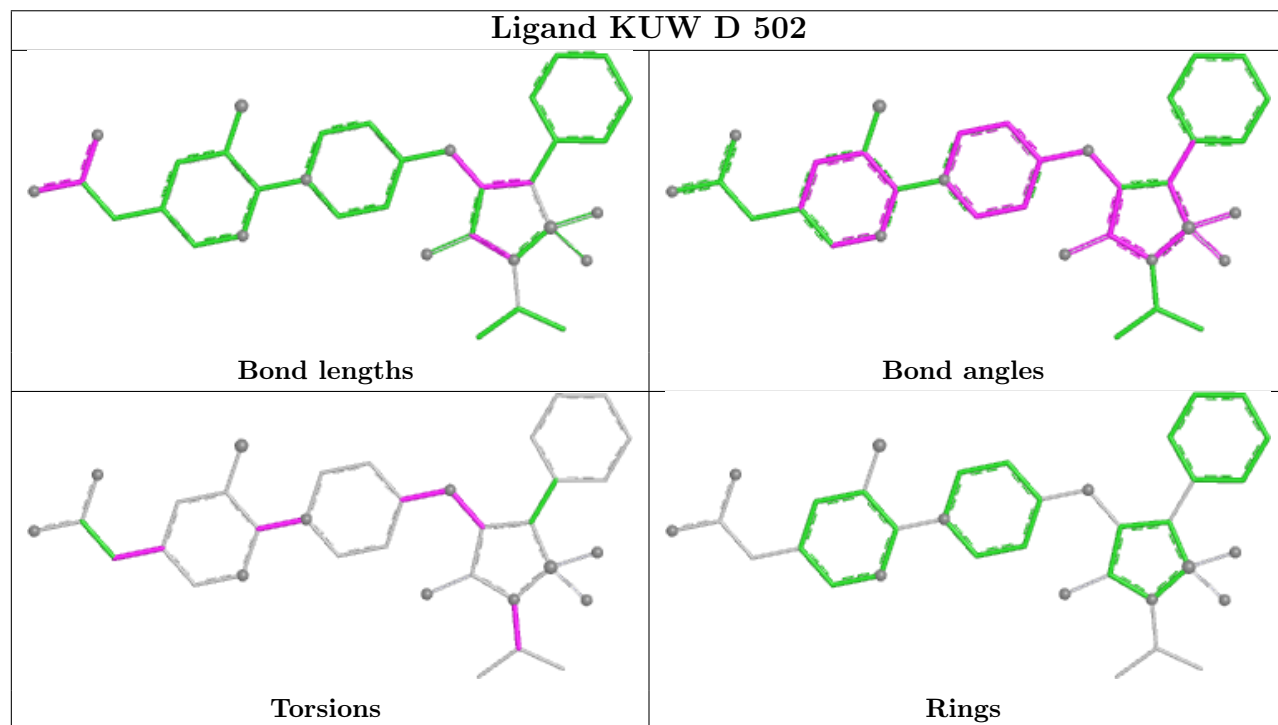


Rings

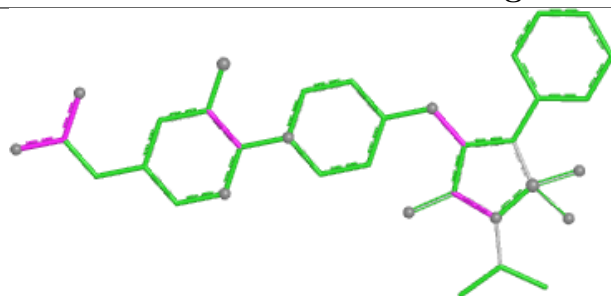
Ligand KUW D 503



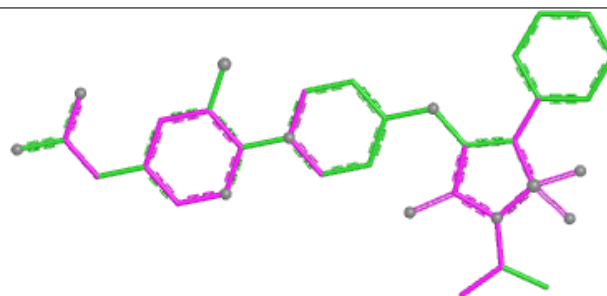
Ligand KUW D 502



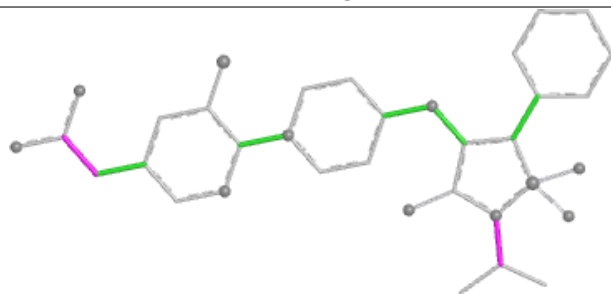
Ligand KUW A 501



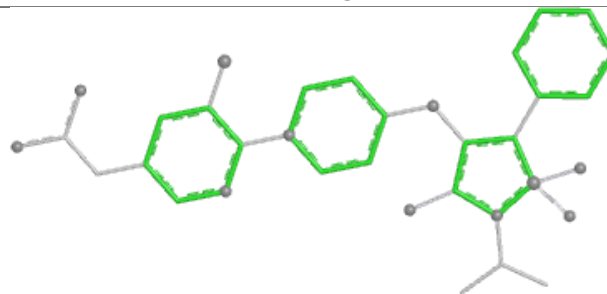
Bond lengths



Bond angles

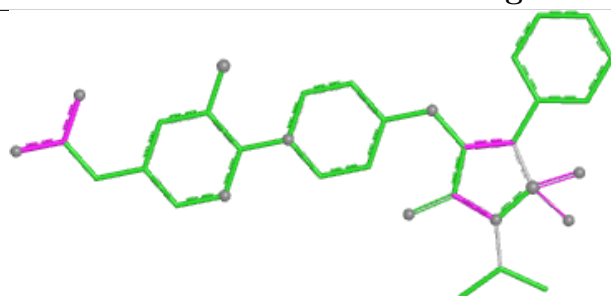


Torsions

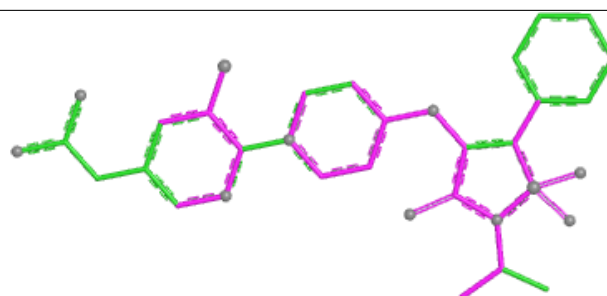


Rings

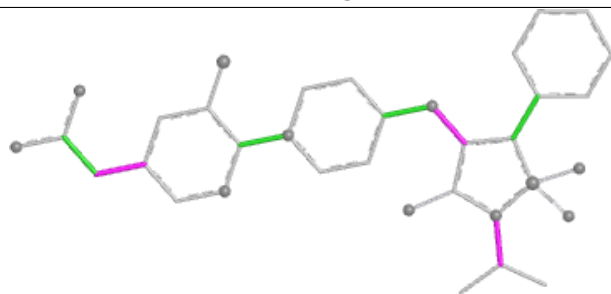
Ligand KUW B 502



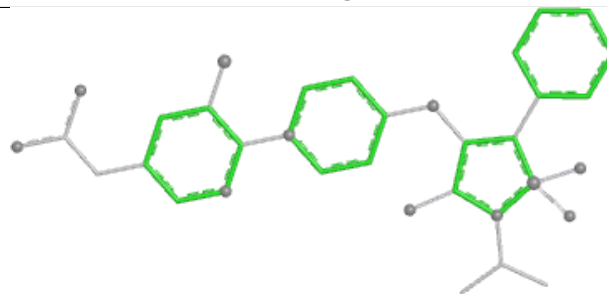
Bond lengths



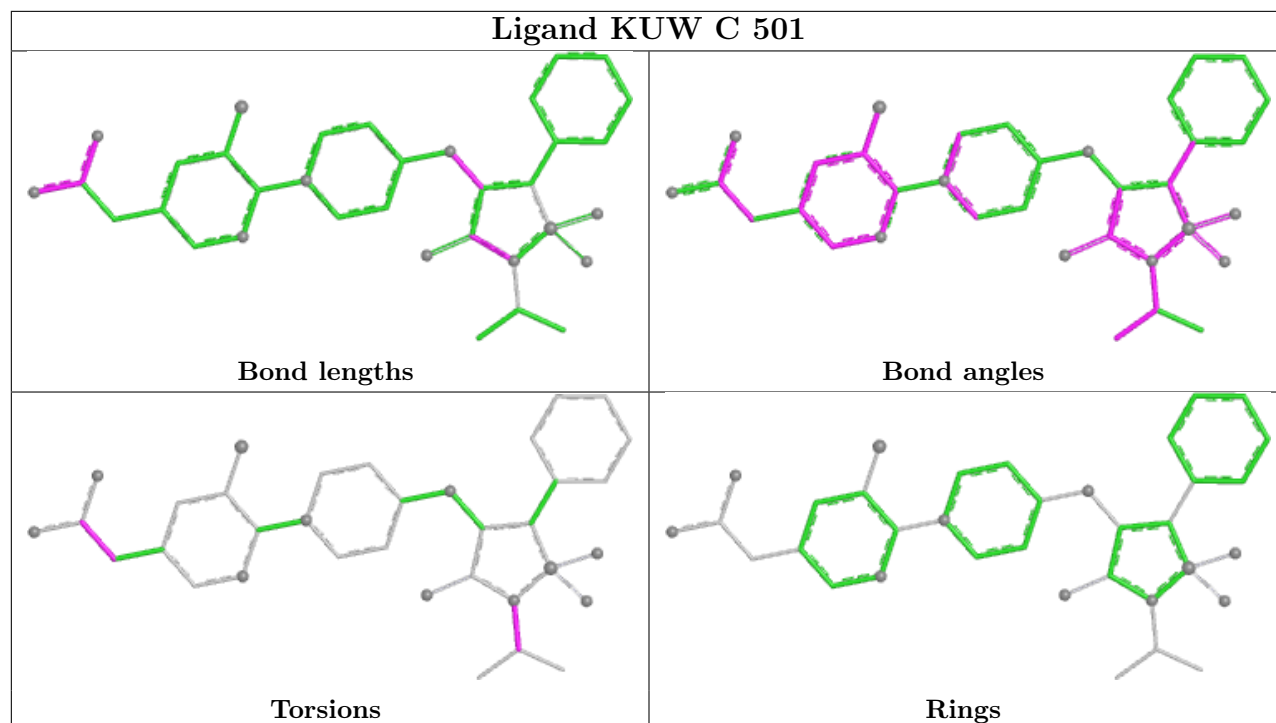
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 ⓘ

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	236/245 (96%)	0.64	20 (8%)	16 17	11, 22, 38, 64	10 (4%)
1	B	233/245 (95%)	0.93	37 (15%)	5 5	13, 24, 47, 75	9 (3%)
1	C	224/245 (91%)	0.75	28 (12%)	8 8	11, 23, 43, 58	7 (3%)
1	D	235/245 (95%)	0.59	19 (8%)	18 19	11, 22, 39, 51	12 (5%)
All	All	928/980 (94%)	0.73	104 (11%)	10 10	11, 23, 43, 75	38 (4%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	PHE	6.2
1	A	243	PHE	6.0
1	A	446	ASP	5.9
1	D	243	PHE	5.8
1	C	323	GLU	5.6
1	B	459	VAL	5.1
1	C	444	LEU	4.7
1	B	254	GLY	4.6
1	B	408	ARG	4.5
1	B	238	CYS	4.4
1	C	265	GLN	4.2
1	B	246	PRO	4.0
1	A	242	SER	4.0
1	A	334	THR	3.9
1	A	459	VAL	3.9
1	C	459	VAL	3.8
1	C	332	ASP	3.7
1	D	247	PRO	3.5
1	C	324	THR	3.5
1	A	444	LEU	3.5
1	C	322	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	239	ASN	3.4
1	B	444	LEU	3.4
1	A	219	GLN	3.4
1	B	236	LEU	3.4
1	C	446	ASP	3.4
1	C	384	PRO	3.1
1	C	244	SER	3.1
1	A	241	ARG	3.1
1	C	338	ASP	3.1
1	B	332	ASP	3.0
1	A	333	PHE	3.0
1	B	244	SER	3.0
1	C	416	LEU	2.9
1	C	237	GLN	2.9
1	B	263	ALA	2.9
1	C	266	GLN	2.9
1	A	238	CYS	2.8
1	B	440	PHE	2.8
1	C	219	GLN	2.8
1	B	412	PRO	2.8
1	B	413	GLN	2.7
1	A	331	LYS	2.7
1	C	243	PHE	2.7
1	B	262	ASP	2.7
1	B	237	GLN	2.7
1	B	265	GLN	2.7
1	B	240	LYS	2.7
1	C	335	TYR	2.7
1	B	334	THR	2.7
1	B	242	SER	2.7
1	C	347[A]	VAL	2.7
1	C	333	PHE	2.6
1	B	410	LYS	2.6
1	B	446	ASP	2.6
1	A	249	LYS	2.6
1	B	415	GLN	2.6
1	D	225	GLU	2.6
1	D	446	ASP	2.6
1	A	338	ASP	2.6
1	D	408	ARG	2.5
1	D	334[A]	THR	2.5
1	D	412	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	321	ASN	2.5
1	D	415	GLN	2.5
1	A	265	GLN	2.5
1	D	241	ARG	2.4
1	B	264	ARG	2.4
1	D	444	LEU	2.4
1	B	225	GLU	2.4
1	D	265	GLN	2.4
1	D	260	SER	2.4
1	A	240	LYS	2.4
1	C	325	GLU	2.3
1	B	409	ILE	2.3
1	C	327	ILE	2.3
1	C	326	CYS	2.3
1	B	363	LEU	2.3
1	B	234	ALA	2.3
1	D	409	ILE	2.3
1	C	443	ARG	2.3
1	D	445	GLN	2.3
1	A	322	HIS	2.2
1	B	347	VAL	2.2
1	D	244	SER	2.2
1	A	443	ARG	2.2
1	B	416	LEU	2.2
1	C	355	GLU	2.1
1	B	220	LEU	2.1
1	B	241	ARG	2.1
1	C	447	LYS	2.1
1	C	342	ARG	2.1
1	B	441	ALA	2.1
1	B	445	GLN	2.1
1	B	443	ARG	2.1
1	C	334	THR	2.1
1	D	413	GLN	2.1
1	A	441	ALA	2.1
1	B	420	ARG	2.1
1	D	307	SER	2.0
1	A	324	THR	2.0
1	A	255	GLY	2.0
1	D	294	GLN	2.0
1	D	335	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

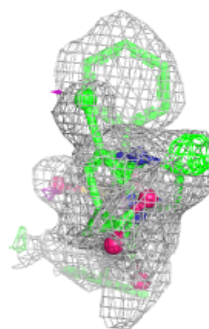
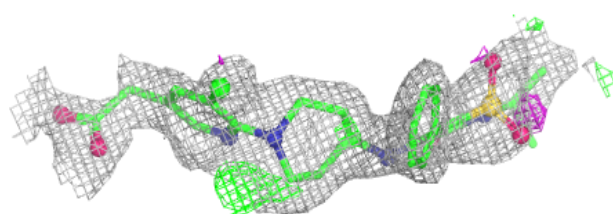
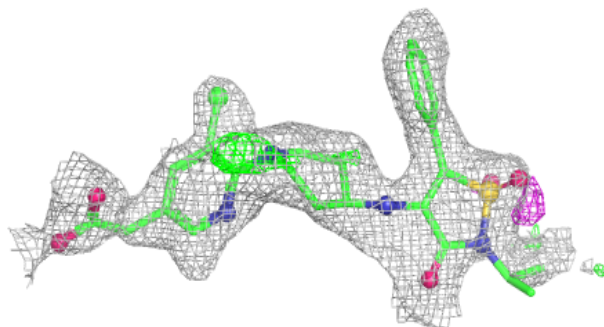
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KUW	D	503	35/35	0.78	0.18	44,51,55,57	0
2	KUW	B	502	35/35	0.84	0.16	31,37,65,73	0
2	KUW	D	502	35/35	0.87	0.14	30,37,58,60	0
2	KUW	A	501	35/35	0.94	0.07	16,18,26,27	0
2	KUW	C	501	35/35	0.95	0.07	18,19,26,28	0
2	KUW	D	501	35/35	0.96	0.07	15,16,22,23	0
2	KUW	B	501	35/35	0.96	0.07	17,18,26,27	0
3	SO4	A	502	5/5	0.96	0.14	26,27,29,31	0

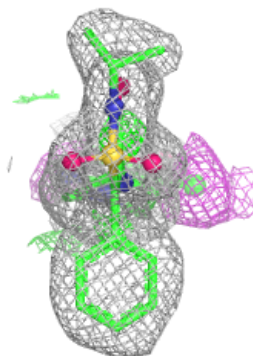
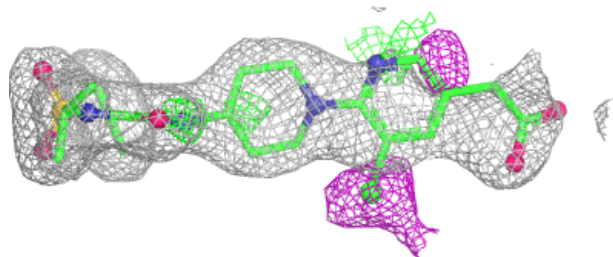
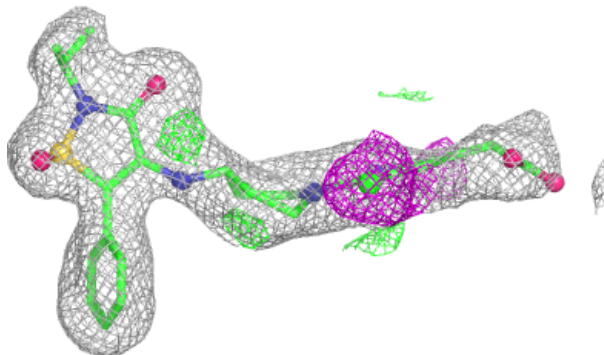
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

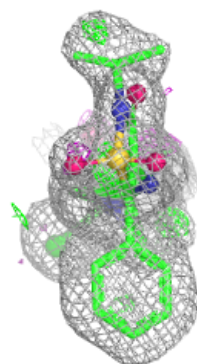
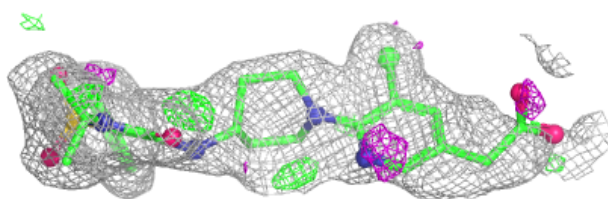
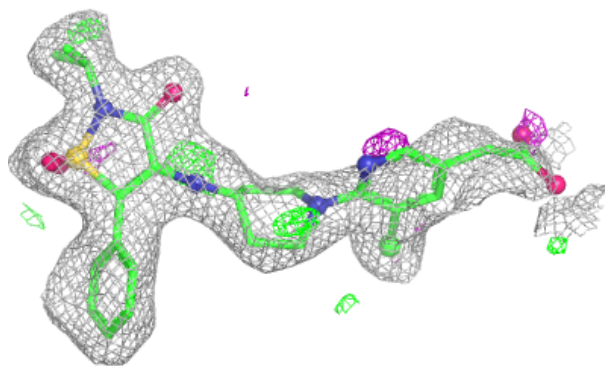
**Electron density around K UW B 502:**

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

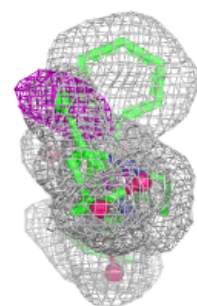
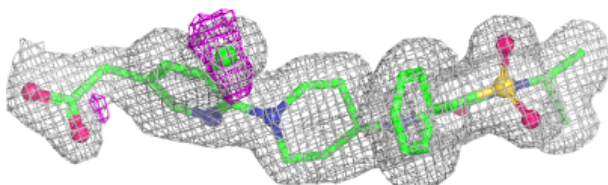
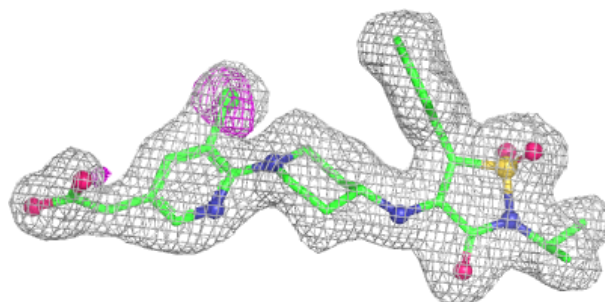


Electron density around K UW D 502:

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

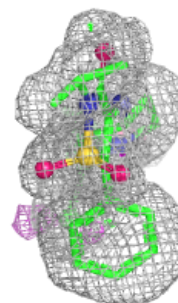
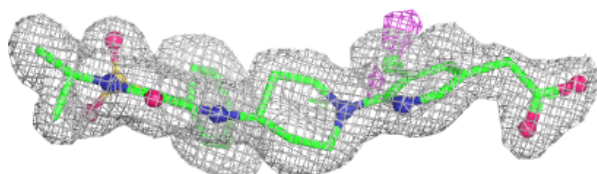
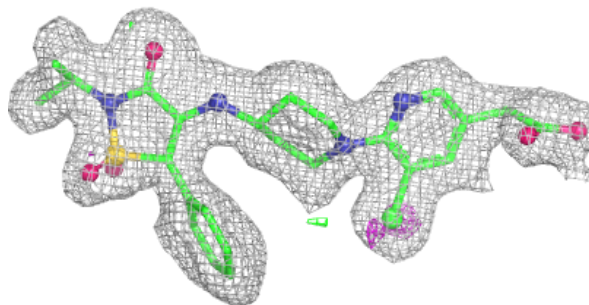
**Electron density around K UW A 501:**

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

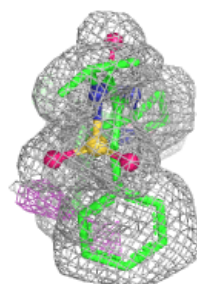
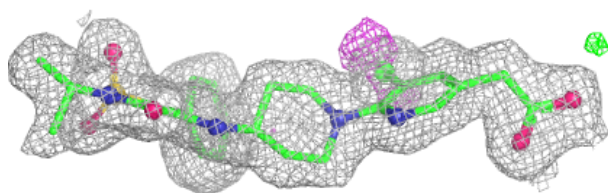
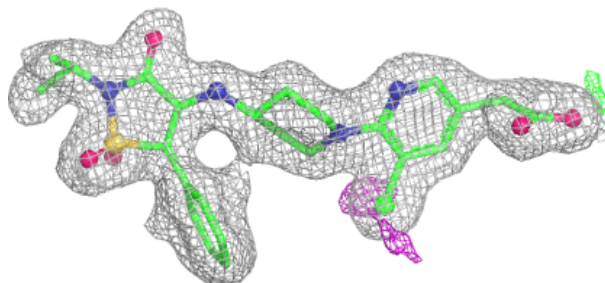


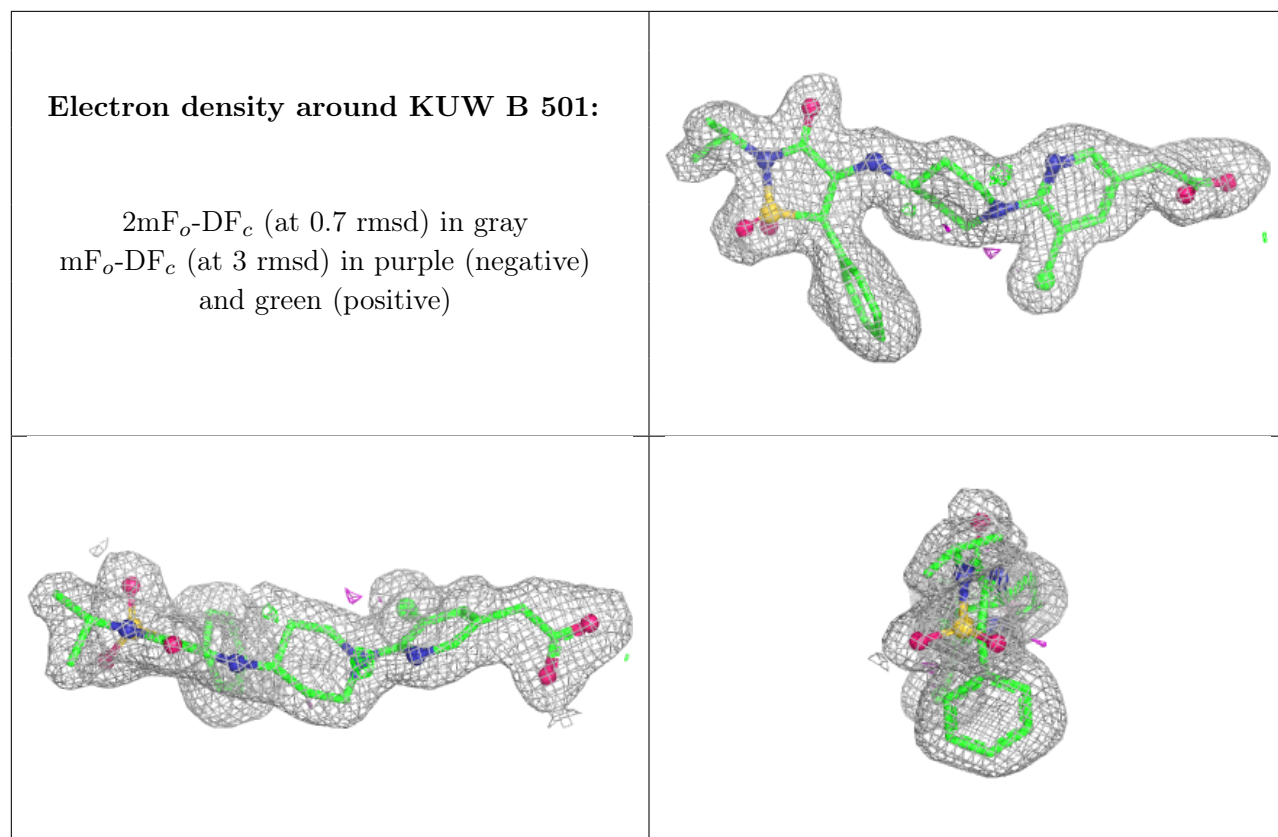
Electron density around K UW C 501:

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

**Electron density around K UW D 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.