Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:46 PM JST

PDB ID	:	5YBF
Title	:	Crystal structure of the GluA2o LBD in complex with glutamate and HBT1
Authors	:	Sogabe, S.; Igaki, S.; Hirokawa, A.; Zama, Y.; Lane, W.; Snell, G.
Deposited on	:	2017-09-04
Resolution	:	1.50 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 (i) 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 (i)) were used in the production of this report:

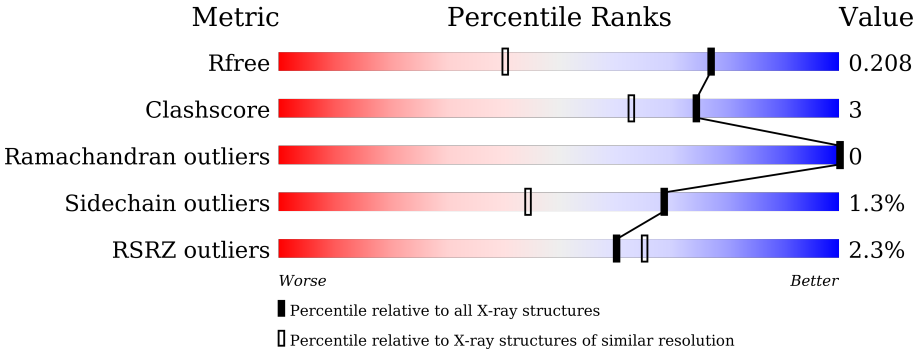
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	263	2% 93% 6% •
1	B	263	7% 94% 5% •
1	C	263	2% 92% 7% •
1	D	263	2% 92% 7% •
1	E	263	% 93% 6% •
1	F	263	92% 6% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14166 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 Glutamate receptor 2,Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2045	1302	342	387	14	0	4	0
1	B	260	2039	1296	342	387	14	0	2	0
1	C	260	2048	1302	343	388	15	0	5	0
1	D	260	2051	1302	344	390	15	0	6	0
1	E	260	2054	1307	346	387	14	0	6	0
1	F	260	2042	1297	343	388	14	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

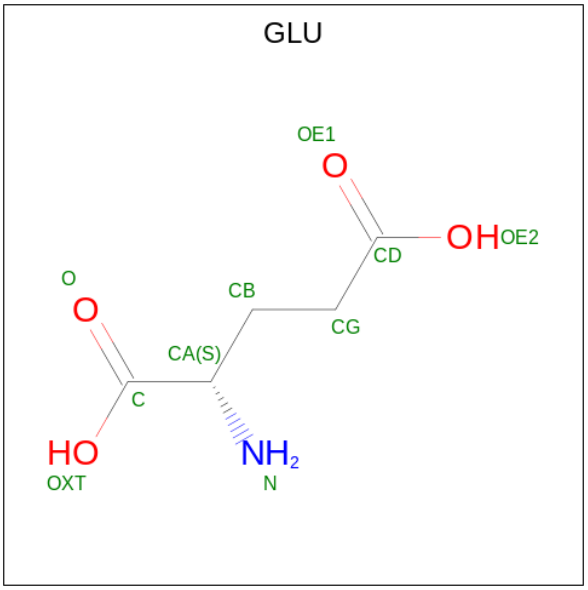
Chain	Residue	Modelled	Actual	Comment	Reference
A	411	GLY	-	expression tag	UNP P42262
A	412	SER	-	expression tag	UNP P42262
A	641	GLY	-	linker	UNP P42262
A	642	THR	-	linker	UNP P42262
B	411	GLY	-	expression tag	UNP P42262
B	412	SER	-	expression tag	UNP P42262
B	641	GLY	-	linker	UNP P42262
B	642	THR	-	linker	UNP P42262
C	411	GLY	-	expression tag	UNP P42262
C	412	SER	-	expression tag	UNP P42262
C	641	GLY	-	linker	UNP P42262
C	642	THR	-	linker	UNP P42262
D	411	GLY	-	expression tag	UNP P42262
D	412	SER	-	expression tag	UNP P42262
D	641	GLY	-	linker	UNP P42262
D	642	THR	-	linker	UNP P42262
E	411	GLY	-	expression tag	UNP P42262

Continued on next page...

Continued from previous page...

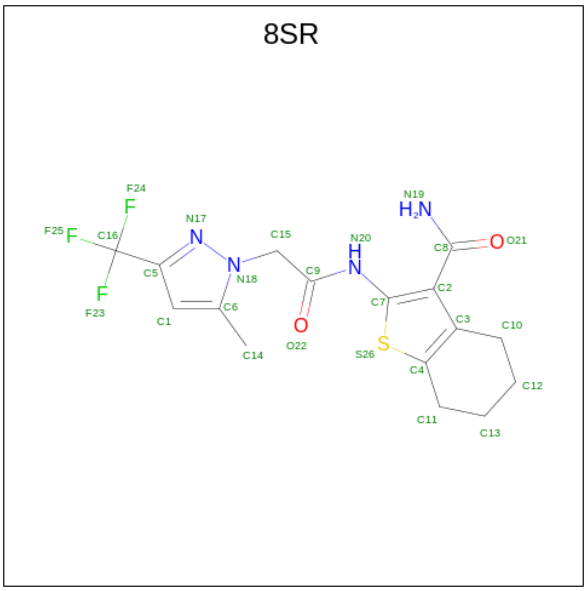
Chain	Residue	Modelled	Actual	Comment	Reference
E	412	SER	-	expression tag	UNP P42262
E	641	GLY	-	linker	UNP P42262
E	642	THR	-	linker	UNP P42262
F	411	GLY	-	expression tag	UNP P42262
F	412	SER	-	expression tag	UNP P42262
F	641	GLY	-	linker	UNP P42262
F	642	THR	-	linker	UNP P42262

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	5	1	4	0	0
2	B	1	10	5	1	4	0	0
2	C	1	10	5	1	4	0	0
2	D	1	10	5	1	4	0	0
2	E	1	10	5	1	4	0	0
2	F	1	10	5	1	4	0	0

- Molecule 3 is 2-[2-[5-methyl-3-(trifluoromethyl)pyrazol-1-yl]ethanoylamino]-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxamide (three-letter code: 8SR) (formula: $C_{16}H_{17}F_3N_4O_2S$).

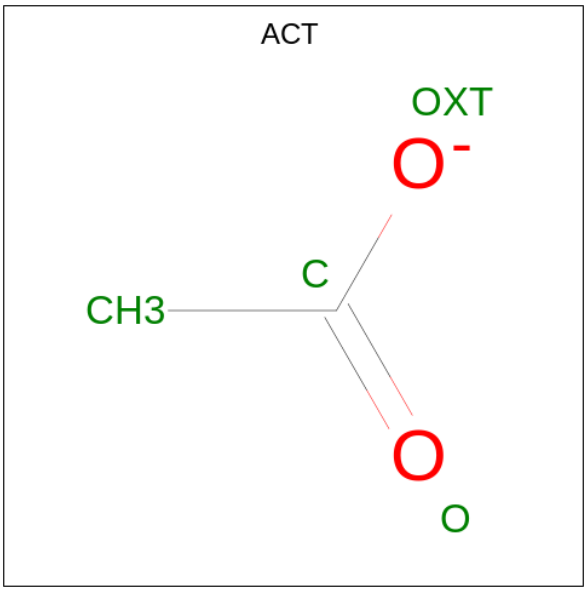


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	52	32	6	8	4	2	0	1
			Total	C	F	N	O	S		
3	C	1	52	32	6	8	4	2	0	1
			Total	C	F	N	O	S		
3	E	1	52	32	6	8	4	2	0	1

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	2	2	2	0	0
			Total	Zn		
4	C	2	2	2	0	0
			Total	Zn		
4	D	3	3	3	0	0
			Total	Zn		
4	F	2	2	2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

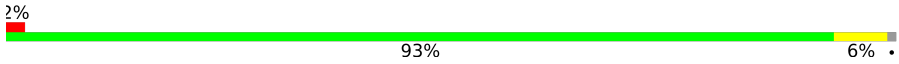
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	240	Total O 240 240	0	0
6	B	208	Total O 208 208	0	0
6	C	317	Total O 317 317	0	0
6	D	337	Total O 337 337	0	0
6	E	301	Total O 301 301	0	0
6	F	250	Total O 250 250	0	0

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.

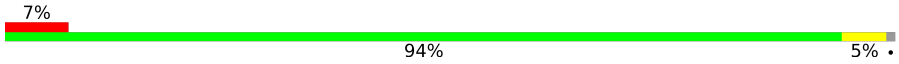
• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

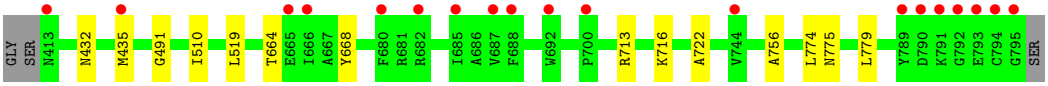
Chain A:



• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

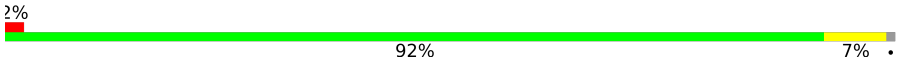
Chain B:





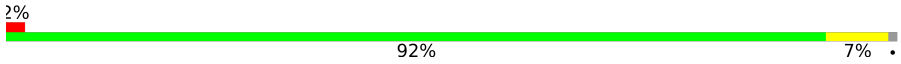
• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

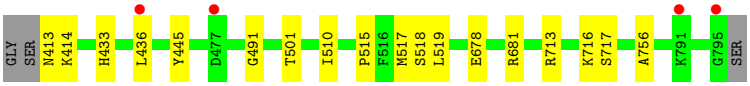
Chain C:



• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

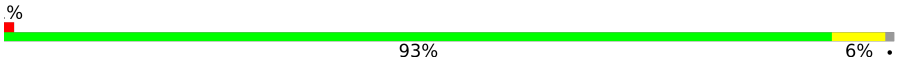
Chain D:





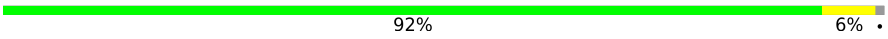
• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

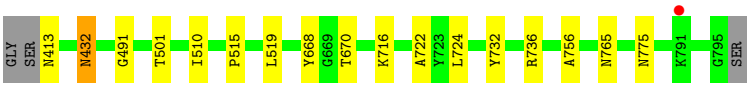
Chain E:



• Molecule 1: Glutamate receptor 2,Glutamate receptor 2

Chain F:


92%
6%


GLY
SER
N413
N432
G491
T501
I510
P515
L519
Y668
G669
T670
K716
A722
Y723
L724
Y732
R736
A756
N765
N775
K791
G795
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.60Å 162.07Å 47.10Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	40.00 – 1.50 42.03 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-1.50) 99.2 (42.03-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.208 0.184 , 0.208	Depositor DCC
R_{free} test set	13397 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14166	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.62% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACT, 8SR

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	0.47	0/2101	0.65	0/2825
1	B	0.45	0/2085	0.65	0/2803
1	C	0.50	0/2109	0.73	0/2835
1	D	0.50	0/2119	0.72	0/2847
1	E	0.47	0/2121	0.66	0/2850
1	F	0.46	0/2093	0.66	0/2814
All	All	0.47	0/12628	0.68	0/16974

There are no bond length outliers.

There are no bond angle outliers.

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	2045	0	2085	17	0
1	B	2039	0	2071	7	0
1	C	2048	0	2085	11	0
1	D	2051	0	2081	10	0
1	E	2054	0	2099	12	0
1	F	2042	0	2073	14	0
2	A	10	0	5	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	5	0	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	1	0
3	A	52	0	0	5	0
3	C	52	0	0	7	0
3	E	52	0	0	8	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	F	2	0	0	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	240	0	0	1	0
6	B	208	0	0	2	0
6	C	317	0	0	3	0
6	D	337	0	0	2	0
6	E	301	0	0	2	0
6	F	250	0	0	4	0
All	All	14166	0	12530	80	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 3.

All (80) 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:C:673:SER:HB3	6:C:2107:HOH:O	1.80	0.80
1:F:432:ASN:HD22	1:F:432:ASN:H	1.26	0.80
1:C:743:LYS:HE2	6:C:2123:HOH:O	1.90	0.69
1:A:453[B]:ILE:HD11	1:A:755:ILE:HD11	1.75	0.69
1:C:474:ARG:HH21	1:C:481:TRP:HE1	1.41	0.69
1:A:453[B]:ILE:HD13	1:A:755:ILE:HD13	1.76	0.68
1:B:432:ASN:HB2	1:B:435:MET:HE2	1.77	0.67
1:E:474:ARG:HD2	1:E:479:LYS:HD3	1.80	0.63
1:C:711:VAL:HG21	1:C:733[A]:ILE:HD13	1.80	0.63
1:F:775:ASN:ND2	6:F:1002:HOH:O	2.33	0.62
1:A:729:MET:O	1:A:733[A]:ILE:HD12	2.01	0.60
1:E:515:PRO:HG3	3:E:902[B]:8SR:S26	2.44	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:HG1	2:A:901:GLU:N	2.03	0.57
1:B:774:LEU:HD22	1:B:779:LEU:HD23	1.87	0.57
1:E:510:ILE:HD12	1:E:756:ALA:HB1	1.86	0.56
1:A:453[B]:ILE:CD1	1:A:755:ILE:CD1	2.84	0.56
1:E:775:ASN:OD1	3:E:902[A]:8SR:C10	2.53	0.56
1:C:501:THR:HG1	2:C:801:GLU:N	2.05	0.55
1:A:775:ASN:ND2	6:A:1001:HOH:O	2.39	0.55
1:A:515:PRO:HG3	3:A:902[B]:8SR:S26	2.48	0.54
1:D:501:THR:HG1	2:D:901:GLU:N	2.07	0.53
1:F:732:TYR:CZ	1:F:736:ARG:HD2	2.44	0.52
1:A:449:LEU:HG	1:A:453[B]:ILE:HD11	1.91	0.52
1:F:501:THR:HG1	2:F:901:GLU:N	2.08	0.52
1:E:452:GLU:HG3	1:E:779:LEU:HD21	1.93	0.51
1:E:501:THR:HG1	2:E:901:GLU:N	2.09	0.51
1:F:765[B]:ASN:ND2	6:F:1004:HOH:O	2.44	0.51
1:E:775:ASN:ND2	6:E:1003:HOH:O	2.43	0.50
1:A:452:GLU:HG3	1:A:779:LEU:HD21	1.93	0.50
1:A:774:LEU:HD22	1:A:779:LEU:HD23	1.93	0.50
1:D:510:ILE:HD12	1:D:756:ALA:HB1	1.93	0.49
1:B:713:ARG:HA	1:B:716:LYS:HE2	1.95	0.49
1:C:510:ILE:HD12	1:C:756:ALA:HB1	1.95	0.49
1:D:716:LYS:HE3	6:D:1251:HOH:O	2.13	0.48
1:C:711:VAL:CG2	1:C:733[A]:ILE:HD13	2.44	0.48
1:A:453[B]:ILE:CD1	1:A:755:ILE:HD11	2.42	0.48
1:A:510:ILE:HD12	1:A:756:ALA:HB1	1.96	0.48
1:D:445:TYR:CZ	1:D:517:MET:HE3	2.49	0.47
1:C:433:HIS:CD2	1:C:436:LEU:HD12	2.50	0.47
3:E:902[B]:8SR:C10	6:E:1073:HOH:O	2.63	0.47
1:A:775:ASN:OD1	3:A:902[A]:8SR:C10	2.63	0.47
1:B:491:GLY:HA2	6:B:1031:HOH:O	2.15	0.46
1:B:510:ILE:HD12	1:B:756:ALA:HB1	1.97	0.46
1:A:515:PRO:HG2	3:A:902[A]:8SR:C7	2.46	0.46
1:C:515:PRO:HG3	3:C:805[A]:8SR:S26	2.54	0.46
3:C:805[B]:8SR:S26	1:D:515:PRO:HG3	2.55	0.46
1:A:449:LEU:HG	1:A:453[B]:ILE:CD1	2.46	0.45
1:F:432:ASN:HD22	1:F:432:ASN:N	2.03	0.45
1:E:774:LEU:HD22	1:E:779:LEU:HD23	1.97	0.45
3:E:902[A]:8SR:S26	1:F:515:PRO:HG3	2.56	0.45
3:A:902[B]:8SR:C10	3:A:902[B]:8SR:N19	2.80	0.45
1:D:491:GLY:HA2	6:D:1072:HOH:O	2.15	0.45
1:F:432:ASN:H	1:F:432:ASN:ND2	2.05	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:GLY:HA2	6:C:2156:HOH:O	2.18	0.44
3:C:805[A]:8SR:S26	3:C:805[A]:8SR:O22	2.75	0.44
1:E:515:PRO:HG2	3:E:902[A]:8SR:C7	2.49	0.43
1:F:670:THR:HG22	1:F:724:LEU:HB2	2.00	0.43
3:C:805[A]:8SR:C10	3:C:805[A]:8SR:N19	2.82	0.43
1:B:668:TYR:HA	1:B:722:ALA:O	2.19	0.43
1:A:668:TYR:HA	1:A:722:ALA:O	2.19	0.43
3:C:805[B]:8SR:C10	3:C:805[B]:8SR:N19	2.82	0.43
1:F:510:ILE:HD12	1:F:756:ALA:HB1	2.01	0.43
1:D:713:ARG:O	1:D:717:SER:HB3	2.18	0.42
1:F:716:LYS:HG3	6:F:1137:HOH:O	2.19	0.42
3:A:902[A]:8SR:O22	3:A:902[A]:8SR:S26	2.77	0.42
1:E:775:ASN:C	1:E:775:ASN:HD22	2.23	0.42
1:F:491:GLY:HA2	6:F:1048:HOH:O	2.17	0.42
1:D:678:GLU:OE1	1:D:681:ARG:NH1	2.51	0.42
3:E:902[A]:8SR:S26	3:E:902[A]:8SR:O22	2.78	0.42
3:E:902[B]:8SR:C7	1:F:515:PRO:HG2	2.49	0.42
1:B:775:ASN:ND2	6:B:1004:HOH:O	2.53	0.42
1:A:453[B]:ILE:HD13	1:A:755:ILE:CD1	2.42	0.42
3:C:805[B]:8SR:C14	1:D:518[B]:SER:HG	2.33	0.41
1:C:713:ARG:O	1:C:717:SER:HB3	2.21	0.41
1:D:433:HIS:CD2	1:D:436:LEU:HD12	2.54	0.41
3:E:902[B]:8SR:C10	3:E:902[B]:8SR:N19	2.84	0.41
3:C:805[B]:8SR:S26	3:C:805[B]:8SR:O22	2.79	0.41
1:E:737:LYS:HG3	1:E:793:GLU:HB3	2.02	0.41
1:F:668:TYR:HA	1:F:722:ALA:O	2.21	0.41
1:E:497:ILE:HG12	1:E:755[B]:ILE:HD12	2.04	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	262/263 (100%)	259 (99%)	3 (1%)	0	100	100
1	B	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
1	C	263/263 (100%)	260 (99%)	3 (1%)	0	100	100
1	D	264/263 (100%)	261 (99%)	3 (1%)	0	100	100
1	E	264/263 (100%)	262 (99%)	2 (1%)	0	100	100
1	F	261/263 (99%)	259 (99%)	2 (1%)	0	100	100
All	All	1574/1578 (100%)	1559 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	223/221 (101%)	221 (99%)	2 (1%)	78	61
1	B	221/221 (100%)	219 (99%)	2 (1%)	78	61
1	C	224/221 (101%)	220 (98%)	4 (2%)	59	30
1	D	225/221 (102%)	222 (99%)	3 (1%)	69	44
1	E	225/221 (102%)	222 (99%)	3 (1%)	69	44
1	F	222/221 (100%)	219 (99%)	3 (1%)	67	42
All	All	1340/1326 (101%)	1323 (99%)	17 (1%)	69	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	519	LEU
1	A	775	ASN
1	B	519	LEU
1	B	664	THR
1	C	413	ASN
1	C	507	GLU
1	C	519	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	672	ASP
1	D	413	ASN
1	D	414	LYS
1	D	519	LEU
1	E	413	ASN
1	E	519	LEU
1	E	775	ASN
1	F	413	ASN
1	F	432	ASN
1	F	519	LEU

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

Mol	Chain	Res	Type
1	A	775	ASN
1	C	775	ASN
1	D	785	ASN
1	E	775	ASN
1	E	777	GLN
1	F	775	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)

Of 24 ligands modelled in this entry, 10 are monoatomic - leaving 14 for Mogul analysis.

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	GLU	C	801	-	8,9,9	1.00	0	10,11,11	1.25	2 (20%)
2	GLU	A	901	-	8,9,9	1.07	0	10,11,11	1.06	1 (10%)
3	8SR	A	902[A]	-	24,28,28	1.71	3 (12%)	26,42,42	1.28	2 (7%)
2	GLU	E	901	-	8,9,9	1.01	0	10,11,11	1.08	0
3	8SR	E	902[B]	-	24,28,28	1.74	5 (20%)	26,42,42	1.37	3 (11%)
5	ACT	D	904	-	3,3,3	0.78	0	3,3,3	0.65	0
5	ACT	C	804	-	3,3,3	0.80	0	3,3,3	0.58	0
3	8SR	C	805[B]	-	24,28,28	1.56	6 (25%)	26,42,42	1.46	5 (19%)
2	GLU	F	901	-	8,9,9	1.14	1 (12%)	10,11,11	1.17	0
3	8SR	E	902[A]	-	24,28,28	1.75	4 (16%)	26,42,42	1.17	3 (11%)
2	GLU	B	901	-	8,9,9	1.13	1 (12%)	10,11,11	1.10	0
2	GLU	D	901	-	8,9,9	1.02	0	10,11,11	1.22	2 (20%)
3	8SR	A	902[B]	-	24,28,28	1.70	6 (25%)	26,42,42	1.42	4 (15%)
3	8SR	C	805[A]	-	24,28,28	1.60	4 (16%)	26,42,42	1.48	3 (11%)

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	GLU	C	801	-	-	2/9/9/9	-
2	GLU	A	901	-	-	1/9/9/9	-
3	8SR	A	902[A]	-	-	0/12/25/25	0/3/3/3
2	GLU	E	901	-	-	0/9/9/9	-
3	8SR	E	902[B]	-	-	0/12/25/25	0/3/3/3
3	8SR	C	805[B]	-	-	0/12/25/25	0/3/3/3
2	GLU	F	901	-	-	1/9/9/9	-
3	8SR	E	902[A]	-	-	0/12/25/25	0/3/3/3
2	GLU	B	901	-	-	1/9/9/9	-
2	GLU	D	901	-	-	2/9/9/9	-
3	8SR	A	902[B]	-	-	1/12/25/25	0/3/3/3
3	8SR	C	805[A]	-	-	0/12/25/25	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902[A]	8SR	C11-C4	-4.51	1.47	1.50
3	E	902[A]	8SR	C11-C4	-4.47	1.47	1.50
3	A	902[B]	8SR	C2-C8	-4.32	1.43	1.51
3	E	902[B]	8SR	C2-C8	-4.25	1.43	1.51
3	C	805[B]	8SR	C2-C8	-4.16	1.43	1.51
3	A	902[A]	8SR	C2-C8	-4.09	1.43	1.51
3	E	902[A]	8SR	C2-C8	-3.97	1.44	1.51
3	C	805[A]	8SR	C2-C8	-3.91	1.44	1.51
3	A	902[B]	8SR	C11-C4	-3.70	1.48	1.50
3	E	902[B]	8SR	C11-C4	-3.69	1.48	1.50
3	E	902[B]	8SR	C10-C3	-3.59	1.45	1.51
3	C	805[A]	8SR	C11-C4	-3.48	1.48	1.50
3	E	902[A]	8SR	C10-C3	-3.46	1.46	1.51
3	A	902[B]	8SR	C10-C3	-3.03	1.46	1.51
3	A	902[A]	8SR	C10-C3	-3.00	1.46	1.51
3	C	805[A]	8SR	C10-C3	-2.93	1.46	1.51
3	C	805[B]	8SR	C10-C3	-2.91	1.46	1.51
3	C	805[B]	8SR	C11-C4	-2.69	1.48	1.50
3	C	805[A]	8SR	C16-C5	-2.38	1.47	1.50
3	A	902[B]	8SR	C8-N19	2.36	1.37	1.33
2	F	901	GLU	OXT-C	-2.33	1.22	1.30
3	C	805[B]	8SR	C16-C5	-2.29	1.47	1.50
2	B	901	GLU	OXT-C	-2.25	1.23	1.30
3	E	902[A]	8SR	C8-N19	2.16	1.37	1.33
3	E	902[B]	8SR	C1-C5	2.15	1.42	1.39
3	A	902[B]	8SR	C16-C5	-2.12	1.47	1.50
3	E	902[B]	8SR	C8-N19	2.08	1.36	1.33
3	A	902[B]	8SR	C1-C5	2.08	1.42	1.39
3	C	805[B]	8SR	C1-C5	2.04	1.42	1.39
3	C	805[B]	8SR	C2-C7	-2.02	1.37	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	805[B]	8SR	C6-N18-N17	3.98	115.01	111.93
3	A	902[B]	8SR	C6-N18-N17	3.94	114.98	111.93
3	C	805[A]	8SR	C6-N18-N17	3.91	114.96	111.93
3	E	902[B]	8SR	C6-N18-N17	3.79	114.86	111.93
3	E	902[A]	8SR	C13-C11-C4	-3.40	107.94	113.53
3	A	902[A]	8SR	C13-C11-C4	-3.32	108.07	113.53
3	A	902[B]	8SR	C13-C11-C4	-3.16	108.34	113.53
3	C	805[A]	8SR	C13-C11-C4	-3.13	108.38	113.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902[A]	8SR	C6-N18-N17	3.02	114.27	111.93
3	E	902[B]	8SR	C13-C11-C4	-3.00	108.60	113.53
3	C	805[A]	8SR	C5-N17-N18	-2.51	102.48	104.37
3	E	902[B]	8SR	C14-C6-C1	2.51	133.32	128.72
3	E	902[A]	8SR	C6-N18-N17	2.41	113.80	111.93
2	C	801	GLU	OE2-CD-CG	2.39	121.72	114.03
3	C	805[B]	8SR	C13-C11-C4	-2.39	109.61	113.53
2	D	901	GLU	OE2-CD-CG	2.26	121.28	114.03
3	C	805[B]	8SR	C5-N17-N18	-2.25	102.68	104.37
3	C	805[B]	8SR	O21-C8-N19	2.23	125.74	122.58
3	A	902[B]	8SR	O21-C8-N19	2.22	125.73	122.58
2	D	901	GLU	OE1-CD-CG	-2.20	116.02	123.08
3	C	805[B]	8SR	C2-C8-N19	-2.19	111.93	116.87
2	C	801	GLU	OE1-CD-CG	-2.18	116.06	123.08
3	A	902[B]	8SR	C14-C6-C1	2.16	132.69	128.72
2	A	901	GLU	OE2-CD-CG	2.04	120.57	114.03
3	E	902[A]	8SR	O21-C8-C2	2.01	122.92	120.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GLU	O-C-CA-N
2	C	801	GLU	O-C-CA-N
2	D	901	GLU	O-C-CA-N
3	A	902[B]	8SR	O22-C9-N20-C7
2	B	901	GLU	OXT-C-CA-CB
2	D	901	GLU	OE2-CD-CG-CB
2	F	901	GLU	OE2-CD-CG-CB
2	C	801	GLU	OE2-CD-CG-CB

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	GLU	1	0
2	A	901	GLU	1	0
3	A	902[A]	8SR	3	0
2	E	901	GLU	1	0
3	E	902[B]	8SR	4	0
3	C	805[B]	8SR	4	0

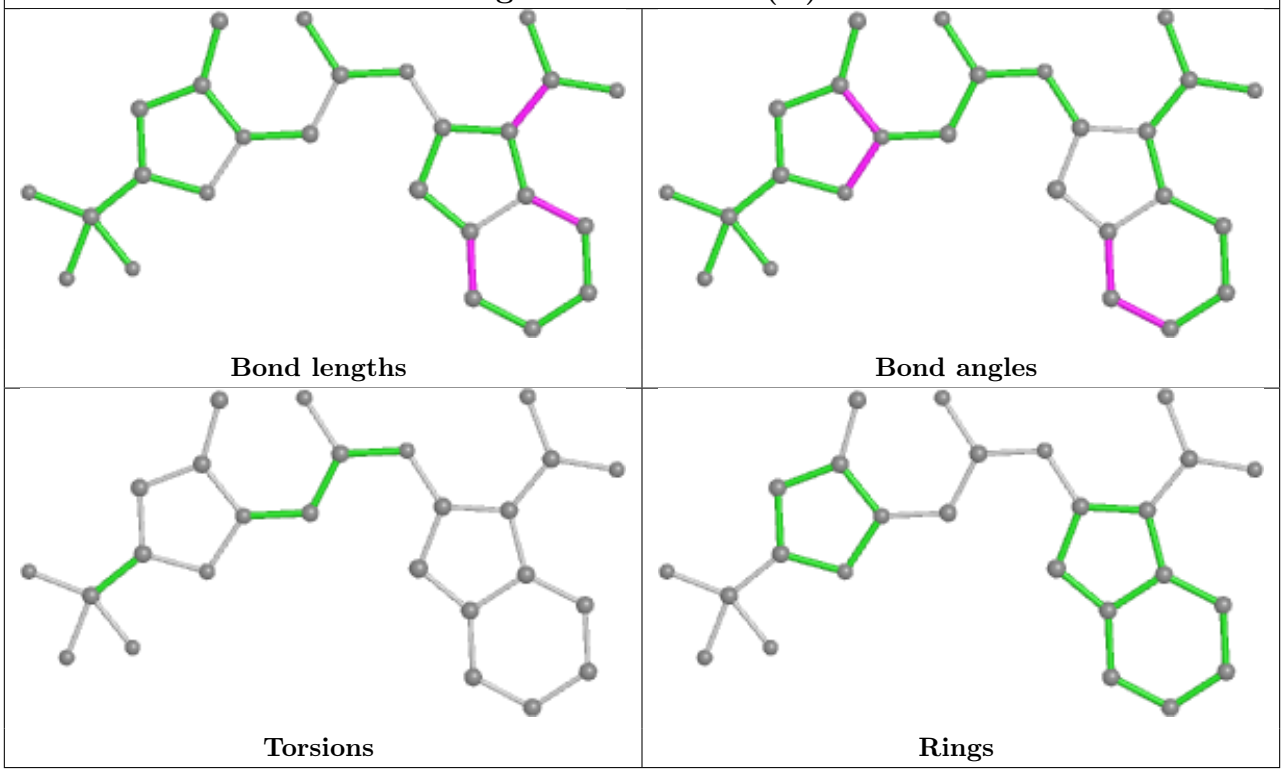
Continued on next page...

Continued from previous page...

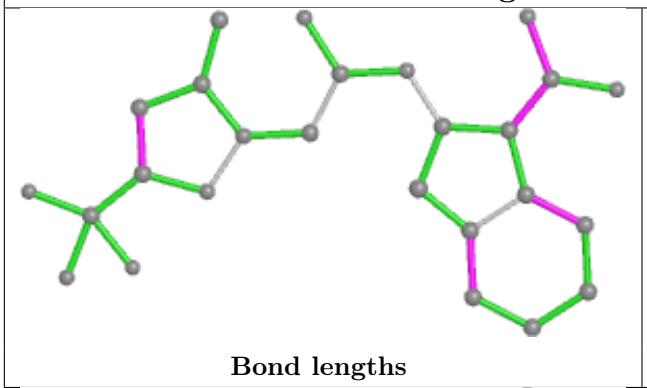
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	GLU	1	0
3	E	902[A]	8SR	4	0
2	D	901	GLU	1	0
3	A	902[B]	8SR	2	0
3	C	805[A]	8SR	3	0

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 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.

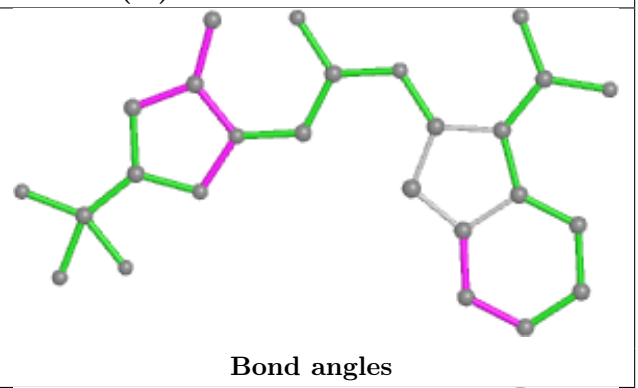
Ligand 8SR A 902 (A)



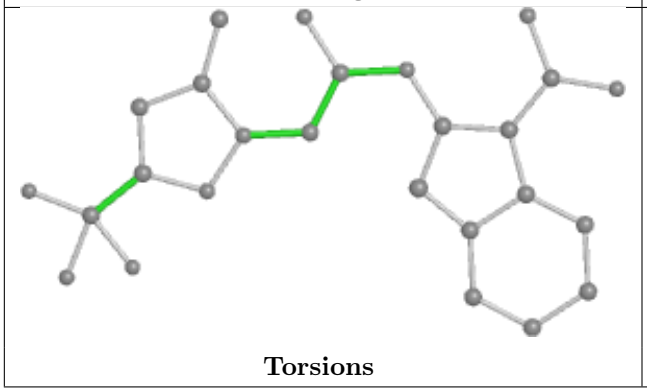
Ligand 8SR E 902 (B)



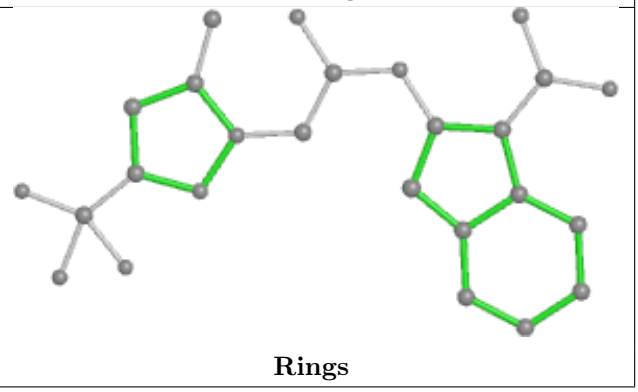
Bond lengths



Bond angles

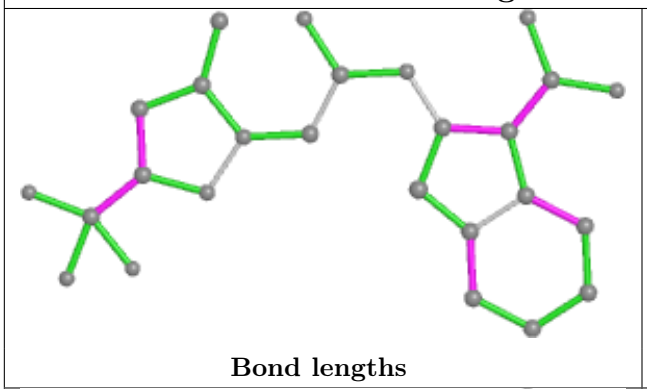


Torsions

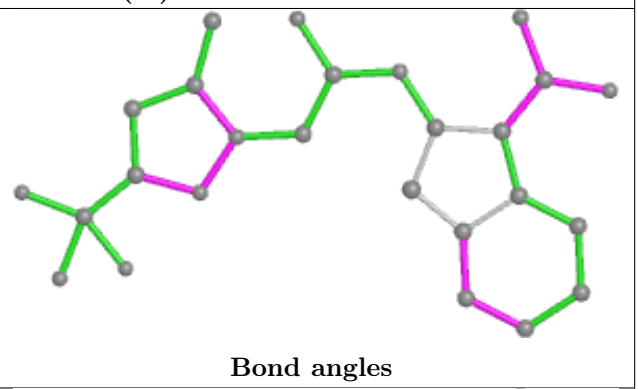


Rings

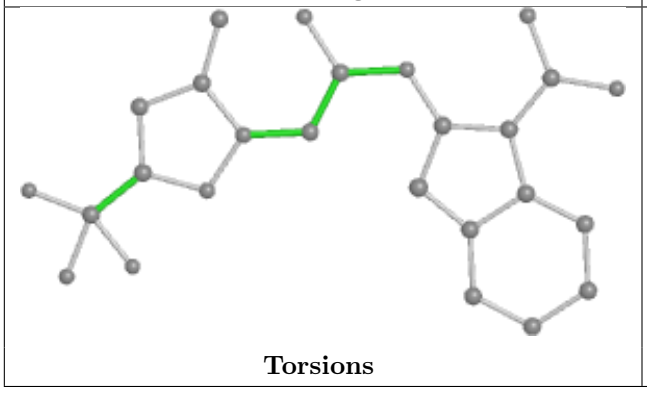
Ligand 8SR C 805 (B)



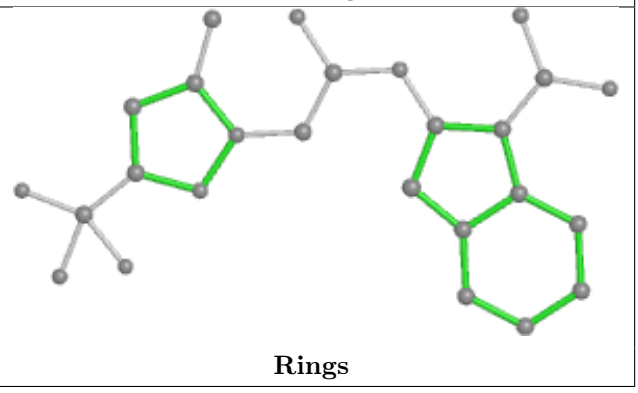
Bond lengths



Bond angles

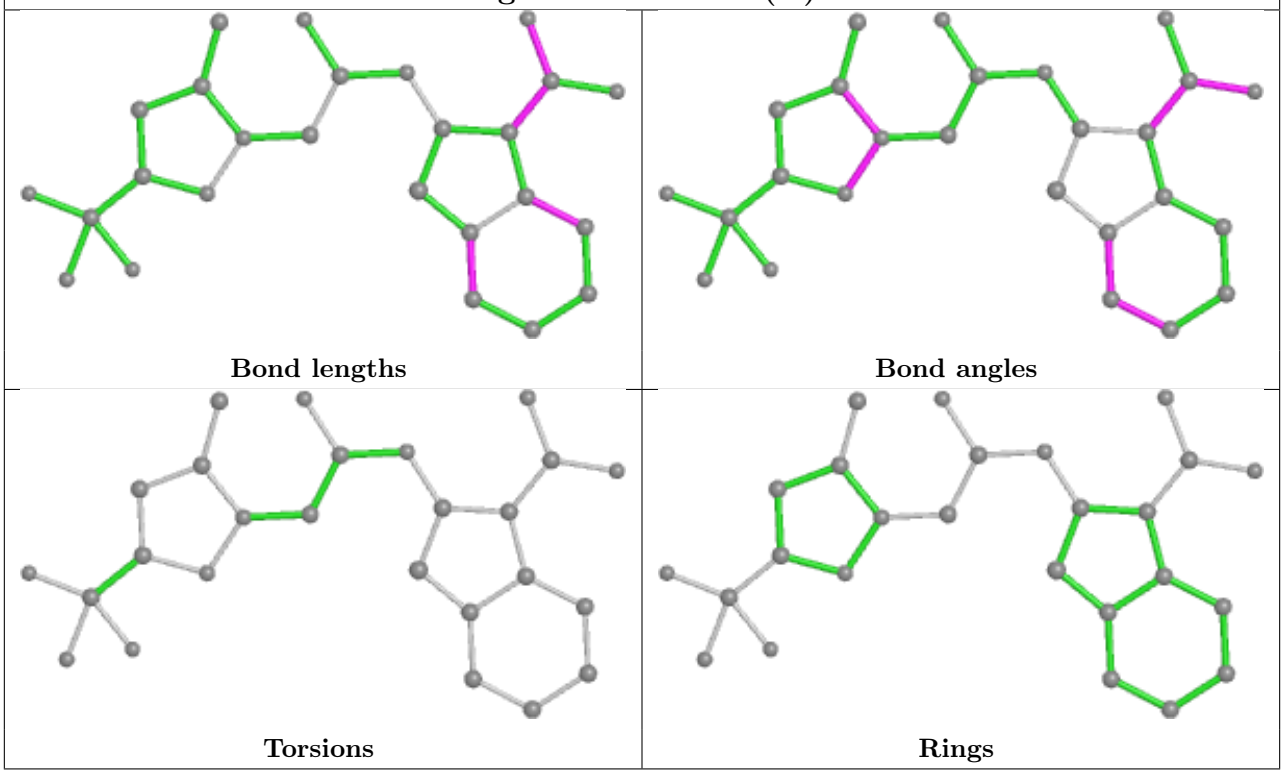


Torsions

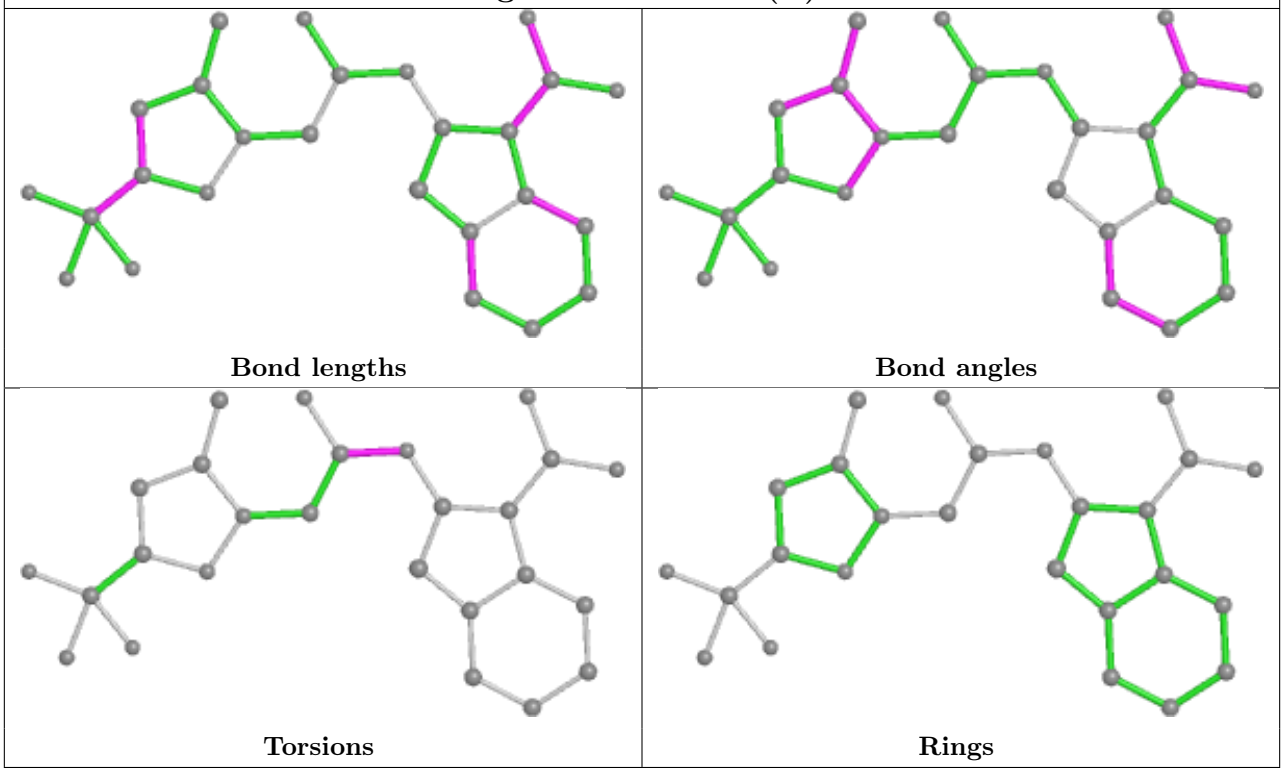


Rings

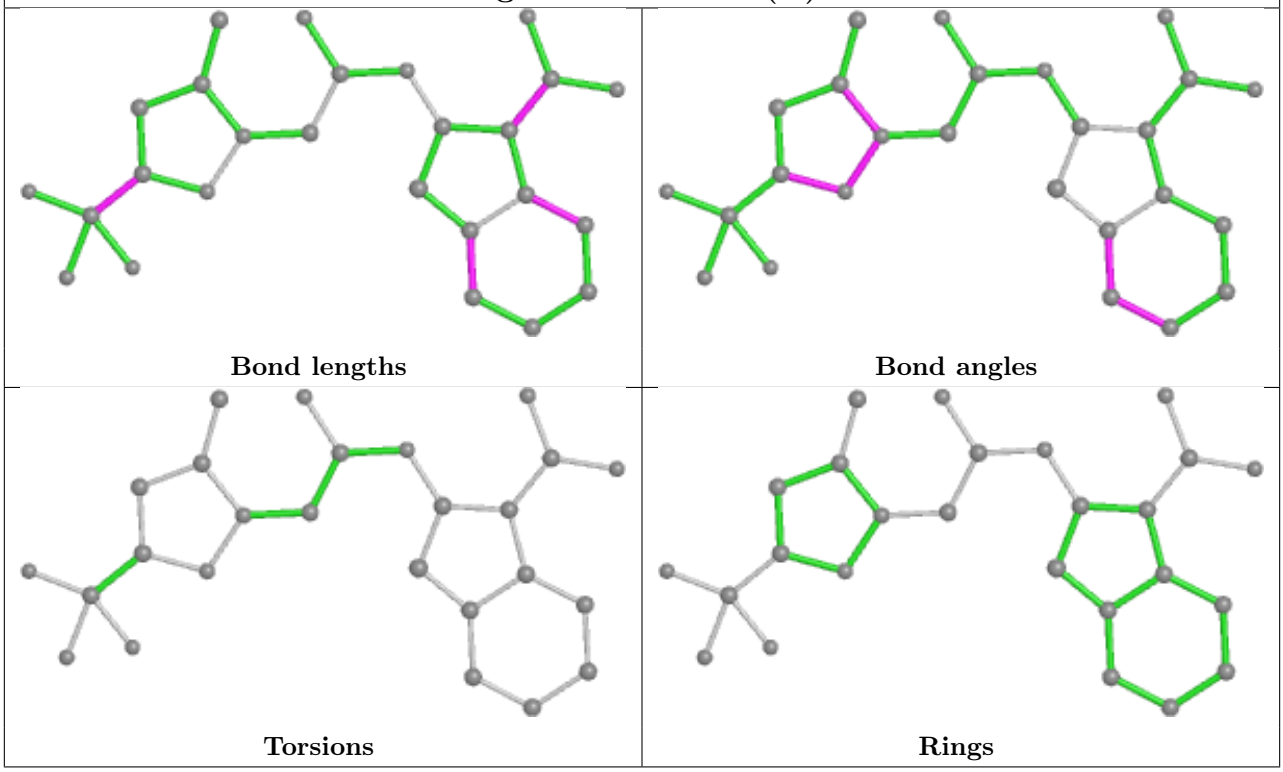
Ligand 8SR E 902 (A)



Ligand 8SR A 902 (B)



Ligand 8SR C 805 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/263 (98%)	-0.05	4 (1%)	73	78	13, 22, 41, 59	0
1	B	260/263 (98%)	0.20	19 (7%)	15	16	14, 25, 48, 69	0
1	C	260/263 (98%)	-0.22	5 (1%)	66	71	11, 18, 37, 62	0
1	D	260/263 (98%)	-0.16	4 (1%)	73	78	11, 18, 38, 62	0
1	E	260/263 (98%)	-0.06	3 (1%)	79	82	12, 21, 39, 58	0
1	F	260/263 (98%)	0.05	1 (0%)	92	94	14, 23, 46, 62	0
All	All	1560/1578 (98%)	-0.04	36 (2%)	60	65	11, 21, 42, 69	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	791	LYS	6.7
1	B	792	GLY	6.6
1	C	791	LYS	5.8
1	B	794	CYS	5.0
1	B	789	TYR	4.6
1	B	795	GLY	4.1
1	B	791	LYS	3.8
1	D	477	ASP	3.2
1	B	793	GLU	3.1
1	E	794	CYS	3.1
1	B	790	ASP	3.1
1	B	680	PHE	3.0
1	D	795	GLY	3.0
1	B	687	VAL	2.9
1	C	436	LEU	2.8
1	A	413	ASN	2.8
1	F	791	LYS	2.7
1	B	665	GLU	2.6
1	A	477	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	435	MET	2.6
1	A	672	ASP	2.6
1	B	666	ILE	2.6
1	E	795	GLY	2.5
1	B	692	TRP	2.4
1	B	682	ARG	2.4
1	B	413	ASN	2.4
1	E	672	ASP	2.4
1	B	685	ILE	2.3
1	C	795	GLY	2.3
1	B	688	PHE	2.2
1	B	435	MET	2.2
1	B	744	VAL	2.2
1	D	436	LEU	2.1
1	A	664	THR	2.1
1	B	700	PRO	2.0
1	C	789	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	C	804	4/4	0.82	0.16	24,27,31,36	0
5	ACT	D	904	4/4	0.83	0.14	25,26,31,36	0
4	ZN	B	903	1/1	0.94	0.08	42,42,42,42	0
4	ZN	F	903	1/1	0.94	0.04	41,41,41,41	0
3	8SR	A	902[A]	26/26	0.95	0.11	14,16,21,25	26
3	8SR	A	902[B]	26/26	0.95	0.11	16,18,23,24	26

Continued on next page...

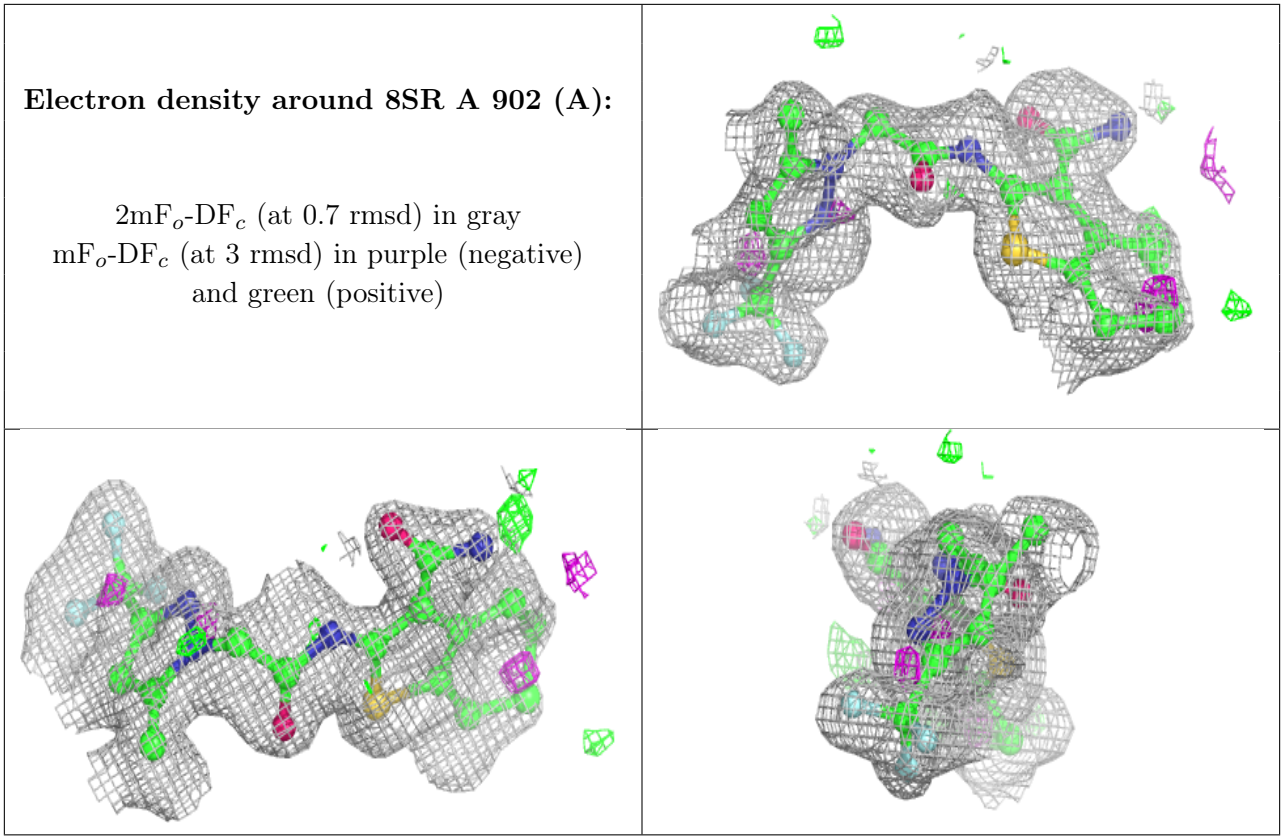
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLU	B	901	10/10	0.96	0.06	15,16,19,19	0
4	ZN	B	902	1/1	0.96	0.04	24,24,24,24	0
2	GLU	A	901	10/10	0.96	0.07	14,15,17,18	0
3	8SR	E	902[B]	26/26	0.97	0.10	15,17,23,24	26
2	GLU	E	901	10/10	0.97	0.07	13,15,16,17	0
2	GLU	F	901	10/10	0.97	0.07	14,15,17,18	0
3	8SR	C	805[A]	26/26	0.97	0.09	11,14,18,22	26
3	8SR	C	805[B]	26/26	0.97	0.09	11,13,18,22	26
3	8SR	E	902[A]	26/26	0.97	0.10	14,15,20,23	26
4	ZN	C	803	1/1	0.98	0.04	20,20,20,20	0
4	ZN	F	902	1/1	0.98	0.04	24,24,24,24	0
4	ZN	A	903	1/1	0.98	0.05	18,18,18,18	0
2	GLU	C	801	10/10	0.98	0.06	11,12,13,14	0
2	GLU	D	901	10/10	0.98	0.06	11,12,13,13	0
4	ZN	C	802	1/1	0.99	0.05	21,21,21,21	0
4	ZN	D	902	1/1	0.99	0.03	22,22,22,22	0
4	ZN	D	903	1/1	0.99	0.05	20,20,20,20	0
4	ZN	D	905	1/1	0.99	0.05	18,18,18,18	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.

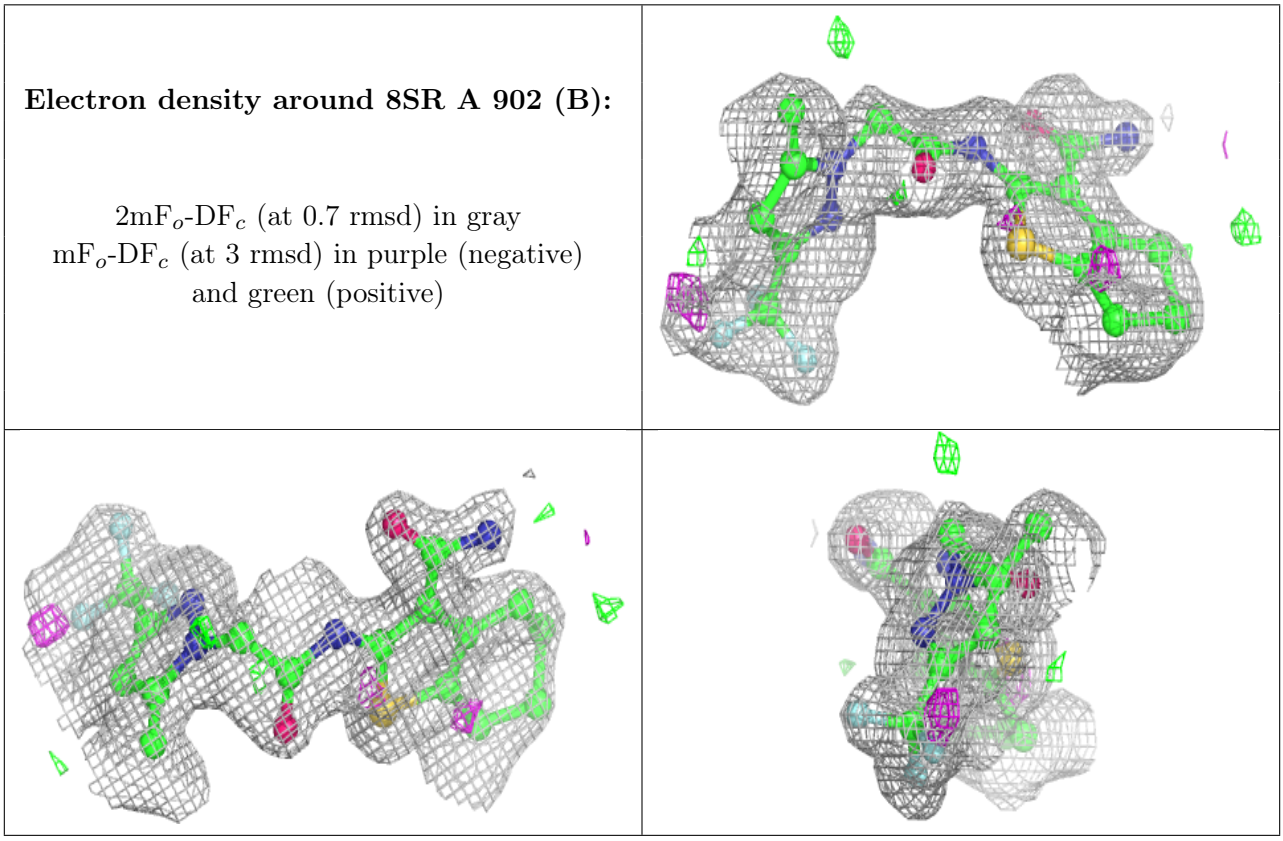
Electron density around 8SR A 902 (A):

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



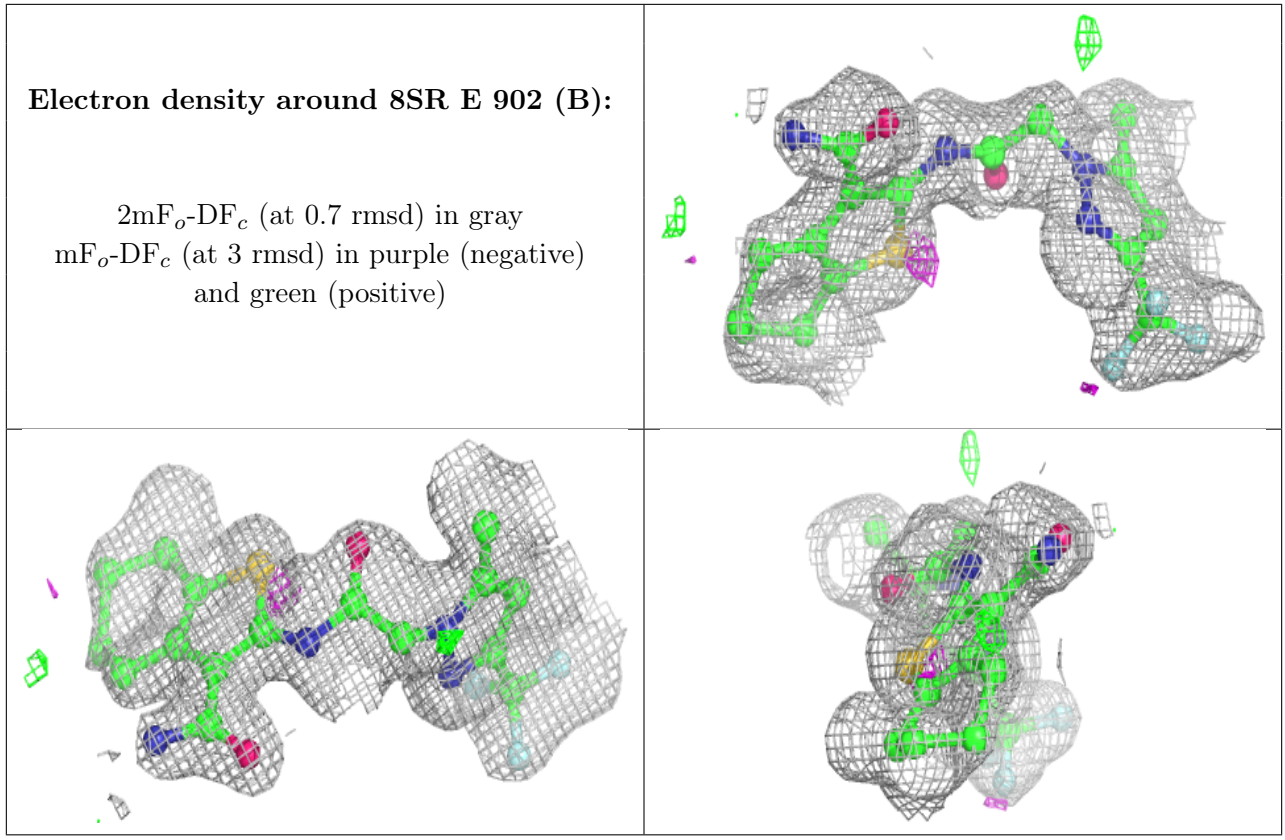
Electron density around 8SR A 902 (B):

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



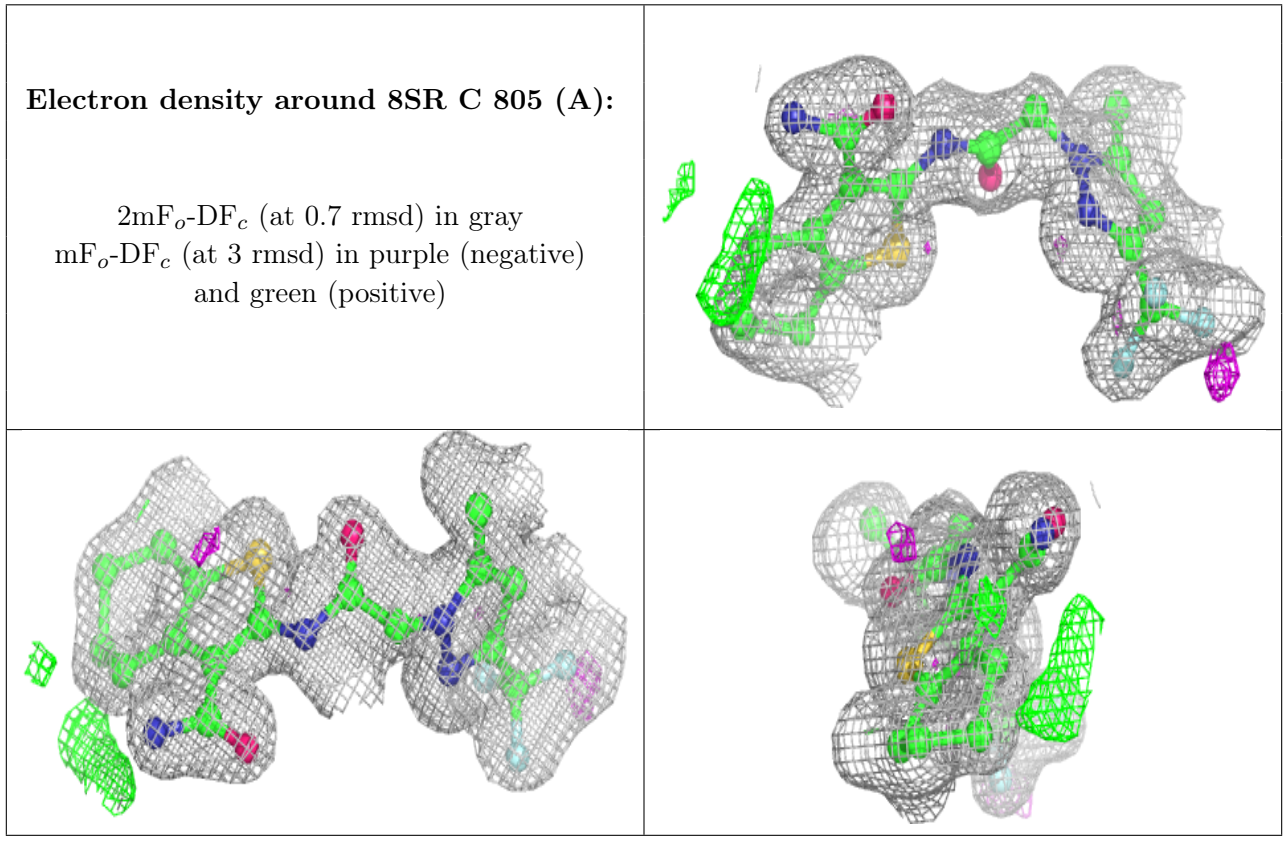
Electron density around 8SR E 902 (B):

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



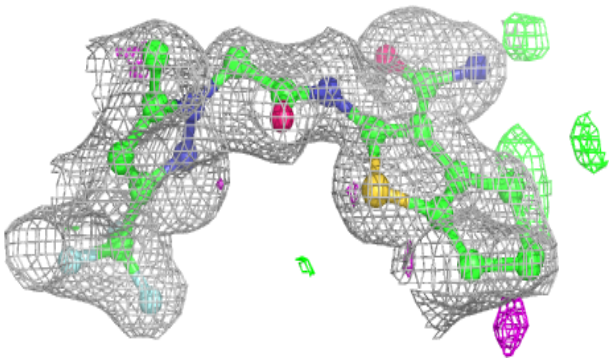
Electron density around 8SR C 805 (A):

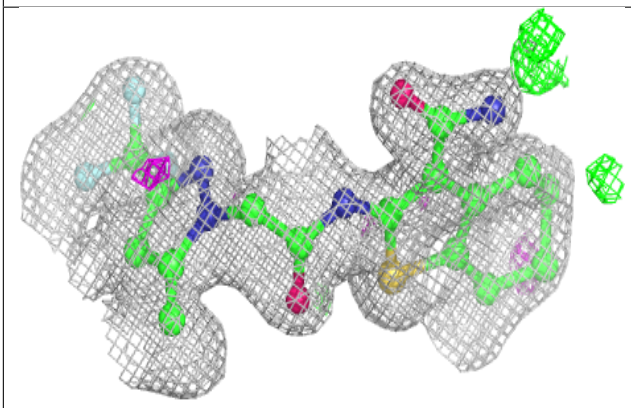
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

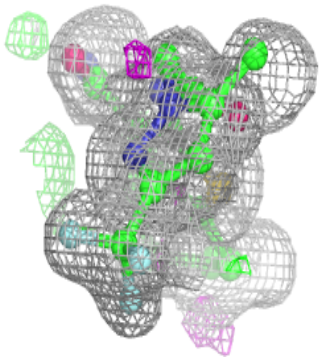


Electron density around 8SR C 805 (B):

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

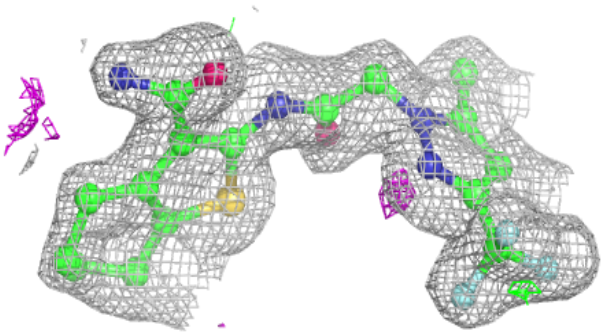


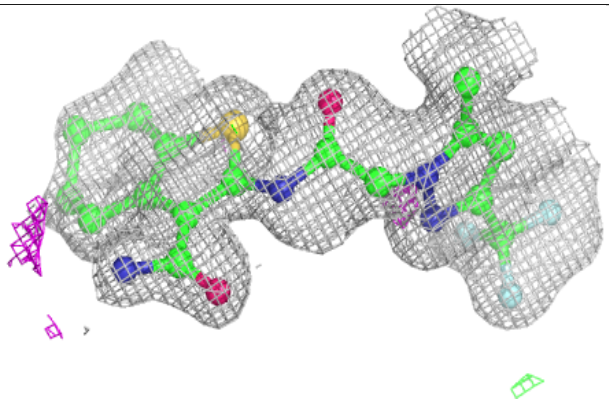


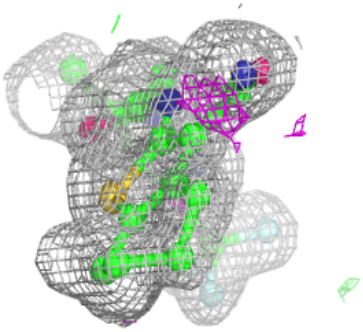


Electron density around 8SR E 902 (A):

$2mF_o$-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.