



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 2FDC / pdb_00002fdc
Title : Structural Basis of DNA Damage Recognition and Processing by UvrB: crystal structure of a UvrB/DNA complex
Authors : Truglio, J.J.; Kisker, C.
Deposited on : 2005-12-13
Resolution : 3.30 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

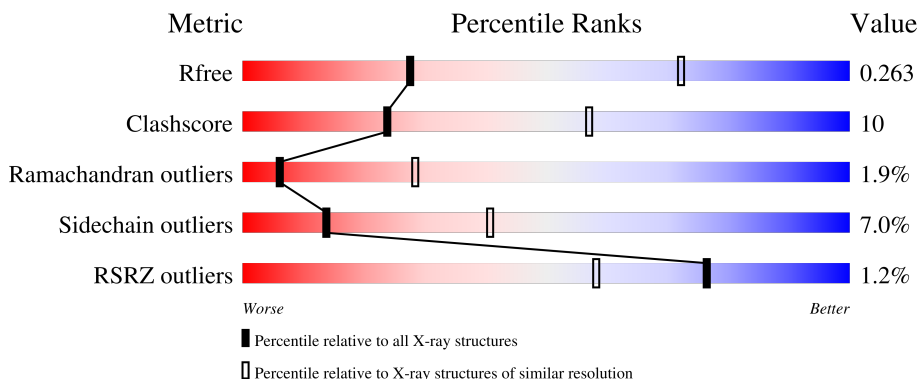
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	C	20	
1	D	20	
2	A	658	
2	B	658	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9178 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 DNA chain called 5'-D(P*CP*GP*GP*CP*TP*CP*CP*AP*TP*CP*TP*C P*TP*AP*CP*CP*GP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	12	243	115	44	72	12	0	0	0
1	D	5	100	47	19	29	5	0	0	0

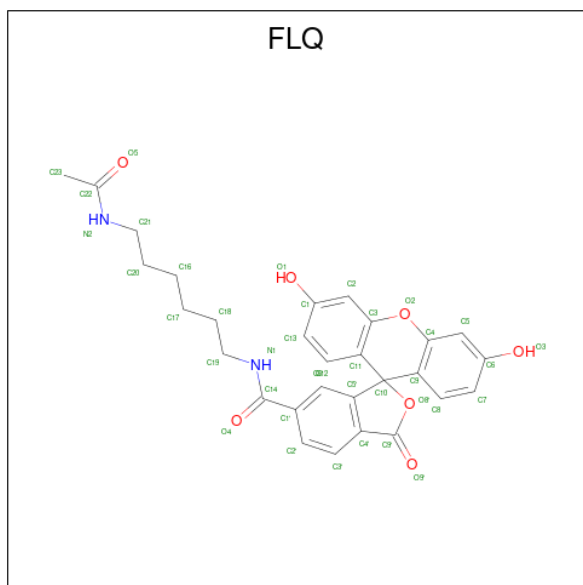
- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	505	4072	2574	718	770	10	0	0	0
2	B	585	4731	2983	844	892	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	ARG	-	SEE REMARK 999	UNP P56981
A	233	GLU	LYS	SEE REMARK 999	UNP P56981
B	189	ARG	-	SEE REMARK 999	UNP P56981
B	233	GLU	LYS	SEE REMARK 999	UNP P56981

- Molecule 3 is N-[6-(ACETYLAMINO)HEXYL]-3',6'-DIHYDROXY-3-OXO-3H-SPIRO[2-BENZOFURAN-1,9'-XANTHENE]-6-CARBOXAMIDE (CCD ID: FLQ) (formula: C₂₉H₂₈N₂O₇).

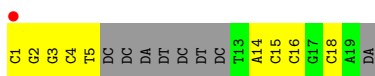
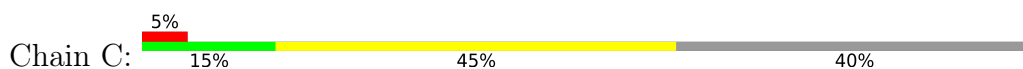


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	32	25	1	6	0	0

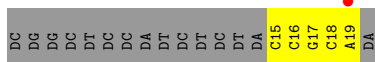
3 Residue-property plots [i](#)

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.

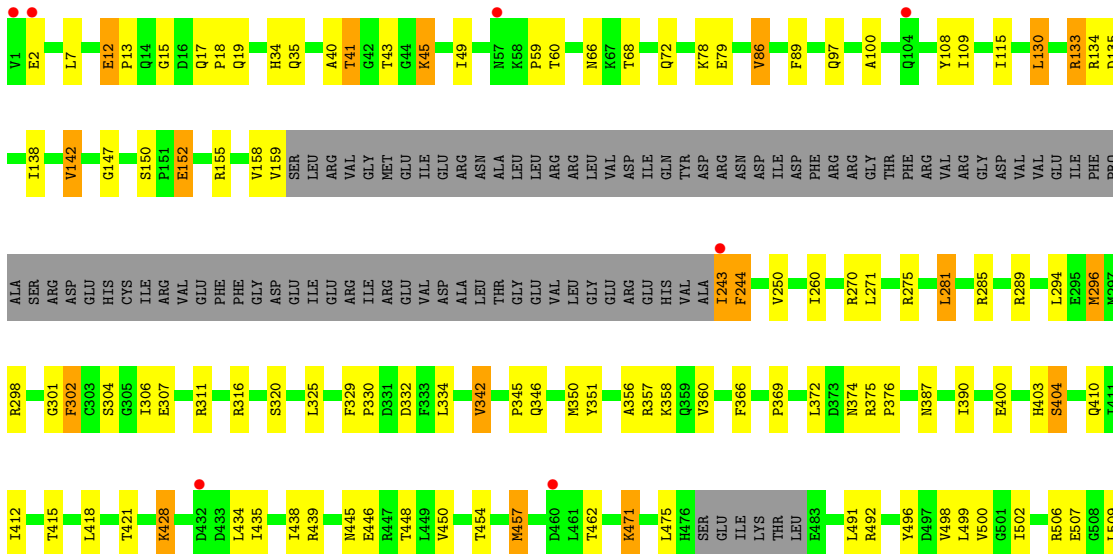
- Molecule 1: 5'-D(P*CP*GP*GP*CP*TP*CP*CP*AP*TP*CP*TP*CP*TP*AP*CP*CP*GP*CP*AP*A)-3'

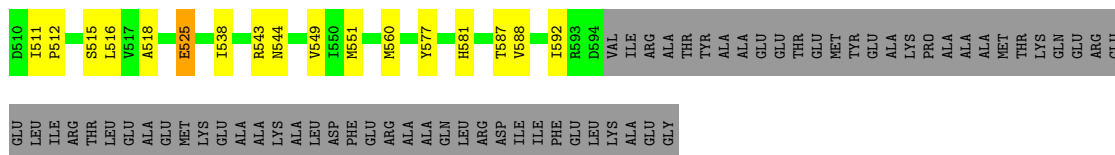


- Molecule 1: 5'-D(P*CP*GP*GP*CP*TP*CP*CP*AP*TP*CP*TP*CP*TP*AP*CP*CP*GP*CP*AP*A)-3'

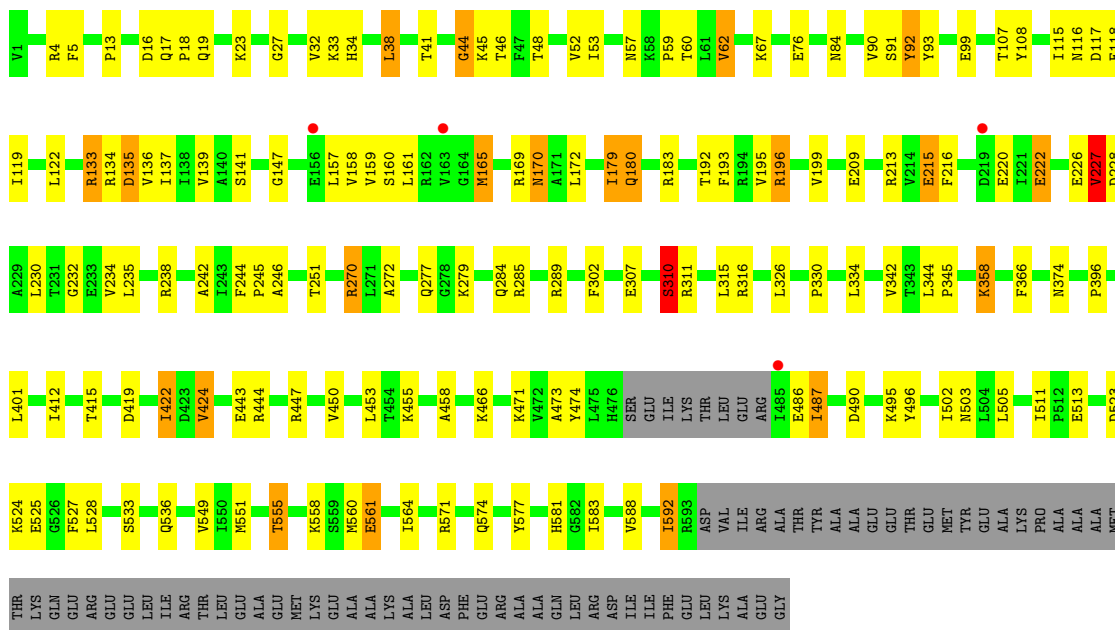


- Molecule 2: UvrABC system protein B





• Molecule 2: UvrABC system protein B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.26Å 153.26Å 160.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.30 10.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-3.30) 96.1 (10.00-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.12Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.258 0.215 , 0.263	Depositor DCC
R_{free} test set	2009 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9178	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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 25.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4044e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	C	0.89	0/270	1.24	0/411
1	D	0.80	0/111	1.24	0/168
2	A	1.07	2/4143 (0.0%)	0.91	2/5601 (0.0%)
2	B	1.15	6/4812 (0.1%)	0.93	7/6502 (0.1%)
All	All	1.11	8/9336 (0.1%)	0.94	9/12682 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	251	THR	CA-CB	5.85	1.60	1.53
2	A	41	THR	CA-CB	5.70	1.63	1.53
2	B	511	ILE	C-N	5.36	1.39	1.33
2	B	487	ILE	CA-CB	5.36	1.61	1.54
2	B	272	ALA	CA-CB	-5.34	1.45	1.53
2	A	115	ILE	CA-CB	5.34	1.59	1.54
2	B	536	GLN	CG-CD	5.33	1.65	1.52
2	B	487	ILE	N-CA	5.22	1.52	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	147	GLY	N-CA-C	6.28	119.15	111.93
2	A	152	GLU	N-CA-C	-6.25	104.09	111.03
2	B	527	PHE	N-CA-C	-6.18	104.63	111.36
2	B	238	ARG	N-CA-C	6.15	118.74	108.96
2	B	495	LYS	N-CA-C	-5.99	104.83	111.36
2	B	147	GLY	N-CA-C	5.64	118.42	111.93
2	B	44	GLY	N-CA-C	5.63	119.70	112.83
2	B	133	ARG	N-CA-C	5.33	117.97	110.14
2	B	235	LEU	N-CA-C	5.10	116.65	111.14

There are no chirality outliers.

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	C	243	0	136	11	0
1	D	100	0	56	6	0
2	A	4072	0	4108	83	0
2	B	4731	0	4761	92	0
3	C	32	0	17	1	0
All	All	9178	0	9078	184	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 10.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:450:VAL:HG12	2:A:518:ALA:HB3	1.52	0.92
2:B:17:GLN:HE21	2:B:44:GLY:HA3	1.44	0.81
2:B:5:PHE:H	2:B:57:ASN:HD21	1.34	0.74
2:A:311:ARG:HD3	2:A:316:ARG:O	1.90	0.72
2:A:133:ARG:HH11	2:A:133:ARG:HG3	1.54	0.72
2:A:454:THR:OG1	2:A:457:MET:HB2	1.90	0.72
2:B:5:PHE:HA	2:B:84:ASN:ND2	2.07	0.70
2:A:400:GLU:O	2:A:404:SER:HB2	1.93	0.69
2:B:422:ILE:HG23	2:B:549:VAL:HB	1.75	0.69
2:B:159:VAL:HG13	2:B:179:ILE:HD12	1.76	0.68
2:B:116:ASN:HD22	2:B:119:ILE:H	1.43	0.67
2:A:438:ILE:HD13	2:A:498:VAL:HG21	1.78	0.66
2:B:571:ARG:HA	2:B:574:GLN:HE21	1.59	0.66
2:B:60:THR:HG22	2:B:334:LEU:HB3	1.78	0.65
2:B:17:GLN:NE2	2:B:44:GLY:HA3	2.12	0.65
1:C:5:DT:H5''	2:B:345:PRO:HB3	1.79	0.65
2:A:68:THR:HG22	2:A:72:GLN:NE2	2.12	0.64
2:A:68:THR:HG22	2:A:72:GLN:HE21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:LEU:HD21	2:B:172:LEU:HD13	1.80	0.63
2:B:455:LYS:HA	2:B:502:ILE:HD11	1.81	0.63
2:B:118:GLU:O	2:B:122:LEU:HG	1.99	0.62
2:B:419:ASP:H	2:B:574:GLN:HE22	1.44	0.62
2:A:475:LEU:HD13	2:A:499:LEU:HD21	1.82	0.62
2:B:310:SER:CB	2:B:374:ASN:HD22	2.14	0.60
1:C:2:DG:H1'	1:C:3:DG:C8	2.36	0.60
2:A:138:ILE:HD12	2:A:329:PHE:CZ	2.37	0.60
2:B:571:ARG:HA	2:B:574:GLN:NE2	2.17	0.59
1:D:18:DC:H3'	2:A:307:GLU:CG	2.34	0.57
2:B:179:ILE:HG23	2:B:245:PRO:HA	1.86	0.57
2:A:133:ARG:HH11	2:A:133:ARG:CG	2.17	0.57
2:A:159:VAL:HB	2:A:243:ILE:N	2.20	0.57
2:A:40:ALA:O	2:A:43:THR:HG22	2.04	0.57
1:C:4:DC:H42	1:C:14:DA:H61	1.54	0.56
2:B:412:ILE:HD13	2:B:577:TYR:CD1	2.41	0.56
1:C:1:DC:P	1:C:1:DC:H3'	2.45	0.56
2:B:33:LYS:HG2	2:B:34:HIS:CD2	2.41	0.55
2:A:60:THR:HG22	2:A:334:LEU:HB3	1.88	0.55
2:B:183:ARG:HG2	2:B:193:PHE:CZ	2.42	0.55
2:B:315:LEU:HD12	2:B:315:LEU:N	2.22	0.55
2:B:46:THR:HG21	2:B:76:GLU:OE1	2.07	0.55
2:B:44:GLY:O	2:B:46:THR:N	2.40	0.55
2:B:27:GLY:O	2:B:32:VAL:HG23	2.06	0.54
1:D:15:DC:H5''	2:A:66:ASN:HA	1.90	0.54
2:A:457:MET:HA	2:A:457:MET:HE2	1.89	0.54
1:C:3:DG:H2''	1:C:4:DC:C6	2.42	0.54
2:A:100:ALA:HB2	2:A:357:ARG:HD2	1.90	0.54
2:A:492:ARG:HG2	2:A:511:ILE:HG23	1.90	0.53
2:B:358:LYS:NZ	2:B:374:ASN:O	2.39	0.53
2:B:92:TYR:HE2	2:B:93:TYR:CE2	2.27	0.53
2:B:48:THR:O	2:B:52:VAL:HG23	2.08	0.52
2:B:310:SER:CB	2:B:374:ASN:ND2	2.73	0.52
1:D:16:DC:H2'	1:D:17:DG:C8	2.44	0.51
2:A:434:LEU:HD21	2:A:450:VAL:HG11	1.92	0.51
2:A:551:MET:CE	2:A:560:MET:HG2	2.41	0.51
2:A:158:VAL:HG23	2:A:244:PHE:HA	1.92	0.51
2:A:281:LEU:HD13	2:A:281:LEU:C	2.35	0.51
2:B:183:ARG:HG2	2:B:193:PHE:CE2	2.45	0.51
2:B:419:ASP:H	2:B:574:GLN:NE2	2.08	0.51
2:B:60:THR:OG1	2:B:137:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASN:HD22	2:B:135:ASP:HB2	1.76	0.50
2:A:296:MET:HA	2:A:296:MET:HE2	1.94	0.50
2:B:108:TYR:CD1	2:B:366:PHE:CE1	3.00	0.50
2:B:116:ASN:O	2:B:117:ASP:HB2	2.11	0.50
2:B:277:GLN:HE21	2:B:279:LYS:HZ2	1.58	0.50
2:A:97:GLN:NE2	2:A:109:ILE:HG21	2.27	0.50
2:A:97:GLN:HE21	2:A:109:ILE:HG21	1.77	0.49
2:A:351:TYR:C	2:A:351:TYR:CD2	2.90	0.49
2:B:59:PRO:HG3	2:B:330:PRO:HG2	1.94	0.49
2:A:142:VAL:HG21	2:A:346:GLN:CD	2.37	0.49
2:A:448:THR:HG23	2:A:516:LEU:HG	1.95	0.49
2:A:475:LEU:HD23	2:A:506:ARG:NH1	2.27	0.49
2:A:471:LYS:HB3	2:A:496:TYR:HA	1.94	0.48
2:B:159:VAL:HG23	2:B:159:VAL:O	2.13	0.48
2:B:270:ARG:HH11	2:B:270:ARG:HG2	1.78	0.48
2:B:422:ILE:CG2	2:B:549:VAL:HB	2.43	0.48
2:B:513:GLU:N	2:B:513:GLU:OE2	2.47	0.48
2:A:332:ASP:HA	2:A:387:ASN:ND2	2.28	0.48
2:A:302:PHE:CD1	2:A:302:PHE:C	2.91	0.48
2:A:271:LEU:O	2:A:275:ARG:HB2	2.14	0.48
2:A:108:TYR:CD1	2:A:366:PHE:CE1	3.02	0.47
2:B:226:GLU:O	2:B:227:VAL:HG22	2.15	0.47
2:A:78:LYS:HA	2:A:86:VAL:HG21	1.96	0.47
2:B:180:GLN:O	2:B:246:ALA:HB3	2.15	0.47
2:B:396:PRO:HG2	2:B:401:LEU:HD21	1.97	0.47
1:C:14:DA:O4'	3:C:473:FLQ:H5	2.15	0.46
2:A:45:LYS:H	2:A:410:GLN:HE22	1.63	0.46
2:A:375:ARG:HB2	2:A:376:PRO:HD2	1.98	0.46
2:B:13:PRO:HB2	2:B:18:PRO:HG3	1.96	0.46
2:B:92:TYR:HD2	2:B:92:TYR:C	2.24	0.46
2:A:43:THR:CG2	2:A:410:GLN:HE21	2.28	0.46
2:B:215:GLU:HB3	2:B:222:GLU:HB2	1.97	0.46
2:A:17:GLN:HB2	2:A:18:PRO:HD3	1.98	0.46
2:B:4:ARG:HD3	2:B:57:ASN:ND2	2.31	0.46
2:B:92:TYR:C	2:B:92:TYR:CD2	2.93	0.46
2:B:285:ARG:HD3	2:B:366:PHE:CD1	2.50	0.46
2:A:260:ILE:HG23	2:A:294:LEU:HD22	1.97	0.46
2:A:369:PRO:O	2:A:372:LEU:HD12	2.15	0.46
2:B:443:GLU:HB3	2:B:444:ARG:HH21	1.81	0.46
2:B:447:ARG:HG2	2:B:513:GLU:HB3	1.98	0.45
2:B:342:VAL:C	2:B:345:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:316:ARG:NH2	2:A:320:SER:HB3	2.32	0.45
2:A:446:GLU:HB3	2:A:515:SER:HB3	1.99	0.45
2:B:170:ASN:HD22	2:B:170:ASN:N	2.13	0.45
2:B:38:LEU:HD22	2:B:396:PRO:HG3	1.99	0.45
2:B:560:MET:O	2:B:561:GLU:C	2.60	0.45
2:A:89:PHE:CD2	2:A:325:LEU:HD22	2.51	0.45
2:B:525:GLU:OE2	2:B:525:GLU:HA	2.16	0.45
2:B:92:TYR:HE2	2:B:93:TYR:CZ	2.35	0.45
2:B:523:ASP:OD2	2:B:555:THR:HG22	2.17	0.45
2:A:509:LEU:HA	2:A:511:ILE:CD1	2.47	0.45
2:B:551:MET:CE	2:B:564:ILE:HD11	2.46	0.45
2:B:67:LYS:HD3	2:B:90:VAL:HG13	1.99	0.44
2:B:277:GLN:HE21	2:B:279:LYS:NZ	2.15	0.44
2:B:424:VAL:HA	2:B:551:MET:O	2.18	0.44
2:A:155:ARG:O	2:A:158:VAL:HG12	2.18	0.44
2:A:551:MET:HE2	2:A:560:MET:HE3	1.99	0.44
2:A:59:PRO:HG3	2:A:330:PRO:HG2	2.00	0.44
2:A:511:ILE:HD12	2:A:511:ILE:N	2.32	0.44
2:A:346:GLN:O	2:A:350:MET:HE3	2.18	0.44
1:C:18:DC:H5'	2:B:307:GLU:HG2	2.00	0.44
1:D:15:DC:C5'	2:A:66:ASN:HA	2.47	0.43
2:B:117:ASP:O	2:B:118:GLU:C	2.59	0.43
2:B:160:SER:HA	2:B:242:ALA:HA	2.00	0.43
2:B:503:ASN:HD21	2:B:505:LEU:HB2	1.83	0.43
2:B:158:VAL:HG22	2:B:244:PHE:CD2	2.53	0.43
2:B:344:LEU:N	2:B:345:PRO:CD	2.82	0.43
2:B:581:HIS:HB2	2:B:583:ILE:HG12	2.00	0.43
2:A:134:ARG:NH1	2:A:134:ARG:HB3	2.33	0.43
2:A:150:SER:OG	2:A:152:GLU:OE1	2.37	0.43
1:C:3:DG:C2'	1:C:4:DC:C6	3.02	0.43
2:A:358:LYS:NZ	2:A:374:ASN:O	2.52	0.43
2:B:172:LEU:HD12	2:B:172:LEU:O	2.19	0.43
2:B:473:ALA:HB2	2:B:496:TYR:CG	2.54	0.43
2:B:453:LEU:HD11	2:B:524:LYS:HB2	2.01	0.43
2:B:62:VAL:HG13	2:B:139:VAL:HA	2.01	0.42
1:C:16:DC:OP1	2:B:141:SER:OG	2.33	0.42
2:A:152:GLU:H	2:A:152:GLU:CD	2.24	0.42
2:A:450:VAL:CG2	2:A:500:VAL:HG22	2.49	0.42
2:A:135:ASP:O	2:A:135:ASP:CG	2.63	0.42
2:A:577:TYR:CE1	2:A:581:HIS:CE1	3.07	0.42
2:B:134:ARG:O	2:B:136:VAL:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:ILE:O	2:A:439:ARG:HG2	2.18	0.42
2:B:115:ILE:HG22	2:B:116:ASN:N	2.35	0.42
2:B:289:ARG:NH1	2:B:366:PHE:O	2.52	0.42
2:A:250:VAL:O	2:A:250:VAL:HG23	2.20	0.42
2:B:116:ASN:ND2	2:B:119:ILE:HG13	2.35	0.42
2:B:159:VAL:HG13	2:B:179:ILE:CD1	2.47	0.42
1:C:15:DC:H2'	1:C:16:DC:C6	2.55	0.42
1:D:19:DA:N3	2:A:304:SER:HB3	2.35	0.42
2:A:152:GLU:OE1	2:A:152:GLU:N	2.34	0.42
2:A:450:VAL:HG23	2:A:500:VAL:HA	2.01	0.42
2:B:169:ARG:HA	2:B:216:PHE:CZ	2.55	0.42
2:B:196:ARG:HB3	2:B:199:VAL:HG13	2.01	0.42
2:A:130:LEU:HD21	2:A:329:PHE:CD2	2.55	0.41
2:B:53:ILE:HG21	2:B:137:ILE:HD11	2.02	0.41
2:B:458:ALA:HB1	2:B:474:TYR:CE1	2.55	0.41
2:B:213:ARG:HB2	2:B:227:VAL:HG21	2.02	0.41
2:A:285:ARG:HD3	2:A:366:PHE:CD1	2.55	0.41
2:A:538:ILE:HG23	2:A:549:VAL:HG21	2.02	0.41
2:B:99:GLU:OE2	2:B:289:ARG:NH2	2.53	0.41
2:A:15:GLY:HA2	2:A:412:ILE:HG22	2.01	0.41
2:A:133:ARG:HG3	2:A:133:ARG:NH1	2.27	0.41
2:A:544:ASN:HA	2:A:587:THR:HG23	2.02	0.41
2:B:502:ILE:CG2	2:B:528:LEU:HD11	2.51	0.41
1:D:18:DC:H3'	2:A:307:GLU:HG2	2.01	0.41
2:A:356:ALA:O	2:A:360:VAL:HG23	2.21	0.41
2:A:342:VAL:C	2:A:345:PRO:HD2	2.45	0.41
2:A:289:ARG:NH1	2:A:366:PHE:O	2.54	0.41
2:A:40:ALA:O	2:A:41:THR:C	2.63	0.41
2:B:16:ASP:HB2	2:B:19:GLN:HE21	1.86	0.41
1:C:1:DC:H2'	1:C:2:DG:C8	2.56	0.40
2:A:294:LEU:O	2:A:298:ARG:HG3	2.20	0.40
2:B:5:PHE:HA	2:B:84:ASN:HD21	1.85	0.40
2:B:60:THR:CG2	2:B:334:LEU:HD23	2.51	0.40
2:A:108:TYR:CD1	2:A:366:PHE:CD1	3.10	0.40
2:A:491:LEU:HD23	2:A:511:ILE:HG12	2.03	0.40
2:A:512:PRO:HA	2:A:543:ARG:HB3	2.03	0.40
2:B:90:VAL:O	2:B:91:SER:C	2.64	0.40
2:B:270:ARG:HH11	2:B:270:ARG:CG	2.34	0.40
2:A:475:LEU:HD23	2:A:506:ARG:HH11	1.85	0.40
2:B:311:ARG:HD3	2:B:316:ARG:O	2.20	0.40
2:A:12:GLU:HG2	2:A:13:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:34:HIS:HB2	2:A:403:HIS:O	2.21	0.40
2:A:35:GLN:O	2:A:390:ILE:HA	2.22	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	
2	A	499/658 (76%)	456 (91%)	36 (7%)	7 (1%)	9	33
2	B	581/658 (88%)	541 (93%)	27 (5%)	13 (2%)	5	26
All	All	1080/1316 (82%)	997 (92%)	63 (6%)	20 (2%)	6	28

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	45	LYS
2	A	79	GLU
2	A	428	LYS
2	A	525	GLU
2	B	45	LYS
2	B	230	LEU
2	B	486	GLU
2	B	487	ILE
2	B	165	MET
2	B	310	SER
2	B	135	ASP
2	B	180	GLN
2	B	227	VAL
2	A	301	GLY
2	A	502	ILE
2	B	222	GLU

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Mol	Chain	Res	Type
2	A	2	GLU
2	B	234	VAL
2	B	592	ILE
2	B	232	GLY

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	
2	A	442/570 (78%)	413 (93%)	29 (7%)	15	43
2	B	512/570 (90%)	474 (93%)	38 (7%)	13	38
All	All	954/1140 (84%)	887 (93%)	67 (7%)	14	41

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	7	LEU
2	A	12	GLU
2	A	19	GLN
2	A	49	ILE
2	A	86	VAL
2	A	130	LEU
2	A	133	ARG
2	A	142	VAL
2	A	243	ILE
2	A	244	PHE
2	A	270	ARG
2	A	281	LEU
2	A	296	MET
2	A	302	PHE
2	A	306	ILE
2	A	342	VAL
2	A	404	SER
2	A	415	THR
2	A	418	LEU

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Mol	Chain	Res	Type
2	A	421	THR
2	A	428	LYS
2	A	445	ASN
2	A	457	MET
2	A	462	THR
2	A	471	LYS
2	A	507	GLU
2	A	525	GLU
2	A	588	VAL
2	A	592	ILE
2	B	23	LYS
2	B	38	LEU
2	B	41	THR
2	B	62	VAL
2	B	92	TYR
2	B	107	THR
2	B	133	ARG
2	B	157	LEU
2	B	165	MET
2	B	170	ASN
2	B	179	ILE
2	B	192	THR
2	B	195	VAL
2	B	196	ARG
2	B	209	GLU
2	B	215	GLU
2	B	220	GLU
2	B	227	VAL
2	B	228	ASP
2	B	270	ARG
2	B	284	GLN
2	B	302	PHE
2	B	310	SER
2	B	326	LEU
2	B	358	LYS
2	B	415	THR
2	B	422	ILE
2	B	424	VAL
2	B	450	VAL
2	B	466	LYS
2	B	471	LYS
2	B	490	ASP

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Mol	Chain	Res	Type
2	B	533	SER
2	B	555	THR
2	B	558	LYS
2	B	561	GLU
2	B	588	VAL
2	B	592	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	6	GLN
2	A	14	GLN
2	A	19	GLN
2	A	65	HIS
2	A	72	GLN
2	A	83	HIS
2	A	97	GLN
2	A	248	HIS
2	A	308	ASN
2	A	341	HIS
2	A	374	ASN
2	A	387	ASN
2	A	410	GLN
2	A	503	ASN
2	A	536	GLN
2	A	565	GLN
2	A	581	HIS
2	B	19	GLN
2	B	57	ASN
2	B	84	ASN
2	B	116	ASN
2	B	170	ASN
2	B	265	GLN
2	B	277	GLN
2	B	364	HIS
2	B	374	ASN
2	B	387	ASN
2	B	388	GLN
2	B	403	HIS
2	B	445	ASN
2	B	503	ASN
2	B	565	GLN

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Mol	Chain	Res	Type
2	B	574	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](#)

1 ligand is 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	FLQ	C	473	-	36,36,42	2.62	12 (33%)	53,54,61	1.45	9 (16%)

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	FLQ	C	473	-	-	1/9/40/46	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	473	FLQ	O1-C1	-6.95	1.21	1.37
3	C	473	FLQ	O8'-C9'	6.33	1.46	1.36
3	C	473	FLQ	C4'-C5'	5.07	1.46	1.39
3	C	473	FLQ	C6'-C5'	-5.00	1.32	1.39
3	C	473	FLQ	O2-C4	4.22	1.45	1.38
3	C	473	FLQ	O2-C3	4.16	1.45	1.38
3	C	473	FLQ	C6'-C1'	-4.09	1.33	1.39
3	C	473	FLQ	C4-C9	3.38	1.46	1.39
3	C	473	FLQ	C8-C9	2.33	1.42	1.39
3	C	473	FLQ	C12-C11	2.25	1.42	1.39
3	C	473	FLQ	C3'-C4'	-2.18	1.36	1.39
3	C	473	FLQ	C2'-C1'	2.08	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	473	FLQ	O8'-C9'-O9'	3.48	124.87	121.12
3	C	473	FLQ	C2'-C3'-C4'	-3.11	115.72	120.86
3	C	473	FLQ	O8'-C10-C11	-2.78	103.53	107.65
3	C	473	FLQ	O8'-C10-C5'	2.62	103.78	101.65
3	C	473	FLQ	C5-C4-C9	-2.61	119.42	122.11
3	C	473	FLQ	C1'-C14-N1	2.58	122.49	117.12
3	C	473	FLQ	C2-C3-C11	-2.53	119.50	122.11
3	C	473	FLQ	C12-C11-C3	2.46	119.58	116.44
3	C	473	FLQ	O8'-C9'-C4'	-2.33	106.45	108.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	473	FLQ	C16-C17-C18-C19

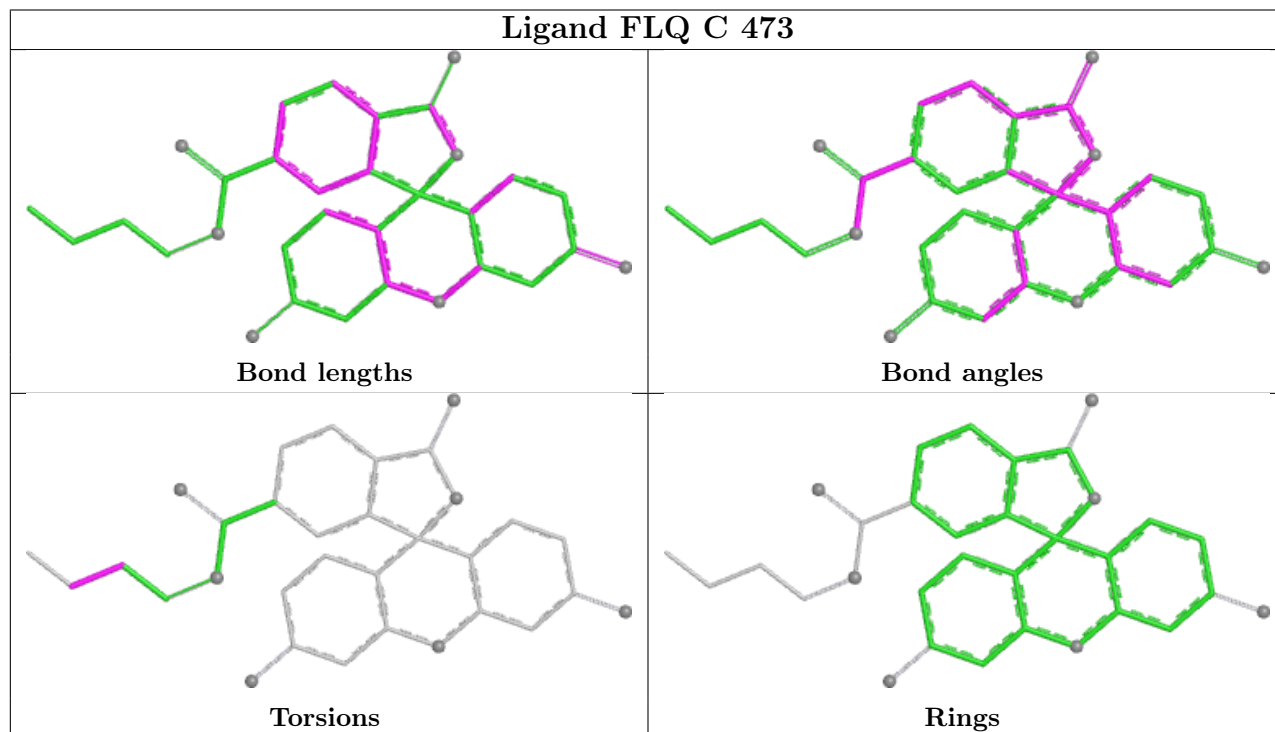
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	473	FLQ	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 [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	C	12/20 (60%)	0.50	1 (8%) 17 13	51, 84, 93, 96	0
1	D	5/20 (25%)	1.50	1 (20%) 3 2	70, 73, 75, 98	0
2	A	505/658 (76%)	-0.10	7 (1%) 73 55	47, 76, 102, 130	0
2	B	585/658 (88%)	-0.28	4 (0%) 84 70	38, 63, 120, 141	0
All	All	1107/1356 (81%)	-0.18	13 (1%) 76 58	38, 70, 113, 141	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	DA	4.2
2	B	156	GLU	3.5
2	A	1	VAL	3.0
2	B	219	ASP	2.9
2	A	2	GLU	2.9
2	A	432	ASP	2.7
2	A	243	ILE	2.5
2	B	485	ILE	2.5
2	A	57	ASN	2.3
2	A	460	ASP	2.1
1	C	1	DC	2.1
2	A	104	GLN	2.1
2	B	163	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

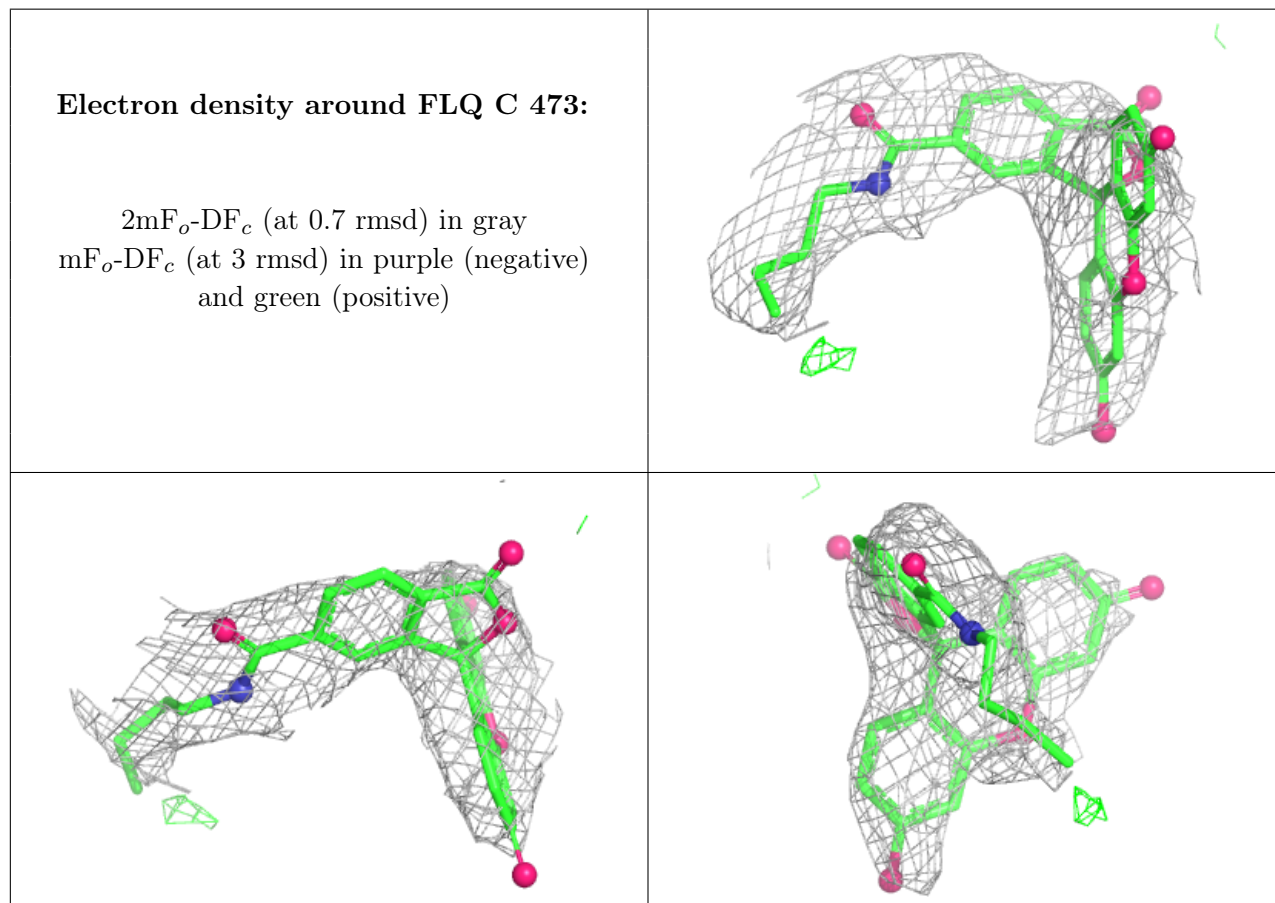
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FLQ	C	473	32/38	0.88	0.12	91,92,93,94	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.