Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 09:45 pm GMT

PDB ID	:	8BDX
Title	:	Ternary complex between VCB, BRD4-BD2 and PROTAC 48
Authors	:	Sorrell, F.J.; Mueller, J.E.; Lehmann, M.; Wegener, A.
Deposited on	:	2022-10-20
Resolution	:	2.93 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:

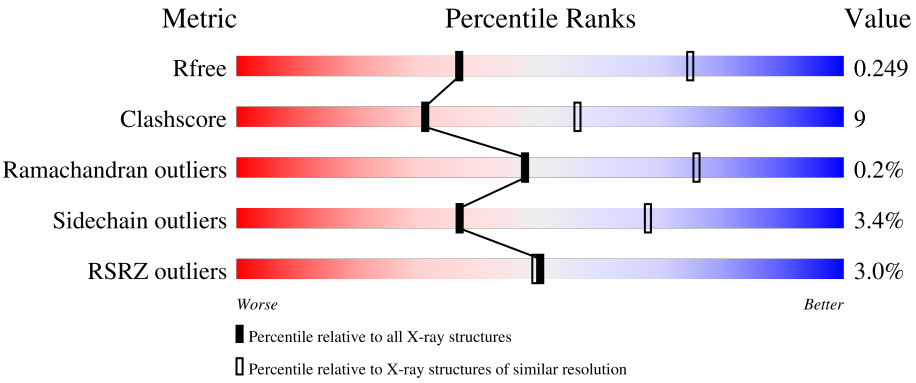
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 <=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	129	2% 60% 24% 16%
1	E	129	67% 17% 16%
2	B	104	81% 17%
2	F	104	11% 80% 19%
3	C	97	2% 90% 10%

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Mol	Chain	Length	Quality of chain
3	G	97	5% 69% 19% 11%
4	D	162	% 73% 19% 8%
4	H	162	4% 77% 14% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7156 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			845	542	136	157	10			
1	E	109	Total	C	N	O	S	0	0	0
			845	542	134	158	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	GLY	-	expression tag	UNP O60885
E	332	GLY	-	expression tag	UNP O60885

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			804	509	133	158	4			
2	F	104	Total	C	N	O	S	0	0	0
			731	461	117	149	4			

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	S	0	0	0
			742	474	118	144	6			
3	G	86	Total	C	N	O	S	0	0	0
			669	433	102	128	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
G	16	MET	-	initiating methionine	UNP Q15369

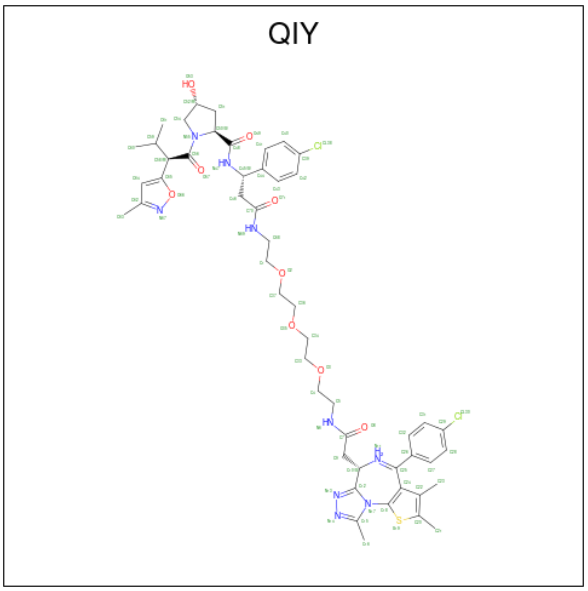
- Molecule 4 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	149	Total	C	N	O	S	0	1	0
			1205	767	217	219	2			
4	H	149	Total	C	N	O	S	0	0	0
			1171	747	208	214	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	52	GLY	-	expression tag	UNP P40337
D	53	SER	-	expression tag	UNP P40337
H	52	GLY	-	expression tag	UNP P40337
H	53	SER	-	expression tag	UNP P40337

- Molecule 5 is (2S,4R)-N-[(1S)-1-(4-chlorophenyl)-3-[2-[2-[2-[2-[2-[(9S)-7-(4-chlorophenyl)-4,5,13-trimethyl-3-thia-1,8$l^{5},11,12-tetrazatricyclo[8.3.0.0^{2,6}]trideca-2(6),4,7,10,12-pentaen-9-yl]ethanoylamino]ethoxy]ethoxy]ethoxy]ethylamino]-3-oxidanylidene-propyl]-1-[(2R)-3-methyl-2-(3-methyl-1,2-oxazol-5-yl)butanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: QIY) (formula: $C_{50}H_{63}Cl_2N_9O_9S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total	C	Cl	N	O	S	0	0
			71	50	2	9	9	1		
5	H	1	Total	C	Cl	N	O	S	0	0
			71	50	2	9	9	1		

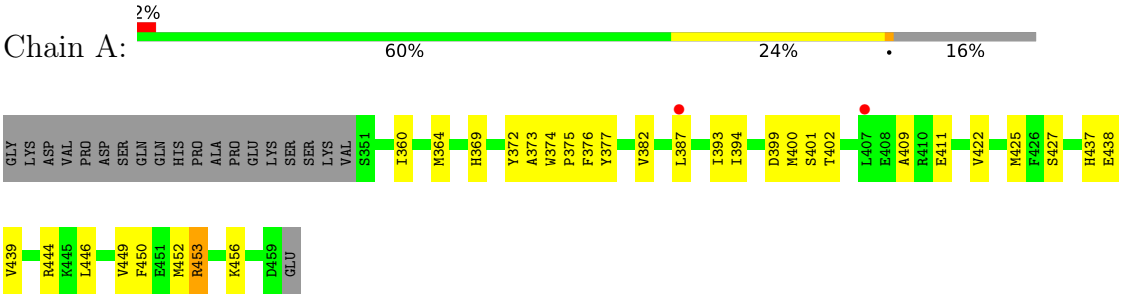
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O 1 1	0	0
6	G	1	Total O 1 1	0	0

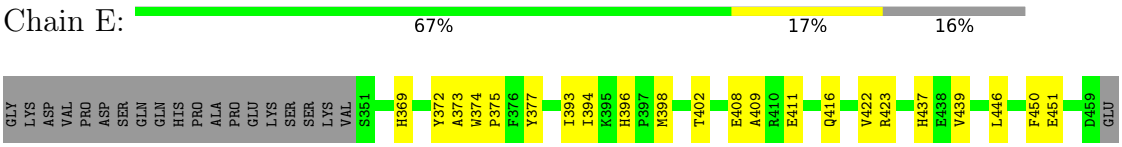
3 Residue-property plots (i)

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.

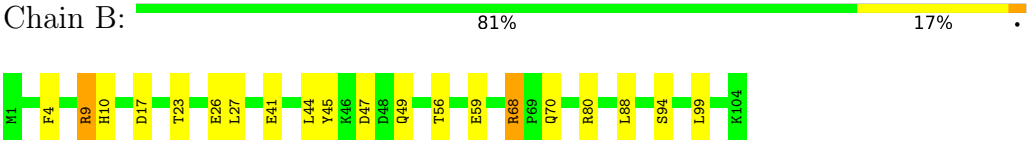
• Molecule 1: Bromodomain-containing protein 4



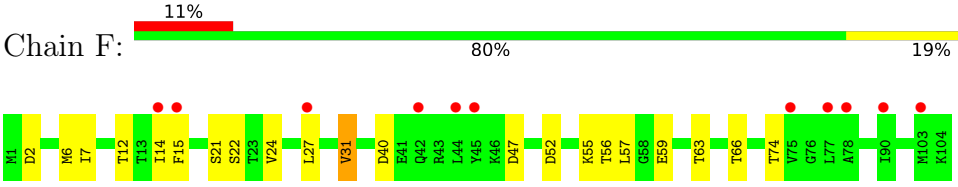
• Molecule 1: Bromodomain-containing protein 4



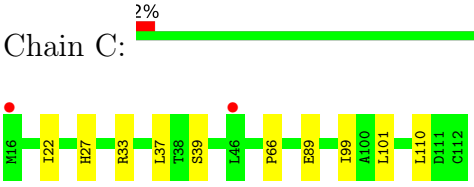
• Molecule 2: Elongin-B



• Molecule 2: Elongin-B

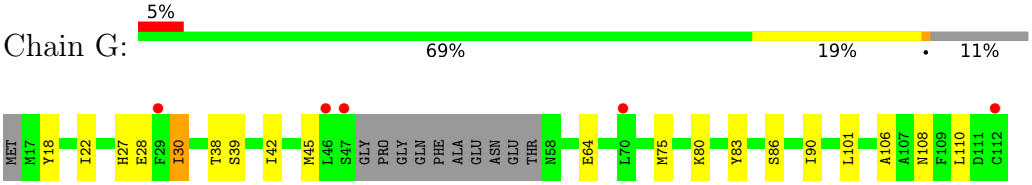


• Molecule 3: Elongin-C



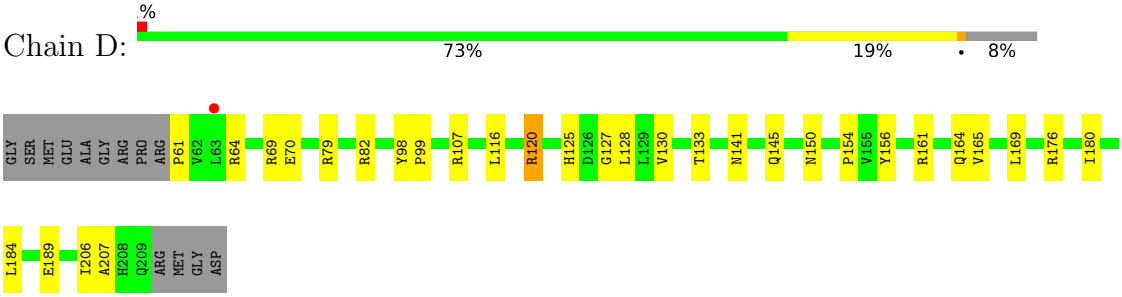
• Molecule 3: Elongin-C

Chain G:



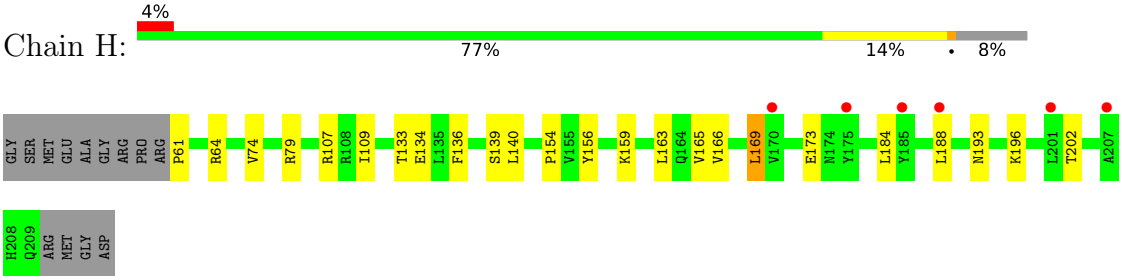
• Molecule 4: von Hippel-Lindau disease tumor suppressor

Chain D:



• Molecule 4: von Hippel-Lindau disease tumor suppressor

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	82.34Å 82.34Å 168.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.31 – 2.93 71.31 – 2.93	Depositor EDS
% Data completeness (in resolution range)	91.5 (71.31-2.93) 91.5 (71.31-2.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.185 , 0.258 0.188 , 0.249	Depositor DCC
R_{free} test set	1342 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	106.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.045 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7156	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.39	0/868	0.70	0/1177
1	E	0.36	0/868	0.71	0/1177
2	B	0.35	0/820	0.69	0/1111
2	F	0.30	0/746	0.65	0/1025
3	C	0.43	0/758	0.70	0/1029
3	G	0.38	0/683	0.64	0/925
4	D	0.36	0/1236	0.73	0/1689
4	H	0.33	0/1202	0.71	1/1648 (0.1%)
All	All	0.36	0/7181	0.70	1/9781 (0.0%)

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	2
2	B	0	1
4	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	107	ARG	NE-CZ-NH2	-5.49	117.55	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	ARG	Sidechain
1	A	453	ARG	Sidechain
2	B	9	ARG	Sidechain
4	D	107	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	845	0	770	23	0
1	E	845	0	770	16	0
2	B	804	0	784	14	0
2	F	731	0	644	13	0
3	C	742	0	709	7	0
3	G	669	0	648	17	0
4	D	1205	0	1188	24	0
4	H	1171	0	1130	20	0
5	D	71	0	0	0	0
5	H	71	0	0	1	0
6	E	1	0	0	1	0
6	G	1	0	0	0	0
All	All	7156	0	6643	126	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 (126) 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:438:GLU:OE2	4:D:69[A]:ARG:NH1	1.95	0.99
4:D:120:ARG:NH1	4:D:125:HIS:O	2.03	0.92
2:B:41:GLU:HG2	2:B:80:ARG:HH12	1.31	0.91
3:G:108:ASN:ND2	4:H:184:LEU:HD21	1.87	0.90
2:F:22:SER:O	2:F:57:LEU:HD12	1.76	0.84
2:F:12:THR:HG22	3:G:28:GLU:HB2	1.59	0.84
4:H:74:VAL:CG1	4:H:109:ILE:HG23	2.11	0.81
4:D:150:ASN:OD1	4:H:79:ARG:NH2	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:THR:H	2:F:66:THR:HG22	1.46	0.77
4:D:141:ASN:ND2	4:D:145:GLN:O	2.16	0.77
1:A:382:VAL:HG22	1:A:387:LEU:O	1.88	0.74
4:H:61:PRO:O	4:H:64:ARG:HD3	1.88	0.73
1:E:398:MET:CE	1:E:402:THR:HB	2.21	0.71
3:G:106:ALA:O	3:G:110:LEU:HD12	1.91	0.69
3:G:38:THR:HG23	3:G:80:LYS:HD2	1.75	0.69
4:D:161:ARG:HH11	4:D:164:GLN:NE2	1.92	0.66
4:D:165:VAL:O	4:D:169:LEU:CD2	2.45	0.65
2:F:22:SER:O	2:F:57:LEU:CD1	2.44	0.65
1:E:398:MET:HE3	1:E:402:THR:HB	1.79	0.64
1:E:393:ILE:HG22	1:E:394:ILE:CD1	2.30	0.62
1:E:393:ILE:HG22	1:E:394:ILE:HD12	1.81	0.61
1:E:398:MET:HE3	1:E:402:THR:CG2	2.32	0.60
1:A:376:PHE:HB2	1:A:400:MET:CE	2.32	0.60
1:A:393:ILE:HG22	1:A:394:ILE:CD1	2.33	0.59
4:H:165:VAL:O	4:H:169:LEU:HD12	2.03	0.59
1:E:423:ARG:NH1	1:E:451:GLU:OE2	2.35	0.59
4:H:64:ARG:HH11	4:H:64:ARG:HG2	1.67	0.59
4:D:128:LEU:HA	4:D:154:PRO:HD3	1.85	0.58
4:H:74:VAL:HG12	4:H:109:ILE:HG23	1.84	0.58
4:D:165:VAL:O	4:D:169:LEU:HD22	2.04	0.58
1:E:422:VAL:HG11	1:E:450:PHE:CD1	2.39	0.58
1:A:422:VAL:HG11	1:A:450:PHE:CD1	2.39	0.57
1:A:400:MET:HB2	1:A:425:MET:HE1	1.87	0.57
4:H:74:VAL:HG13	4:H:109:ILE:HG23	1.85	0.57
4:D:176:ARG:NH2	4:D:189:GLU:OE1	2.35	0.57
4:H:74:VAL:HG13	4:H:109:ILE:CG2	2.34	0.57
3:C:22:ILE:HD12	3:C:22:ILE:N	2.19	0.56
2:B:68:ARG:NH1	2:B:70:GLN:HE22	2.04	0.56
4:H:133:THR:HG22	4:H:134:GLU:H	1.71	0.56
3:G:22:ILE:HD12	3:G:22:ILE:N	2.21	0.56
2:F:14:ILE:HG23	3:G:30:ILE:HD11	1.89	0.55
1:A:399:ASP:CA	1:A:425:MET:HE3	2.37	0.55
1:A:393:ILE:HG22	1:A:394:ILE:HD12	1.88	0.54
1:A:399:ASP:HA	1:A:425:MET:CE	2.37	0.54
4:D:161:ARG:NH1	4:D:164:GLN:NE2	2.56	0.54
1:A:399:ASP:O	1:A:401:SER:N	2.37	0.53
2:F:63:THR:H	2:F:66:THR:CG2	2.21	0.53
3:G:106:ALA:O	3:G:110:LEU:CD1	2.57	0.52
1:A:399:ASP:HA	1:A:425:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:ARG:HG3	4:H:79:ARG:NH2	2.25	0.52
3:G:83:TYR:HB3	3:G:90:ILE:HD12	1.90	0.52
4:H:133:THR:HG22	4:H:134:GLU:N	2.25	0.52
2:B:56:THR:HG22	2:B:59:GLU:CD	2.31	0.51
4:D:180:ILE:HD12	4:D:184:LEU:HB2	1.91	0.51
3:G:18:TYR:CD2	3:G:30:ILE:HD12	2.46	0.51
4:H:154:PRO:HG2	4:H:156:TYR:CE1	2.46	0.51
1:E:398:MET:HE3	1:E:402:THR:CB	2.40	0.50
3:G:108:ASN:HD22	4:H:184:LEU:HD21	1.73	0.49
1:A:437:HIS:ND1	1:A:439:VAL:HG12	2.27	0.49
2:B:94:SER:OG	3:C:66:PRO:HB2	2.13	0.49
2:B:56:THR:HG23	2:B:59:GLU:H	1.78	0.48
1:A:360:ILE:HG22	1:A:364:MET:CE	2.44	0.48
1:A:382:VAL:CG2	1:A:387:LEU:O	2.60	0.48
2:B:68:ARG:NH1	2:B:70:GLN:NE2	2.62	0.48
4:D:161:ARG:NH1	4:D:164:GLN:HE21	2.10	0.48
4:D:206:ILE:C	4:D:206:ILE:HD12	2.34	0.48
2:F:56:THR:HG23	2:F:59:GLU:H	1.79	0.47
5:H:301:QIY:O57	5:H:301:QIY:C48	2.60	0.47
4:D:61:PRO:O	4:D:64:ARG:HD3	2.15	0.47
4:D:165:VAL:O	4:D:169:LEU:HD23	2.13	0.47
1:E:437:HIS:ND1	1:E:439:VAL:HG12	2.29	0.47
2:B:9:ARG:NH1	2:B:10:HIS:NE2	2.63	0.47
2:B:41:GLU:HG2	2:B:80:ARG:NH1	2.13	0.47
4:D:82:ARG:HH22	4:D:164:GLN:NE2	2.14	0.46
1:E:409:ALA:HB3	1:E:411:GLU:HG3	1.96	0.46
3:G:83:TYR:O	3:G:86:SER:HB3	2.16	0.46
1:A:374:TRP:N	1:A:375:PRO:CD	2.78	0.46
4:H:163:LEU:HD22	4:H:188:LEU:HD23	1.97	0.46
4:H:74:VAL:HG21	4:H:136:PHE:CE2	2.51	0.45
1:A:409:ALA:HB3	1:A:411:GLU:HG3	1.98	0.45
1:A:360:ILE:HG22	1:A:364:MET:HE2	1.99	0.45
3:G:64:GLU:HA	3:G:64:GLU:OE2	2.17	0.45
2:B:23:THR:HG23	2:B:26:GLU:H	1.80	0.45
1:A:373:ALA:HB2	1:A:446:LEU:HD13	1.99	0.44
2:B:27:LEU:HD23	2:B:44:LEU:HD23	1.98	0.44
2:B:45:TYR:CG	2:B:88:LEU:HD22	2.53	0.44
4:D:154:PRO:HG2	4:D:156:TYR:CE1	2.53	0.44
2:F:14:ILE:HG23	3:G:30:ILE:CD1	2.48	0.44
4:H:166:VAL:CG2	4:H:188:LEU:HD21	2.48	0.43
2:B:4:PHE:CD2	2:B:17:ASP:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ALA:HB2	1:E:446:LEU:HD13	1.99	0.43
4:H:74:VAL:HG21	4:H:136:PHE:HE2	1.83	0.43
1:E:369:HIS:HD1	1:E:372:TYR:HH	1.62	0.43
1:A:369:HIS:HD1	1:A:372:TYR:HH	1.65	0.43
1:E:374:TRP:N	1:E:375:PRO:CD	2.81	0.43
4:D:82:ARG:NH2	4:D:164:GLN:HE22	2.17	0.43
2:F:7:ILE:HB	2:F:14:ILE:HD12	1.99	0.42
4:H:193:ASN:HD22	4:H:196:LYS:H	1.67	0.42
4:D:206:ILE:HD12	4:D:207:ALA:N	2.35	0.42
1:A:374:TRP:HA	1:A:377:TYR:CE2	2.54	0.42
1:A:449:VAL:O	1:A:453:ARG:HG3	2.20	0.42
1:E:374:TRP:HA	1:E:377:TYR:CD2	2.55	0.42
3:C:101:LEU:HD23	3:C:101:LEU:HA	1.86	0.42
2:B:80:ARG:HG2	2:B:80:ARG:HH11	1.84	0.42
3:G:39:SER:HB3	3:G:42:ILE:HB	2.02	0.42
3:C:37:LEU:HD13	3:C:37:LEU:HA	1.91	0.42
4:D:120:ARG:HD2	4:D:127:GLY:HA2	2.02	0.42
2:F:24:VAL:HG23	2:F:55:LYS:O	2.19	0.42
1:E:396:HIS:CE1	6:E:501:HOH:O	2.73	0.42
1:E:398:MET:HE3	1:E:402:THR:HG21	2.01	0.42
3:C:39:SER:OG	3:C:110:LEU:O	2.32	0.41
4:D:130:VAL:O	4:D:133:THR:HG22	2.19	0.41
1:A:399:ASP:OD2	1:A:402:THR:OG1	2.30	0.41
3:G:22:ILE:HA	3:G:27:HIS:O	2.20	0.41
4:D:82:ARG:HH22	4:D:164:GLN:HE22	1.67	0.41
2:F:27:LEU:O	2:F:31:VAL:HG13	2.20	0.41
3:G:18:TYR:CD2	3:G:30:ILE:CD1	3.04	0.41
3:C:22:ILE:HA	3:C:27:HIS:O	2.21	0.41
4:H:159:LYS:O	4:H:163:LEU:HG	2.21	0.41
1:A:452:MET:O	1:A:456:LYS:HG3	2.20	0.41
4:D:98:TYR:HB3	4:D:99:PRO:CD	2.51	0.40
2:F:6:MET:CE	2:F:15:PHE:CZ	3.05	0.40
2:F:6:MET:HE2	2:F:15:PHE:CZ	2.56	0.40
3:G:101:LEU:HD23	3:G:101:LEU:HA	1.95	0.40
2:B:56:THR:HG22	2:B:59:GLU:CG	2.52	0.40
3:C:33:ARG:O	3:C:37:LEU:HD23	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	
1	A	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
1	E	107/129 (83%)	105 (98%)	2 (2%)	0	100	100
2	B	102/104 (98%)	96 (94%)	5 (5%)	1 (1%)	15	43
2	F	102/104 (98%)	95 (93%)	6 (6%)	1 (1%)	15	43
3	C	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
3	G	82/97 (84%)	79 (96%)	3 (4%)	0	100	100
4	D	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
4	H	147/162 (91%)	142 (97%)	5 (3%)	0	100	100
All	All	890/984 (90%)	853 (96%)	35 (4%)	2 (0%)	47	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	ASP
2	F	47	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	84/113 (74%)	83 (99%)	1 (1%)	71	89
1	E	85/113 (75%)	83 (98%)	2 (2%)	49	77
2	B	87/92 (95%)	84 (97%)	3 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	71/92 (77%)	65 (92%)	6 (8%)	10 29
3	C	80/86 (93%)	78 (98%)	2 (2%)	47 76
3	G	74/86 (86%)	71 (96%)	3 (4%)	30 61
4	D	135/148 (91%)	132 (98%)	3 (2%)	52 78
4	H	128/148 (86%)	123 (96%)	5 (4%)	32 63
All	All	744/878 (85%)	719 (97%)	25 (3%)	37 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	SER
2	B	49	GLN
2	B	68	ARG
2	B	99	LEU
3	C	89	GLU
3	C	99	ILE
4	D	70	GLU
4	D	116	LEU
4	D	120	ARG
1	E	408	GLU
1	E	416	GLN
2	F	2	ASP
2	F	21	SER
2	F	31	VAL
2	F	40	ASP
2	F	52	ASP
2	F	74	THR
3	G	30	ILE
3	G	45	MET
3	G	75	MET
4	H	139	SER
4	H	140	LEU
4	H	169	LEU
4	H	173	GLU
4	H	202	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	164	GLN
4	D	191	HIS
3	G	58	ASN
3	G	108	ASN
4	H	191	HIS
4	H	193	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
5	QIY	D	301	-	68,77,77	0.86	3 (4%)	77,108,108	0.80	3 (3%)
5	QIY	H	301	-	68,77,77	0.88	4 (5%)	77,108,108	1.02	2 (2%)

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
5	QIY	D	301	-	-	13/52/84/84	0/6/7/7
5	QIY	H	301	-	-	10/52/84/84	0/6/7/7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	QIY	C64-C65	-3.80	1.34	1.39
5	H	301	QIY	C64-C65	-3.75	1.34	1.39
5	H	301	QIY	C24-C25	-3.43	1.44	1.49
5	D	301	QIY	C24-C25	-3.23	1.44	1.49
5	H	301	QIY	C15-N17	2.55	1.40	1.37
5	H	301	QIY	C24-C22	2.47	1.43	1.39
5	D	301	QIY	C24-C22	2.42	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	301	QIY	C10-N11-C25	6.09	123.53	117.62
5	D	301	QIY	C10-N11-C25	3.45	120.96	117.62
5	H	301	QIY	C12-C10-N11	2.52	110.84	106.72
5	D	301	QIY	C12-C10-N11	2.24	110.38	106.72
5	D	301	QIY	C60-C59-C58	-2.20	107.89	111.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	QIY	C56-C58-C59-C60
5	D	301	QIY	C56-C58-C59-C61
5	D	301	QIY	C65-C58-C59-C60
5	H	301	QIY	O71-C70-N69-C68
5	H	301	QIY	C46-C70-N69-C68
5	D	301	QIY	O71-C70-N69-C68
5	D	301	QIY	C46-C70-N69-C68
5	H	301	QIY	C33-C34-O35-C36
5	D	301	QIY	O2-C1-C68-N69
5	H	301	QIY	C37-C36-O35-C34
5	H	301	QIY	C5-C4-O3-C33
5	H	301	QIY	C34-C33-O3-C4
5	D	301	QIY	C65-C58-C59-C61
5	D	301	QIY	C33-C34-O35-C36
5	D	301	QIY	O35-C36-C37-O2

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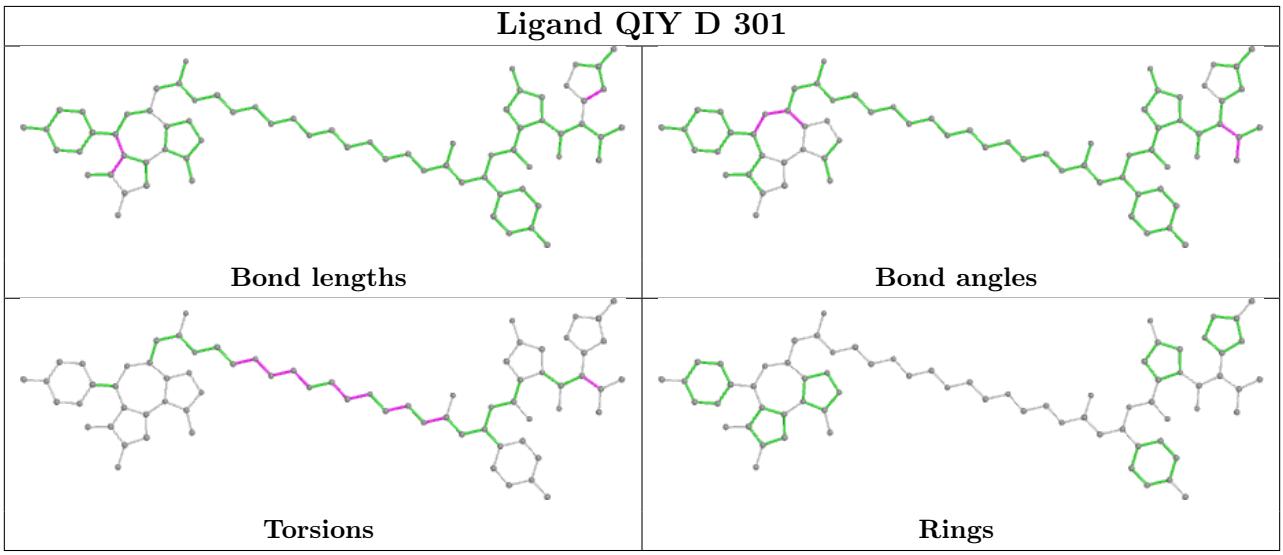
Mol	Chain	Res	Type	Atoms
5	H	301	QIY	O2-C1-C68-N69
5	D	301	QIY	C34-C33-O3-C4
5	D	301	QIY	C36-C37-O2-C1
5	D	301	QIY	O3-C33-C34-O35
5	D	301	QIY	C5-C4-O3-C33
5	H	301	QIY	C45-C46-C70-O71
5	H	301	QIY	O35-C36-C37-O2
5	H	301	QIY	C45-C46-C70-N69

There are no ring outliers.

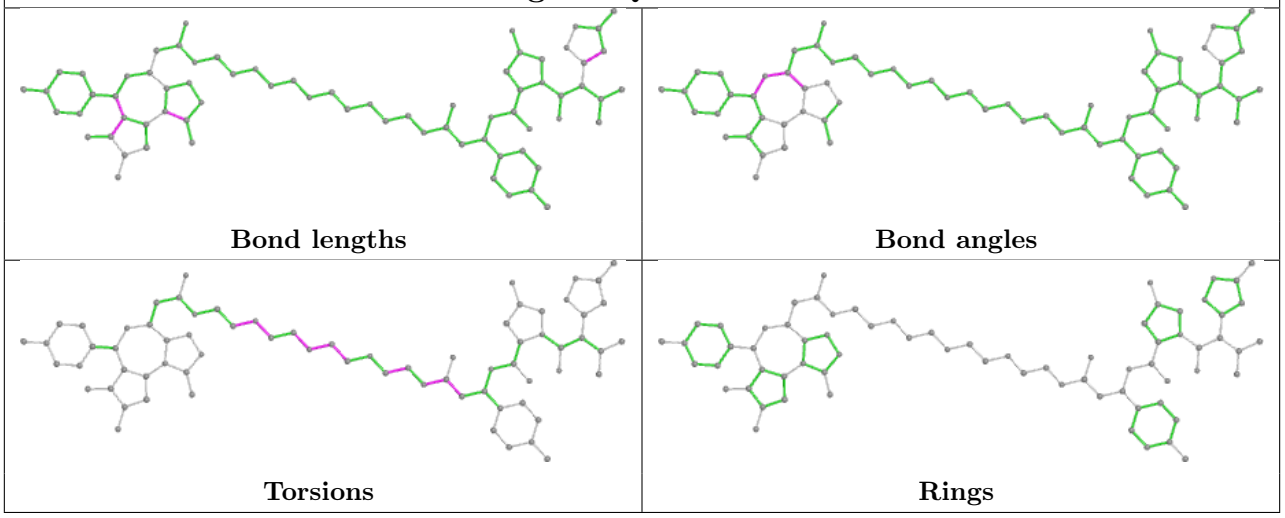
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	QIY	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 QIY H 301



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, 95^{th} 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	109/129 (84%)	0.07	2 (1%) 68 69	85, 106, 142, 157	0
1	E	109/129 (84%)	0.02	0 100 100	79, 99, 139, 164	0
2	B	104/104 (100%)	-0.03	0 100 100	85, 122, 148, 169	0
2	F	104/104 (100%)	0.16	11 (10%) 6 5	110, 149, 186, 208	0
3	C	97/97 (100%)	0.12	2 (2%) 63 64	76, 104, 171, 219	0
3	G	86/97 (88%)	0.41	5 (5%) 23 21	103, 129, 154, 166	0
4	D	149/162 (91%)	0.10	1 (0%) 87 88	79, 103, 137, 166	0
4	H	149/162 (91%)	0.19	6 (4%) 38 37	86, 116, 160, 193	0
All	All	907/984 (92%)	0.12	27 (2%) 50 49	76, 115, 163, 219	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	77	LEU	4.4
2	F	78	ALA	3.9
3	G	47	SER	3.7
4	H	175	TYR	3.6
3	G	46	LEU	3.5
2	F	15	PHE	3.1
3	C	16	MET	2.9
2	F	14	ILE	2.7
3	C	46	LEU	2.7
2	F	45	TYR	2.7
1	A	407	LEU	2.6
3	G	29	PHE	2.5
2	F	42	GLN	2.5
2	F	75	VAL	2.5
4	H	185	TYR	2.5
3	G	70	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	63	LEU	2.4
2	F	103	MET	2.3
1	A	387	LEU	2.3
2	F	44	LEU	2.3
2	F	27	LEU	2.3
3	G	112	CYS	2.3
4	H	188	LEU	2.2
2	F	90	ILE	2.2
4	H	170	VAL	2.2
4	H	201	LEU	2.2
4	H	207	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

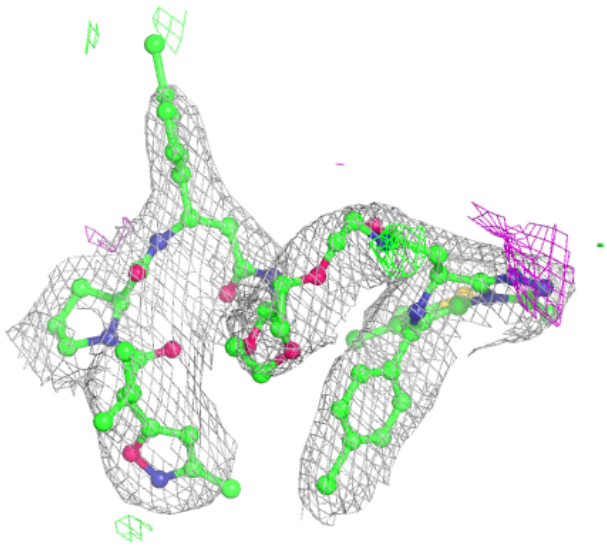
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

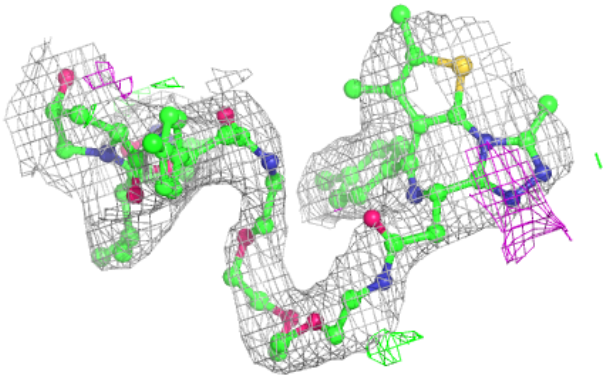
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	QIY	D	301	71/71	0.96	0.30	94,110,137,222	0
5	QIY	H	301	71/71	0.97	0.25	82,107,135,159	0

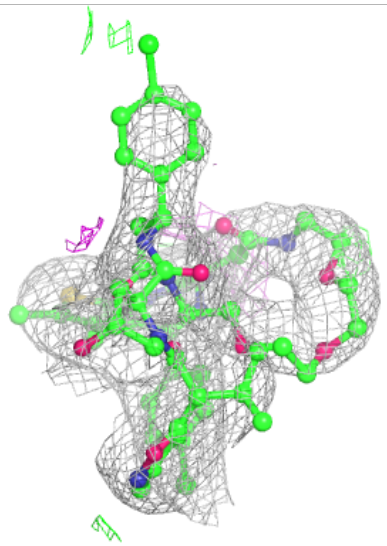
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QIY D 301:

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

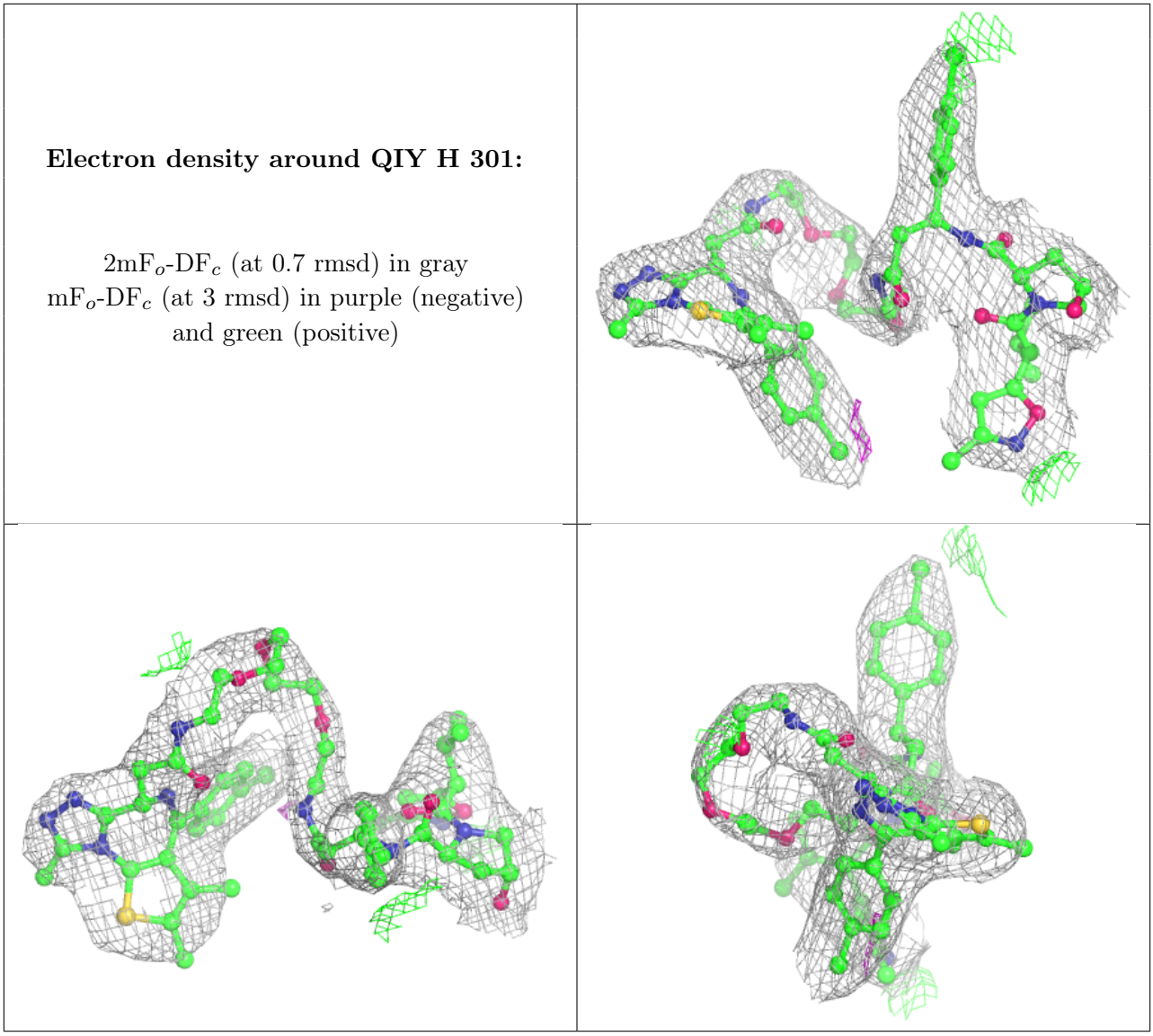






Electron density around QIY H 301:

$2mF_o$-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.