Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 09:34 am BST

PDB ID	:	2FDC
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (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.
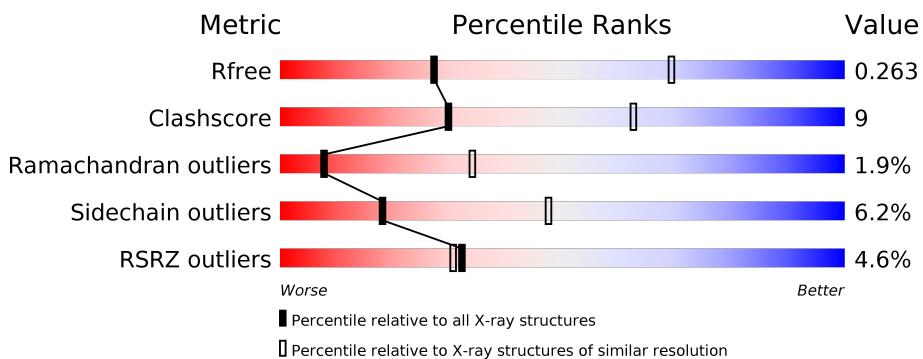
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
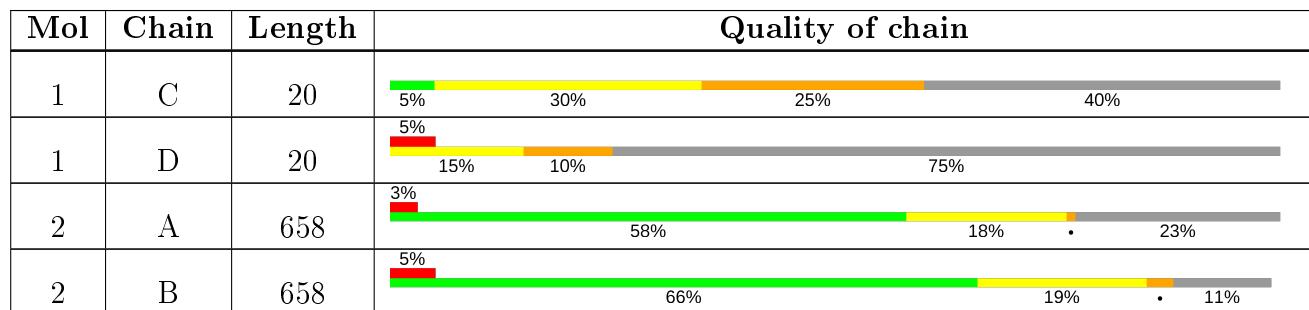
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLQ	C	473	-	-	-	X

2 Entry composition (i)

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
1	C	12	Total 243	C 115	N 44	O 72	P 12	0	0	0
1	D	5	Total 100	C 47	N 19	O 29	P 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	505	Total 4072	C 2574	N 718	O 770	S 10	0	0	0
2	B	585	Total 4731	C 2983	N 844	O 892	S 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-B ENZOFURAN-1,9'-XANTHENE]-6-CARBOXAMIDE (three-letter code: FLQ) (formula: $C_{29}H_{28}N_2O_7$).

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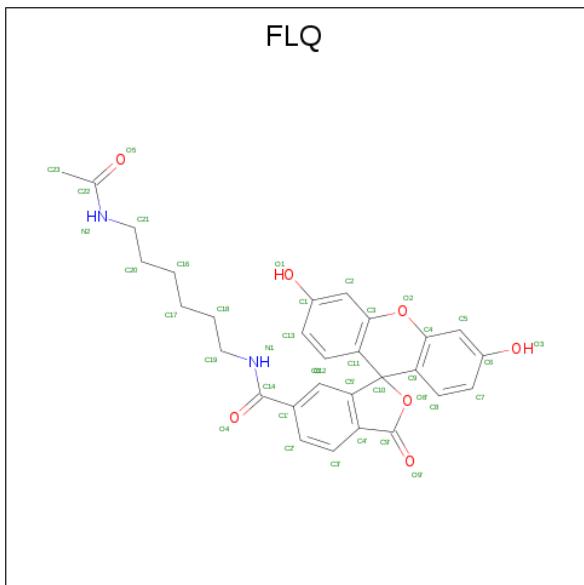
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			32	25	1	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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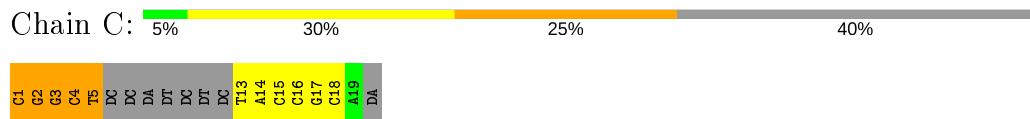
Chain C:

• 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'

Chain D:

• Molecule 2: UvrABC system protein B

Chain A:

● Molecule 2: UvrABC system protein B

Chain B:
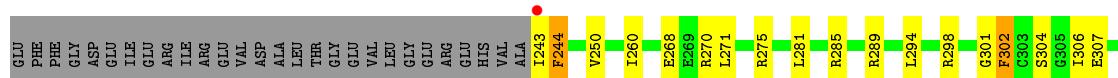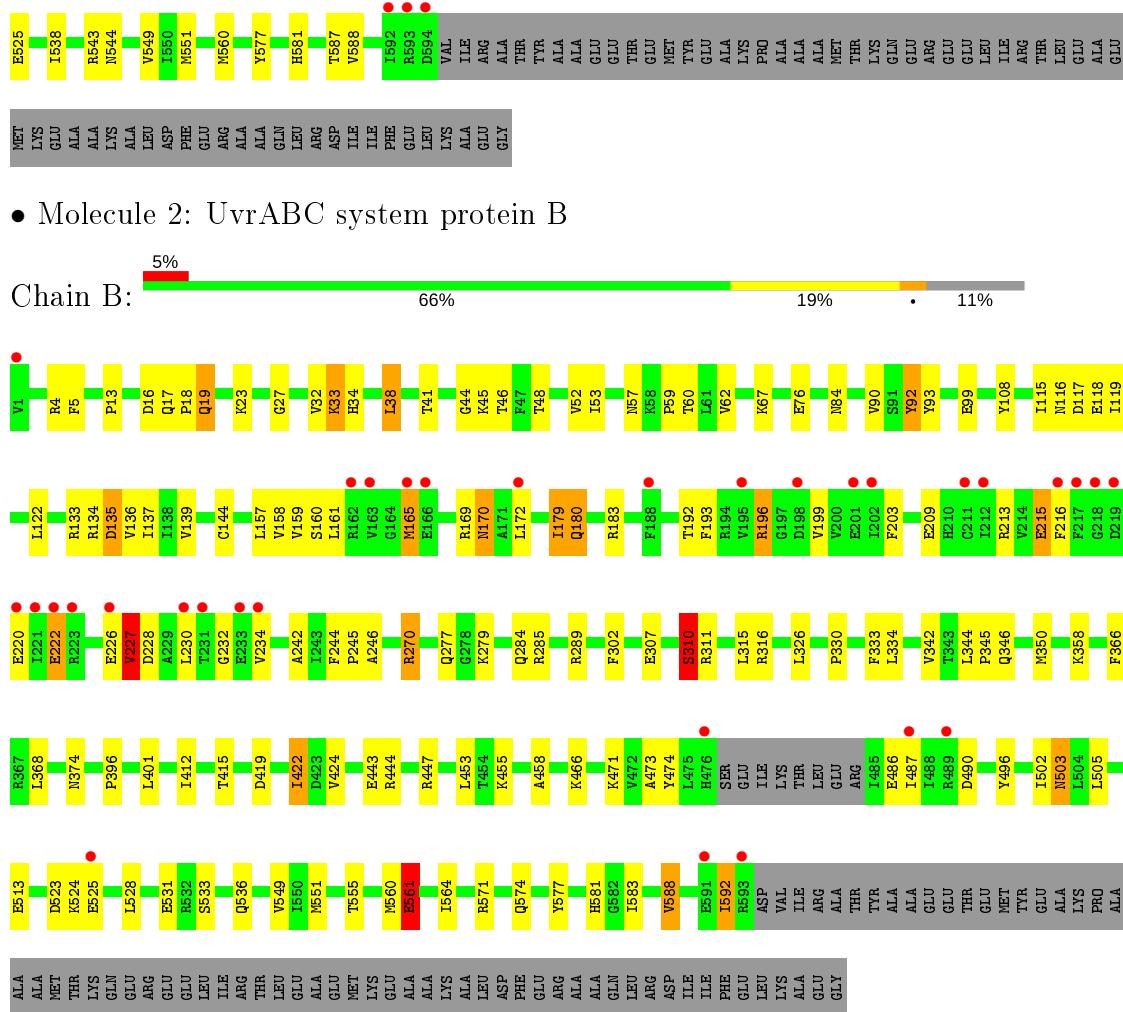
4 Data and refinement statistics (i)

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 37.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-3.30) 99.9 (37.26-3.09)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.258 0.219 , 0.263	Depositor DCC
R_{free} test set	2009 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	63.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.76	2/270 (0.7%)	1.87	10/411 (2.4%)
1	D	1.65	1/111 (0.9%)	1.62	1/168 (0.6%)
2	A	0.84	1/4143 (0.0%)	0.67	1/5601 (0.0%)
2	B	0.91	5/4812 (0.1%)	0.69	0/6502
All	All	0.93	9/9336 (0.1%)	0.77	12/12682 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	144	CYS	CB-SG	-6.48	1.71	1.82
2	B	536	GLN	CG-CD	6.23	1.65	1.51
1	C	3	DG	C3'-O3'	-5.83	1.36	1.44
2	B	588	VAL	CB-CG2	5.83	1.65	1.52
1	D	19	DA	N9-C4	5.72	1.41	1.37
2	A	268	GLU	CB-CG	5.61	1.62	1.52
2	B	561	GLU	CG-CD	5.41	1.60	1.51
2	B	531	GLU	CG-CD	5.28	1.59	1.51
1	C	17	DG	C3'-O3'	-5.11	1.37	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	DG	O4'-C1'-N9	10.77	115.54	108.00
1	C	4	DC	O4'-C4'-C3'	-7.90	101.26	106.00
1	C	1	DC	O4'-C4'-C3'	-7.73	101.36	106.00
1	C	4	DC	O4'-C1'-N1	7.44	113.21	108.00
1	C	13	DT	N3-C4-O4	6.21	123.63	119.90
2	A	133	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	5	DT	C1'-O4'-C4'	-5.44	104.66	110.10
1	C	13	DT	C5-C4-O4	-5.42	121.11	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	DC	P-O3'-C3'	5.40	126.18	119.70
1	C	2	DG	O4'-C1'-N9	5.40	111.78	108.00
1	C	13	DT	O4'-C1'-N1	5.18	111.63	108.00
1	D	18	DC	O4'-C4'-C3'	-5.18	102.43	104.50

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	10	0
1	D	100	0	56	6	0
2	A	4072	0	4108	74	0
2	B	4731	0	4761	89	0
3	C	32	0	17	1	0
All	All	9178	0	9078	172	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 9.

All (172) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:412:ILE:HD13	2:B:577:TYR:CD1	2.41	0.56
1:C:4:DC:H42	1:C:14:DA:H61	1.54	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:N	2:B:315:LEU:HD12	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
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:310:SER:CB	2:B:374:ASN:ND2	2.73	0.52
2:B:48:THR:O	2:B:52:VAL:HG23	2.08	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:DC:H2'	1:D:17:DG:C8	2.44	0.51
2:A:158:VAL:HG23	2:A:244:PHE:HA	1.92	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
2:B:84:ASN:HD22	2:B:135:ASP:HB2	1.76	0.50
2:B:116:ASN:O	2:B:117:ASP:HB2	2.11	0.50
2:B:108:TYR:CD1	2:B:366:PHE:CE1	3.00	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:B:59:PRO:HG3	2:B:330:PRO:HG2	1.94	0.49
2:A:475:LEU:HD23	2:A:506:ARG:NH1	2.27	0.49
2:A:448:THR:HG23	2:A:516:LEU:HG	1.95	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:271:LEU:O	2:A:275:ARG:HB2	2.14	0.48
2:A:281:LEU:HD13	2:A:281:LEU:C	2.35	0.47
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
2:A:45:LYS:H	2:A:410:GLN:HE22	1.63	0.46
1:C:14:DA:O4'	3:C:473:FLQ:H5	2.15	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASN:N	2:B:170:ASN:HD22	2.13	0.45
2:B:346:GLN:O	2:B:350:MET:HE3	2.16	0.45
2:B:38:LEU:HD22	2:B:396:PRO:HG3	1.99	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:A:351:TYR:C	2:A:351:TYR:CD2	2.90	0.45
2:B:523:ASP:OD2	2:B:555:THR:HG22	2.17	0.45
2:B:92:TYR:HE2	2:B:93:TYR:CZ	2.35	0.45
2:A:142:VAL:HG21	2:A:346:GLN:CD	2.37	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:277:GLN:HE21	2:B:279:LYS:NZ	2.15	0.44
2:B:67:LYS:HD3	2:B:90:VAL:HG13	1.99	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:302:PHE:CD1	2:A:302:PHE:C	2.91	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
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: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
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:O	2:B:172:LEU:HD12	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
2:A:450:VAL:CG2	2:A:500:VAL:HG22	2.49	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
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:HG23	2:A:250:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:92:TYR:C	2:B:92:TYR:HD2	2.24	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: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:133:ARG:HG3	2:A:133:ARG:NH1	2.27	0.41
2:A:15:GLY:HA2	2:A:412:ILE:HG22	2.01	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
2:B:92:TYR:C	2:B:92:TYR:CD2	2.93	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:289:ARG:NH1	2:A:366:PHE:O	2.54	0.41
2:B:342:VAL:C	2:B:345:PRO:HD2	2.41	0.41
2:B:16:ASP:HB2	2:B:19:GLN:HE21	1.86	0.41
2:A:294:LEU:O	2:A:298:ARG:HG3	2.20	0.40
2:B:60:THR:CG2	2:B:334:LEU:HD23	2.51	0.40
2:B:5:PHE:HA	2:B:84:ASN:HD21	1.85	0.40
1:C:1:DC:H2'	1:C:2:DG:C8	2.56	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:270:ARG:HH11	2:B:270:ARG:CG	2.34	0.40
2:B:560:MET:O	2:B:561:GLU:C	2.60	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
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%)	11	38
2	B	581/658 (88%)	541 (93%)	27 (5%)	13 (2%)	6	30
All	All	1080/1316 (82%)	997 (92%)	63 (6%)	20 (2%)	8	34

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
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%)	419 (95%)	23 (5%)	23	54
2	B	512/570 (90%)	476 (93%)	36 (7%)	15	43
All	All	954/1140 (84%)	895 (94%)	59 (6%)	18	47

All (59) 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	86	VAL
2	A	130	LEU
2	A	133	ARG
2	A	244	PHE
2	A	270	ARG
2	A	302	PHE
2	A	306	ILE
2	A	333	PHE
2	A	342	VAL
2	A	404	SER
2	A	415	THR
2	A	418	LEU
2	A	419	ASP
2	A	421	THR
2	A	428	LYS
2	A	445	ASN
2	A	457	MET
2	A	464	TYR
2	A	507	GLU
2	A	588	VAL
2	B	19	GLN
2	B	23	LYS
2	B	33	LYS
2	B	38	LEU
2	B	41	THR
2	B	92	TYR
2	B	133	ARG
2	B	157	LEU

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Mol	Chain	Res	Type
2	B	165	MET
2	B	170	ASN
2	B	179	ILE
2	B	192	THR
2	B	196	ARG
2	B	203	PHE
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	333	PHE
2	B	368	LEU
2	B	415	THR
2	B	422	ILE
2	B	466	LYS
2	B	471	LYS
2	B	490	ASP
2	B	503	ASN
2	B	533	SER
2	B	561	GLU
2	B	588	VAL
2	B	592	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	6	GLN
2	A	19	GLN
2	A	65	HIS
2	A	72	GLN
2	A	97	GLN
2	A	374	ASN
2	A	387	ASN
2	A	410	GLN
2	A	503	ASN
2	A	536	GLN

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Mol	Chain	Res	Type
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	277	GLN
2	B	308	ASN
2	B	364	HIS
2	B	374	ASN
2	B	388	GLN
2	B	410	GLN
2	B	503	ASN
2	B	565	GLN
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 carbohydrates 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	2.60	11 (30%)	54,54,61	1.51	10 (18%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	473	FLQ	O1-C1	-6.70	1.21	1.37
3	C	473	FLQ	O8'-C9'	5.74	1.46	1.37
3	C	473	FLQ	C4'-C5'	5.27	1.46	1.39
3	C	473	FLQ	C6'-C5'	-4.73	1.32	1.39
3	C	473	FLQ	O2-C4	4.60	1.45	1.38
3	C	473	FLQ	O2-C3	4.53	1.45	1.38
3	C	473	FLQ	C6'-C1'	-4.10	1.33	1.39
3	C	473	FLQ	C4-C9	3.71	1.46	1.39
3	C	473	FLQ	C8-C9	2.25	1.42	1.39
3	C	473	FLQ	C12-C11	2.17	1.42	1.39
3	C	473	FLQ	C3'-C4'	-2.04	1.36	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	473	FLQ	O8'-C9'-O9'	3.43	124.87	121.11
3	C	473	FLQ	C2'-C3'-C4'	-3.22	115.72	120.94
3	C	473	FLQ	C5-C4-C9	-3.01	119.42	122.20
3	C	473	FLQ	C2-C3-C11	-2.93	119.50	122.20
3	C	473	FLQ	O8'-C10-C11	-2.82	103.53	107.76
3	C	473	FLQ	O8'-C10-C5'	2.82	103.78	101.67
3	C	473	FLQ	C12-C11-C3	2.65	119.58	116.52
3	C	473	FLQ	C1'-C14-N1	2.51	122.49	117.09
3	C	473	FLQ	O8'-C9'-C4'	-2.45	106.45	108.35
3	C	473	FLQ	C8-C9-C4	2.04	118.88	116.52

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 then 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 FLQ C 473

Bond lengths

Bond angles

Torsions

Rings
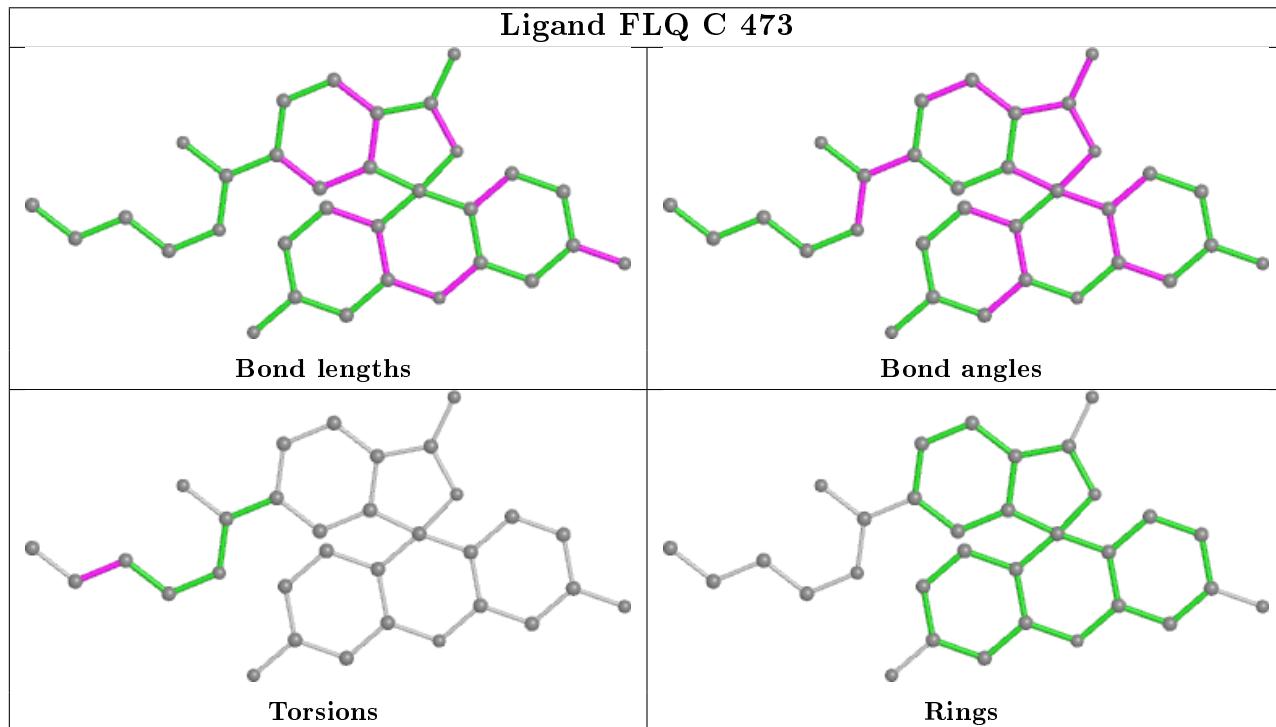
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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(Å²)	Q<0.9
1	C	12/20 (60%)	0.48	0	100	100	51, 84, 93, 96	0
1	D	5/20 (25%)	0.66	1 (20%)	1	1	70, 73, 75, 98	0
2	A	505/658 (76%)	0.04	18 (3%)	42	40	47, 76, 102, 130	0
2	B	585/658 (88%)	-0.02	32 (5%)	25	23	38, 63, 120, 141	0
All	All	1107/1356 (81%)	0.02	51 (4%)	32	30	38, 70, 113, 141	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1	VAL	8.6
2	A	159	VAL	6.6
2	B	219	ASP	6.1
2	B	223	ARG	4.6
2	A	243	ILE	4.6
2	A	2	GLU	4.5
2	B	220	GLU	4.1
2	B	166	GLU	3.9
2	A	486	GLU	3.8
2	B	230	LEU	3.7
2	B	202	ILE	3.6
2	B	487	ILE	3.5
2	B	216	PHE	3.3
2	B	217	PHE	3.3
2	B	221	ILE	3.3
2	B	231	THR	3.2
2	A	594	ASP	3.2
2	B	234	VAL	3.2
2	A	483	GLU	3.1
2	A	485	ILE	3.1
2	A	476	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	212	ILE	3.0
2	B	163	VAL	2.9
1	D	19	DA	2.8
2	B	591	GLU	2.8
2	B	188	PHE	2.7
2	A	474	TYR	2.6
2	B	525	GLU	2.6
2	B	172	LEU	2.5
2	B	222	GLU	2.5
2	A	9	ALA	2.5
2	A	473	ALA	2.5
2	B	195	VAL	2.4
2	B	165	MET	2.4
2	A	593	ARG	2.4
2	B	211	CYS	2.4
2	B	593	ARG	2.4
2	B	233	GLU	2.4
2	A	592	ILE	2.4
2	B	201	GLU	2.4
2	B	198	ASP	2.3
2	A	10	PRO	2.3
2	A	157	LEU	2.3
2	B	476	HIS	2.3
2	B	226	GLU	2.2
2	A	455	LYS	2.2
2	B	489	ARG	2.1
2	B	1	VAL	2.1
2	A	475	LEU	2.1
2	B	218	GLY	2.1
2	B	162	ARG	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 carbohydrates 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
3	FLQ	C	473	32/38	0.73	0.44	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.

Electron density around FLQ C 473:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.