



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 7P6N / pdb_00007p6n
Title : ROCK2 IN COMPLEX WITH COMPOUND 12
Authors : Maillard, M.C.
Deposited on : 2021-07-16
Resolution : 3.00 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)
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

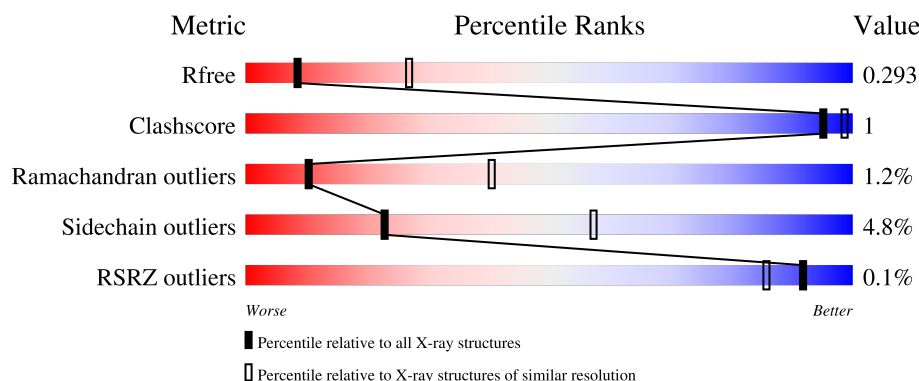
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	399	87% 8% • •
1	B	399	87% 8% • •
1	C	399	85% 9% • 5%
1	D	399	88% 7% • •
1	E	399	88% 8% • •

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Mol	Chain	Length	Quality of chain
1	F	399	89% 7%
1	G	399	87% 8%
1	H	399	81% 8% 8%

2 Entry composition

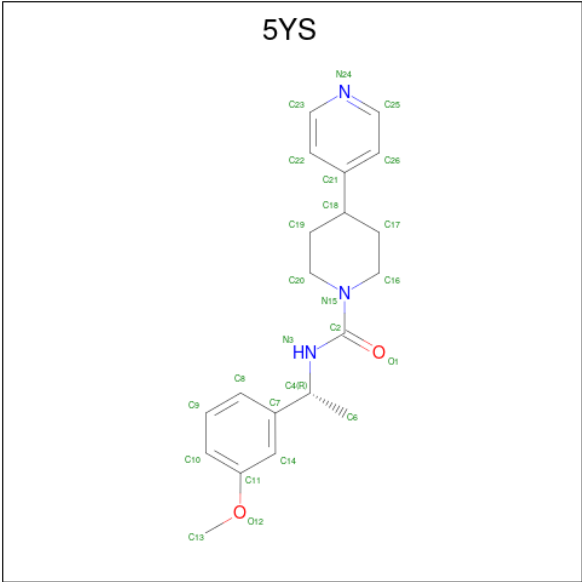
There are 2 unique types of molecules in this entry. The entry contains 25053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3123	2006	524	574	19			
1	B	385	Total	C	N	O	S	0	0	0
			3141	2014	526	581	20			
1	C	378	Total	C	N	O	S	0	0	0
			3082	1982	517	563	20			
1	D	385	Total	C	N	O	S	0	0	0
			3130	2009	524	577	20			
1	E	385	Total	C	N	O	S	0	0	0
			3126	2005	525	576	20			
1	F	384	Total	C	N	O	S	0	0	0
			3124	2006	523	575	20			
1	G	385	Total	C	N	O	S	0	0	0
			3132	2008	525	579	20			
1	H	366	Total	C	N	O	S	0	0	0
			2995	1928	502	548	17			

- Molecule 2 is {N}-[(1 {R})-1-(3-methoxyphenyl)ethyl]-4-pyridin-4-yl-piperidine-1-carboxamide (CCD ID: 5YS) (formula: C₂₀H₂₅N₃O₂) (labeled as "Ligand of Interest" by depositor).

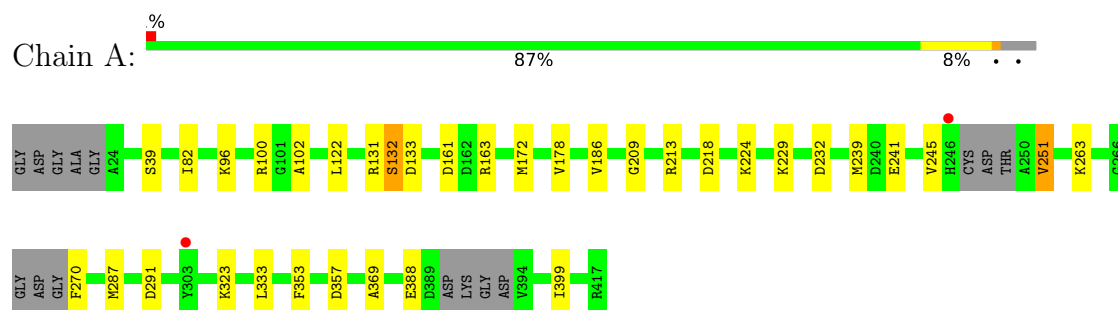


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	3	2		
2	B	1	Total	C	N	O	0	0
			25	20	3	2		
2	C	1	Total	C	N	O	0	0
			25	20	3	2		
2	D	1	Total	C	N	O	0	0
			25	20	3	2		
2	E	1	Total	C	N	O	0	0
			25	20	3	2		
2	F	1	Total	C	N	O	0	0
			25	20	3	2		
2	G	1	Total	C	N	O	0	0
			25	20	3	2		
2	H	1	Total	C	N	O	0	0
			25	20	3	2		

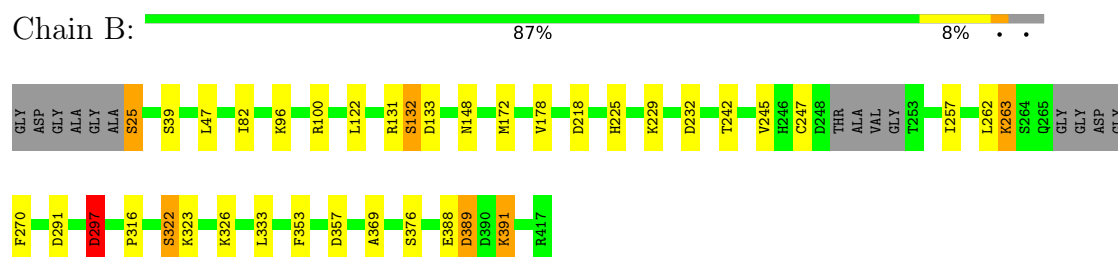
3 Residue-property plots

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.

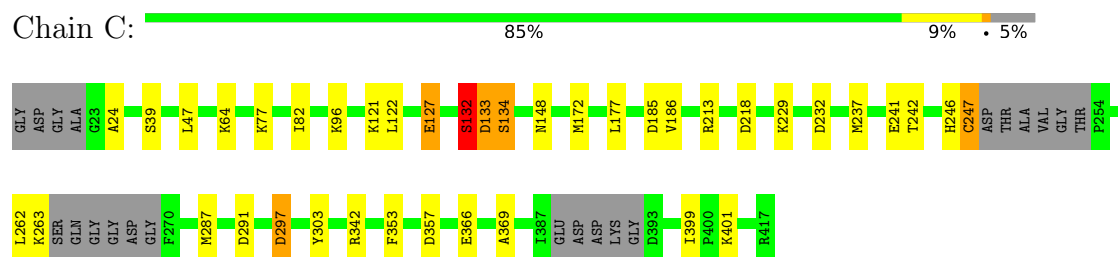
• Molecule 1: Rho-associated protein kinase 2



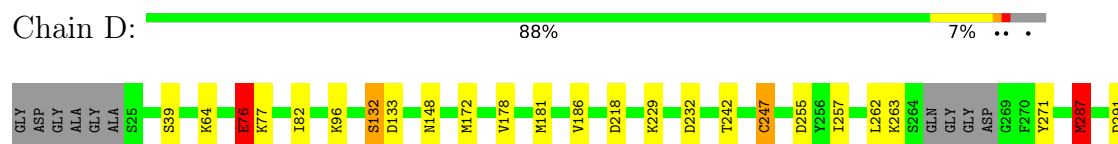
• Molecule 1: Rho-associated protein kinase 2

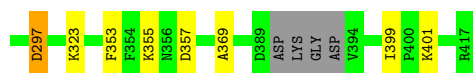


• Molecule 1: Rho-associated protein kinase 2



• Molecule 1: Rho-associated protein kinase 2





- Molecule 1: Rho-associated protein kinase 2

Chain E: 88% 8% . .



- Molecule 1: Rho-associated protein kinase 2

Chain F: 89% 7% . .



- Molecule 1: Rho-associated protein kinase 2

Chain G: 87% 8% . .



- Molecule 1: Rho-associated protein kinase 2

Chain H: 81% 8% . . 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.90Å 101.60Å 102.75Å 83.92° 73.64° 77.71°	Depositor
Resolution (Å)	99.15 – 3.00 99.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (99.15-3.00) 94.8 (99.15-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.185 , 0.288 0.193 , 0.293	Depositor DCC
R_{free} test set	513 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25053	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5YS

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	0.89	1/3199 (0.0%)	1.19	7/4319 (0.2%)
1	B	0.87	1/3218 (0.0%)	1.18	7/4345 (0.2%)
1	C	0.92	2/3158 (0.1%)	1.20	11/4262 (0.3%)
1	D	0.89	2/3207 (0.1%)	1.18	7/4332 (0.2%)
1	E	0.88	0/3203	1.18	7/4323 (0.2%)
1	F	0.89	0/3201	1.18	6/4324 (0.1%)
1	G	0.93	3/3209 (0.1%)	1.21	9/4333 (0.2%)
1	H	0.93	5/3069 (0.2%)	1.23	14/4144 (0.3%)
All	All	0.90	14/25464 (0.1%)	1.19	68/34382 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	1
1	G	0	2
1	H	0	2
All	All	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	246	HIS	CA-C	13.54	1.59	1.52
1	H	199	VAL	C-N	-10.00	1.19	1.33
1	G	133	ASP	CA-CB	7.92	1.63	1.53
1	H	133	ASP	CA-CB	7.18	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	132	SER	N-CA	6.93	1.55	1.46
1	A	251	VAL	CA-C	6.83	1.61	1.52
1	C	133	ASP	N-CA	6.00	1.54	1.46
1	H	319	ALA	N-CA	5.78	1.53	1.46
1	H	200	LEU	N-CA	5.74	1.53	1.46
1	H	272	GLY	N-CA	5.37	1.53	1.45
1	G	133	ASP	CA-C	5.28	1.59	1.52
1	D	133	ASP	CA-CB	5.25	1.59	1.53
1	B	322	SER	CB-OG	-5.20	1.31	1.42
1	D	255	ASP	N-CA	5.17	1.52	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	199	VAL	CB-CA-C	-14.20	96.75	111.80
1	G	246	HIS	CA-C-O	-14.06	110.97	119.55
1	G	133	ASP	CB-CA-C	9.36	126.26	110.81
1	H	133	ASP	CB-CA-C	9.29	126.14	110.81
1	C	342	ARG	CG-CD-NE	-9.03	92.12	112.00
1	F	132	SER	N-CA-C	8.51	128.93	110.80
1	H	199	VAL	N-CA-C	-8.21	95.72	107.37
1	H	200	LEU	N-CA-CB	7.86	123.77	110.49
1	G	247	CYS	N-CA-C	7.16	121.27	111.17
1	C	133	ASP	N-CA-CB	6.74	120.68	110.30
1	C	342	ARG	CB-CA-C	6.72	121.43	110.88
1	E	350	GLN	CA-CB-CG	6.70	127.49	114.10
1	D	64	LYS	CB-CG-CD	6.36	125.92	111.30
1	C	297	ASP	N-CA-C	-6.21	104.14	111.03
1	H	320	GLU	CA-C-O	6.20	129.03	121.72
1	B	132	SER	N-CA-C	6.18	123.96	110.80
1	D	369	ALA	CA-C-N	6.17	125.66	119.24
1	D	369	ALA	C-N-CA	6.17	125.66	119.24
1	F	369	ALA	CA-C-N	6.10	125.59	119.24
1	F	369	ALA	C-N-CA	6.10	125.59	119.24
1	E	132	SER	N-CA-C	6.09	123.78	110.80
1	A	132	SER	N-CA-C	6.09	123.76	110.80
1	B	369	ALA	CA-C-N	6.06	125.55	119.24
1	B	369	ALA	C-N-CA	6.06	125.55	119.24
1	H	369	ALA	CA-C-N	6.06	125.54	119.24
1	H	369	ALA	C-N-CA	6.06	125.54	119.24
1	G	297	ASP	N-CA-C	-5.99	104.38	111.03
1	E	369	ALA	CA-C-N	5.93	125.41	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	369	ALA	C-N-CA	5.93	125.41	119.24
1	C	24	ALA	N-CA-C	5.92	119.60	112.38
1	F	297	ASP	N-CA-C	-5.91	104.47	111.03
1	C	127	GLU	CB-CG-CD	5.90	122.63	112.60
1	C	369	ALA	CA-C-N	5.88	125.36	119.24
1	C	369	ALA	C-N-CA	5.88	125.36	119.24
1	G	369	ALA	CA-C-N	5.81	125.29	119.24
1	G	369	ALA	C-N-CA	5.81	125.29	119.24
1	A	161	ASP	N-CA-CB	-5.80	102.06	111.22
1	H	35	ARG	CA-CB-CG	-5.75	102.61	114.10
1	D	287	MET	CB-CG-SD	5.73	129.90	112.70
1	C	185	ASP	N-CA-C	-5.70	101.41	109.96
1	A	178	VAL	N-CA-C	-5.63	105.24	110.53
1	A	369	ALA	CA-C-N	5.59	125.06	119.24
1	A	369	ALA	C-N-CA	5.59	125.06	119.24
1	G	178	VAL	N-CA-C	-5.56	105.30	110.53
1	E	178	VAL	N-CA-C	-5.49	105.37	110.53
1	E	24	ALA	N-CA-C	5.48	119.47	112.34
1	D	76	GLU	CA-CB-CG	5.40	124.90	114.10
1	A	270	PHE	N-CA-CB	-5.36	101.40	110.50
1	H	178	VAL	N-CA-C	-5.35	105.50	110.53
1	H	237	MET	CG-SD-CE	5.33	112.62	100.90
1	H	274	GLU	CA-CB-CG	5.30	124.70	114.10
1	E	297	ASP	N-CA-C	-5.26	104.45	111.24
1	C	134	SER	CA-CB-OG	5.24	121.59	111.10
1	H	132	SER	N-CA-C	5.22	121.93	110.80
1	B	178	VAL	N-CA-C	-5.21	105.64	110.53
1	H	163	ARG	N-CA-C	5.20	119.62	113.12
1	A	163	ARG	N-CA-C	5.18	119.59	113.12
1	C	247	CYS	N-CA-C	5.17	125.48	111.00
1	B	297	ASP	N-CA-C	-5.15	104.60	111.24
1	B	25	SER	CB-CA-C	5.13	119.85	110.10
1	G	132	SER	N-CA-C	5.13	121.73	110.80
1	B	47	LEU	CB-CG-CD1	5.13	126.08	110.70
1	H	25	SER	CB-CA-C	5.10	119.78	110.10
1	F	178	VAL	N-CA-C	-5.04	105.79	110.53
1	F	224	LYS	CD-CE-NZ	5.04	128.02	111.90
1	D	132	SER	N-CA-C	5.03	121.52	110.80
1	D	178	VAL	N-CA-C	-5.02	105.81	110.53
1	G	247	CYS	CA-CB-SG	-5.00	102.89	114.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	VAL	Peptide
1	A	251	VAL	Peptide
1	A	263	LYS	Peptide
1	B	263	LYS	Peptide
1	B	388	GLU	Peptide
1	C	132	SER	Peptide
1	C	246	HIS	Peptide
1	C	262	LEU	Peptide
1	D	263	LYS	Peptide
1	G	133	ASP	Sidechain
1	G	263	LYS	Peptide
1	H	133	ASP	Sidechain
1	H	271	TYR	Peptide

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	3123	0	3055	9	0
1	B	3141	0	3064	10	0
1	C	3082	0	3018	5	0
1	D	3130	0	3059	7	0
1	E	3126	0	3051	9	0
1	F	3124	0	3054	5	0
1	G	3132	0	3053	8	0
1	H	2995	0	2935	9	0
2	A	25	0	0	1	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
2	E	25	0	0	1	0
2	F	25	0	0	0	0
2	G	25	0	0	0	0
2	H	25	0	0	2	0
All	All	25053	0	24289	57	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 1.

All (57) 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:H:196:ALA:O	1:H:199:VAL:O	1.83	0.96
1:E:29:LYS:NZ	1:G:350:GLN:O	2.24	0.70
1:D:186:VAL:HG11	1:D:287:MET:HE3	1.77	0.67
1:A:209:GLY:HA2	1:A:239:MET:HE2	1.78	0.65
1:H:274:GLU:HG2	1:H:342:ARG:HG2	1.82	0.61
1:E:209:GLY:HA2	1:E:239:MET:HE2	1.82	0.61
1:G:237:MET:HE1	1:G:247:CYS:SG	2.41	0.60
1:G:388:GLU:N	1:G:388:GLU:OE1	2.34	0.59
1:H:274:GLU:CG	1:H:342:ARG:HG2	2.35	0.56
1:A:241:GLU:HB3	1:B:376:SER:HB2	1.89	0.55
1:A:241:GLU:CB	1:B:376:SER:HB2	2.37	0.54
1:D:247:CYS:HG	1:D:271:TYR:HH	1.55	0.53
1:E:186:VAL:HG11	1:E:287:MET:HE2	1.91	0.53
1:G:186:VAL:HG11	1:G:287:MET:HE2	1.91	0.51
1:B:172:MET:HE2	1:B:229:LYS:HB2	1.93	0.50
1:H:103:PHE:H	2:H:501:5YS:C13	2.23	0.50
1:H:186:VAL:HG11	1:H:287:MET:HE2	1.92	0.50
1:D:172:MET:HE2	1:D:229:LYS:HB2	1.94	0.49
1:F:172:MET:HE2	1:F:229:LYS:HB2	1.93	0.49
1:H:172:MET:HE2	1:H:229:LYS:HB2	1.93	0.49
1:B:245:VAL:O	1:B:270:PHE:N	2.45	0.49
1:B:100:ARG:HH22	1:B:389:ASP:HB3	1.78	0.49
1:C:172:MET:HE2	1:C:229:LYS:HB2	1.94	0.49
1:H:321:ILE:HG23	1:H:326:LYS:HE2	1.94	0.49
1:A:186:VAL:HG11	1:A:287:MET:HE2	1.95	0.49
1:G:172:MET:HE2	1:G:229:LYS:HB2	1.94	0.49
1:E:172:MET:HE2	1:E:229:LYS:HB2	1.94	0.48
1:E:239:MET:HE3	1:G:242:THR:HG22	1.96	0.47
1:A:172:MET:HE2	1:A:229:LYS:HB2	1.95	0.47
1:C:186:VAL:HG11	1:C:287:MET:HE2	1.97	0.47
1:E:273:ARG:NH1	1:G:241:GLU:HG2	2.30	0.46
1:D:181:MET:SD	1:D:287:MET:HG2	2.55	0.46
1:H:232:ASP:HB2	2:H:501:5YS:C2	2.46	0.45
1:C:121:LYS:NZ	2:C:501:5YS:O1	2.49	0.45
1:B:100:ARG:NH2	1:B:389:ASP:HB3	2.33	0.44
1:B:131:ARG:O	1:B:133:ASP:N	2.45	0.43
1:E:257:ILE:HG21	1:E:262:LEU:HD21	2.01	0.43
1:A:131:ARG:O	1:A:133:ASP:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD12	1:A:122:LEU:N	2.35	0.42
1:G:257:ILE:HG21	1:G:262:LEU:HD21	2.01	0.42
1:A:100:ARG:NH2	1:A:388:GLU:O	2.53	0.42
1:E:221:LEU:CD1	2:E:501:5YS:C21	2.98	0.41
1:D:76:GLU:HG2	1:D:77:LYS:HG2	2.02	0.41
1:F:122:LEU:N	1:F:122:LEU:HD12	2.35	0.41
1:F:186:VAL:HG11	1:F:287:MET:HE2	2.01	0.41
1:C:122:LEU:N	1:C:122:LEU:HD12	2.35	0.41
1:E:131:ARG:O	1:E:133:ASP:N	2.46	0.41
1:F:257:ILE:HG21	1:F:262:LEU:HD21	2.02	0.41
1:B:257:ILE:HG21	1:B:262:LEU:HD21	2.02	0.41
1:F:131:ARG:O	1:F:133:ASP:N	2.46	0.41
1:D:257:ILE:HG21	1:D:262:LEU:HD21	2.03	0.40
1:C:237:MET:HE1	1:C:247:CYS:HA	2.03	0.40
1:H:131:ARG:O	1:H:133:ASP:N	2.46	0.40
1:A:102:ALA:HB3	2:A:501:5YS:C13	2.50	0.40
1:B:122:LEU:HD12	1:B:122:LEU:N	2.36	0.40
1:B:297:ASP:N	1:B:297:ASP:OD1	2.54	0.40
1:D:297:ASP:N	1:D:297:ASP:OD1	2.55	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	376/399 (94%)	348 (93%)	25 (7%)	3 (1%)	16	50
1	B	379/399 (95%)	350 (92%)	23 (6%)	6 (2%)	7	34
1	C	370/399 (93%)	344 (93%)	21 (6%)	5 (1%)	9	36
1	D	379/399 (95%)	350 (92%)	24 (6%)	5 (1%)	9	38
1	E	379/399 (95%)	349 (92%)	26 (7%)	4 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	378/399 (95%)	349 (92%)	25 (7%)	4 (1%)	11	43
1	G	379/399 (95%)	353 (93%)	22 (6%)	4 (1%)	11	43
1	H	358/399 (90%)	332 (93%)	22 (6%)	4 (1%)	11	43
All	All	2998/3192 (94%)	2775 (93%)	188 (6%)	35 (1%)	10	40

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	B	132	SER
1	E	132	SER
1	F	132	SER
1	G	132	SER
1	H	132	SER
1	B	389	ASP
1	B	391	LYS
1	D	132	SER
1	F	270	PHE
1	H	200	LEU
1	A	232	ASP
1	B	232	ASP
1	C	232	ASP
1	D	232	ASP
1	E	232	ASP
1	E	268	ASP
1	F	232	ASP
1	G	232	ASP
1	G	270	PHE
1	H	232	ASP
1	C	132	SER
1	D	76	GLU
1	A	353	PHE
1	B	148	ASN
1	B	353	PHE
1	C	148	ASN
1	C	353	PHE
1	F	353	PHE
1	C	213	ARG
1	D	148	ASN
1	D	353	PHE
1	E	353	PHE

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Mol	Chain	Res	Type
1	G	353	PHE
1	H	353	PHE

5.3.2 Protein sidechains ⓘ

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	339/347 (98%)	328 (97%)	11 (3%)	34	67
1	B	343/347 (99%)	325 (95%)	18 (5%)	21	55
1	C	335/347 (96%)	314 (94%)	21 (6%)	16	48
1	D	341/347 (98%)	326 (96%)	15 (4%)	25	60
1	E	339/347 (98%)	325 (96%)	14 (4%)	27	61
1	F	340/347 (98%)	325 (96%)	15 (4%)	25	60
1	G	341/347 (98%)	324 (95%)	17 (5%)	22	56
1	H	326/347 (94%)	308 (94%)	18 (6%)	19	53
All	All	2704/2776 (97%)	2575 (95%)	129 (5%)	23	57

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	82	ILE
1	A	96	LYS
1	A	213	ARG
1	A	218	ASP
1	A	224	LYS
1	A	291	ASP
1	A	323	LYS
1	A	333	LEU
1	A	357	ASP
1	A	399	ILE
1	B	25	SER
1	B	39	SER

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Mol	Chain	Res	Type
1	B	82	ILE
1	B	96	LYS
1	B	218	ASP
1	B	225	HIS
1	B	242	THR
1	B	247	CYS
1	B	263	LYS
1	B	291	ASP
1	B	297	ASP
1	B	316	PRO
1	B	322	SER
1	B	323	LYS
1	B	326	LYS
1	B	333	LEU
1	B	357	ASP
1	B	391	LYS
1	C	39	SER
1	C	47	LEU
1	C	64	LYS
1	C	77	LYS
1	C	82	ILE
1	C	96	LYS
1	C	127	GLU
1	C	133	ASP
1	C	134	SER
1	C	177	LEU
1	C	218	ASP
1	C	241	GLU
1	C	242	THR
1	C	263	LYS
1	C	291	ASP
1	C	297	ASP
1	C	303	TYR
1	C	357	ASP
1	C	366	GLU
1	C	399	ILE
1	C	401	LYS
1	D	39	SER
1	D	76	GLU
1	D	82	ILE
1	D	96	LYS
1	D	218	ASP

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Mol	Chain	Res	Type
1	D	242	THR
1	D	247	CYS
1	D	287	MET
1	D	291	ASP
1	D	297	ASP
1	D	323	LYS
1	D	355	LYS
1	D	357	ASP
1	D	399	ILE
1	D	401	LYS
1	E	29	LYS
1	E	35	ARG
1	E	39	SER
1	E	47	LEU
1	E	82	ILE
1	E	96	LYS
1	E	218	ASP
1	E	238	LYS
1	E	291	ASP
1	E	297	ASP
1	E	303	TYR
1	E	342	ARG
1	E	355	LYS
1	E	357	ASP
1	F	25	SER
1	F	39	SER
1	F	47	LEU
1	F	82	ILE
1	F	96	LYS
1	F	218	ASP
1	F	224	LYS
1	F	230	LEU
1	F	242	THR
1	F	291	ASP
1	F	297	ASP
1	F	316	PRO
1	F	355	LYS
1	F	357	ASP
1	F	399	ILE
1	G	25	SER
1	G	39	SER
1	G	47	LEU

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Mol	Chain	Res	Type
1	G	80	LYS
1	G	82	ILE
1	G	96	LYS
1	G	133	ASP
1	G	177	LEU
1	G	185	ASP
1	G	213	ARG
1	G	218	ASP
1	G	241	GLU
1	G	248	ASP
1	G	291	ASP
1	G	297	ASP
1	G	326	LYS
1	G	357	ASP
1	H	25	SER
1	H	39	SER
1	H	82	ILE
1	H	96	LYS
1	H	133	ASP
1	H	177	LEU
1	H	200	LEU
1	H	218	ASP
1	H	224	LYS
1	H	225	HIS
1	H	237	MET
1	H	291	ASP
1	H	297	ASP
1	H	323	LYS
1	H	333	LEU
1	H	336	ARG
1	H	357	ASP
1	H	401	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	356	ASN
1	B	324	HIS
1	B	356	ASN
1	C	154	GLN
1	C	324	HIS

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Mol	Chain	Res	Type
1	C	327	ASN
1	C	356	ASN
1	D	154	GLN
1	D	324	HIS
1	D	356	ASN
1	D	358	GLN
1	E	265	GLN
1	E	324	HIS
1	E	356	ASN
1	F	27	GLN
1	F	356	ASN
1	F	358	GLN
1	G	324	HIS
1	G	356	ASN
1	H	324	HIS
1	H	356	ASN
1	H	358	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](#)

8 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	5YS	A	501	-	27,27,27	3.07	3 (11%)	35,36,36	1.02	0
2	5YS	E	501	-	27,27,27	3.08	3 (11%)	35,36,36	1.11	2 (5%)
2	5YS	H	501	-	27,27,27	3.09	3 (11%)	35,36,36	1.02	1 (2%)
2	5YS	B	501	-	27,27,27	3.08	3 (11%)	35,36,36	1.16	3 (8%)
2	5YS	F	501	-	27,27,27	3.08	3 (11%)	35,36,36	1.11	3 (8%)
2	5YS	G	501	-	27,27,27	3.08	3 (11%)	35,36,36	1.09	2 (5%)
2	5YS	C	501	-	27,27,27	3.08	3 (11%)	35,36,36	1.09	1 (2%)
2	5YS	D	501	-	27,27,27	3.07	3 (11%)	35,36,36	1.15	3 (8%)

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	5YS	A	501	-	-	3/18/28/28	0/3/3/3
2	5YS	E	501	-	-	3/18/28/28	0/3/3/3
2	5YS	H	501	-	-	4/18/28/28	0/3/3/3
2	5YS	B	501	-	-	3/18/28/28	0/3/3/3
2	5YS	F	501	-	-	2/18/28/28	0/3/3/3
2	5YS	G	501	-	-	3/18/28/28	0/3/3/3
2	5YS	C	501	-	-	3/18/28/28	0/3/3/3
2	5YS	D	501	-	-	4/18/28/28	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	5YS	C20-N15	9.28	1.63	1.47
2	H	501	5YS	C16-N15	9.28	1.63	1.47
2	H	501	5YS	C20-N15	9.27	1.63	1.47
2	A	501	5YS	C16-N15	9.27	1.63	1.47
2	B	501	5YS	C16-N15	9.26	1.63	1.47
2	C	501	5YS	C16-N15	9.24	1.63	1.47
2	G	501	5YS	C16-N15	9.22	1.63	1.47
2	E	501	5YS	C16-N15	9.18	1.63	1.47
2	H	501	5YS	C2-N15	9.15	1.52	1.36
2	F	501	5YS	C16-N15	9.13	1.63	1.47
2	D	501	5YS	C16-N15	9.10	1.63	1.47
2	E	501	5YS	C20-N15	9.10	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	5YS	C2-N15	9.10	1.52	1.36
2	E	501	5YS	C2-N15	9.09	1.52	1.36
2	B	501	5YS	C20-N15	9.07	1.63	1.47
2	C	501	5YS	C2-N15	9.07	1.52	1.36
2	F	501	5YS	C20-N15	9.06	1.63	1.47
2	G	501	5YS	C2-N15	9.06	1.52	1.36
2	G	501	5YS	C20-N15	9.02	1.63	1.47
2	C	501	5YS	C20-N15	9.00	1.63	1.47
2	A	501	5YS	C20-N15	9.00	1.63	1.47
2	A	501	5YS	C2-N15	8.95	1.52	1.36
2	B	501	5YS	C2-N15	8.94	1.52	1.36
2	D	501	5YS	C2-N15	8.87	1.51	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	5YS	C16-C17-C18	-2.94	107.56	111.00
2	B	501	5YS	C19-C18-C21	-2.46	106.86	112.67
2	D	501	5YS	C20-C19-C18	-2.44	108.15	111.00
2	F	501	5YS	C25-N24-C23	2.30	122.12	116.86
2	B	501	5YS	C25-N24-C23	2.27	122.05	116.86
2	D	501	5YS	C16-C17-C18	-2.16	108.47	111.00
2	D	501	5YS	C25-N24-C23	2.16	121.80	116.86
2	B	501	5YS	C16-C17-C18	-2.15	108.48	111.00
2	G	501	5YS	C25-N24-C23	2.09	121.65	116.86
2	E	501	5YS	C25-N24-C23	2.09	121.64	116.86
2	F	501	5YS	C20-C19-C18	-2.08	108.57	111.00
2	F	501	5YS	C19-C18-C21	-2.07	107.77	112.67
2	H	501	5YS	C25-N24-C23	2.06	121.57	116.86
2	G	501	5YS	C16-C17-C18	-2.01	108.64	111.00
2	C	501	5YS	C25-N24-C23	2.01	121.45	116.86

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	5YS	C7-C4-N3-C2
2	B	501	5YS	C7-C4-N3-C2
2	E	501	5YS	C7-C4-N3-C2
2	G	501	5YS	C7-C4-N3-C2
2	C	501	5YS	C7-C4-N3-C2
2	H	501	5YS	C7-C4-N3-C2

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Mol	Chain	Res	Type	Atoms
2	A	501	5YS	C17-C18-C21-C22
2	G	501	5YS	C17-C18-C21-C22
2	G	501	5YS	C17-C18-C21-C26
2	A	501	5YS	C17-C18-C21-C26
2	D	501	5YS	C17-C18-C21-C26
2	D	501	5YS	C17-C18-C21-C22
2	H	501	5YS	C17-C18-C21-C26
2	E	501	5YS	C17-C18-C21-C22
2	H	501	5YS	C17-C18-C21-C22
2	E	501	5YS	C17-C18-C21-C26
2	D	501	5YS	C6-C4-N3-C2
2	F	501	5YS	C17-C18-C21-C22
2	F	501	5YS	C17-C18-C21-C26
2	D	501	5YS	C7-C4-N3-C2
2	B	501	5YS	C17-C18-C21-C22
2	C	501	5YS	C17-C18-C21-C22
2	B	501	5YS	C17-C18-C21-C26
2	C	501	5YS	C17-C18-C21-C26
2	H	501	5YS	C6-C4-N3-C2

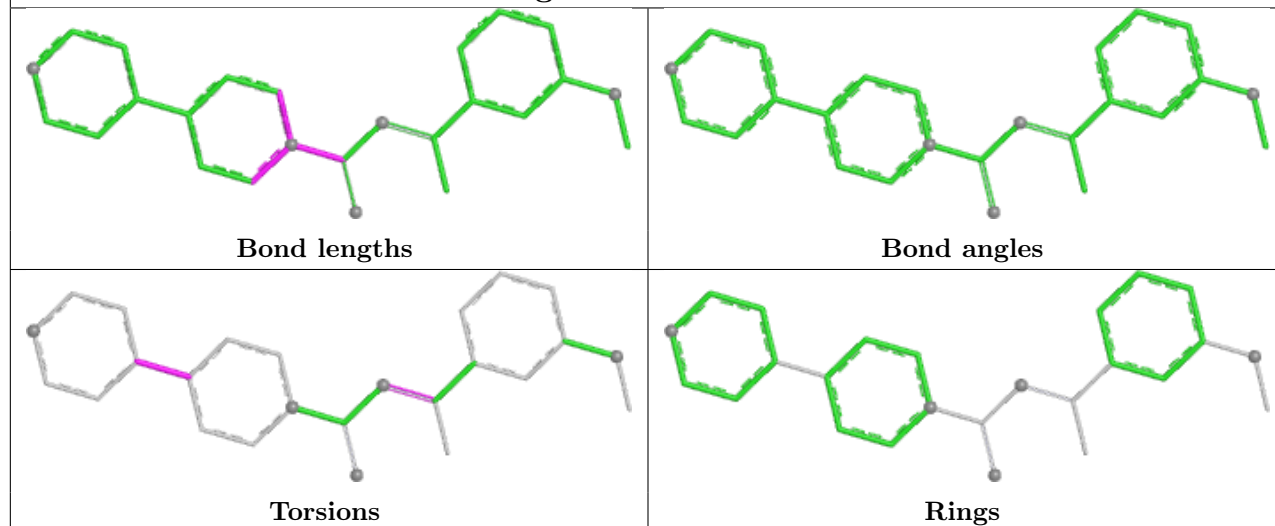
There are no ring outliers.

4 monomers are involved in 5 short contacts:

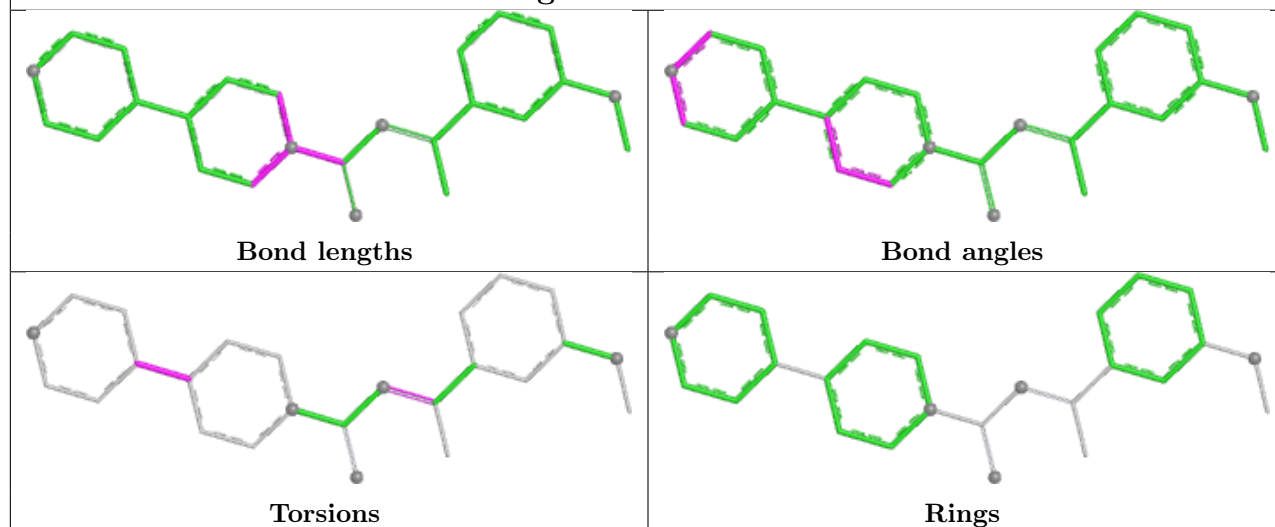
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	5YS	1	0
2	E	501	5YS	1	0
2	H	501	5YS	2	0
2	C	501	5YS	1	0

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.

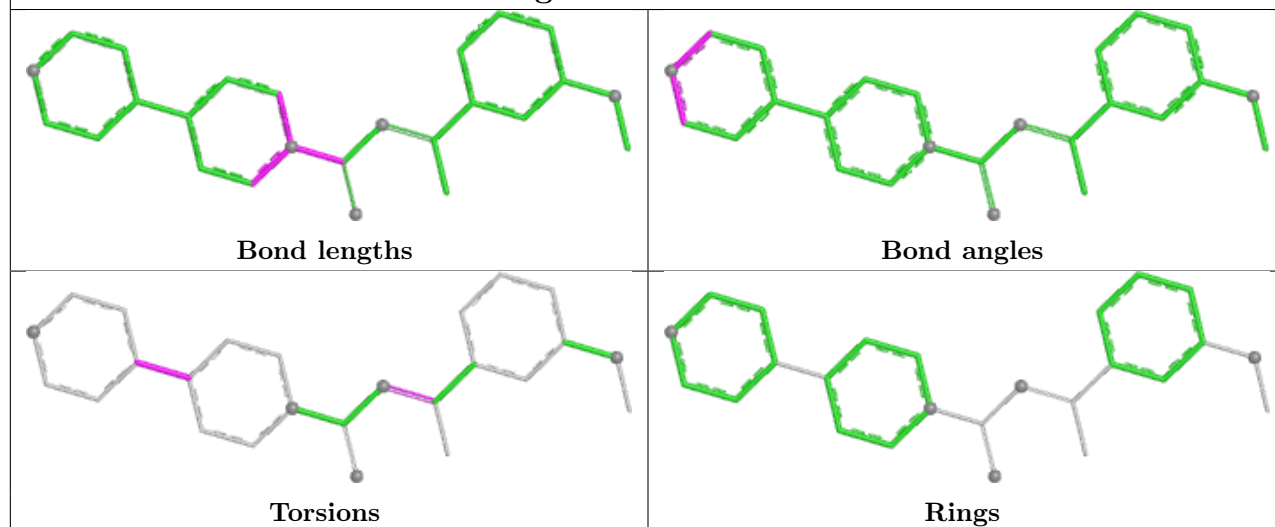
Ligand 5YS A 501



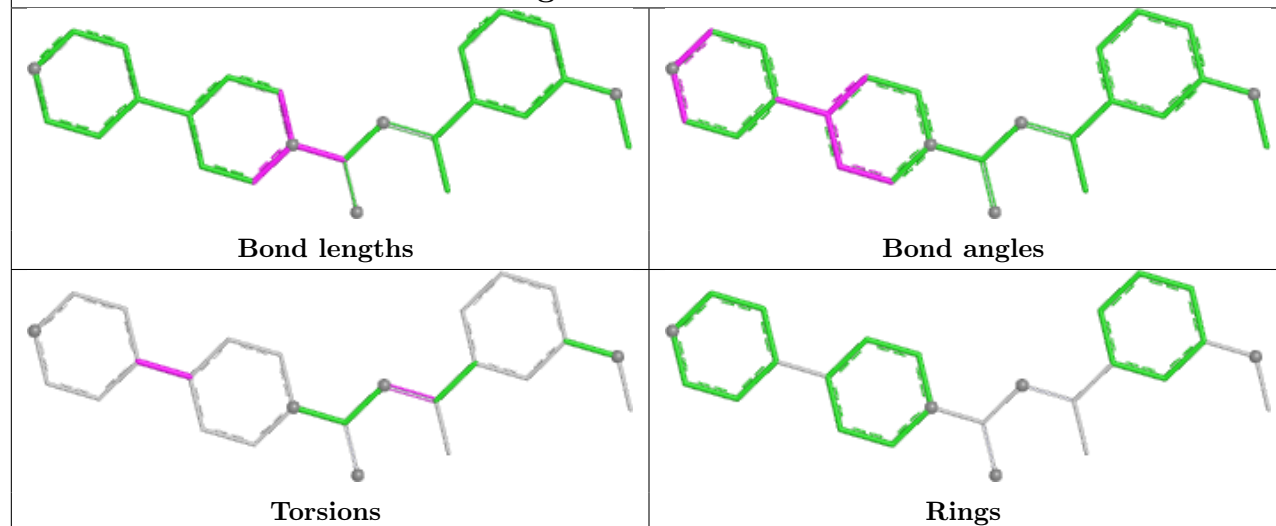
Ligand 5YS E 501



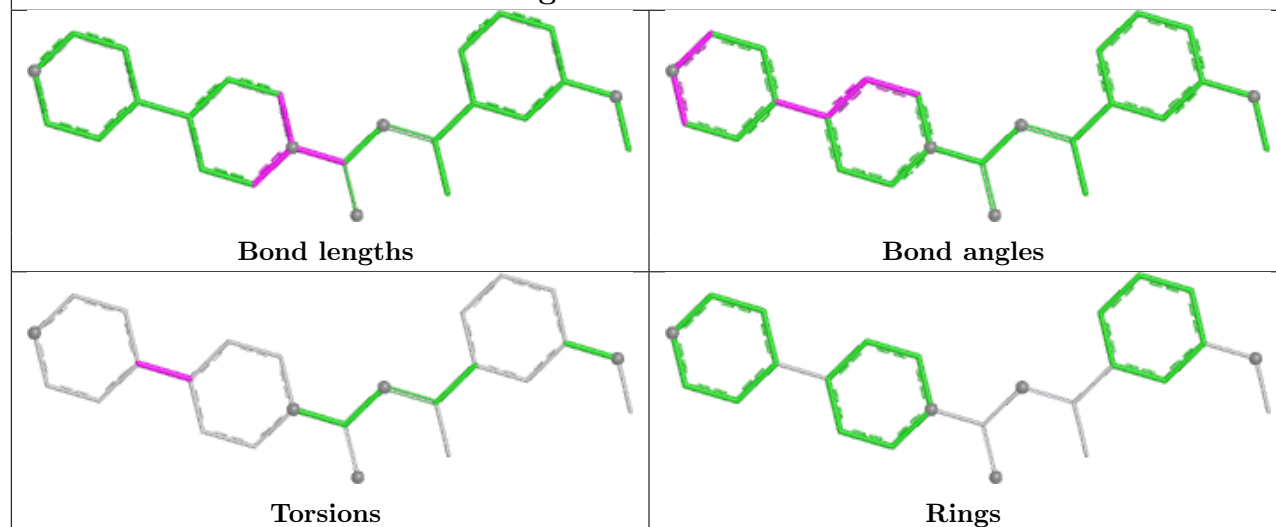
Ligand 5YS H 501



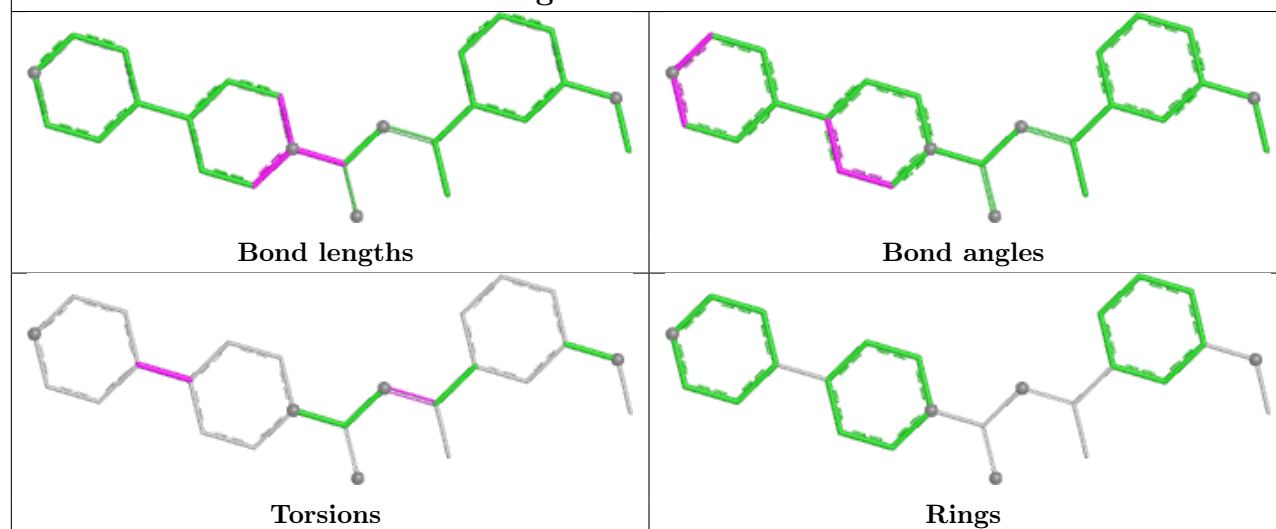
Ligand 5YS B 501

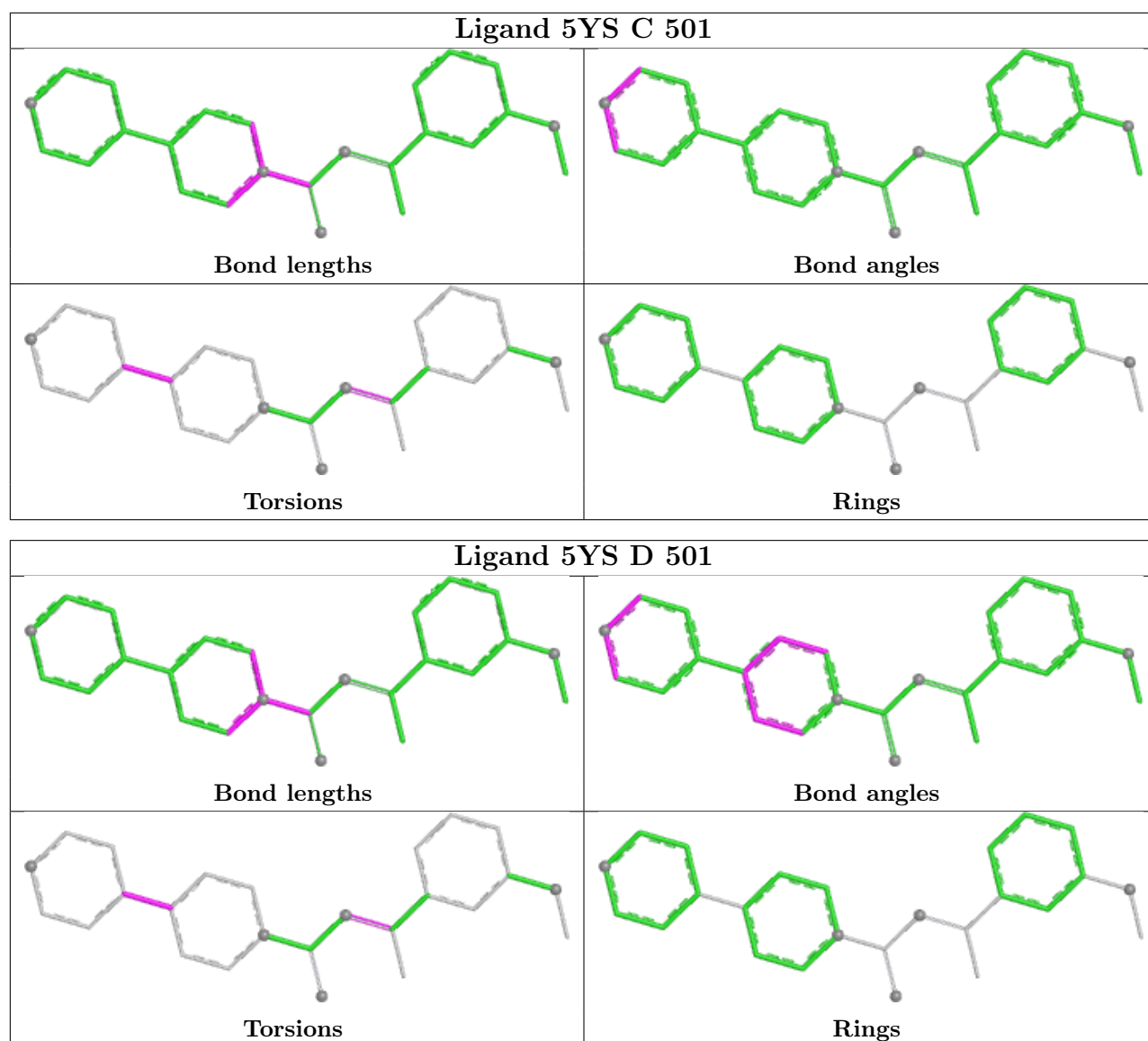


Ligand 5YS F 501



Ligand 5YS G 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	199:VAL	C	200:LEU	N	1.19

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	A	384/399 (96%)	-0.69	2 (0%) 87 72	42, 79, 131, 173	0
1	B	385/399 (96%)	-0.65	0 100 100	58, 95, 152, 224	0
1	C	378/399 (94%)	-0.64	0 100 100	50, 83, 130, 159	0
1	D	385/399 (96%)	-0.64	0 100 100	46, 83, 130, 169	0
1	E	385/399 (96%)	-0.58	0 100 100	58, 94, 138, 231	0
1	F	384/399 (96%)	-0.61	0 100 100	50, 83, 130, 153	0
1	G	385/399 (96%)	-0.59	1 (0%) 90 79	54, 89, 138, 194	0
1	H	366/399 (91%)	-0.46	0 100 100	65, 111, 160, 240	0
All	All	3052/3192 (95%)	-0.61	3 (0%) 92 86	42, 90, 144, 240	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	TYR	3.0
1	A	246	HIS	2.6
1	G	303	TYR	2.3

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](#)

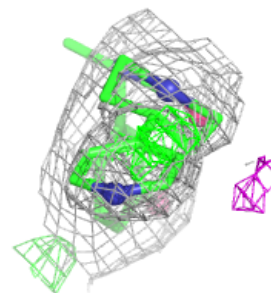
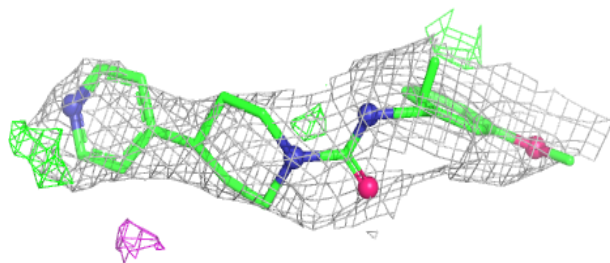
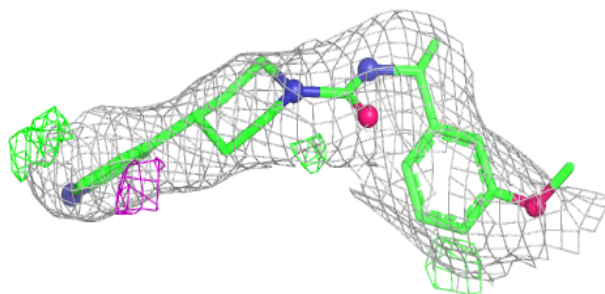
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5YS	H	501	25/25	0.89	0.12	71,100,138,159	0
2	5YS	E	501	25/25	0.94	0.09	43,67,105,155	0
2	5YS	G	501	25/25	0.94	0.09	37,62,81,99	0
2	5YS	C	501	25/25	0.94	0.10	36,56,78,117	0
2	5YS	B	501	25/25	0.95	0.09	45,66,96,159	0
2	5YS	F	501	25/25	0.95	0.10	51,63,85,87	0
2	5YS	A	501	25/25	0.95	0.09	30,54,77,116	0
2	5YS	D	501	25/25	0.95	0.08	39,63,93,141	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.

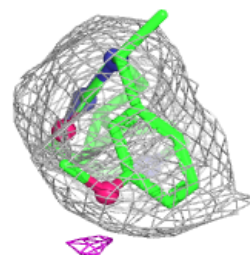
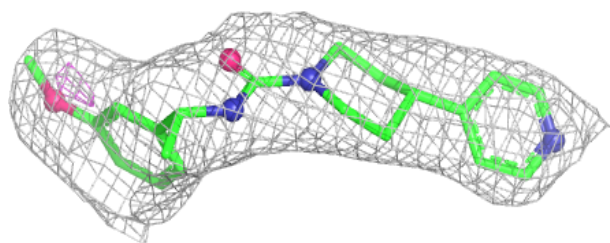
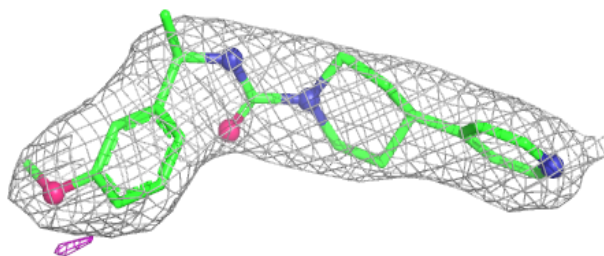
Electron density around 5YS H 501:

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

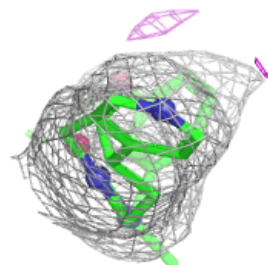
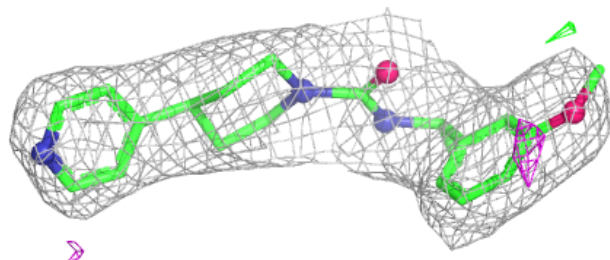
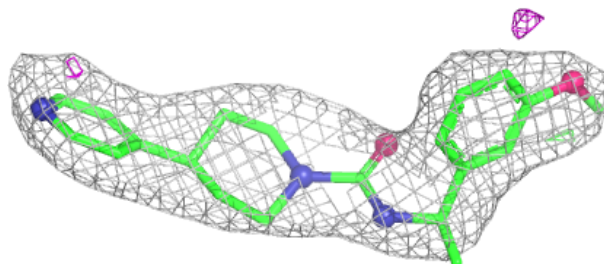


Electron density around 5YS E 501:

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

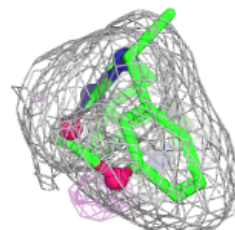
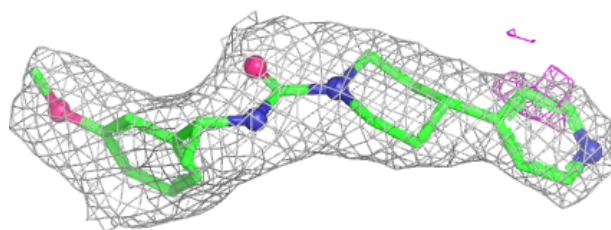
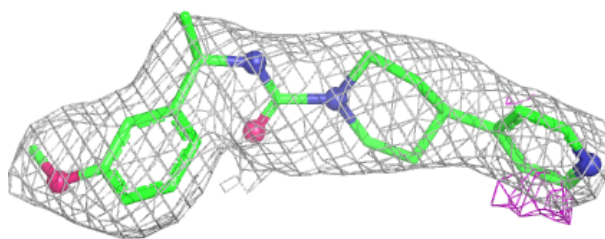
**Electron density around 5YS G 501:**

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

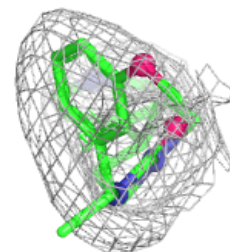
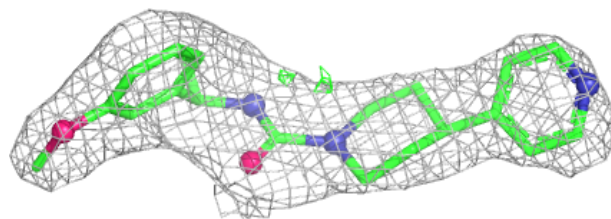
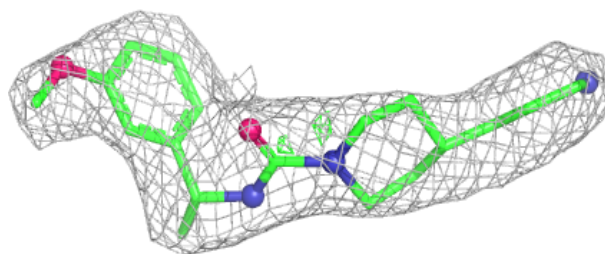


Electron density around 5YS C 501:

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

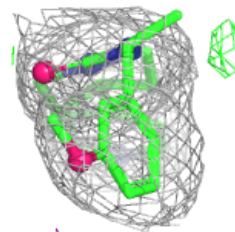
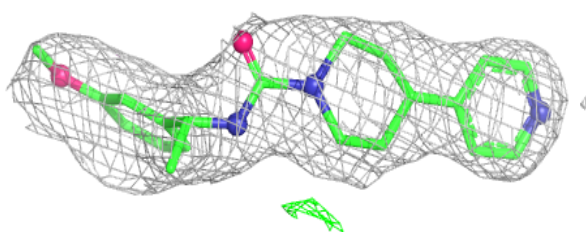
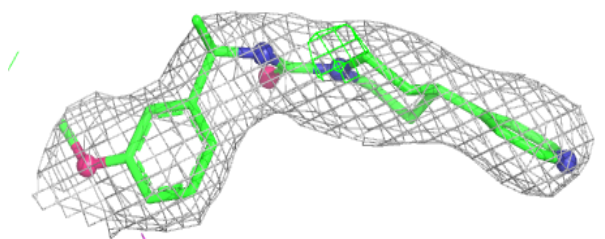
**Electron density around 5YS B 501:**

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

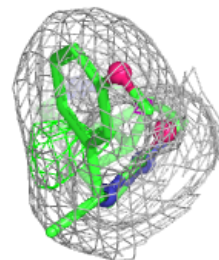
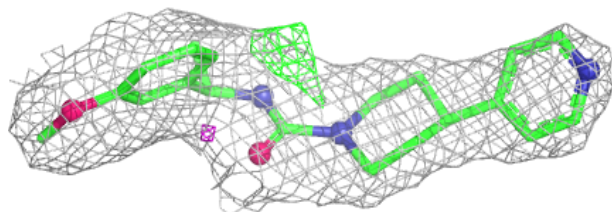
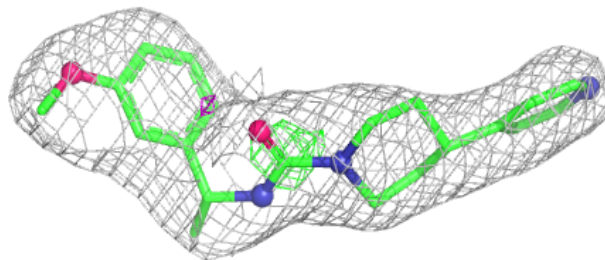


Electron density around 5YS F 501:

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

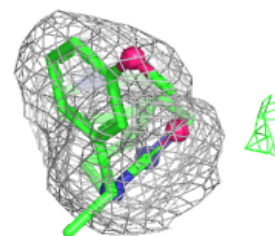
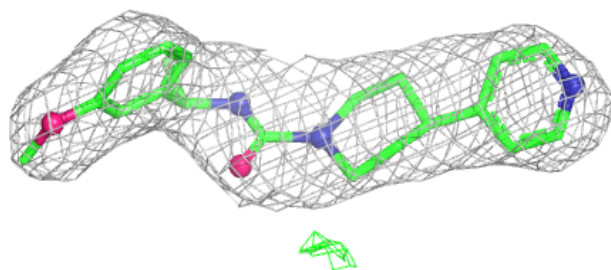
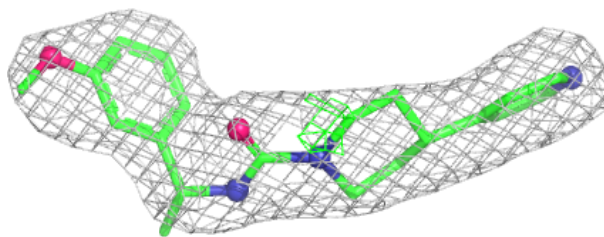
**Electron density around 5YS A 501:**

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



Electron density around 5YS D 501:

$2mF_o-DF_c$ (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.