



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2025 – 12:44 PM EDT

PDB ID : 9DT5 / pdb_00009dt5
Title : Crystal structure of the engineered sulfonyleurea repressor CsR (L4.2-20), bound to chlorsulfuron
Authors : Schreiter, E.R.; Leija, C.; Kakani, N.K.; McBride, K.E.; Looger, L.L.
Deposited on : 2024-09-30
Resolution : 2.00 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

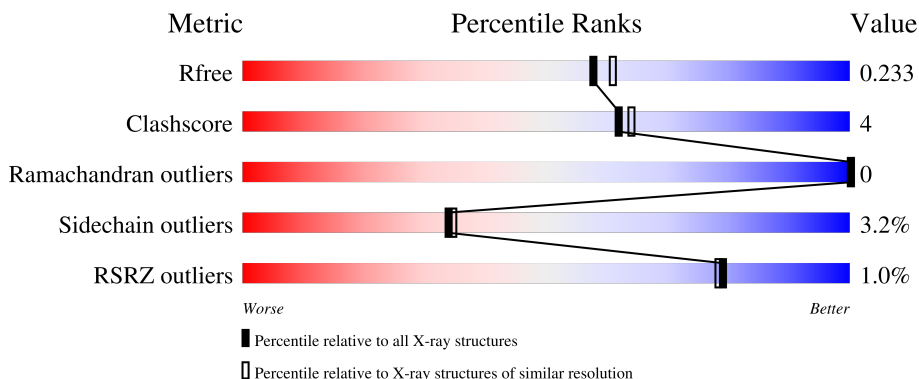
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	207	<div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	B	207	<div> <div>90%</div> <div>6%</div> <div>• •</div> </div>
1	C	207	<div> <div>2%</div> <div>86%</div> <div>7%</div> <div>• •</div> </div>
1	D	207	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6990 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 Sulfonylurea repressor CsR (L4.2-20).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	1	0
			1618	1030	282	302	4			
1	B	203	Total	C	N	O	S	0	0	0
			1631	1036	287	304	4			
1	C	200	Total	C	N	O	S	0	0	0
			1605	1022	281	298	4			
1	D	202	Total	C	N	O	S	0	0	0
			1621	1031	286	300	4			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP P04483
A	60	HIS	LEU	conflict	UNP P04483
A	64	GLN	HIS	conflict	UNP P04483
A	67	TYR	PHE	conflict	UNP P04483
A	68	LEU	CYS	conflict	UNP P04483
A	82	PHE	ASN	conflict	UNP P04483
A	86	MET	PHE	conflict	UNP P04483
A	88	LEU	CYS	conflict	UNP P04483
A	100	SER	HIS	conflict	UNP P04483
A	105	TRP	PRO	conflict	UNP P04483
A	108	GLN	LYS	conflict	UNP P04483
A	113	ALA	LEU	conflict	UNP P04483
A	116	MET	GLN	conflict	UNP P04483
A	121	THR	CYS	conflict	UNP P04483
A	134	THR	LEU	conflict	UNP P04483
A	135	ASP	SER	conflict	UNP P04483
A	138	ARG	GLY	conflict	UNP P04483
A	139	VAL	HIS	conflict	UNP P04483
A	144	ALA	CYS	conflict	UNP P04483
A	147	LEU	GLU	conflict	UNP P04483
A	151	GLN	HIS	conflict	UNP P04483

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	PRO	THR	conflict	UNP P04483
A	174	TRP	ILE	conflict	UNP P04483
A	177	LYS	PHE	conflict	UNP P04483
A	178	VAL	ASP	conflict	UNP P04483
A	195	ALA	CYS	conflict	UNP P04483
A	203	ARG	CYS	conflict	UNP P04483
B	2	ALA	SER	conflict	UNP P04483
B	60	HIS	LEU	conflict	UNP P04483
B	64	GLN	HIS	conflict	UNP P04483
B	67	TYR	PHE	conflict	UNP P04483
B	68	LEU	CYS	conflict	UNP P04483
B	82	PHE	ASN	conflict	UNP P04483
B	86	MET	PHE	conflict	UNP P04483
B	88	LEU	CYS	conflict	UNP P04483
B	100	SER	HIS	conflict	UNP P04483
B	105	TRP	PRO	conflict	UNP P04483
B	108	GLN	LYS	conflict	UNP P04483
B	113	ALA	LEU	conflict	UNP P04483
B	116	MET	GLN	conflict	UNP P04483
B	121	THR	CYS	conflict	UNP P04483
B	134	THR	LEU	conflict	UNP P04483
B	135	ASP	SER	conflict	UNP P04483
B	138	ARG	GLY	conflict	UNP P04483
B	139	VAL	HIS	conflict	UNP P04483
B	144	ALA	CYS	conflict	UNP P04483
B	147	LEU	GLU	conflict	UNP P04483
B	151	GLN	HIS	conflict	UNP P04483
B	163	PRO	THR	conflict	UNP P04483
B	174	TRP	ILE	conflict	UNP P04483
B	177	LYS	PHE	conflict	UNP P04483
B	178	VAL	ASP	conflict	UNP P04483
B	195	ALA	CYS	conflict	UNP P04483
B	203	ARG	CYS	conflict	UNP P04483
C	2	ALA	SER	conflict	UNP P04483
C	60	HIS	LEU	conflict	UNP P04483
C	64	GLN	HIS	conflict	UNP P04483
C	67	TYR	PHE	conflict	UNP P04483
C	68	LEU	CYS	conflict	UNP P04483
C	82	PHE	ASN	conflict	UNP P04483
C	86	MET	PHE	conflict	UNP P04483
C	88	LEU	CYS	conflict	UNP P04483
C	100	SER	HIS	conflict	UNP P04483

Continued on next page...

Continued from previous page...

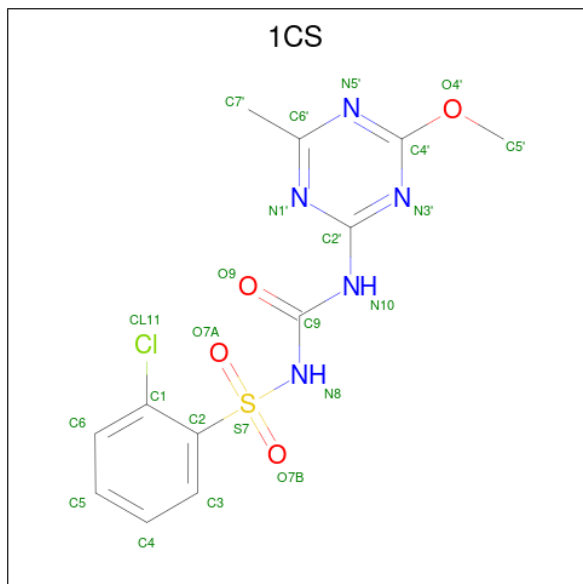
Chain	Residue	Modelled	Actual	Comment	Reference
C	105	TRP	PRO	conflict	UNP P04483
C	108	GLN	LYS	conflict	UNP P04483
C	113	ALA	LEU	conflict	UNP P04483
C	116	MET	GLN	conflict	UNP P04483
C	121	THR	CYS	conflict	UNP P04483
C	134	THR	LEU	conflict	UNP P04483
C	135	ASP	SER	conflict	UNP P04483
C	138	ARG	GLY	conflict	UNP P04483
C	139	VAL	HIS	conflict	UNP P04483
C	144	ALA	CYS	conflict	UNP P04483
C	147	LEU	GLU	conflict	UNP P04483
C	151	GLN	HIS	conflict	UNP P04483
C	163	PRO	THR	conflict	UNP P04483
C	174	TRP	ILE	conflict	UNP P04483
C	177	LYS	PHE	conflict	UNP P04483
C	178	VAL	ASP	conflict	UNP P04483
C	195	ALA	CYS	conflict	UNP P04483
C	203	ARG	CYS	conflict	UNP P04483
D	2	ALA	SER	conflict	UNP P04483
D	60	HIS	LEU	conflict	UNP P04483
D	64	GLN	HIS	conflict	UNP P04483
D	67	TYR	PHE	conflict	UNP P04483
D	68	LEU	CYS	conflict	UNP P04483
D	82	PHE	ASN	conflict	UNP P04483
D	86	MET	PHE	conflict	UNP P04483
D	88	LEU	CYS	conflict	UNP P04483
D	100	SER	HIS	conflict	UNP P04483
D	105	TRP	PRO	conflict	UNP P04483
D	108	GLN	LYS	conflict	UNP P04483
D	113	ALA	LEU	conflict	UNP P04483
D	116	MET	GLN	conflict	UNP P04483
D	121	THR	CYS	conflict	UNP P04483
D	134	THR	LEU	conflict	UNP P04483
D	135	ASP	SER	conflict	UNP P04483
D	138	ARG	GLY	conflict	UNP P04483
D	139	VAL	HIS	conflict	UNP P04483
D	144	ALA	CYS	conflict	UNP P04483
D	147	LEU	GLU	conflict	UNP P04483
D	151	GLN	HIS	conflict	UNP P04483
D	163	PRO	THR	conflict	UNP P04483
D	174	TRP	ILE	conflict	UNP P04483
D	177	LYS	PHE	conflict	UNP P04483

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	178	VAL	ASP	conflict	UNP P04483
D	195	ALA	CYS	conflict	UNP P04483
D	203	ARG	CYS	conflict	UNP P04483

- Molecule 2 is 1-(2-CHLOROPHENYLSULFONYL)-3-(4-METHOXY-6-METHYL-L,3,5-TRIAZIN-2-YL)UREA (CCD ID: 1CS) (formula: $C_{12}H_{12}ClN_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0
2	B	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0
2	C	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0
2	D	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	126	Total	O	0	0
			126	126		
3	C	104	Total	O	0	0
			104	104		

Continued on next page...

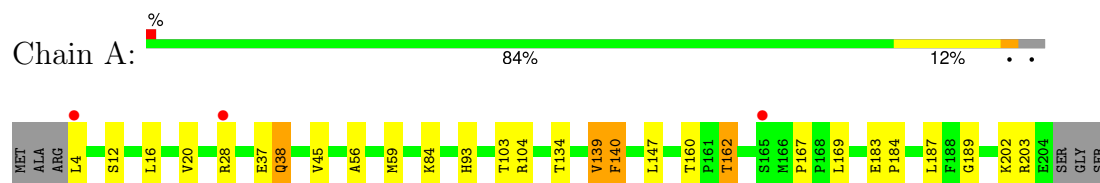
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	106	Total 106	O 106	0	0

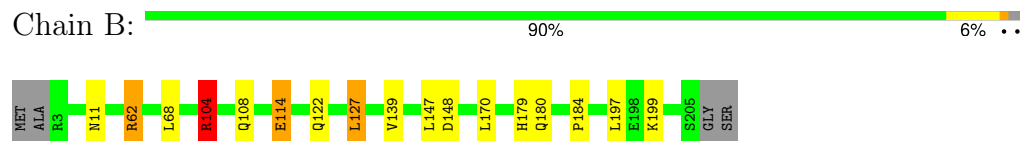
3 Residue-property plots

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.

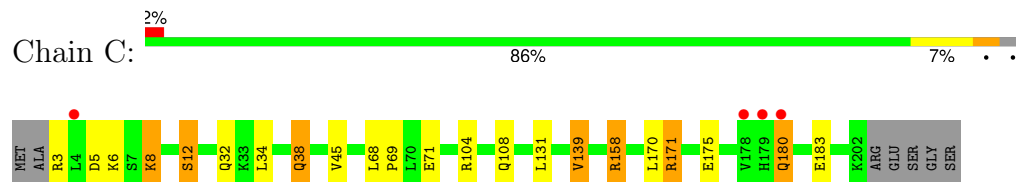
- Molecule 1: Sulfonyleurea repressor CsR (L4.2-20)



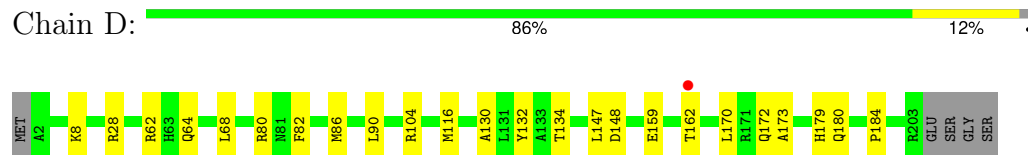
- Molecule 1: Sulfonyleurea repressor CsR (L4.2-20)



- Molecule 1: Sulfonyleurea repressor CsR (L4.2-20)



- Molecule 1: Sulfonyleurea repressor CsR (L4.2-20)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.01Å 109.09Å 129.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.00) 99.6 (19.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.178 , 0.228 0.186 , 0.233	Depositor DCC
R_{free} test set	3048 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.9	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	0.95	EDS
Total number of atoms	6990	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: 1CS

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	0.58	0/1652	1.09	4/2235 (0.2%)
1	B	0.61	0/1662	1.14	4/2247 (0.2%)
1	C	0.59	0/1636	1.08	4/2213 (0.2%)
1	D	0.60	0/1652	1.09	4/2234 (0.2%)
All	All	0.60	0/6602	1.10	16/8929 (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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	GLU	CB-CA-C	-7.51	98.80	110.81
1	B	62	ARG	CB-CA-C	-6.92	99.31	110.79
1	B	148	ASP	CA-CB-CG	6.44	119.04	112.60
1	D	148	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	45	VAL	N-CA-CB	-6.08	104.32	112.10
1	A	139	VAL	N-CA-CB	6.05	119.65	110.58
1	D	80	ARG	N-CA-CB	5.90	118.79	110.12
1	D	172	GLN	N-CA-CB	5.43	118.11	110.12
1	C	5	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	140	PHE	CA-CB-CG	-5.35	108.45	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	HIS	CA-CB-CG	-5.29	108.51	113.80
1	C	139	VAL	N-CA-CB	5.20	118.37	110.58
1	D	62	ARG	CB-CA-C	5.19	120.63	110.67
1	A	162	THR	CB-CA-C	5.18	115.30	110.17
1	C	158	ARG	N-CA-CB	-5.17	101.91	111.52
1	C	71	GLU	CB-CA-C	-5.02	103.63	109.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	ARG	Sidechain
1	C	3	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	1618	0	1631	15	0
1	B	1631	0	1642	11	0
1	C	1605	0	1618	17	0
1	D	1621	0	1636	18	0
2	A	23	0	12	2	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	1	0
3	A	87	0	0	0	0
3	B	126	0	0	1	0
3	C	104	0	0	3	0
3	D	106	0	0	6	0
All	All	6990	0	6575	53	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 4.

All (53) 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:179:HIS:HB2	3:D:460:HOH:O	1.79	0.82
1:D:68:LEU:HD23	3:D:443:HOH:O	1.80	0.79
1:A:167:PRO:HG2	1:B:114:GLU:HG2	1.66	0.76
1:D:82:PHE:CZ	1:D:86:MET:CE	2.69	0.75
1:C:171:ARG:CG	1:C:171:ARG:HH11	2.01	0.74
1:D:64:GLN:OE1	3:D:401:HOH:O	2.11	0.68
1:C:32:GLN:HB3	3:C:460:HOH:O	1.96	0.66
1:B:11:ASN:OD1	1:B:62:ARG:NH2	2.35	0.59
1:B:108:GLN:HG3	1:B:108:GLN:O	2.02	0.59
1:B:104:ARG:N	1:B:104:ARG:HD3	2.22	0.55
1:D:68:LEU:CD2	3:D:443:HOH:O	2.49	0.55
1:B:68:LEU:HD23	3:B:468:HOH:O	2.06	0.54
1:C:171:ARG:HH11	1:C:171:ARG:HG2	1.74	0.52
1:D:8:LYS:HD2	3:D:453:HOH:O	2.10	0.52
1:D:180:GLN:HB3	1:D:184:PRO:HG2	1.92	0.52
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.92	0.51
1:C:171:ARG:HH11	1:C:171:ARG:HG3	1.76	0.51
1:D:28:ARG:NH1	3:D:406:HOH:O	2.44	0.50
1:A:84:LYS:HE2	1:A:187:LEU:HD21	1.93	0.50
1:C:170:LEU:HG	2:D:301:1CS:H6	1.94	0.50
1:C:139:VAL:HG12	1:D:147:LEU:HD22	1.94	0.50
1:A:134[A]:THR:HG22	2:A:301:1CS:H5'1	1.94	0.49
1:D:82:PHE:CZ	1:D:86:MET:HE1	2.46	0.49
1:C:8:LYS:HE2	1:C:8:LYS:HA	1.95	0.49
1:C:180:GLN:HG2	1:D:132:TYR:OH	2.13	0.48
1:A:169:LEU:HD22	1:B:127:LEU:HD13	1.95	0.48
1:D:162:THR:O	1:D:162:THR:OG1	2.31	0.48
1:A:56:ALA:CB	1:A:103:THR:HG21	2.45	0.47
1:C:158:ARG:HD3	1:D:104:ARG:CZ	2.44	0.47
2:C:301:1CS:H6	1:D:170:LEU:HG	1.97	0.47
1:D:130:ALA:O	1:D:134:THR:HG23	2.15	0.47
1:A:28:ARG:CZ	1:A:28:ARG:HB3	2.46	0.45
1:C:12:SER:OG	1:C:34:LEU:HD21	2.17	0.44
1:B:180:GLN:HB3	1:B:184:PRO:HG2	2.00	0.44
1:A:139:VAL:HG12	1:B:147:LEU:HD22	1.99	0.43
1:A:140:PHE:CZ	1:A:189:GLY:HA3	2.53	0.43
1:C:8:LYS:HA	1:C:8:LYS:CE	2.48	0.43
1:C:68:LEU:HA	1:C:69:PRO:HD3	1.91	0.43
1:C:131:LEU:HD13	1:D:173:ALA:HB1	2.00	0.43
1:C:8:LYS:O	1:C:12:SER:OG	2.35	0.43
1:C:38:GLN:HG3	3:C:441:HOH:O	2.19	0.42
1:D:82:PHE:CZ	1:D:86:MET:HE2	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HG3	3:C:481:HOH:O	2.19	0.42
1:A:147:LEU:HD22	1:B:139:VAL:HG22	2.02	0.42
1:A:59:MET:HG2	1:A:93:HIS:CD2	2.54	0.42
1:D:86:MET:O	1:D:90:LEU:HG	2.20	0.41
1:A:202:LYS:O	1:A:203:ARG:C	2.63	0.41
1:C:171:ARG:O	1:C:175:GLU:HG2	2.20	0.41
1:A:37:GLU:O	1:A:38:GLN:C	2.64	0.40
1:A:84:LYS:HE2	1:A:187:LEU:CD2	2.50	0.40
1:A:16:LEU:O	1:A:20:VAL:HG22	2.21	0.40
2:A:301:1CS:H6	1:B:170:LEU:HG	2.04	0.40
1:B:104:ARG:HD3	1:B:104:ARG:H	1.85	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	200/207 (97%)	200 (100%)	0	0	100	100
1	B	201/207 (97%)	201 (100%)	0	0	100	100
1	C	198/207 (96%)	197 (100%)	1 (0%)	0	100	100
1	D	200/207 (97%)	200 (100%)	0	0	100	100
All	All	799/828 (96%)	798 (100%)	1 (0%)	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	172/175 (98%)	166 (96%)	6 (4%)	31	31
1	B	173/175 (99%)	168 (97%)	5 (3%)	37	39
1	C	170/175 (97%)	161 (95%)	9 (5%)	19	16
1	D	171/175 (98%)	169 (99%)	2 (1%)	67	73
All	All	686/700 (98%)	664 (97%)	22 (3%)	34	35

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	12	SER
1	A	38	GLN
1	A	104	ARG
1	A	160	THR
1	A	162	THR
1	B	104	ARG
1	B	122	GLN
1	B	127	LEU
1	B	197	LEU
1	B	199	LYS
1	C	6	LYS
1	C	8	LYS
1	C	12	SER
1	C	38	GLN
1	C	45	VAL
1	C	104	ARG
1	C	171	ARG
1	C	180	GLN
1	C	183	GLU
1	D	116	MET
1	D	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	129	ASN
1	A	149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	GLN
1	B	122	GLN
1	B	123	GLN
1	C	32	GLN
1	C	44	HIS
1	C	122	GLN
1	C	179	HIS
1	D	32	GLN
1	D	38	GLN
1	D	172	GLN
1	D	179	HIS

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](#)

4 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	1CS	C	301	-	24,24,24	2.14	5 (20%)	34,34,34	3.24	13 (38%)
2	1CS	A	301	-	24,24,24	1.70	5 (20%)	34,34,34	3.27	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1CS	B	301	-	24,24,24	2.12	3 (12%)	34,34,34	3.18	16 (47%)
2	1CS	D	301	-	24,24,24	2.07	4 (16%)	34,34,34	3.03	15 (44%)

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	1CS	C	301	-	-	1/17/17/17	0/2/2/2
2	1CS	A	301	-	-	1/17/17/17	0/2/2/2
2	1CS	B	301	-	-	1/17/17/17	0/2/2/2
2	1CS	D	301	-	-	1/17/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	1CS	O7B-S7	7.63	1.52	1.43
2	B	301	1CS	O7A-S7	6.86	1.51	1.43
2	D	301	1CS	O7A-S7	5.65	1.50	1.43
2	B	301	1CS	O7B-S7	5.27	1.49	1.43
2	D	301	1CS	O7B-S7	4.82	1.49	1.43
2	A	301	1CS	C2'-N10	-4.72	1.32	1.38
2	D	301	1CS	C2'-N10	-4.61	1.32	1.38
2	B	301	1CS	C2'-N10	-4.36	1.33	1.38
2	C	301	1CS	C2'-N10	-4.24	1.33	1.38
2	A	301	1CS	C2-S7	2.97	1.81	1.77
2	A	301	1CS	C9-N8	-2.83	1.33	1.39
2	D	301	1CS	C9-N8	-2.78	1.33	1.39
2	C	301	1CS	C9-N10	-2.63	1.31	1.37
2	A	301	1CS	C1-C2	-2.54	1.37	1.40
2	C	301	1CS	C9-N8	-2.21	1.34	1.39
2	A	301	1CS	C3-C2	-2.20	1.36	1.39
2	C	301	1CS	O7A-S7	2.09	1.46	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	1CS	C4'-N3'-C2'	10.48	121.41	112.86
2	D	301	1CS	C4'-N3'-C2'	10.48	121.41	112.86
2	B	301	1CS	O7B-S7-O7A	-8.67	108.99	119.52
2	A	301	1CS	C4'-N3'-C2'	8.41	119.73	112.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	1CS	C4'-N3'-C2'	8.12	119.49	112.86
2	A	301	1CS	O7B-S7-O7A	-8.01	109.79	119.52
2	B	301	1CS	C5'-O4'-C4'	-7.95	105.01	117.56
2	A	301	1CS	C5'-O4'-C4'	-7.51	105.69	117.56
2	C	301	1CS	O7B-S7-O7A	-7.22	110.75	119.52
2	D	301	1CS	C2-C1-CL11	-5.93	117.23	121.52
2	C	301	1CS	C1-C2-S7	-5.89	119.13	123.19
2	C	301	1CS	C5'-O4'-C4'	-5.80	108.40	117.56
2	A	301	1CS	C2'-N10-C9	-5.50	124.67	130.34
2	D	301	1CS	O7B-S7-O7A	-5.10	113.32	119.52
2	C	301	1CS	C2'-N10-C9	-4.94	125.26	130.34
2	A	301	1CS	N3'-C2'-N1'	-4.91	118.21	126.26
2	B	301	1CS	C1-C2-S7	-4.74	119.92	123.19
2	D	301	1CS	N3'-C2'-N1'	-4.65	118.64	126.26
2	A	301	1CS	C7'-C6'-N1'	4.48	123.83	117.13
2	C	301	1CS	N3'-C4'-N5'	-4.21	120.00	127.65
2	B	301	1CS	N3'-C2'-N1'	-4.20	119.37	126.26
2	A	301	1CS	C2'-N1'-C6'	4.12	120.76	114.61
2	C	301	1CS	N3'-C2'-N1'	-3.81	120.02	126.26
2	D	301	1CS	N3'-C4'-N5'	-3.74	120.86	127.65
2	D	301	1CS	O7B-S7-C2	3.71	113.81	107.68
2	D	301	1CS	C2'-N1'-C6'	3.68	120.09	114.61
2	A	301	1CS	C6-C1-C2	3.68	122.44	120.04
2	B	301	1CS	C7'-C6'-N1'	3.63	122.56	117.13
2	D	301	1CS	O7A-S7-C2	-3.31	102.21	107.68
2	B	301	1CS	C2-S7-N8	3.23	109.98	105.96
2	B	301	1CS	C2'-N10-C9	-3.18	127.07	130.34
2	B	301	1CS	C2'-N1'-C6'	3.13	119.27	114.61
2	B	301	1CS	N3'-C4'-N5'	-3.07	122.07	127.65
2	C	301	1CS	C3-C2-S7	3.03	121.86	117.51
2	D	301	1CS	N8-C9-N10	-3.03	110.07	114.87
2	C	301	1CS	C7'-C6'-N1'	3.02	121.66	117.13
2	A	301	1CS	N3'-C4'-N5'	-3.01	122.19	127.65
2	C	301	1CS	N10-C2'-N1'	2.99	125.11	116.44
2	A	301	1CS	N1'-C6'-N5'	-2.94	120.58	125.77
2	B	301	1CS	O7A-S7-N8	2.87	114.97	106.77
2	A	301	1CS	C3-C2-C1	-2.80	117.05	119.05
2	B	301	1CS	C6-C1-C2	2.78	121.85	120.04
2	B	301	1CS	C2-C1-CL11	-2.78	119.51	121.52
2	A	301	1CS	N10-C2'-N1'	2.72	124.34	116.44
2	A	301	1CS	O7B-S7-C2	2.70	112.13	107.68
2	C	301	1CS	C2'-N1'-C6'	2.66	118.57	114.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	1CS	N1'-C6'-N5'	-2.52	121.32	125.77
2	C	301	1CS	C2-C1-CL11	-2.50	119.71	121.52
2	C	301	1CS	N1'-C6'-N5'	-2.32	121.67	125.77
2	B	301	1CS	N1'-C6'-N5'	-2.28	121.75	125.77
2	D	301	1CS	C2-S7-N8	2.21	108.70	105.96
2	A	301	1CS	C2-S7-N8	2.14	108.62	105.96
2	D	301	1CS	C6-C1-C2	2.13	121.43	120.04
2	D	301	1CS	C2'-N10-C9	-2.11	128.16	130.34
2	B	301	1CS	C3-C2-S7	2.10	120.53	117.51
2	D	301	1CS	N10-C2'-N1'	2.10	122.53	116.44
2	B	301	1CS	N10-C2'-N1'	2.04	122.38	116.44
2	D	301	1CS	C5'-O4'-C4'	-2.04	114.34	117.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	1CS	N8-C9-N10-C2'
2	B	301	1CS	N8-C9-N10-C2'
2	C	301	1CS	N8-C9-N10-C2'
2	D	301	1CS	N8-C9-N10-C2'

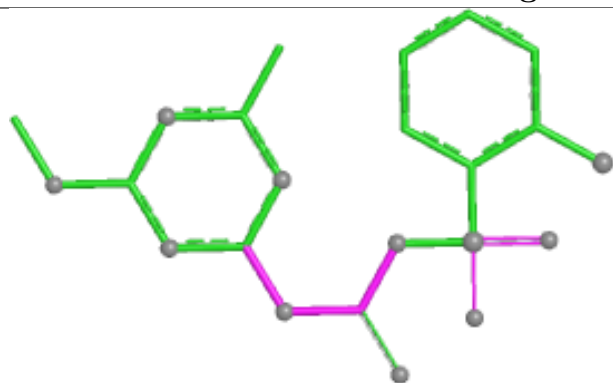
There are no ring outliers.

3 monomers are involved in 4 short contacts:

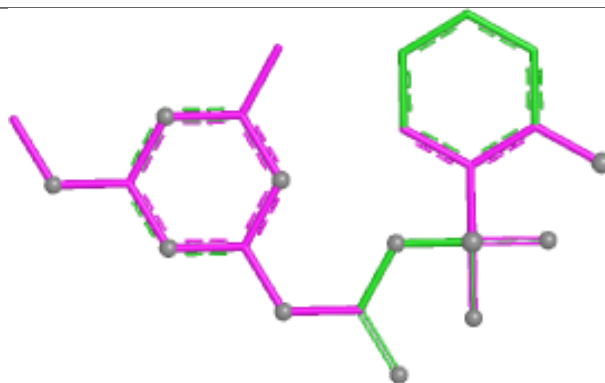
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	1CS	1	0
2	A	301	1CS	2	0
2	D	301	1CS	1	0

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.

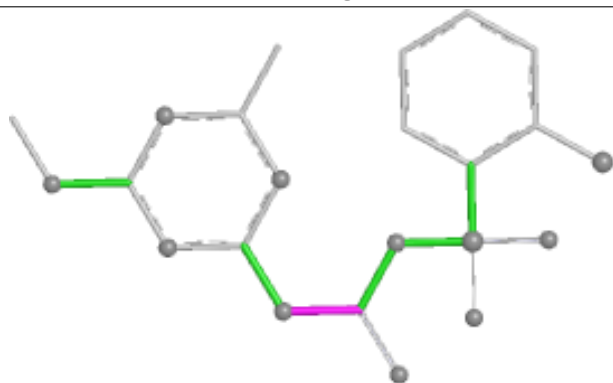
Ligand 1CS C 301



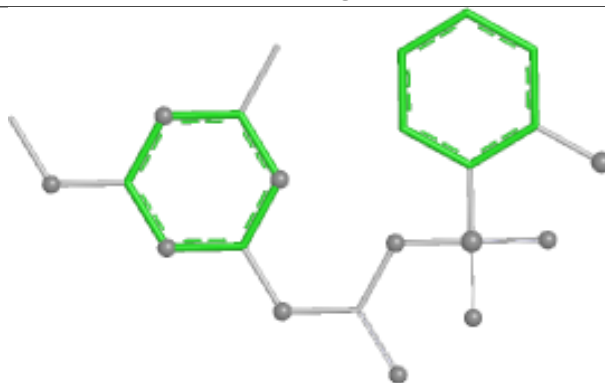
Bond lengths



Bond angles

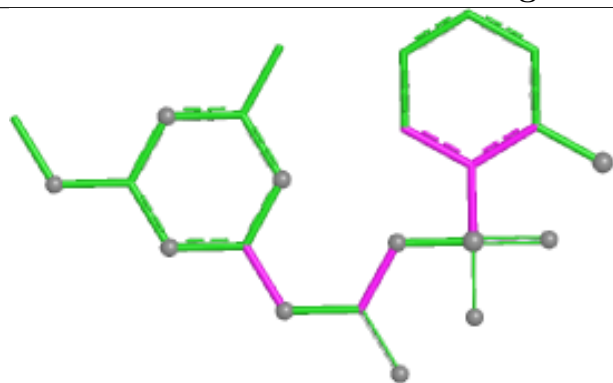


Torsions

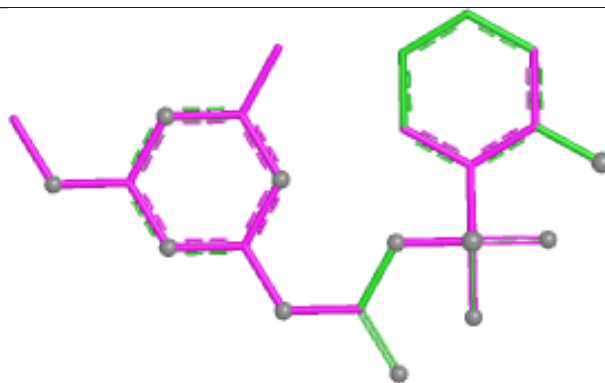


Rings

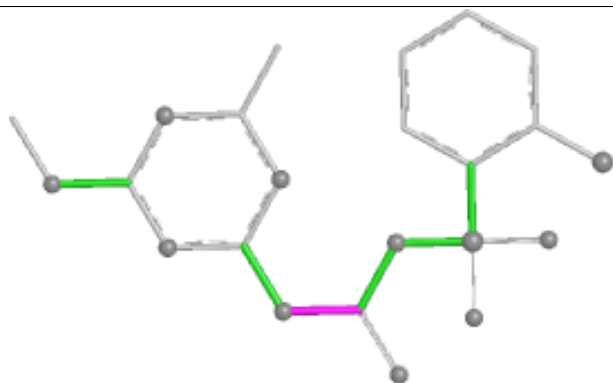
Ligand 1CS A 301



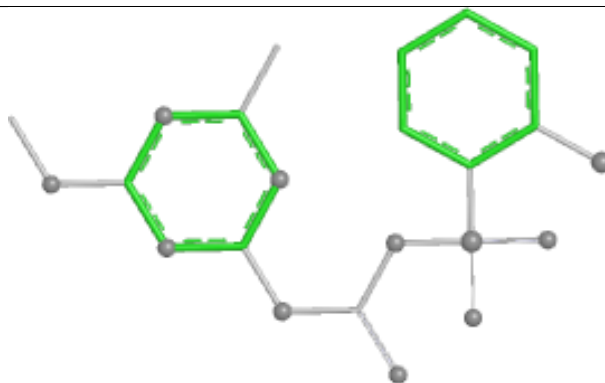
Bond lengths



Bond angles

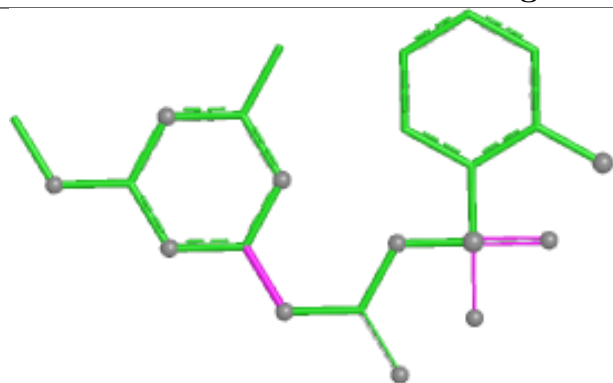


Torsions

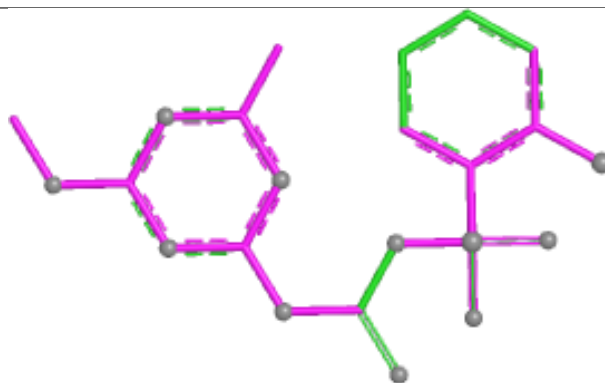


Rings

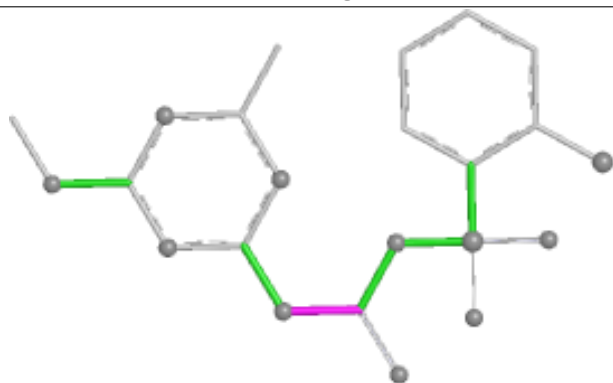
Ligand 1CS B 301



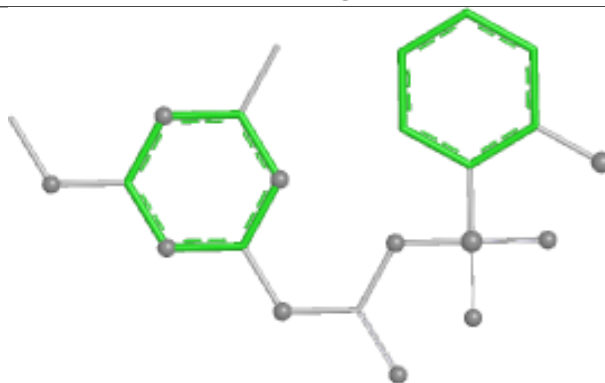
Bond lengths



Bond angles

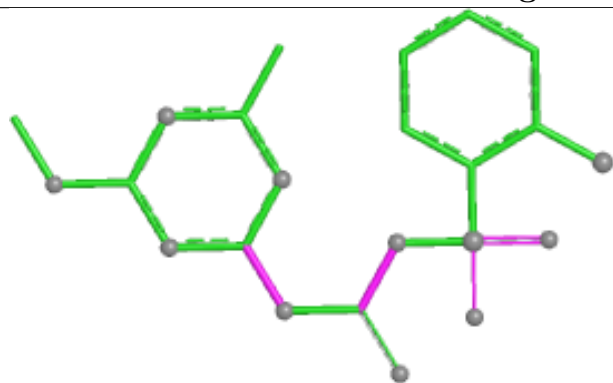


Torsions

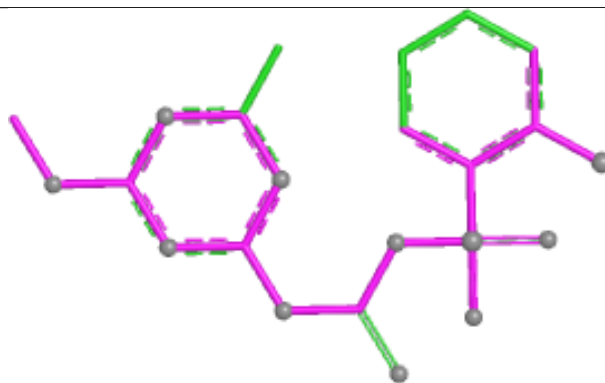


Rings

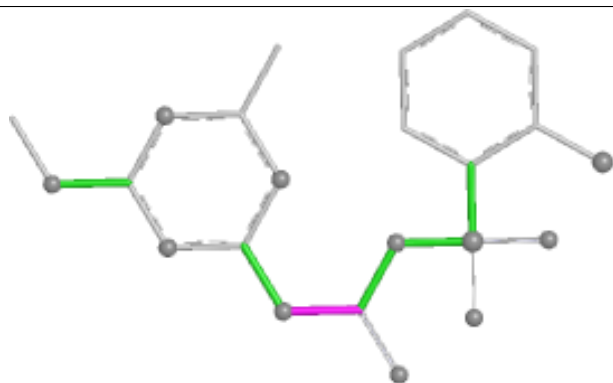
Ligand 1CS D 301



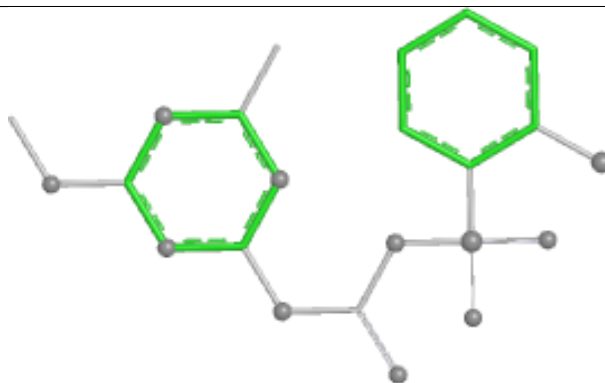
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	201/207 (97%)	-0.15	3 (1%) 71 70	11, 26, 51, 79	1 (0%)
1	B	203/207 (98%)	-0.33	0 100 100	15, 25, 42, 58	0
1	C	200/207 (96%)	-0.19	4 (2%) 64 63	15, 27, 52, 70	0
1	D	202/207 (97%)	-0.27	1 (0%) 87 86	14, 25, 43, 75	0
All	All	806/828 (97%)	-0.23	8 (0%) 79 78	11, 26, 48, 79	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	4.0
1	C	4	LEU	3.2
1	C	178	VAL	2.4
1	D	162	THR	2.4
1	C	180	GLN	2.4
1	A	28	ARG	2.3
1	A	165	SER	2.1
1	C	179	HIS	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](#)

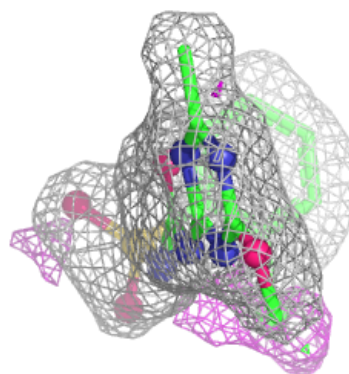
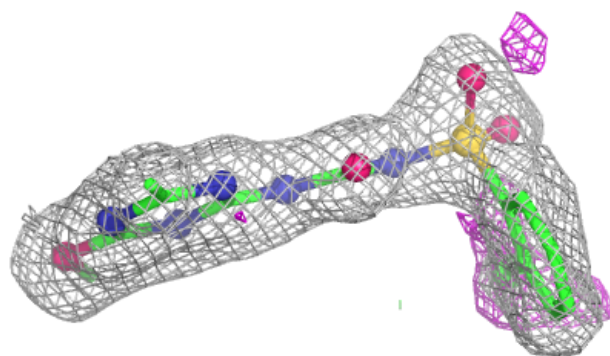
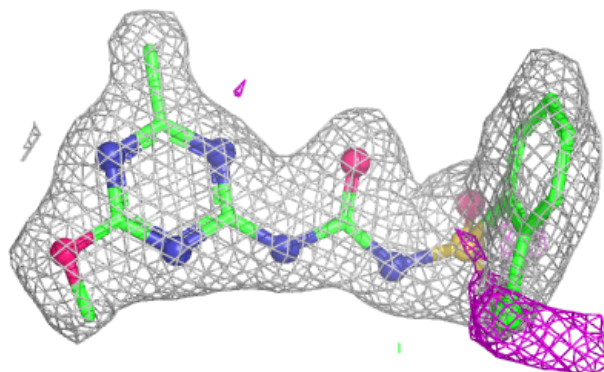
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	1CS	B	301	23/23	0.93	0.10	20,28,36,62	0
2	1CS	C	301	23/23	0.94	0.07	19,24,32,68	0
2	1CS	A	301	23/23	0.96	0.07	18,22,29,61	0
2	1CS	D	301	23/23	0.96	0.06	18,24,29,59	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.

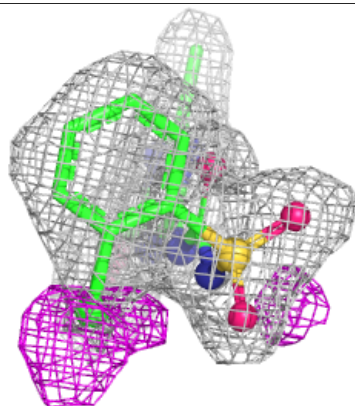
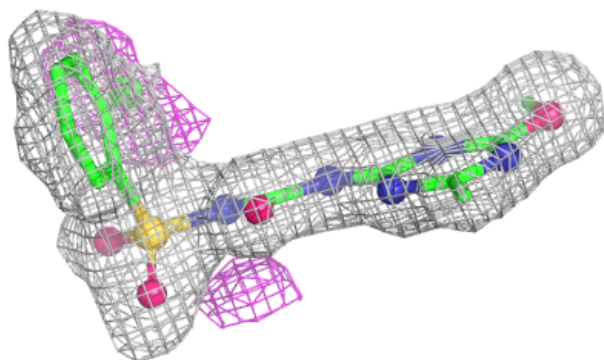
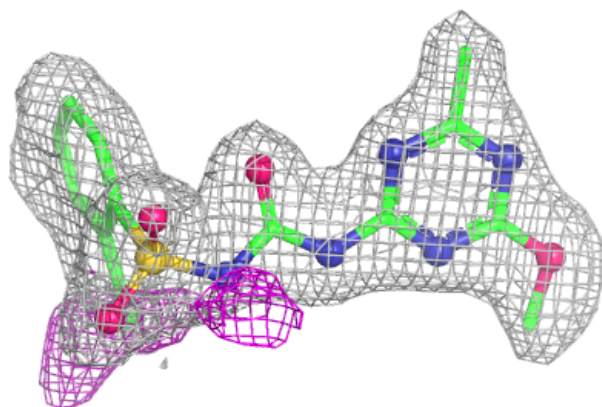
Electron density around 1CS B 301:

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

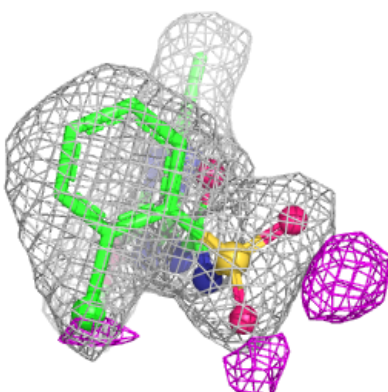
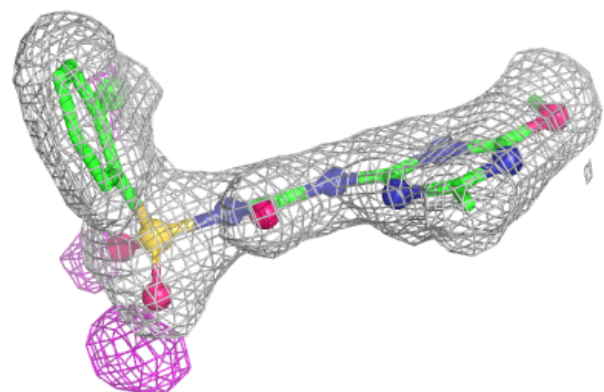
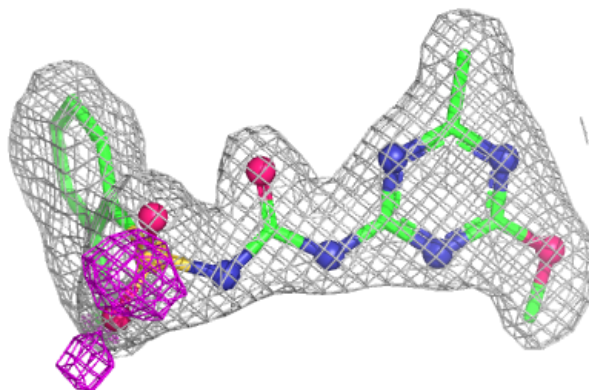


Electron density around 1CS C 301:

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

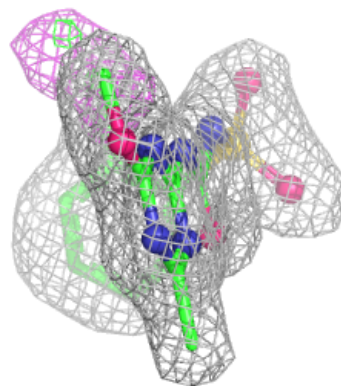
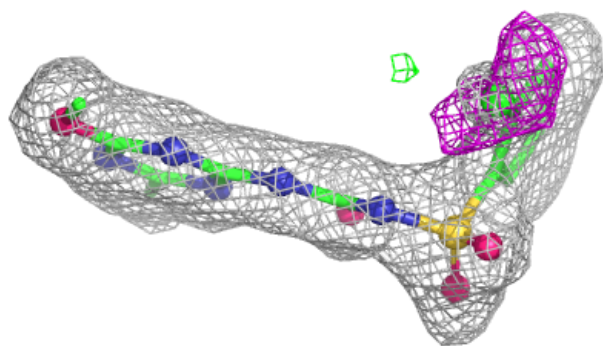
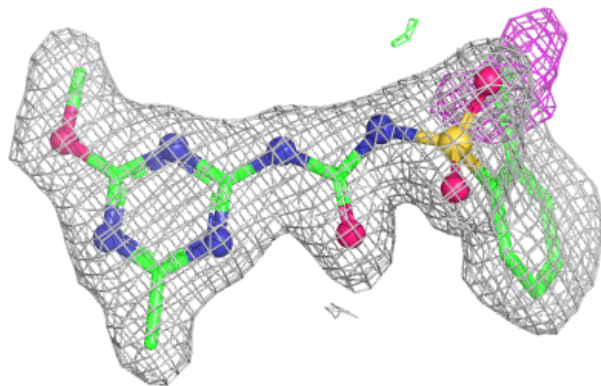
**Electron density around 1CS A 301:**

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



Electron density around 1CS D 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.