



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:05 AM UTC

PDB ID : 9ESP / pdb_00009esp
Title : CDK2-cyclin A in complex with FragLite 26
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on : 2024-03-26
Resolution : 2.38 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

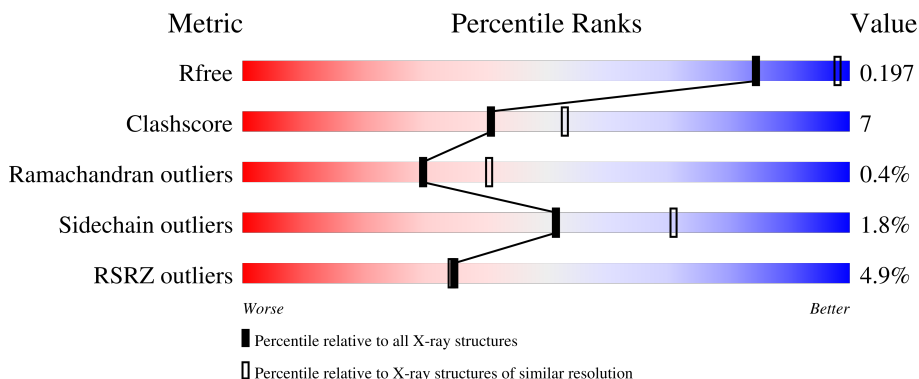
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	302	 4% 77% 18% ..
1	C	302	 6% 79% 17% ..
2	B	268	 % 87% 10% .
2	D	268	 7% 85% 12% ..

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9356 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	293	Total	C	N	O	P	S	0	1	0
			2356	1526	398	423	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	Total	C	N	O	S	0	2	0
			2124	1373	346	394	11			
2	D	262	Total	C	N	O	S	0	1	0
			2119	1371	345	393	10			

There are 14 discrepancies between the modelled and reference sequences:

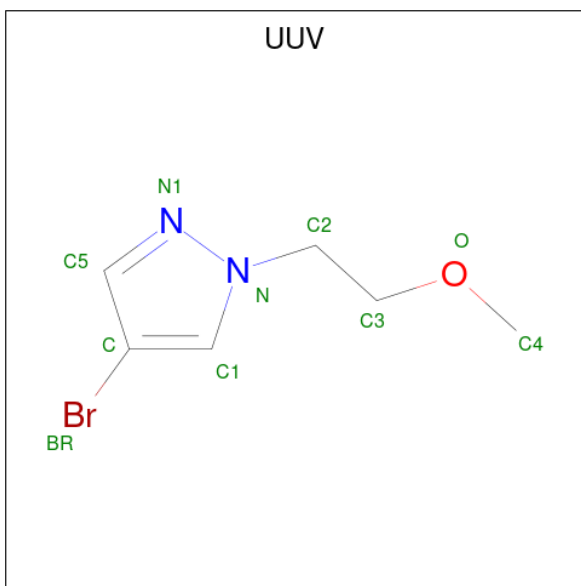
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is 4-bromo-1-(2-methoxyethyl)-1H-pyrazole (CCD ID: UUV) (formula: C₆H₉BrN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	10	1	6	2	1	0	0
3	B	1	10	1	6	2	1	0	0
3	C	1	10	1	6	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		

Continued on next page...

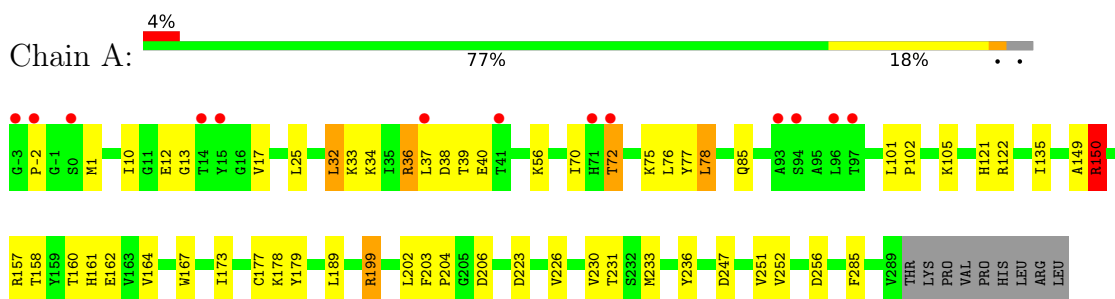
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	113	Total 113	O 113	0	0
4	C	57	Total 57	O 57	0	0
4	D	49	Total 49	O 49	0	0

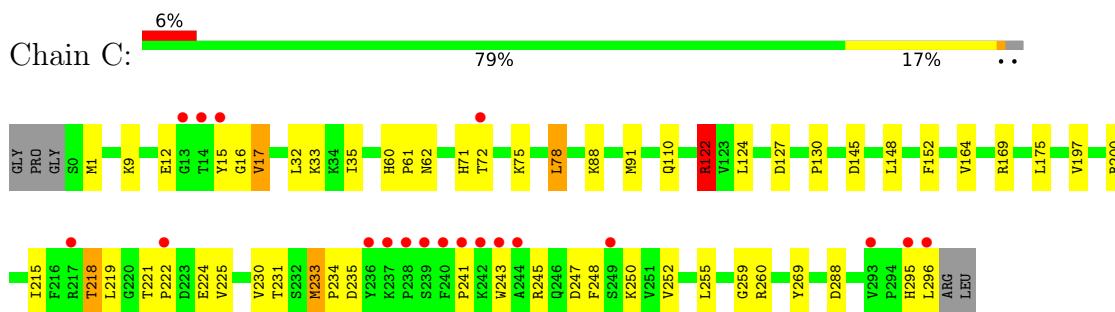
3 Residue-property plots [i](#)

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.

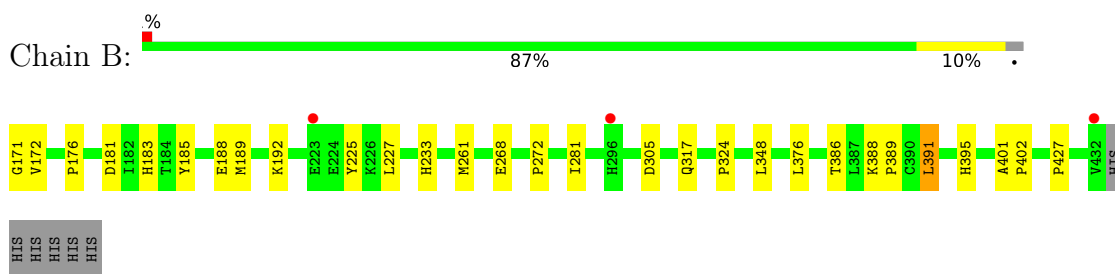
- Molecule 1: Cyclin-dependent kinase 2



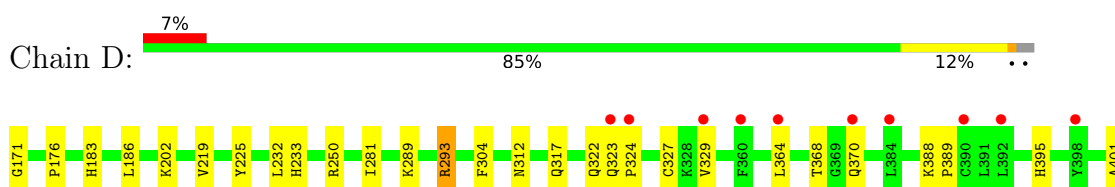
- Molecule 1: Cyclin-dependent kinase 2

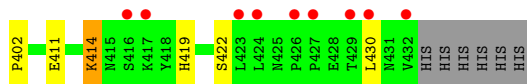


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.06Å 133.71Å 147.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.33 – 2.38 99.14 – 2.38	Depositor EDS
% Data completeness (in resolution range)	94.1 (99.33-2.38) 93.9 (99.14-2.38)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.209 , 0.212 0.196 , 0.197	Depositor DCC
R_{free} test set	2959 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtrriage
Anisotropy	0.163	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9356	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.72	4/2404 (0.2%)	1.16	1/3260 (0.0%)
1	C	0.64	0/2438	1.14	1/3308 (0.0%)
2	B	0.63	0/2174	1.15	3/2956 (0.1%)
2	D	0.60	0/2169	1.18	2/2949 (0.1%)
All	All	0.65	4/9185 (0.0%)	1.16	7/12473 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	4
2	D	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ALA	C-N	-8.86	1.22	1.33
1	A	150	ARG	C-N	-7.73	1.22	1.33
1	A	33	LYS	C-N	-6.16	1.24	1.33
1	A	32	LEU	C-N	-5.73	1.24	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	ASP	CA-CB-CG	5.86	118.46	112.60
2	D	414	LYS	N-CA-C	-5.71	106.08	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ASP	CB-CA-C	5.60	118.72	109.70
1	C	72	THR	N-CA-C	-5.57	101.00	108.86
2	B	272	PRO	N-CA-CB	5.39	106.02	103.22
2	D	411	GLU	CB-CA-C	-5.37	102.44	110.88
2	B	391	LEU	N-CA-CB	-5.20	102.48	110.12

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ARG	Sidechain
1	A	199	ARG	Sidechain
1	A	36	ARG	Sidechain
1	C	122	ARG	Sidechain
1	C	169	ARG	Sidechain
1	C	200	ARG	Sidechain
1	C	245	ARG	Sidechain
2	D	250	ARG	Sidechain
2	D	293	ARG	Sidechain

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	2356	0	2385	41	0
1	C	2388	0	2430	42	0
2	B	2124	0	2135	20	0
2	D	2119	0	2133	20	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	A	120	0	0	2	0
4	B	113	0	0	3	0
4	C	57	0	0	0	0
4	D	49	0	0	1	0
All	All	9356	0	9083	118	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 7.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:HG2	1:A:13:GLY:H	0.98	1.10
1:A:177:CYS:SG	1:A:233:MET:HE3	1.92	1.09
2:D:289:LYS:HE2	2:D:293:ARG:NH1	1.80	0.95
1:A:12:GLU:HG2	1:A:13:GLY:N	1.81	0.93
1:C:15:TYR:HB3	1:C:35:ILE:HG12	1.53	0.90
1:A:12:GLU:CG	1:A:13:GLY:H	1.83	0.90
2:D:289:LYS:HE2	2:D:293:ARG:HH11	1.34	0.88
2:D:289:LYS:CE	2:D:293:ARG:NH1	2.42	0.82
1:C:247:ASP:H	1:C:250:LYS:HE3	1.46	0.81
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.66	0.76
1:C:12:GLU:HG3	1:C:16:GLY:O	1.86	0.75
1:A:177:CYS:SG	1:A:233:MET:CE	2.74	0.74
1:C:15:TYR:CD2	1:C:33:LYS:HD3	2.23	0.74
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.22	0.69
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.74	0.69
1:A:157:ARG:NH1	2:B:268:GLU:OE2	2.25	0.69
1:C:15:TYR:CB	1:C:35:ILE:HG12	2.24	0.67
1:A:78:LEU:N	1:A:78:LEU:HD23	2.09	0.67
1:A:121:HIS:O	1:A:122:ARG:HG3	1.95	0.67
1:A:161:HIS:HE1	1:A:173:ILE:O	1.79	0.65
2:B:233:HIS:HD2	4:B:656:HOH:O	1.80	0.64
1:C:15:TYR:HD2	1:C:33:LYS:HD3	1.61	0.64
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.32	0.63
1:C:15:TYR:HB3	1:C:35:ILE:CG1	2.29	0.61
1:C:15:TYR:CG	1:C:35:ILE:HG12	2.37	0.60
2:D:233:HIS:HD2	4:D:517:HOH:O	1.85	0.59
1:A:105:LYS:HE2	1:A:285:PHE:O	2.02	0.59
2:B:188:GLU:HG2	2:B:189:MET:HE2	1.87	0.57
1:C:215:ILE:HG23	1:C:219:LEU:HD12	1.85	0.57
1:A:121:HIS:C	1:A:122:ARG:HG3	2.30	0.56
1:A:177:CYS:SG	1:A:233:MET:HG2	2.47	0.55
1:A:10:ILE:HD12	3:A:1501:UUV:C2	2.37	0.55
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.88	0.54
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.42	0.54
2:B:171:GLY:O	2:B:176:PRO:HD3	2.07	0.54
1:A:72:THR:HB	1:A:75:LYS:H	1.74	0.53
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:HB2	4:A:1625:HOH:O	2.08	0.53
1:C:175:LEU:HA	1:C:235:ASP:HB2	1.91	0.53
2:B:185:TYR:CE1	2:B:189:MET:HE3	2.44	0.53
2:B:189:MET:CE	2:B:192:LYS:HE2	2.39	0.52
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.74	0.52
2:D:322:GLN:HB3	2:D:324:PRO:O	2.09	0.52
1:C:127:ASP:HB2	1:C:148:LEU:HD12	1.91	0.51
2:D:329:VAL:HG11	2:D:364:LEU:HD12	1.93	0.50
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.94	0.49
2:B:189:MET:HE1	2:B:192:LYS:CE	2.42	0.49
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.77	0.48
1:C:218:THR:HG22	1:C:219:LEU:HG	1.94	0.48
2:D:327:CYS:HB2	2:D:419:HIS:CE1	2.49	0.48
2:B:395:HIS:HE1	2:B:427:PRO:O	1.97	0.48
2:D:225:TYR:HE2	2:D:281:ILE:HG21	1.79	0.48
1:C:1:MET:HE1	1:C:32:LEU:HD13	1.95	0.48
1:C:241:PRO:HB2	1:C:243:TRP:CZ2	2.49	0.48
1:A:231:THR:HA	1:A:236:TYR:CD2	2.49	0.48
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.96	0.47
2:B:401:ALA:N	2:B:402:PRO:CD	2.77	0.47
1:A:36:ARG:HB3	1:A:39:THR:HG22	1.95	0.47
1:A:223:ASP:H	1:A:226:VAL:HG12	1.80	0.47
2:B:386:THR:HB	4:B:605:HOH:O	2.14	0.47
2:D:395:HIS:HB2	2:D:430:LEU:HD11	1.97	0.47
1:A:177:CYS:SG	1:A:233:MET:SD	3.12	0.47
2:B:189:MET:HE1	2:B:192:LYS:HE2	1.96	0.46
1:C:197:VAL:CG1	1:C:252:VAL:HG13	2.39	0.46
2:B:225:TYR:HE2	2:B:281:ILE:HG21	1.80	0.46
1:C:295:HIS:O	1:C:296:LEU:C	2.58	0.46
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.96	0.46
1:C:78:LEU:HD23	1:C:78:LEU:N	2.30	0.46
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.98	0.45
1:C:124:LEU:HG	1:C:152:PHE:CD2	2.51	0.45
1:A:78:LEU:N	1:A:78:LEU:CD2	2.78	0.45
1:A:34:LYS:HD2	1:A:75:LYS:HD3	1.97	0.45
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.52	0.45
1:A:230:VAL:HA	1:A:233:MET:SD	2.56	0.45
1:C:248:PHE:CB	1:C:260:ARG:HD2	2.47	0.45
1:C:230:VAL:HA	1:C:233:MET:SD	2.57	0.44
1:C:255:LEU:HG	1:C:259:GLY:HA3	2.00	0.44
1:C:9:LYS:HG3	1:C:17:VAL:CG2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:HIS:CG	1:A:162:GLU:N	2.86	0.44
1:A:36:ARG:O	1:A:40:GLU:HG2	2.18	0.44
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.99	0.44
1:A:77:TYR:C	1:A:78:LEU:HD23	2.43	0.43
1:C:71:HIS:CE1	2:D:304:PHE:HE1	2.36	0.43
2:D:368:THR:HB	2:D:370:GLN:NE2	2.33	0.43
2:D:323:GLN:O	2:D:323:GLN:HG3	2.19	0.43
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.82	0.43
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.33	0.43
1:A:157:ARG:HG3	1:A:158:THR:N	2.34	0.42
1:A:38:ASP:OD1	1:A:38:ASP:N	2.52	0.42
1:C:248:PHE:HB3	1:C:260:ARG:HD2	2.02	0.42
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.94	0.42
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.42
2:D:233:HIS:CE1	2:D:312:ASN:OD1	2.73	0.42
2:B:183:HIS:HD2	4:B:621:HOH:O	2.03	0.42
2:D:171:GLY:O	2:D:176:PRO:HD3	2.19	0.42
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.01	0.41
1:A:256:ASP:HA	4:A:1705:HOH:O	2.19	0.41
2:B:348:LEU:HD23	2:B:348:LEU:HA	1.93	0.41
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.48	0.41
1:C:224:GLU:HG2	1:C:231:THR:HG23	2.03	0.41
1:C:127:ASP:CB	1:C:148:LEU:HD12	2.50	0.41
2:D:388:LYS:O	2:D:389:PRO:C	2.64	0.41
1:A:56:LYS:CD	2:B:305[B]:ASP:OD1	2.68	0.41
1:C:233:MET:HA	1:C:234:PRO:HD3	1.97	0.41
1:A:37:LEU:HD11	1:A:76:LEU:HB2	2.03	0.41
1:A:56:LYS:HD3	2:B:305[B]:ASP:OD1	2.21	0.41
1:A:105:LYS:HG3	1:A:285:PHE:CE2	2.56	0.41
1:A:202:LEU:HD23	1:A:203:PHE:CE2	2.55	0.41
1:C:241:PRO:HB2	1:C:243:TRP:CH2	2.56	0.41
1:C:288:ASP:OD1	1:C:288:ASP:N	2.53	0.41
1:A:85:GLN:HE21	1:A:135:ILE:HD11	1.87	0.40
1:C:122:ARG:HD2	2:D:186:LEU:HD21	2.03	0.40
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.97	0.40
1:C:221:THR:HA	1:C:222:PRO:HD2	1.92	0.40
2:D:414:LYS:HG3	2:D:422:SER:OG	2.22	0.40
2:D:401:ALA:HB3	2:D:402:PRO:HD3	2.03	0.40
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.88	0.40
2:D:219:VAL:HG22	2:D:232:LEU:HD21	2.03	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	291/302 (96%)	280 (96%)	9 (3%)	2 (1%)	18	26
1	C	294/302 (97%)	280 (95%)	12 (4%)	2 (1%)	18	26
2	B	262/268 (98%)	259 (99%)	3 (1%)	0	100	100
2	D	261/268 (97%)	255 (98%)	6 (2%)	0	100	100
All	All	1108/1140 (97%)	1074 (97%)	30 (3%)	4 (0%)	30	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
1	C	145	ASP
1	A	-2	PRO

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	256/264 (97%)	249 (97%)	7 (3%)	39	59
1	C	261/264 (99%)	254 (97%)	7 (3%)	39	59
2	B	236/240 (98%)	233 (99%)	3 (1%)	61	78
2	D	235/240 (98%)	234 (100%)	1 (0%)	84	91
All	All	988/1008 (98%)	970 (98%)	18 (2%)	51	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	70	ILE
1	A	72	THR
1	A	78	LEU
1	A	150	ARG
1	A	199	ARG
1	A	206	ASP
2	B	172	VAL
2	B	324	PRO
2	B	391	LEU
1	C	17	VAL
1	C	75	LYS
1	C	78	LEU
1	C	122	ARG
1	C	218	THR
1	C	225	VAL
1	C	233	MET
2	D	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	161	HIS
1	A	265	GLN
2	B	179	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	425	ASN
1	C	287	GLN
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	370	GLN
2	D	395	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	431	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	C	160	1	8,10,11	0.76	0	10,14,16	0.86	0
1	TPO	A	160	1	8,10,11	0.71	0	10,14,16	0.98	1 (10%)

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
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-2.35	118.73	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	UUV	B	501	-	10,10,10	0.40	0	12,12,12	0.74	0
3	UUV	A	1501	-	10,10,10	0.69	0	12,12,12	0.77	1 (8%)
3	UUV	C	501	-	10,10,10	0.29	0	12,12,12	0.72	0

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
3	UUV	B	501	-	-	1/4/4/4	0/1/1/1
3	UUV	A	1501	-	-	2/4/4/4	0/1/1/1
3	UUV	C	501	-	-	2/4/4/4	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	UUV	BR-C-C5	2.05	129.65	127.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

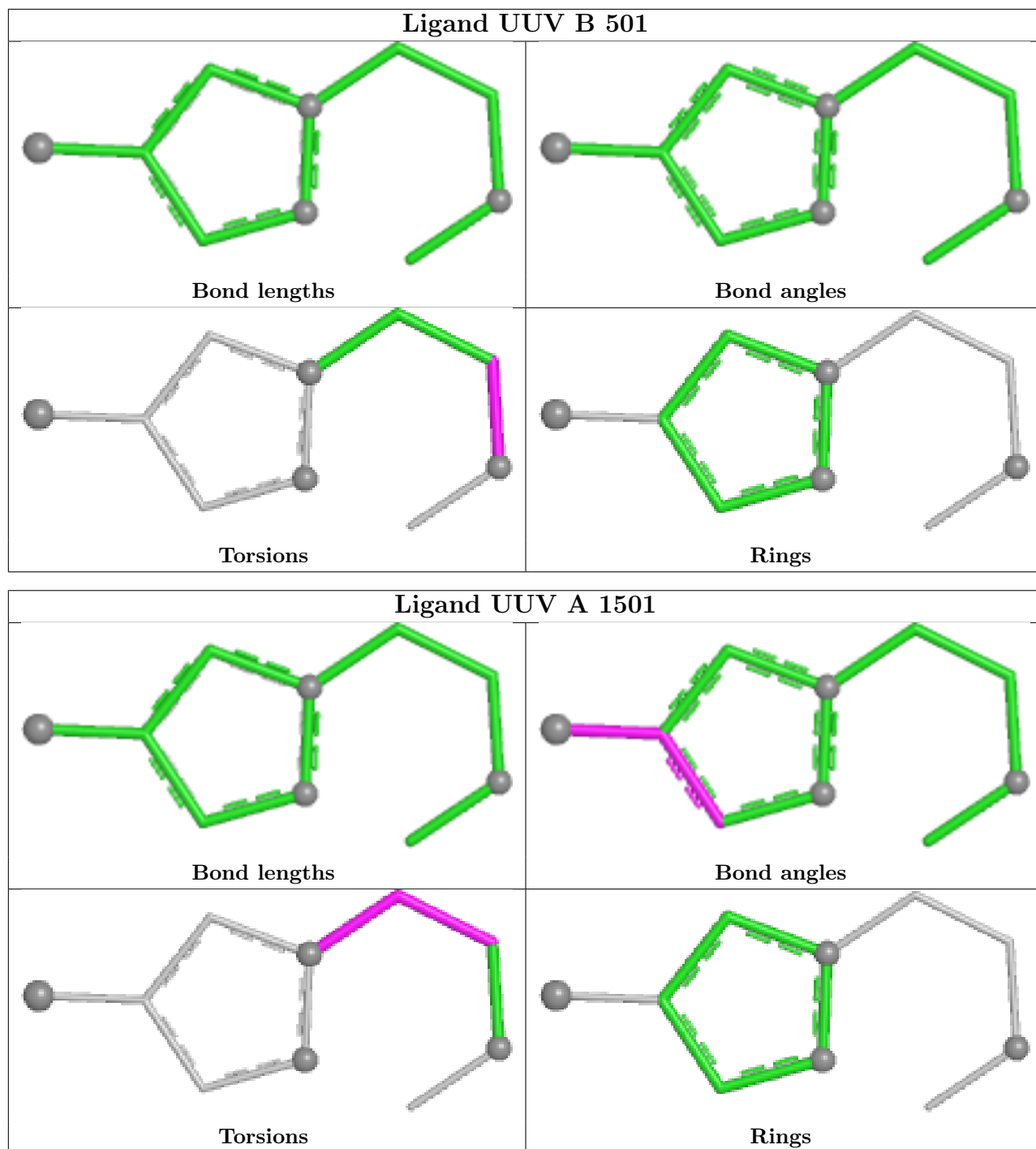
Mol	Chain	Res	Type	Atoms
3	A	1501	UUV	N-C2-C3-O
3	C	501	UUV	N-C2-C3-O
3	B	501	UUV	C2-C3-O-C4
3	C	501	UUV	C2-C3-O-C4
3	A	1501	UUV	C3-C2-N-N1

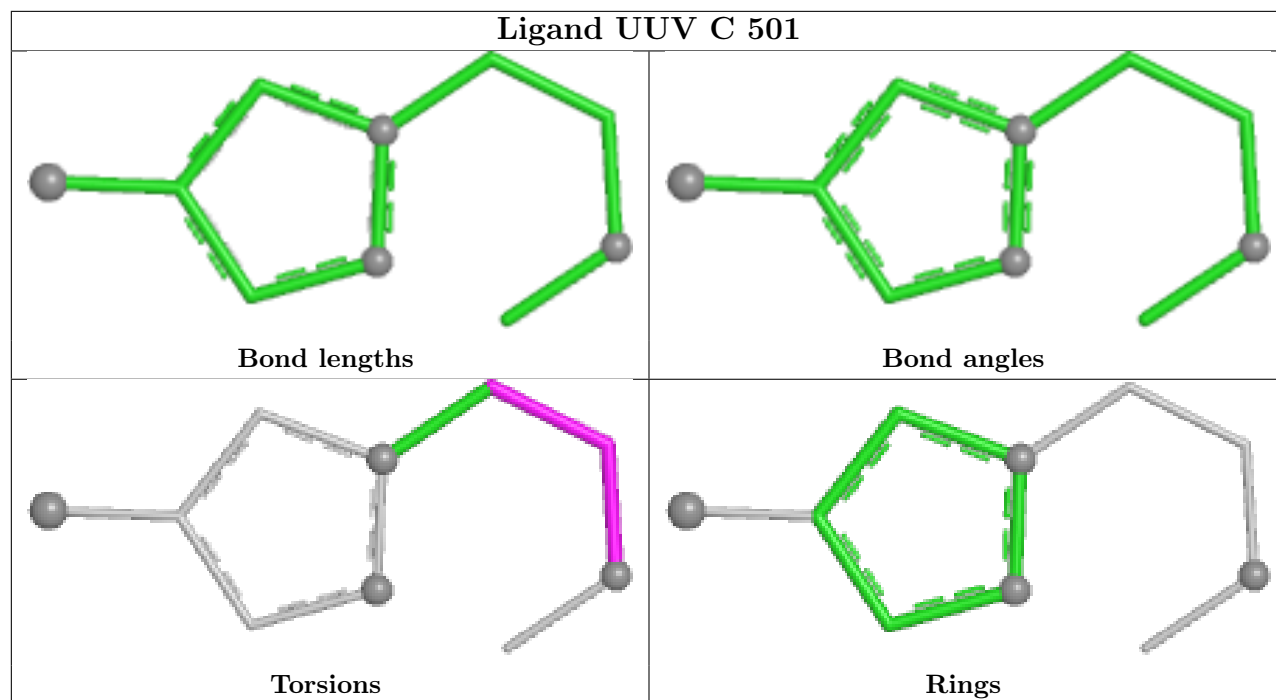
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	UUV	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	292/302 (96%)	-0.03	13 (4%) 38 37	31, 47, 103, 172	1 (0%)
1	C	296/302 (98%)	0.32	19 (6%) 25 24	39, 60, 110, 146	0
2	B	262/268 (97%)	-0.20	3 (1%) 78 77	26, 50, 79, 112	2 (0%)
2	D	262/268 (97%)	0.40	19 (7%) 21 20	29, 64, 106, 152	1 (0%)
All	All	1112/1140 (97%)	0.12	54 (4%) 35 34	26, 55, 105, 172	4 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	VAL	6.0
1	A	71	HIS	5.8
1	A	15	TYR	5.3
1	C	296	LEU	4.9
1	A	-3	GLY	3.6
1	A	96	LEU	3.6
1	C	14	THR	3.6
1	C	295	HIS	3.4
1	A	94	SER	3.3
1	A	-2	PRO	3.2
1	C	237	LYS	3.2
2	D	430	LEU	3.2
1	C	241	PRO	3.1
1	C	243	TRP	3.0
2	B	296	HIS	2.9
2	B	432	VAL	2.9
1	C	239	SER	2.9
1	A	0	SER	2.8
1	C	238	PRO	2.8
2	D	360	PHE	2.7
2	D	424	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	13	GLY	2.7
1	C	240	PHE	2.6
1	A	97	THR	2.6
1	C	222	PRO	2.6
1	C	15	TYR	2.6
2	D	384	LEU	2.5
1	C	244	ALA	2.5
1	C	242	LYS	2.5
1	A	14	THR	2.5
1	C	236	TYR	2.5
2	D	398	TYR	2.4
1	C	72	THR	2.4
2	D	426	PRO	2.4
2	D	416	SER	2.4
2	D	329	VAL	2.3
2	D	417	LYS	2.3
1	C	217	ARG	2.3
2	D	323	GLN	2.3
1	C	293	VAL	2.3
2	D	370	GLN	2.2
1	A	72	THR	2.2
1	C	249	SER	2.2
2	D	324	PRO	2.2
2	B	223	GLU	2.2
2	D	390	CYS	2.2
2	D	423	LEU	2.1
1	A	41	THR	2.1
1	A	37	LEU	2.1
2	D	364	LEU	2.1
2	D	392	LEU	2.1
2	D	429	THR	2.0
1	A	93	ALA	2.0
2	D	427	PRO	2.0

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

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(\AA^2)	Q<0.9
1	TPO	A	160	11/12	0.97	0.06	39,46,49,49	0
1	TPO	C	160	11/12	0.98	0.06	46,52,60,60	0

6.3 Carbohydrates [i](#)

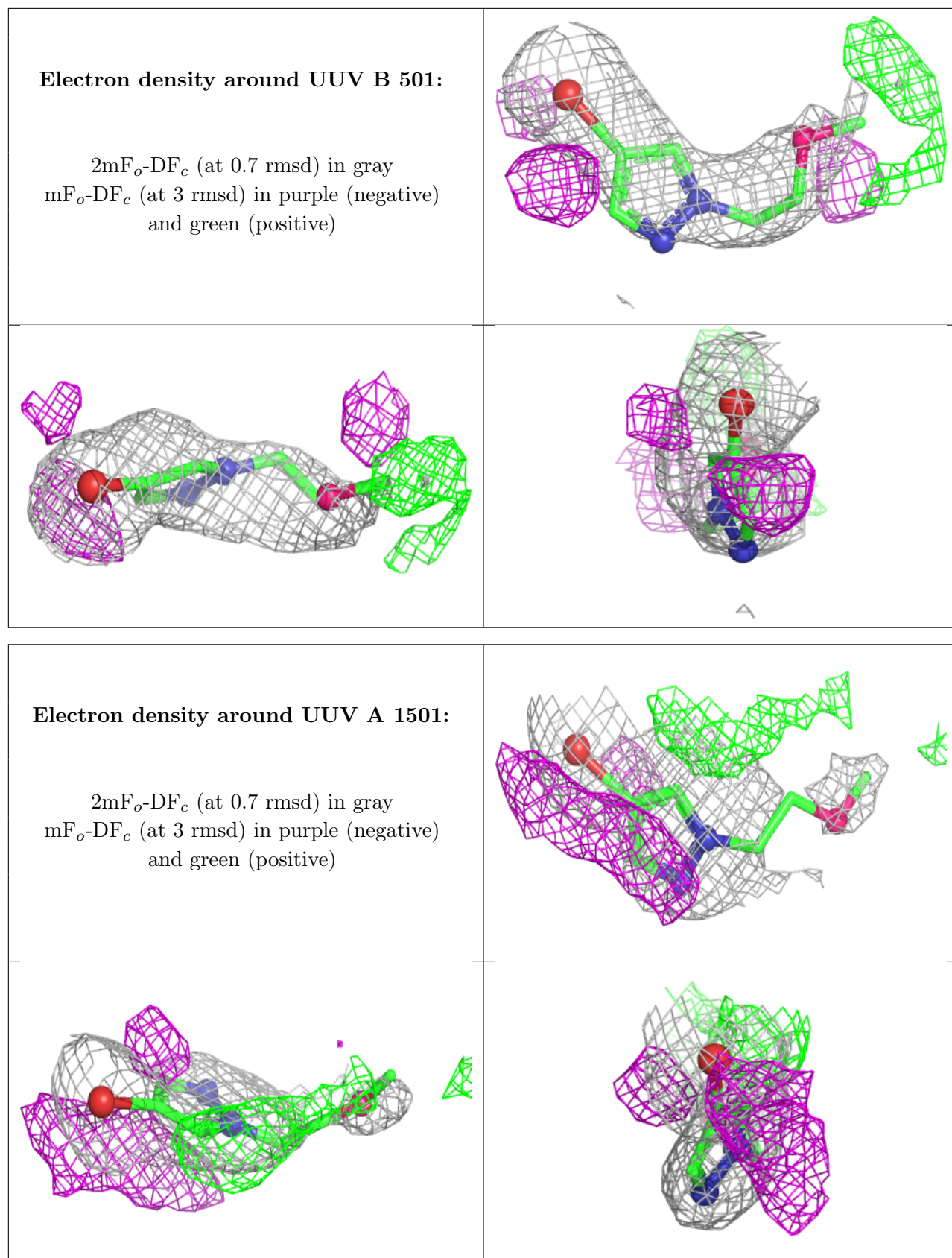
There are no oligosaccharides in this entry.

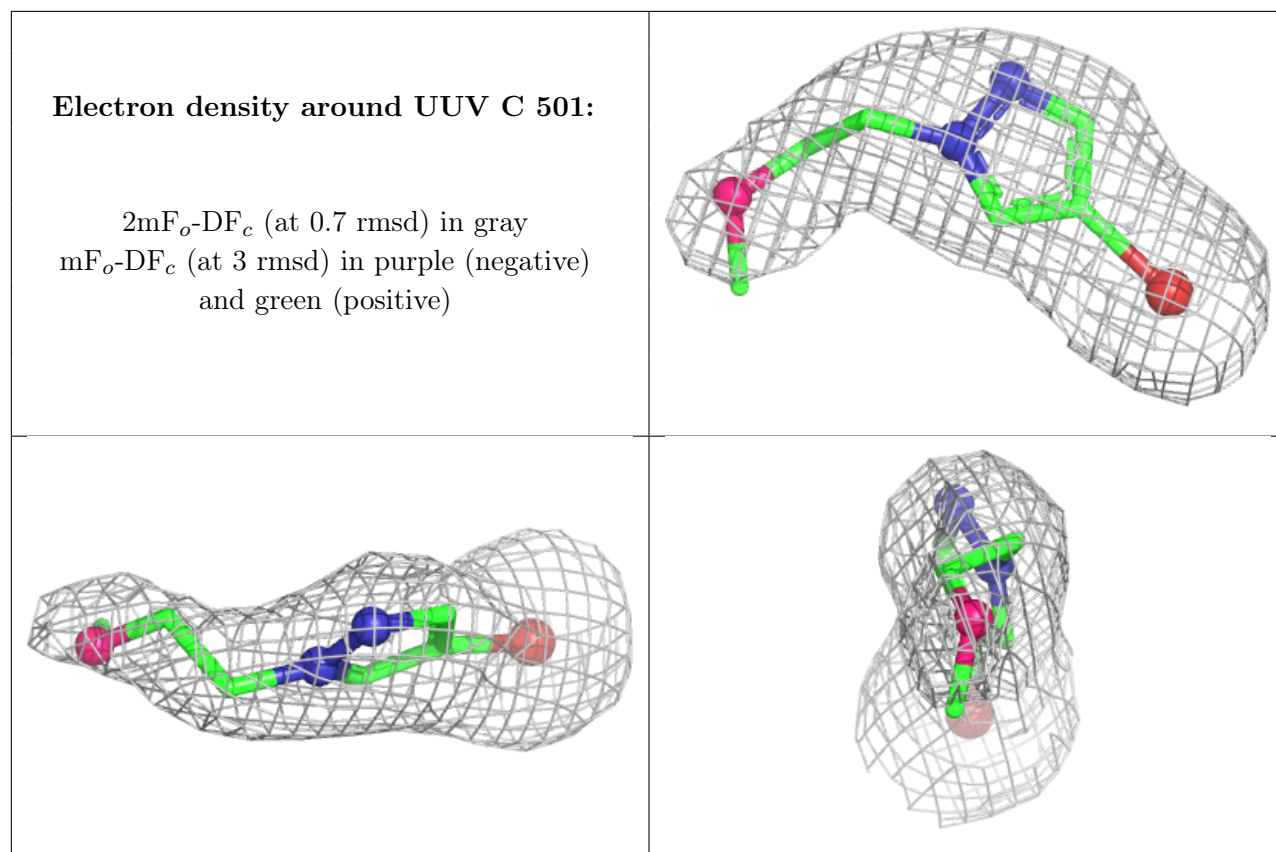
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UUV	B	501	10/10	0.82	0.24	95,120,138,144	0
3	UUV	A	1501	10/10	0.84	0.25	78,98,111,120	0
3	UUV	C	501	10/10	0.97	0.11	64,75,88,94	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.