



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:53 AM UTC

PDB ID : 9CJQ / pdb\_00009cjq  
Title : X-ray crystal structure of SARS-CoV-2 main protease quadruple mutants in complex with Ensitrelvir  
Authors : Esler, M.A.; Shi, K.; Harris, R.S.; Aihara, H.  
Deposited on : 2024-07-07  
Resolution : 2.24 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](mailto: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>.

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

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

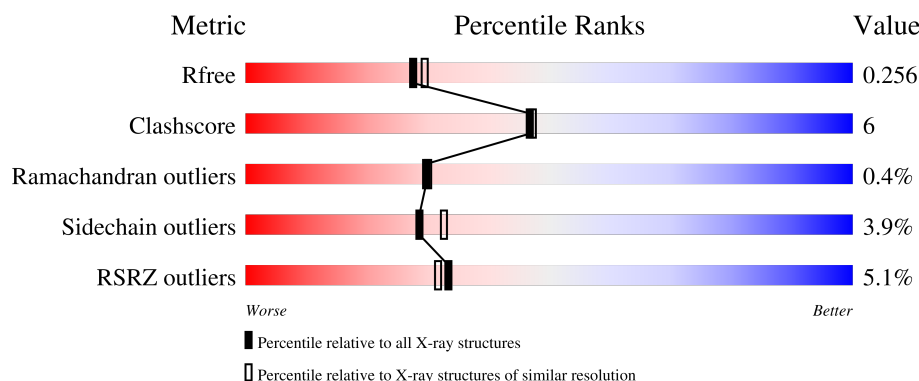
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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  $\geq 3$ , 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	307	<div> <div>7%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	B	307	<div> <div>7%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	307	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	D	307	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9699 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.

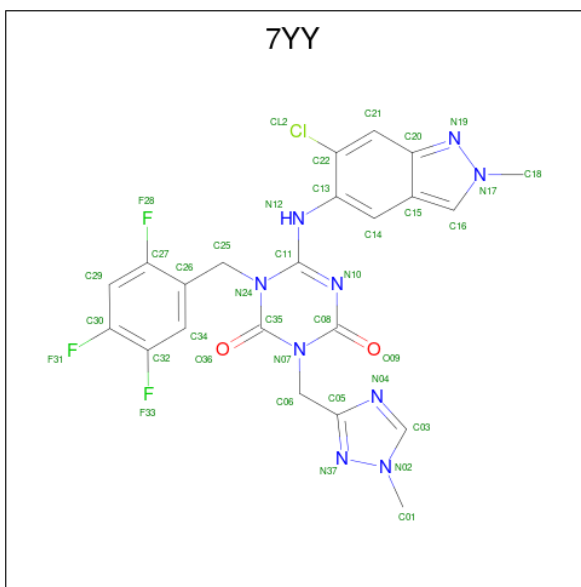
- Molecule 1 is a protein called main protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2359	1499	400	438	22			
1	B	299	Total	C	N	O	S	0	1	0
			2332	1484	396	430	22			
1	C	300	Total	C	N	O	S	0	0	0
			2324	1476	395	431	22			
1	D	304	Total	C	N	O	S	0	0	0
			2353	1496	399	436	22			

There are 16 discrepancies between the modelled and reference sequences:

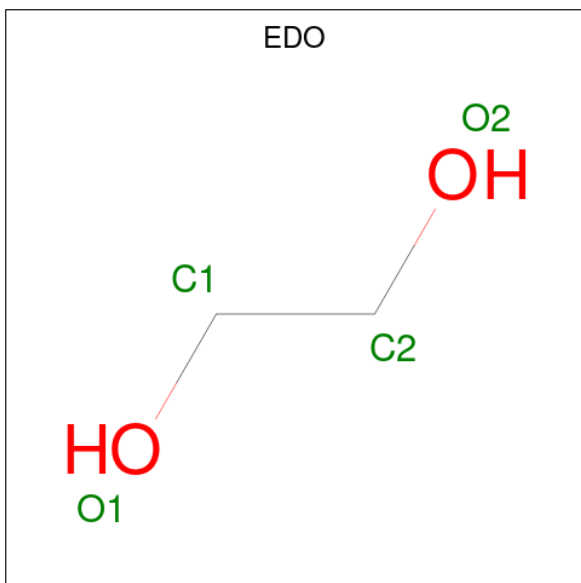
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	THR	engineered mutation	UNP P0DTD1
A	50	PHE	LEU	engineered mutation	UNP P0DTD1
A	144	ALA	SER	engineered mutation	UNP P0DTD1
A	166	VAL	GLU	engineered mutation	UNP P0DTD1
B	21	ILE	THR	engineered mutation	UNP P0DTD1
B	50	PHE	LEU	engineered mutation	UNP P0DTD1
B	144	ALA	SER	engineered mutation	UNP P0DTD1
B	166	VAL	GLU	engineered mutation	UNP P0DTD1
C	21	ILE	THR	engineered mutation	UNP P0DTD1
C	50	PHE	LEU	engineered mutation	UNP P0DTD1
C	144	ALA	SER	engineered mutation	UNP P0DTD1
C	166	VAL	GLU	engineered mutation	UNP P0DTD1
D	21	ILE	THR	engineered mutation	UNP P0DTD1
D	50	PHE	LEU	engineered mutation	UNP P0DTD1
D	144	ALA	SER	engineered mutation	UNP P0DTD1
D	166	VAL	GLU	engineered mutation	UNP P0DTD1

- Molecule 2 is 6-[(6-chloranyl-2-methyl-indazol-5-yl)amino]-3-[(1-methyl-1,2,4-triazol-3-yl)methyl]-1-[[2,4,5-tris(fluoranyl)phenyl)methyl]-1,3,5-triazine-2,4-dione (CCD ID: 7YY) (formula: C<sub>22</sub>H<sub>17</sub>ClF<sub>3</sub>N<sub>9</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 37	C 22	Cl 1	F 3	N 9	O 2	0	0
2	B	1	Total 37	C 22	Cl 1	F 3	N 9	O 2	0	0
2	C	1	Total 37	C 22	Cl 1	F 3	N 9	O 2	0	0
2	D	1	Total 37	C 22	Cl 1	F 3	N 9	O 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

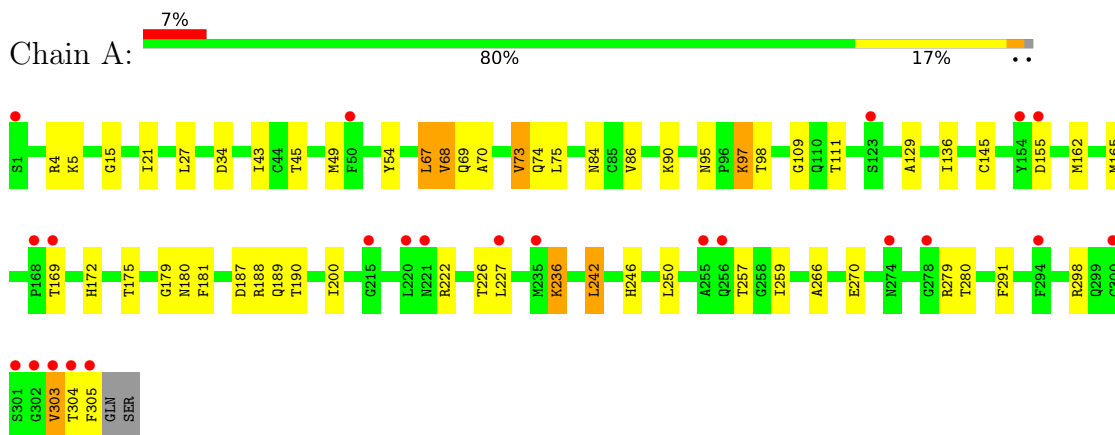
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	44	Total	O	0	0
			44	44		
4	C	56	Total	O	0	0
			56	56		
4	D	41	Total	O	0	0
			41	41		

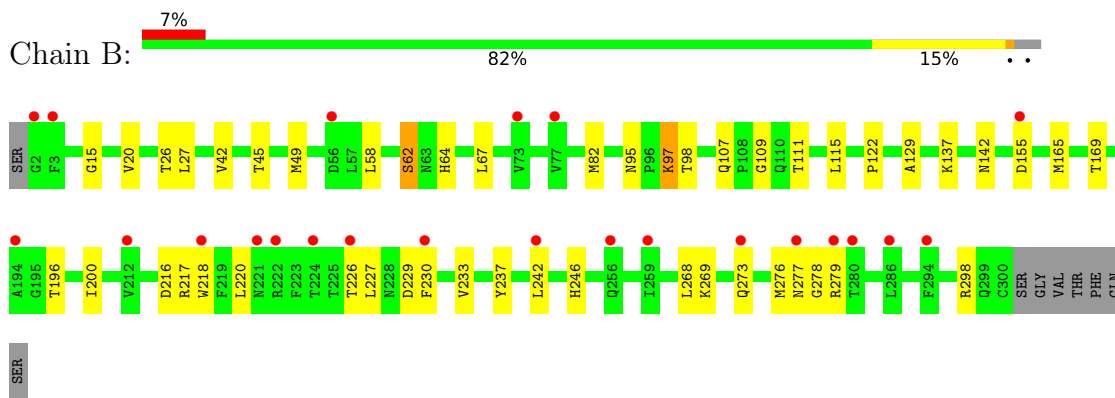
### 3 Residue-property plots [i](#)

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.

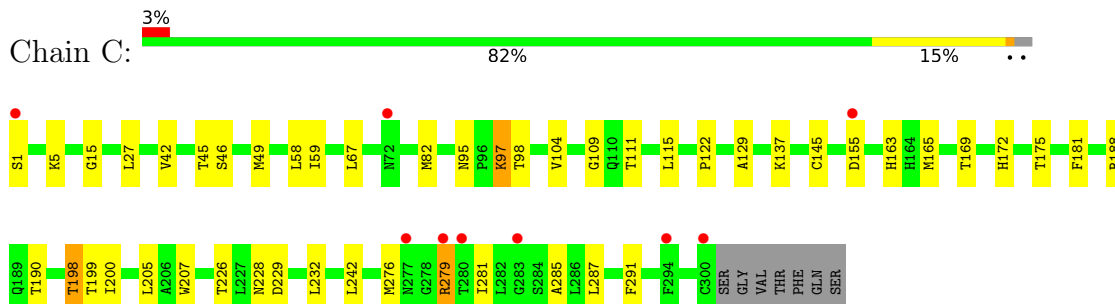
- Molecule 1: main protease



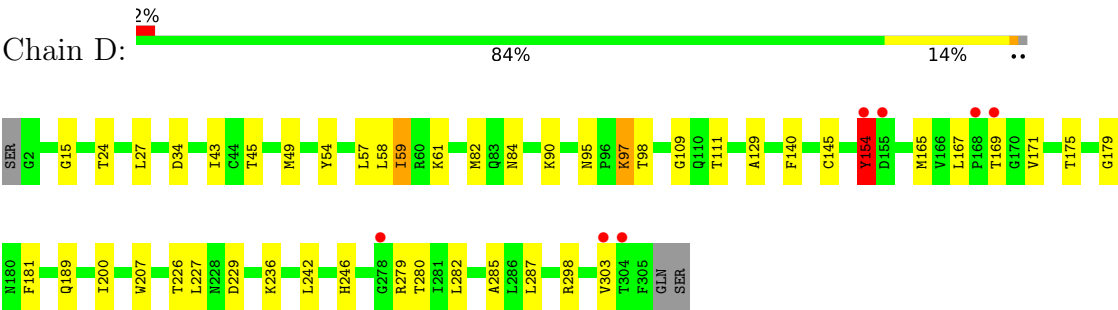
- Molecule 1: main protease



- Molecule 1: main protease



● Molecule 1: main protease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.02Å 106.99Å 116.52Å 90.00° 99.34° 90.00°	Depositor
Resolution (Å)	78.33 – 2.24 78.33 – 2.24	Depositor EDS
% Data completeness (in resolution range)	64.7 (78.33-2.24) 65.5 (78.33-2.24)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.221 , 0.258 0.221 , 0.256	Depositor DCC
$R_{free}$ test set	1688 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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 77.46 % 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 8.4748e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7YY, EDO

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	0.17	0/2413	0.38	0/3280
1	B	0.15	0/2387	0.37	0/3246
1	C	0.20	0/2377	0.39	1/3231 (0.0%)
1	D	0.15	0/2407	0.43	4/3272 (0.1%)
All	All	0.17	0/9584	0.39	5/13029 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	TYR	CA-CB-CG	8.79	129.72	113.90
1	D	154	TYR	CB-CA-C	-5.69	99.10	110.42
1	C	279	ARG	CG-CD-NE	5.61	124.33	112.00
1	D	154	TYR	CA-C-N	5.33	130.75	122.49
1	D	154	TYR	C-N-CA	5.33	130.75	122.49

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	A	2359	0	2311	35	0
1	B	2332	0	2279	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2324	0	2278	24	0
1	D	2353	0	2303	27	0
2	A	37	0	0	3	0
2	B	37	0	0	1	0
2	C	37	0	0	2	0
2	D	37	0	0	3	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
4	A	34	0	0	0	0
4	B	44	0	0	1	0
4	C	56	0	0	0	0
4	D	41	0	0	0	0
All	All	9699	0	9183	107	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 6.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HD21	2:D:401:7YY:CL2	2.23	0.75
1:A:165:MET:HE1	1:A:187:ASP:HA	1.71	0.73
1:C:27:LEU:HD21	2:C:401:7YY:CL2	2.25	0.73
1:D:189:GLN:NE2	2:D:401:7YY:F28	2.12	0.71
1:A:27:LEU:HD21	2:A:401:7YY:CL2	2.28	0.71
1:B:226:THR:HG23	1:B:229:ASP:H	1.56	0.69
1:C:15:GLY:HA3	1:C:97:LYS:HD2	1.77	0.66
1:C:46:SER:HA	1:C:49:MET:HE2	1.78	0.64
1:A:15:GLY:HA3	1:A:97:LYS:HD2	1.80	0.64
1:A:70:ALA:HB3	1:A:73:VAL:HG22	1.82	0.62
1:C:226:THR:HG23	1:C:229:ASP:H	1.63	0.62
1:A:189:GLN:NE2	2:A:401:7YY:F28	2.23	0.61
1:B:15:GLY:HA3	1:B:97:LYS:HD2	1.83	0.61
1:C:5:LYS:HG2	1:C:291:PHE:CZ	2.37	0.60
1:B:276:MET:O	1:B:278:GLY:N	2.34	0.59
1:A:67:LEU:HD11	1:A:74:GLN:HE22	1.67	0.59
1:D:226:THR:HG23	1:D:229:ASP:H	1.68	0.59
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.86	0.57
1:D:227:LEU:HD11	1:D:242:LEU:HD22	1.88	0.56
1:A:34:ASP:OD2	1:A:90:LYS:NZ	2.34	0.55
1:D:298:ARG:HG3	1:D:303:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HB	1:B:27:LEU:HD12	1.90	0.54
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.90	0.53
1:A:111:THR:HG22	1:A:129:ALA:HB2	1.89	0.52
1:D:45:THR:O	1:D:49:MET:HG3	2.10	0.52
1:D:57:LEU:O	1:D:61:LYS:HG2	2.09	0.52
1:D:58:LEU:HD22	1:D:82:MET:HB2	1.92	0.52
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.92	0.51
1:C:165:MET:HA	2:C:401:7YY:O36	2.10	0.51
1:B:165:MET:HA	2:B:401:7YY:O36	2.10	0.51
1:C:188:ARG:HG3	1:C:190:THR:HG22	1.93	0.51
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.92	0.50
1:B:111:THR:HG22	1:B:129:ALA:HB2	1.94	0.50
1:D:15:GLY:HA3	1:D:97:LYS:HD2	1.92	0.50
1:A:188:ARG:HG3	1:A:190:THR:HG22	1.94	0.50
1:A:180:ASN:OD1	1:C:228:ASN:ND2	2.36	0.49
1:A:257:THR:O	1:A:259:ILE:HD12	2.12	0.49
1:C:285:ALA:HB3	1:D:285:ALA:HB3	1.95	0.49
1:A:227:LEU:HD11	1:A:242:LEU:HD22	1.93	0.49
1:B:217:ARG:HB3	1:B:220:LEU:HD12	1.94	0.49
1:B:227:LEU:HD11	1:B:242:LEU:HD22	1.94	0.49
1:A:4:ARG:NH1	1:B:137:LYS:O	2.47	0.48
1:A:5:LYS:HG2	1:A:291:PHE:CZ	2.49	0.48
1:A:68:VAL:HG13	1:A:75:LEU:HB2	1.96	0.47
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.96	0.47
1:A:43:ILE:HD11	1:A:54:TYR:HD1	1.80	0.46
1:C:205:LEU:HD11	1:C:242:LEU:HD11	1.98	0.46
1:C:175:THR:HG22	1:C:181:PHE:HA	1.96	0.46
1:D:165:MET:HA	2:D:401:7YY:O36	2.15	0.46
1:C:45:THR:O	1:C:49:MET:HG3	2.16	0.46
1:A:298:ARG:HD2	1:A:305:PHE:CE2	2.51	0.46
1:A:27:LEU:HD22	1:A:145:CYS:HB3	1.98	0.46
1:C:111:THR:HG22	1:C:129:ALA:HB2	1.98	0.46
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.16	0.46
1:A:175:THR:HG22	1:A:181:PHE:HA	1.98	0.46
1:A:45:THR:O	1:A:49:MET:HG3	2.16	0.45
1:C:27:LEU:HD22	1:C:145:CYS:HB3	1.98	0.45
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.16	0.45
1:D:111:THR:HG22	1:D:129:ALA:HB2	1.97	0.45
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.17	0.45
1:A:21:ILE:HB	1:A:67:LEU:HB3	1.99	0.45
1:A:136:ILE:HG13	1:A:172:HIS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:TYR:OH	1:B:273:GLN:HA	2.18	0.44
1:B:298:ARG:NH2	4:B:506:HOH:O	2.50	0.44
1:C:27:LEU:HD12	1:C:42:VAL:HB	2.00	0.44
1:D:43:ILE:HD11	1:D:54:TYR:HD1	1.82	0.44
1:D:109:GLY:HA2	1:D:200:ILE:HD13	2.00	0.44
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.80	0.43
1:A:84:ASN:HB2	1:A:179:GLY:HA3	1.99	0.43
1:A:165:MET:HA	2:A:401:7YY:O36	2.18	0.43
1:D:34:ASP:OD2	1:D:90:LYS:HE3	2.18	0.43
1:D:59:ILE:HA	1:D:59:ILE:HD12	1.73	0.43
1:D:84:ASN:HB2	1:D:179:GLY:HA3	1.99	0.43
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.99	0.43
1:D:167:LEU:HB2	1:D:171:VAL:HG23	2.01	0.43
1:A:236:LYS:HB2	1:A:236:LYS:HE3	1.70	0.43
1:C:276:MET:HE3	1:C:281:ILE:HG13	2.00	0.43
1:D:242:LEU:HD23	1:D:246:HIS:HB2	2.00	0.43
1:A:242:LEU:HD23	1:A:246:HIS:HB2	2.00	0.43
1:D:27:LEU:HD22	1:D:145:CYS:HB3	2.00	0.43
1:B:107:GLN:OE1	1:B:107:GLN:N	2.52	0.42
1:D:175:THR:HG22	1:D:181:PHE:HA	2.01	0.42
1:B:242:LEU:HD23	1:B:246:HIS:HB2	2.00	0.42
1:A:86:VAL:HG22	1:A:162:MET:HE1	2.00	0.42
1:C:58:LEU:HD22	1:C:82:MET:HB2	2.01	0.42
1:C:95:ASN:HB3	1:C:98:THR:OG1	2.19	0.42
1:A:86:VAL:HG22	1:A:162:MET:CE	2.50	0.42
1:D:207:TRP:HZ3	1:D:287:LEU:HD23	1.83	0.42
1:B:45:THR:O	1:B:49:MET:HG3	2.19	0.42
1:D:165:MET:HE2	1:D:181:PHE:CZ	2.55	0.42
1:B:62:SER:HB2	1:B:64:HIS:CD2	2.54	0.42
1:B:58:LEU:HD22	1:B:82:MET:HB2	2.02	0.42
1:B:233:VAL:HG11	1:B:269:LYS:HG3	2.01	0.42
1:B:269:LYS:HE3	1:B:273:GLN:HE22	1.83	0.42
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.89	0.42
1:C:163:HIS:CE1	1:C:172:HIS:HB3	2.55	0.41
1:C:198:THR:OG1	1:C:199:THR:N	2.53	0.41
1:B:216:ASP:HA	1:B:218[B]:TRP:CZ3	2.55	0.41
1:B:115:LEU:HD11	1:B:122:PRO:HB3	2.03	0.41
1:B:279:ARG:HD2	1:B:279:ARG:HA	1.84	0.41
1:A:27:LEU:CD2	1:A:145:CYS:HB3	2.51	0.41
1:A:266:ALA:O	1:A:270:GLU:HG2	2.21	0.41
1:C:207:TRP:HZ3	1:C:287:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HA	1:D:27:LEU:HD23	1.76	0.41
1:B:230:PHE:HZ	1:B:268:LEU:HD23	1.85	0.40
1:A:187:ASP:OD1	1:A:187:ASP:N	2.54	0.40
1:C:1:SER:HA	1:D:140:PHE:O	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	303/307 (99%)	289 (95%)	12 (4%)	2 (1%)	18	16
1	B	298/307 (97%)	285 (96%)	12 (4%)	1 (0%)	36	38
1	C	298/307 (97%)	289 (97%)	9 (3%)	0	100	100
1	D	302/307 (98%)	288 (95%)	12 (4%)	2 (1%)	18	16
All	All	1201/1228 (98%)	1151 (96%)	45 (4%)	5 (0%)	30	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ARG
1	B	277	ASN
1	D	279	ARG
1	A	303	VAL
1	D	154	TYR

### 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	261/263 (99%)	246 (94%)	15 (6%)	18	17
1	B	257/263 (98%)	249 (97%)	8 (3%)	35	41
1	C	257/263 (98%)	247 (96%)	10 (4%)	28	33
1	D	260/263 (99%)	253 (97%)	7 (3%)	39	47
All	All	1035/1052 (98%)	995 (96%)	40 (4%)	28	33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	68	VAL
1	A	69	GLN
1	A	73	VAL
1	A	97	LYS
1	A	155	ASP
1	A	169	THR
1	A	222	ARG
1	A	226	THR
1	A	236	LYS
1	A	242	LEU
1	A	250	LEU
1	A	280	THR
1	A	303	VAL
1	A	304	THR
1	B	26	THR
1	B	62	SER
1	B	67	LEU
1	B	97	LYS
1	B	142	ASN
1	B	155	ASP
1	B	169	THR
1	B	196	THR
1	C	59	ILE
1	C	67	LEU
1	C	97	LYS
1	C	104	VAL
1	C	137	LYS
1	C	155	ASP
1	C	169	THR

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Mol	Chain	Res	Type
1	C	198	THR
1	C	232	LEU
1	C	279	ARG
1	D	24	THR
1	D	59	ILE
1	D	97	LYS
1	D	154	TYR
1	D	169	THR
1	D	236	LYS
1	D	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	189	GLN
1	A	274	ASN
1	B	64	HIS
1	B	69	GLN
1	B	72	ASN
1	B	83	GLN
1	B	180	ASN
1	B	189	GLN
1	B	214	ASN
1	B	238	ASN
1	C	69	GLN
1	C	72	ASN
1	C	74	GLN
1	C	107	GLN
1	C	180	ASN
1	D	83	GLN
1	D	180	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

6 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
2	7YY	D	401	-	39,41,41	0.80	2 (5%)	48,61,61	1.27	7 (14%)
2	7YY	B	401	-	39,41,41	0.78	2 (5%)	48,61,61	1.30	7 (14%)
2	7YY	C	401	-	39,41,41	0.80	2 (5%)	48,61,61	1.33	7 (14%)
3	EDO	C	402	-	3,3,3	0.43	0	2,2,2	0.31	0
2	7YY	A	401	-	39,41,41	0.79	1 (2%)	48,61,61	1.28	7 (14%)
3	EDO	A	402	-	3,3,3	0.40	0	2,2,2	0.36	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
2	7YY	D	401	-	-	3/12/12/12	0/5/5/5
2	7YY	B	401	-	-	4/12/12/12	0/5/5/5
2	7YY	C	401	-	-	3/12/12/12	0/5/5/5
3	EDO	C	402	-	-	0/1/1/1	-
2	7YY	A	401	-	-	4/12/12/12	0/5/5/5
3	EDO	A	402	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7YY	C05-N04	-2.15	1.33	1.37
2	A	401	7YY	C05-N04	-2.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	7YY	C05-N04	-2.10	1.33	1.37
2	D	401	7YY	C14-C13	-2.10	1.38	1.40
2	C	401	7YY	C05-N04	-2.08	1.33	1.37
2	B	401	7YY	C14-C13	-2.06	1.38	1.40
2	C	401	7YY	C14-C13	-2.05	1.38	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	7YY	C03-N04-C05	3.32	106.01	102.88
2	A	401	7YY	C03-N04-C05	3.31	106.01	102.88
2	D	401	7YY	C03-N04-C05	3.31	106.01	102.88
2	B	401	7YY	C14-C13-C22	3.26	121.55	118.21
2	B	401	7YY	C03-N04-C05	3.19	105.90	102.88
2	C	401	7YY	C14-C13-C22	3.17	121.45	118.21
2	D	401	7YY	C14-C13-C22	3.13	121.41	118.21
2	A	401	7YY	C14-C13-C22	3.04	121.32	118.21
2	C	401	7YY	N37-C05-N04	-2.90	111.41	115.26
2	C	401	7YY	C06-N07-C35	2.90	120.20	116.71
2	A	401	7YY	N37-C05-N04	-2.90	111.42	115.26
2	D	401	7YY	N37-C05-N04	-2.87	111.45	115.26
2	B	401	7YY	N37-C05-N04	-2.76	111.59	115.26
2	D	401	7YY	C01-N02-N37	2.74	122.36	119.57
2	B	401	7YY	C01-N02-N37	2.61	122.22	119.57
2	A	401	7YY	C01-N02-N37	2.60	122.22	119.57
2	C	401	7YY	C01-N02-N37	2.58	122.20	119.57
2	B	401	7YY	C15-C16-N17	-2.41	106.29	108.08
2	A	401	7YY	N24-C11-N10	-2.38	122.69	124.07
2	C	401	7YY	C15-C16-N17	-2.30	106.37	108.08
2	D	401	7YY	C15-C16-N17	-2.28	106.38	108.08
2	A	401	7YY	C15-C16-N17	-2.26	106.40	108.08
2	B	401	7YY	C06-N07-C35	2.25	119.42	116.71
2	A	401	7YY	C06-N07-C35	2.21	119.38	116.71
2	B	401	7YY	N24-C11-N10	-2.10	122.85	124.07
2	C	401	7YY	N24-C11-N10	-2.09	122.85	124.07
2	D	401	7YY	C06-N07-C35	2.07	119.21	116.71
2	D	401	7YY	N24-C11-N10	-2.03	122.89	124.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

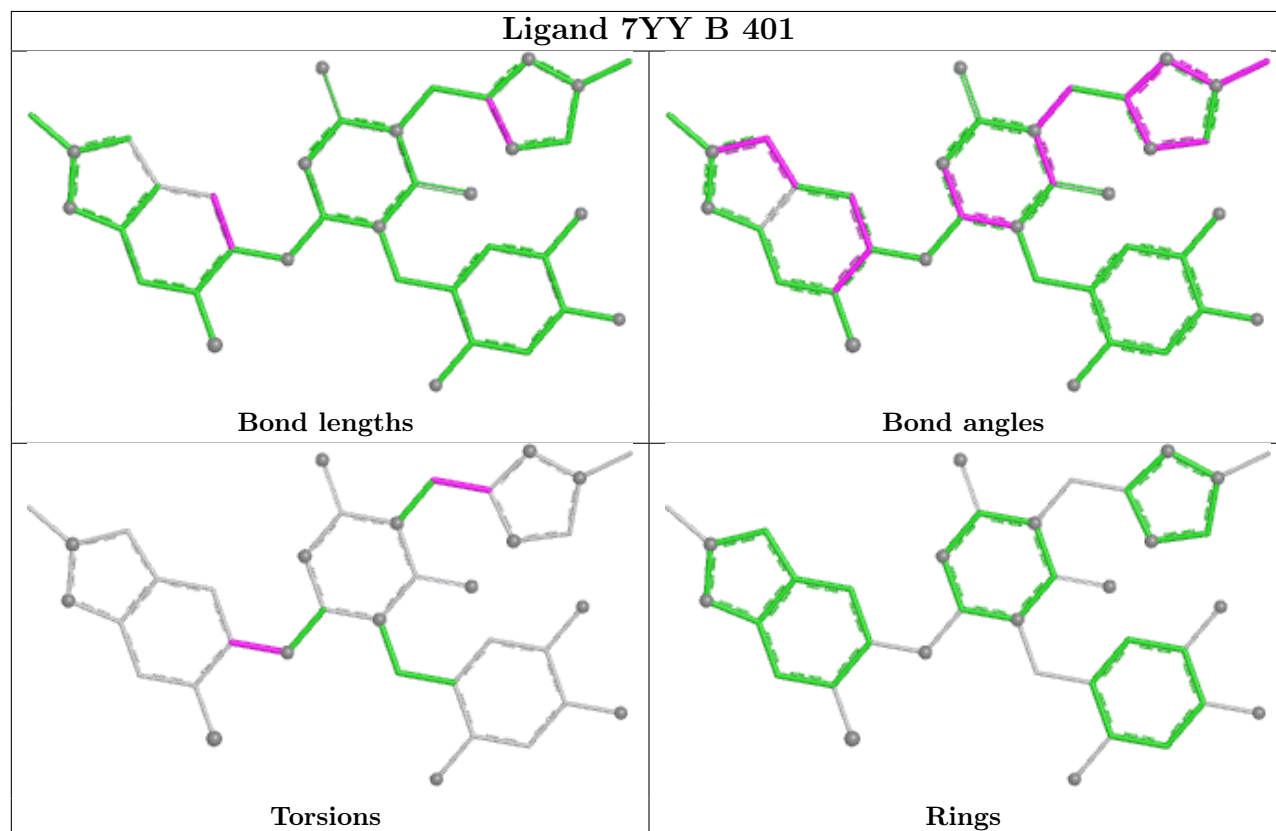
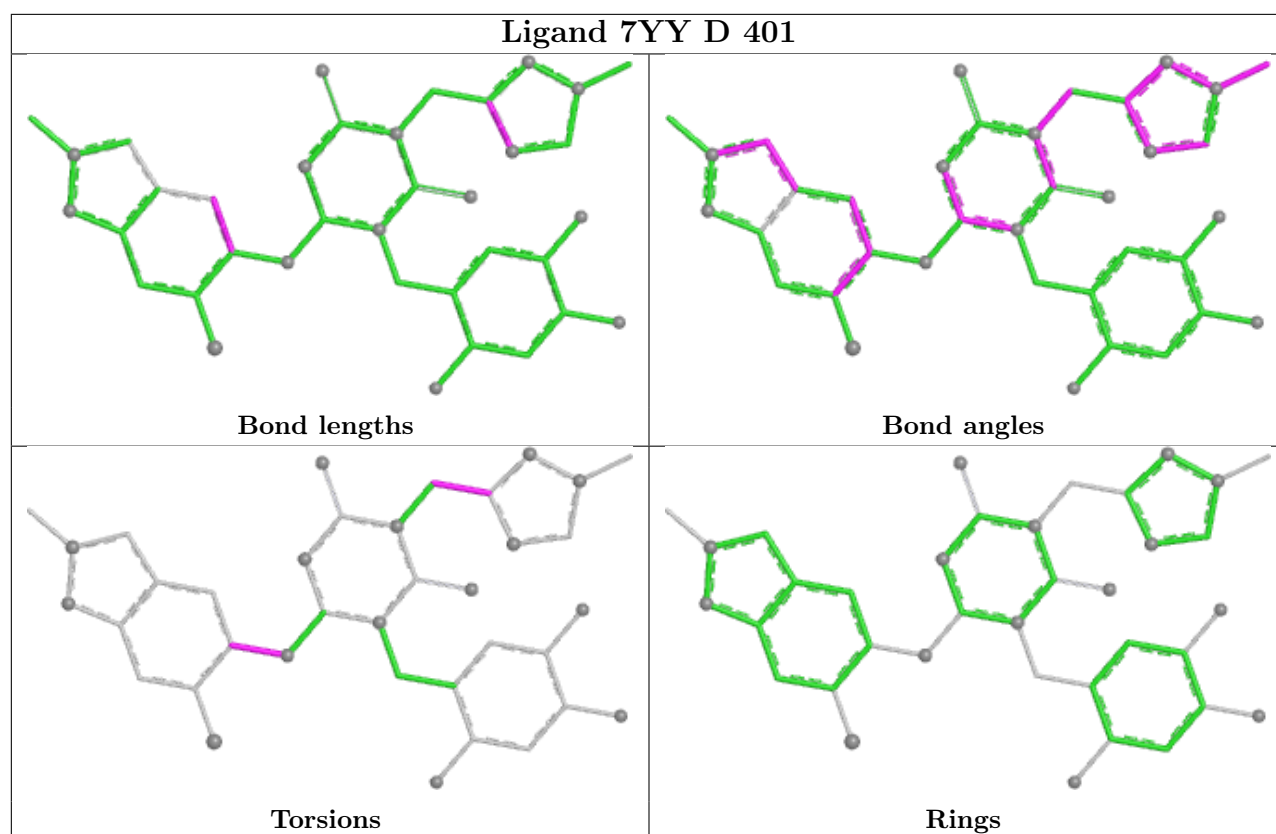
Mol	Chain	Res	Type	Atoms
2	A	401	7YY	N04-C05-C06-N07
2	B	401	7YY	N04-C05-C06-N07
2	C	401	7YY	N04-C05-C06-N07
2	D	401	7YY	N04-C05-C06-N07
2	A	401	7YY	C22-C13-N12-C11
2	B	401	7YY	C22-C13-N12-C11
2	C	401	7YY	C22-C13-N12-C11
2	D	401	7YY	C22-C13-N12-C11
2	B	401	7YY	C14-C13-N12-C11
2	A	401	7YY	C14-C13-N12-C11
2	A	401	7YY	N37-C05-C06-N07
2	B	401	7YY	N37-C05-C06-N07
2	C	401	7YY	N37-C05-C06-N07
2	D	401	7YY	C14-C13-N12-C11

There are no ring outliers.

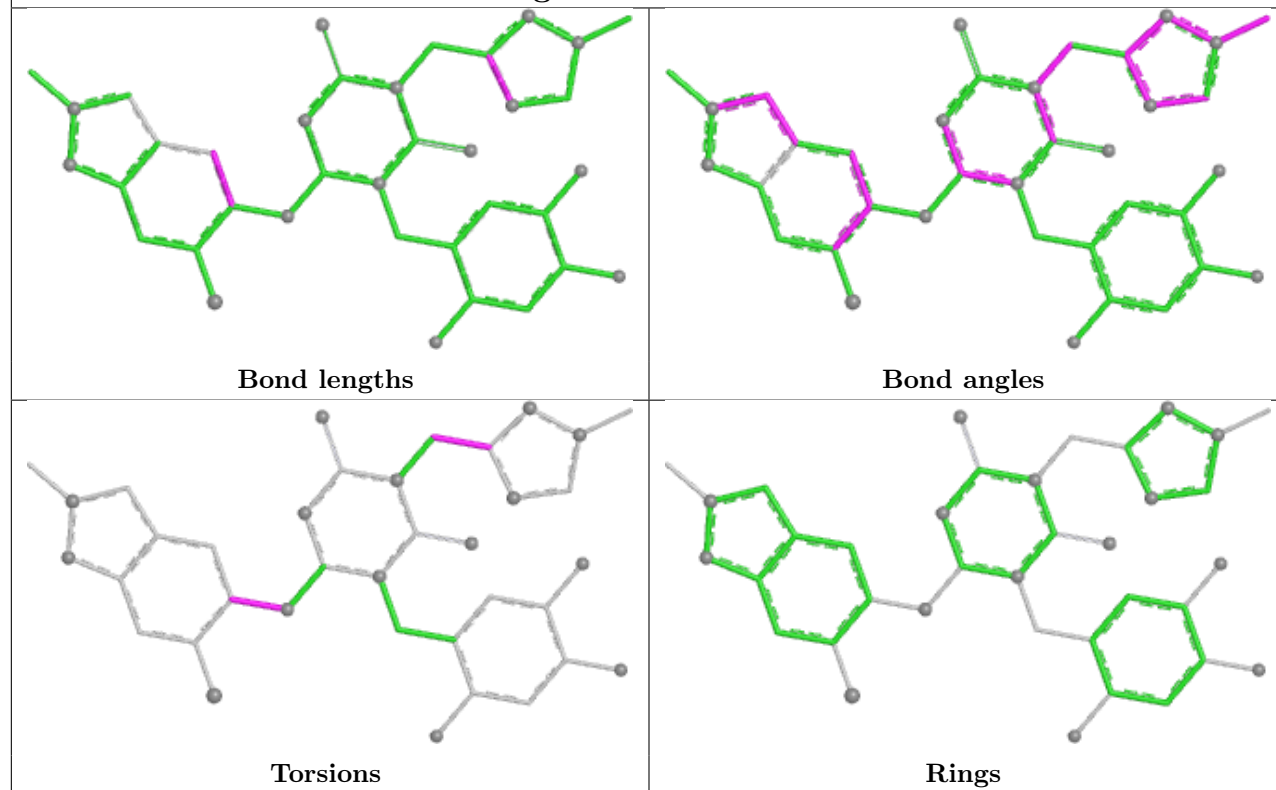
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	7YY	3	0
2	B	401	7YY	1	0
2	C	401	7YY	2	0
2	A	401	7YY	3	0

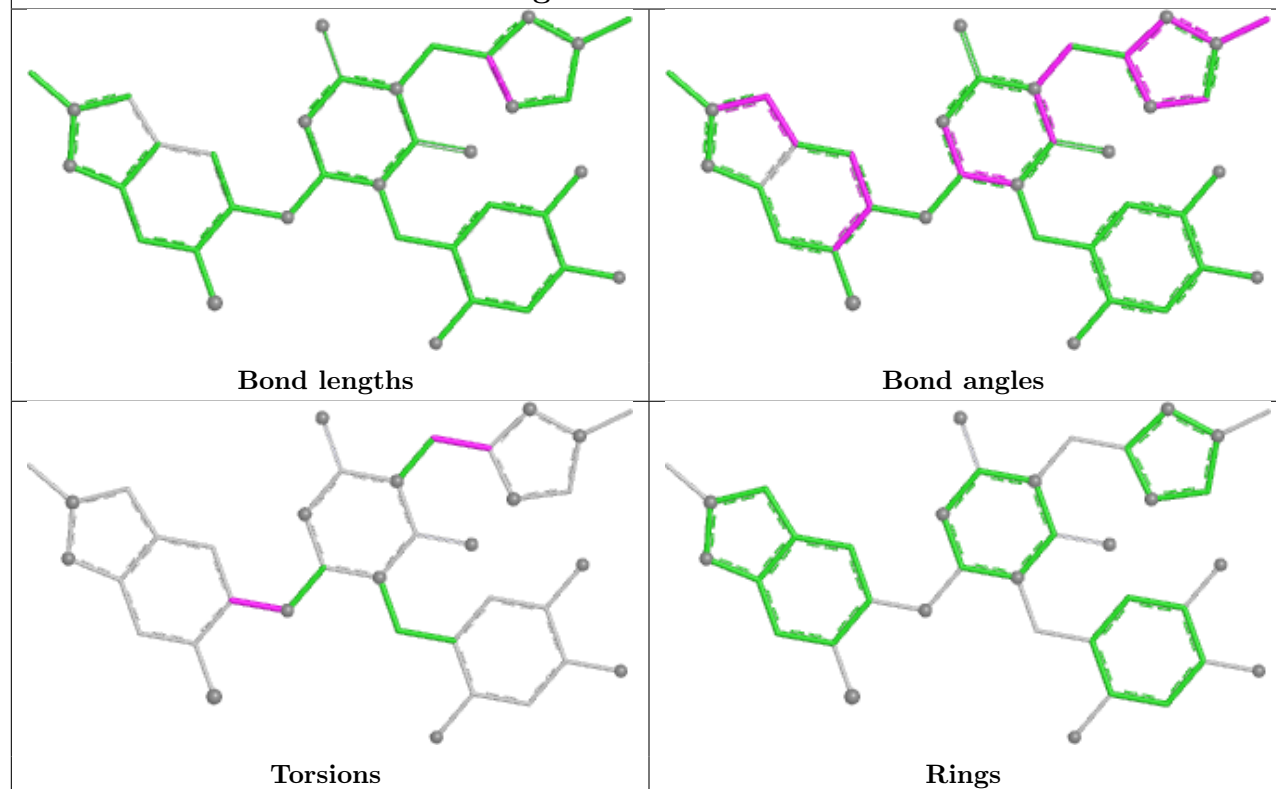
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand 7YY C 401



## Ligand 7YY A 401



## 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	305/307 (99%)	0.90	23 (7%)	20 18	36, 53, 80, 113	0
1	B	299/307 (97%)	0.82	23 (7%)	19 17	31, 51, 75, 132	1 (0%)
1	C	300/307 (97%)	0.00	9 (3%)	52 52	22, 33, 58, 87	0
1	D	304/307 (99%)	0.04	7 (2%)	61 62	24, 36, 59, 94	0
All	All	1208/1228 (98%)	0.44	62 (5%)	33 32	22, 44, 72, 132	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	TYR	6.0
1	A	305	PHE	5.8
1	B	218[A]	TRP	5.5
1	A	303	VAL	5.0
1	A	304	THR	4.9
1	A	154	TYR	4.4
1	B	279	ARG	4.4
1	A	301	SER	3.5
1	A	300	CYS	3.4
1	B	2	GLY	3.3
1	B	280	THR	3.3
1	B	294	PHE	3.2
1	B	155	ASP	3.1
1	A	294	PHE	3.1
1	B	256	GLN	3.1
1	A	168	PRO	3.0
1	D	304	THR	3.0
1	B	194	ALA	2.9
1	A	302	GLY	2.8
1	B	286	LEU	2.8
1	A	255	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	ASN	2.6
1	D	169	THR	2.6
1	B	273	GLN	2.6
1	C	300	CYS	2.6
1	C	155	ASP	2.6
1	A	220	LEU	2.5
1	C	279	ARG	2.5
1	B	230	PHE	2.5
1	C	1	SER	2.5
1	B	221	ASN	2.5
1	C	283	GLY	2.5
1	C	277	ASN	2.5
1	B	3	PHE	2.4
1	A	169	THR	2.4
1	B	226	THR	2.4
1	B	73	VAL	2.4
1	A	278	GLY	2.4
1	A	256	GLN	2.3
1	A	274	ASN	2.3
1	C	72	ASN	2.3
1	B	77	VAL	2.3
1	B	222	ARG	2.3
1	B	212	VAL	2.3
1	A	235	MET	2.3
1	A	215	GLY	2.2
1	A	227	LEU	2.2
1	A	50	PHE	2.2
1	A	1	SER	2.2
1	B	224	THR	2.2
1	A	155	ASP	2.1
1	B	277	ASN	2.1
1	D	155	ASP	2.1
1	D	278	GLY	2.1
1	B	259	ILE	2.1
1	C	294	PHE	2.1
1	C	280	THR	2.1
1	B	242	LEU	2.1
1	D	168	PRO	2.1
1	D	303	VAL	2.1
1	A	123	SER	2.1
1	B	56	ASP	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 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, 95<sup>th</sup> 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.

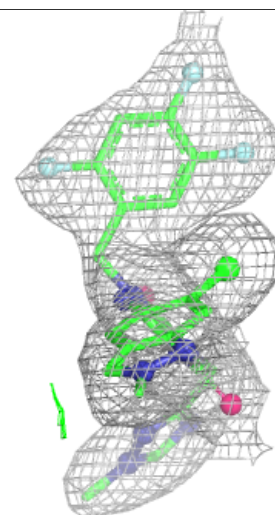
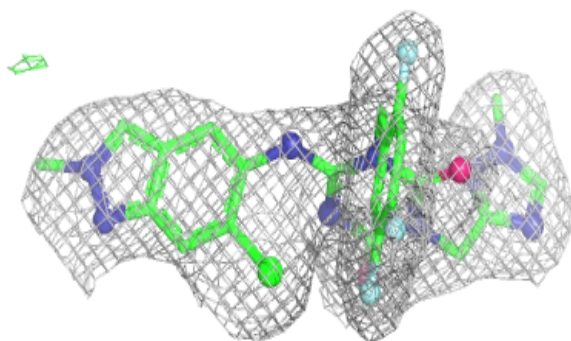
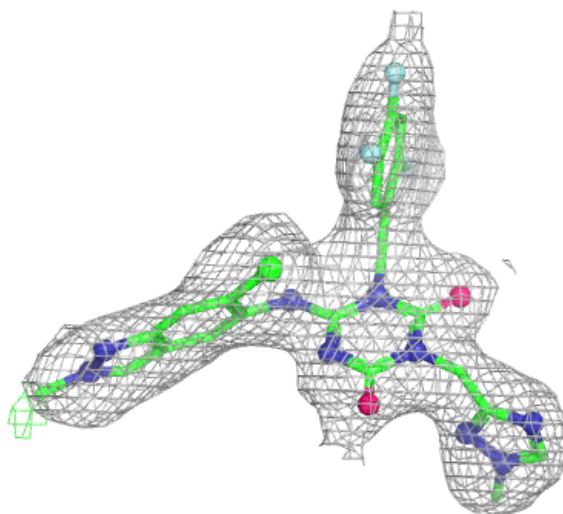
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	402	4/4	0.70	0.15	46,47,50,55	0
3	EDO	C	402	4/4	0.73	0.13	45,53,56,57	0
2	7YY	A	401	37/37	0.93	0.07	32,42,49,53	0
2	7YY	B	401	37/37	0.93	0.07	25,35,44,51	0
2	7YY	C	401	37/37	0.94	0.07	15,27,39,45	0
2	7YY	D	401	37/37	0.94	0.07	23,32,40,41	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.



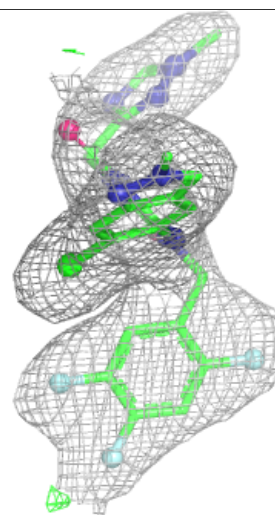
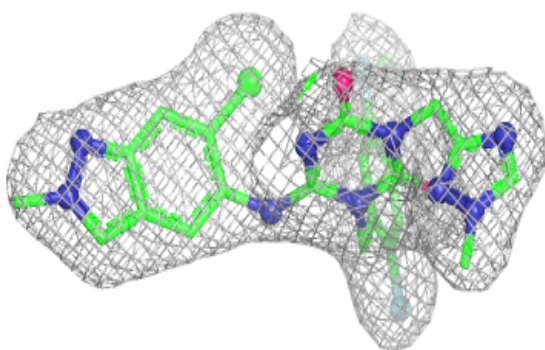
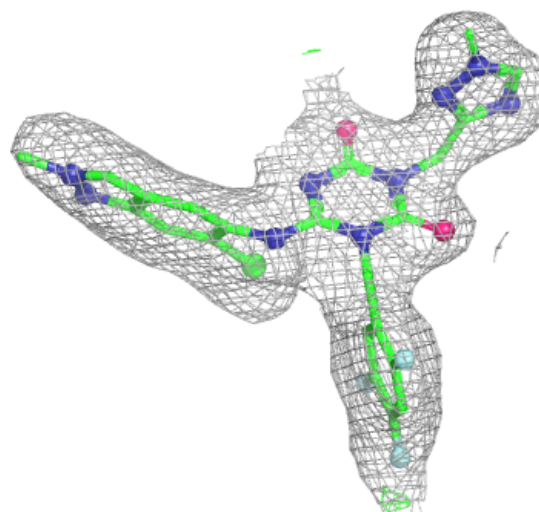
**Electron density around 7YY A 401:**

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



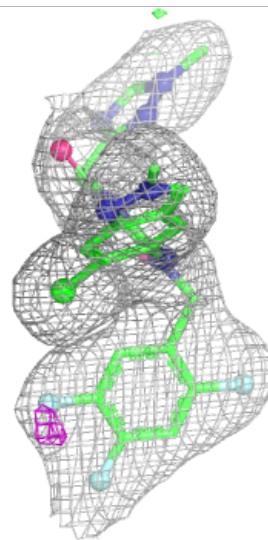
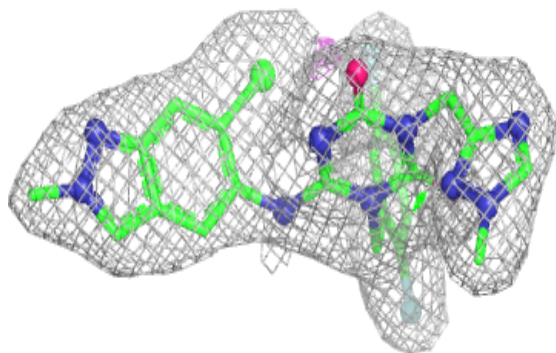
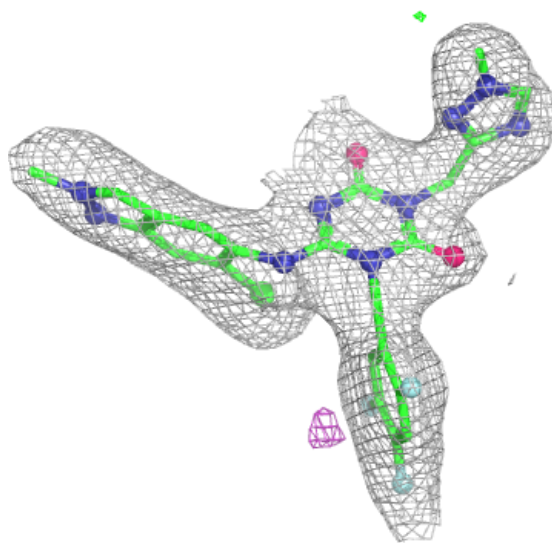
**Electron density around 7YY B 401:**

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



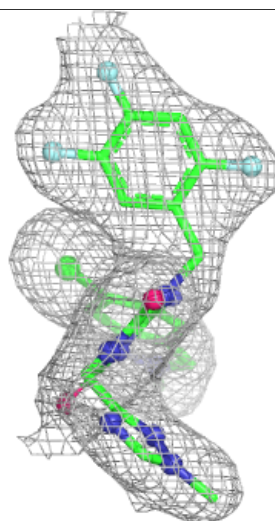
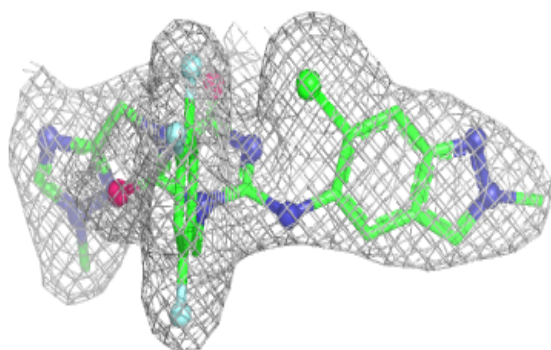
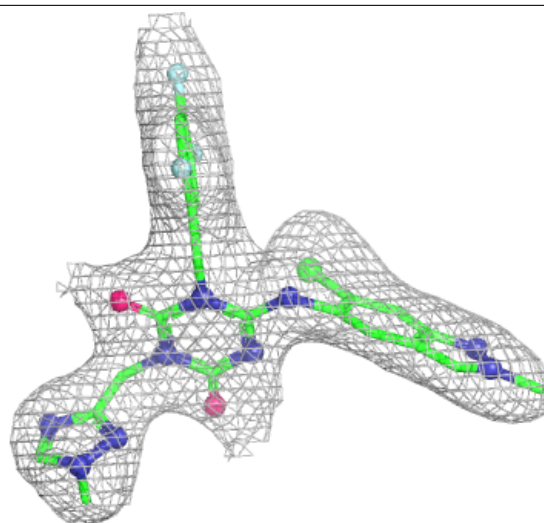
**Electron density around 7YY C 401:**

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



**Electron density around 7YY D 401:**

$2mF_o-DF_c$  (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.