WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 10:01 PM EDT

PDB ID	:	5Q01
Title	:	Human liver fructose-1,6-bisphosphatase 1 (fructose 1,6-bisphosphate 1-phosphatase, E.C.3.1.3.11) complexed with the allosteric inhibitor 1-(5-bromo-1,3-thiazol-2-yl)-3-[4-(4,5-dichloro-2-methylpyrazol-3-yl)oxyphenyl]sulfonylurea
Authors	:	Ruf, A.; Joseph, C.; Alker, A.; Banner, D.; Tetaz, T.; Benz, J.; Kuhn, B.; Rudolph, M.G.; Yang, H.; Shao, C.; Burley, S.K.
Deposited on	:	2017-04-18
Resolution	:	2.60 Å(reported)

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

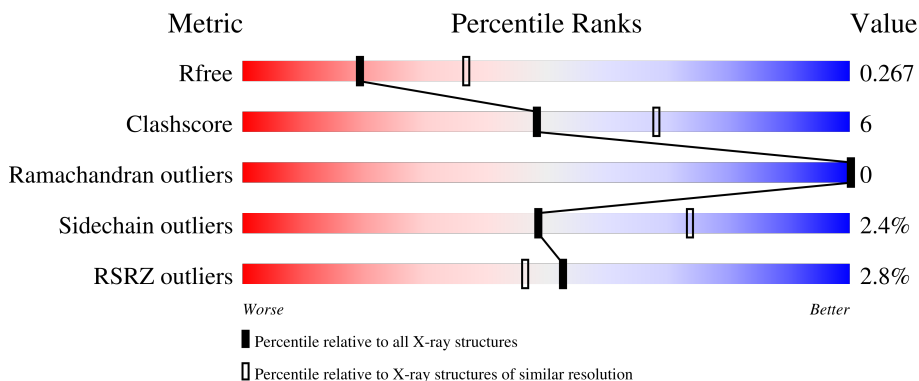|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.60 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.4%
RSRZ outliers		2.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

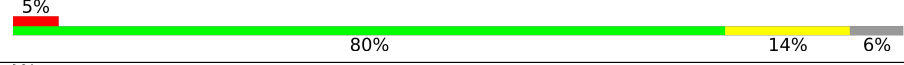| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	338	4% / 80% 14% · 6%
1	B	338	2% / 76% 17% · 6%
1	C	338	% / 80% 14% 6%

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Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

WORLDWIDE wwPDB PROTEIN DATA BANK

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| Mol	Chain	Length	Quality of chain
1	D	338	% 81% 13% 6%
1	E	338	4% 80% 14% 6%
1	F	338	5% 80% 14% 6%
1	G	338	2% 76% 17% 6%
1	H	338	2% 80% 14% 6%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 20072 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 Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	1	0
			2446	1558	412	459	17			
1	B	317	Total	C	N	O	S	0	1	0
			2431	1548	409	457	17			
1	C	317	Total	C	N	O	S	0	0	0
			2425	1545	406	457	17			
1	D	317	Total	C	N	O	S	0	1	0
			2431	1548	409	457	17			
1	E	319	Total	C	N	O	S	0	1	0
			2447	1559	412	459	17			
1	F	317	Total	C	N	O	S	0	1	0
			2430	1547	409	457	17			
1	G	317	Total	C	N	O	S	0	1	0
			2430	1547	409	457	17			
1	H	317	Total	C	N	O	S	0	0	0
			2425	1545	406	457	17			

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-4-[(3,4-dichloro-1-methyl-1H-pyrazol-5-yl)oxy]benzene-1-sulfonamide (three-letter code: 95G) (formula: $C_{14}H_{10}BrCl_2N_5O_4S_2$).

95G
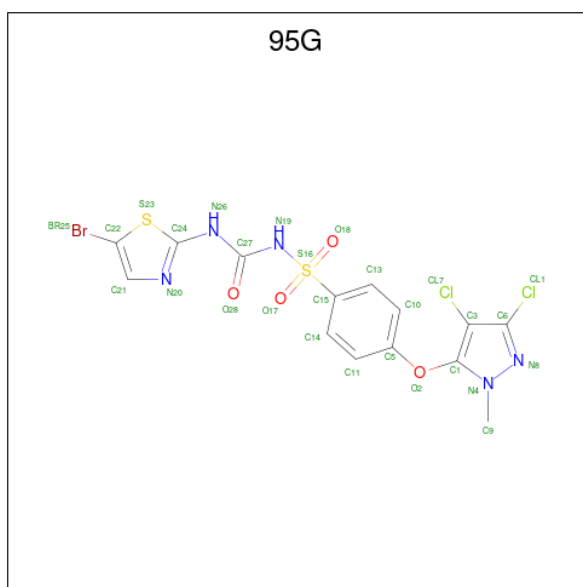
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	B	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	C	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	D	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	E	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	F	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	G	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		
2	H	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	14	2	5	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	32	Total	O	0	0
			32	32		
3	C	54	Total	O	0	0
			54	54		
3	D	75	Total	O	0	0
			75	75		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	27	Total 27	O 27	0	0
3	F	15	Total 15	O 15	0	0
3	G	73	Total 73	O 73	0	0
3	H	65	Total 65	O 65	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.
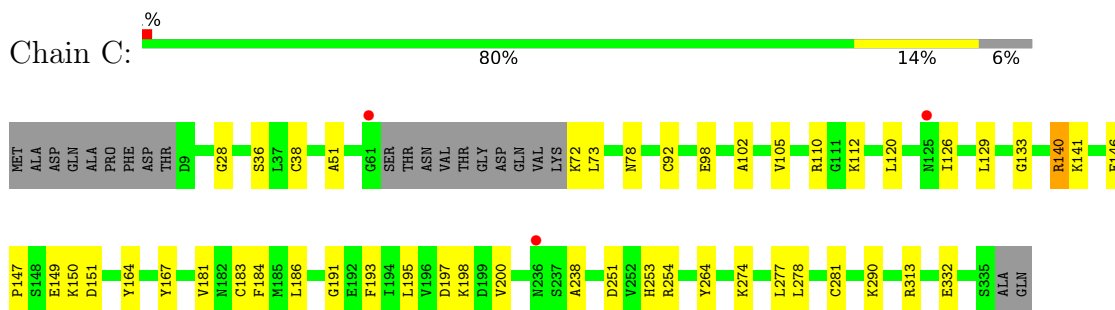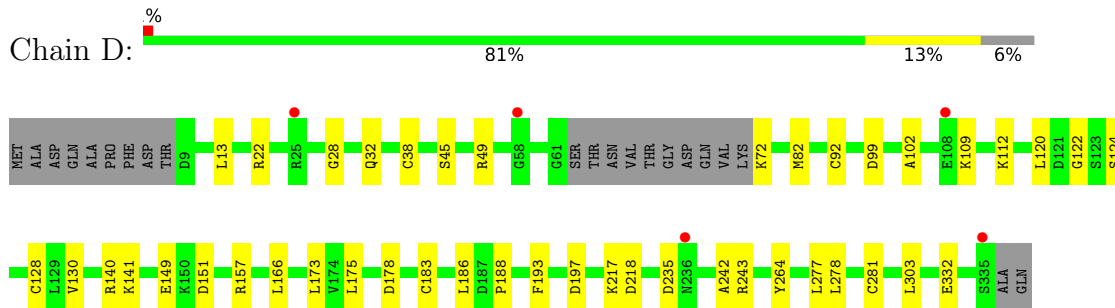
- Molecule 1: Fructose-1,6-bisphosphatase 1
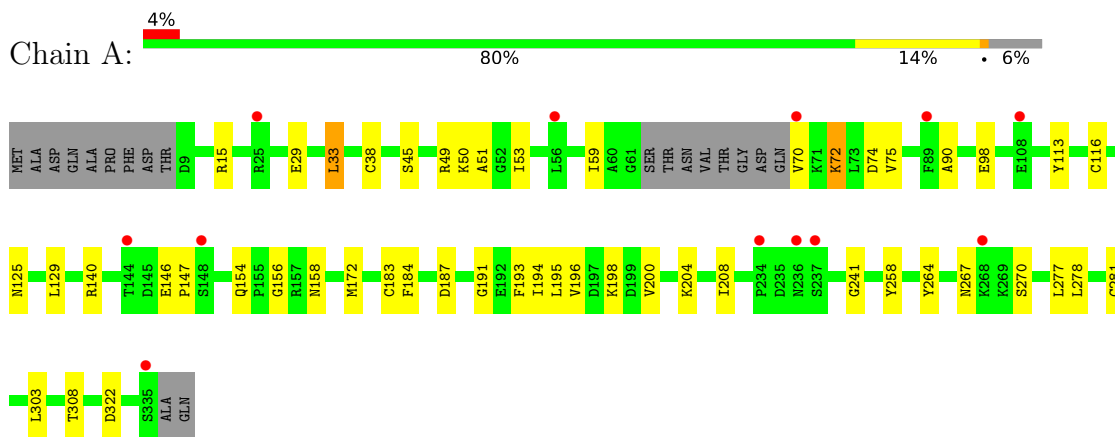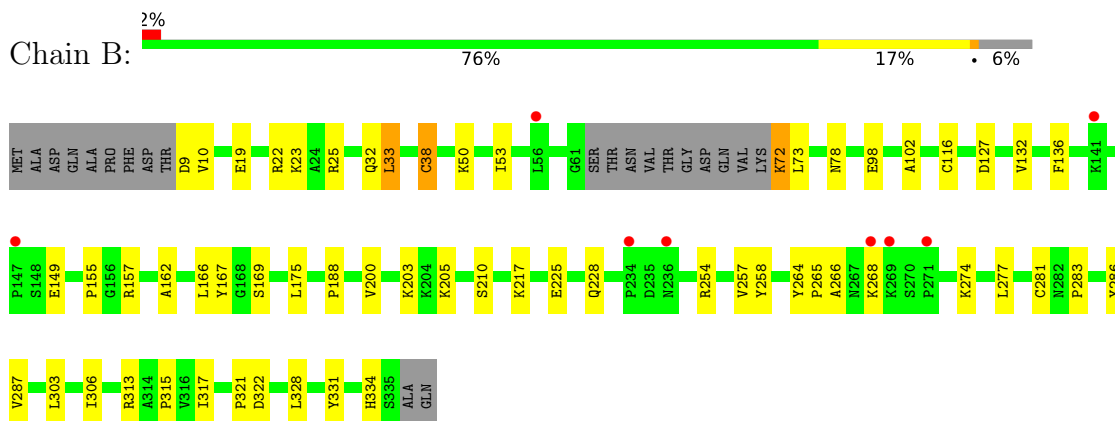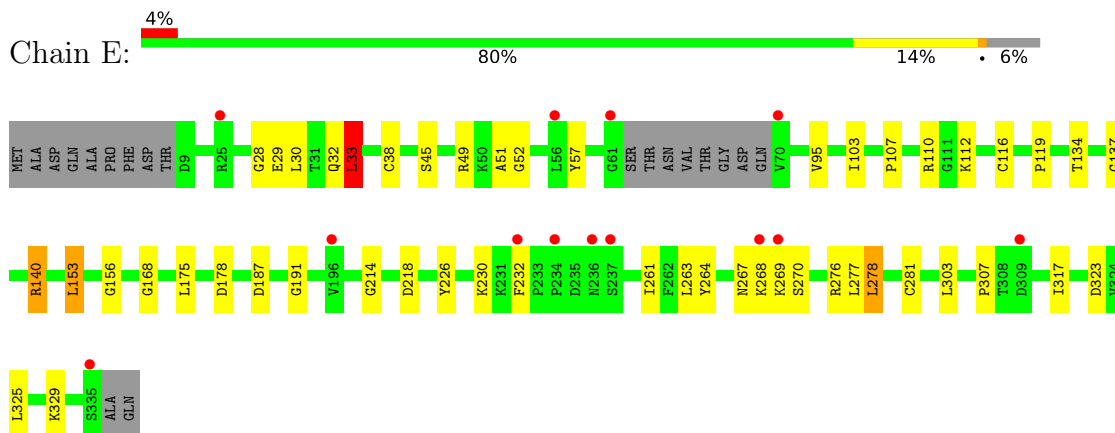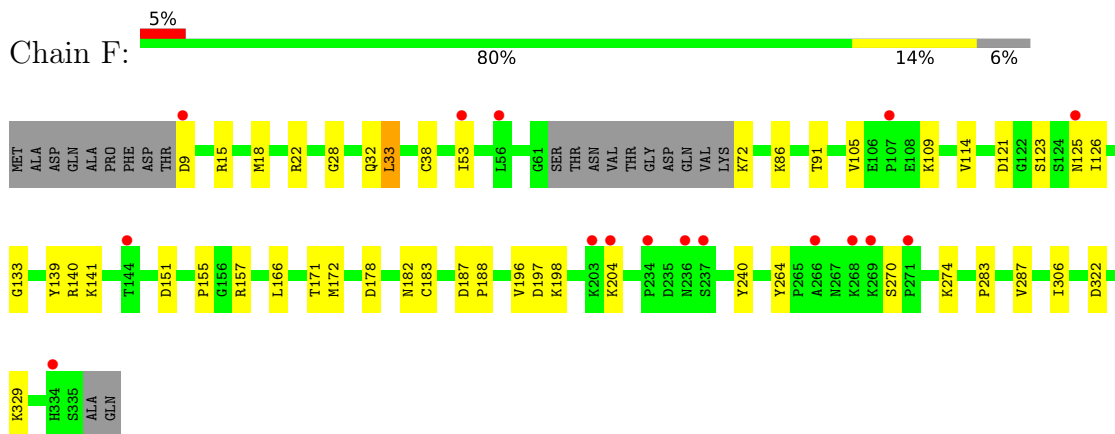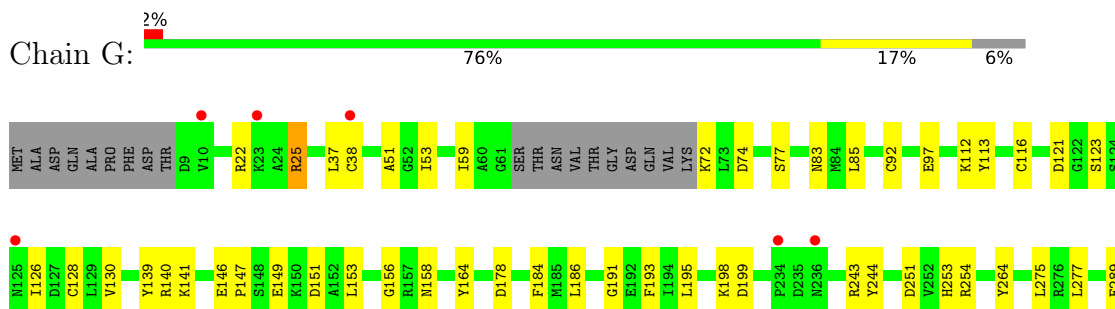

- Molecule 1: Fructose-1,6-bisphosphatase 1

- Molecule 1: Fructose-1,6-bisphosphatase 1

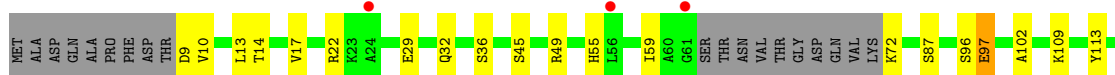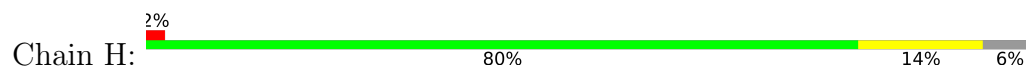• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain D:

• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain E:

• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain F:

• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain G:

G293 P307 I310 R313 V316 P321 K329 E332 K333 H334 S335 ALA GLN

• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H:

2%

80%   14%   6%

MET ALA ASP GLN ALA PRO PHE ASP THR D9 V10 L13 T14 V17 R22 K23 A24 E29 Q32 S36 S45 R49 H55 L56 I59 A60 G61 SER THR ASN VAL THR GLY ASP GLN VAL LYS K72 S87 S96 E97 A102 K109 Y113

F117 D121 S124 D127 G133 Y139 D145 E149 P155 L159 L173 M177 D178 C179 N182 C183 D187 P188 L195 V196 D197 K198 D199 V200 K217 N236 S237 Y264 N267 K268 K274 Y279 L303 I306 R313 S335

ALA GLN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.44Å 294.19Å 83.57Å 90.00° 97.56° 90.00°	Depositor
Resolution (Å)	30.41 – 2.60 30.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	78.8 (30.41-2.60) 78.9 (30.41-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.187 , 0.267 0.187 , 0.267	Depositor DCC
R_{free} test set	3777 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20072	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 95G

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	0.42	0/2495	0.63	1/3368 (0.0%)
1	B	0.40	0/2479	0.64	1/3347 (0.0%)
1	C	0.46	0/2468	0.65	0/3333
1	D	0.46	0/2479	0.66	0/3347
1	E	0.42	1/2495 (0.0%)	0.63	1/3368 (0.0%)
1	F	0.37	0/2479	0.61	1/3347 (0.0%)
1	G	0.49	1/2479 (0.0%)	0.64	0/3347
1	H	0.44	0/2468	0.65	2/3333 (0.1%)
All	All	0.44	2/19842 (0.0%)	0.64	6/26790 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	CYS	CB-SG	7.07	1.94	1.82
1	E	153	LEU	C-N	-6.09	1.20	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	33	LEU	CA-CB-CG	6.86	131.09	115.30
1	F	33	LEU	CA-CB-CG	6.34	129.89	115.30
1	H	173	LEU	CA-CB-CG	5.08	126.97	115.30
1	H	173	LEU	CB-CG-CD2	-5.07	102.37	111.00

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	2446	0	2496	30	1
1	B	2431	0	2478	36	0
1	C	2425	0	2469	35	0
1	D	2431	0	2478	28	1
1	E	2447	0	2500	31	0
1	F	2430	0	2474	31	1
1	G	2430	0	2474	40	1
1	H	2425	0	2469	33	0
2	A	28	0	0	0	0
2	B	28	0	0	1	0
2	C	28	0	0	2	0
2	D	28	0	0	2	0
2	E	28	0	0	3	0
2	F	28	0	0	2	0
2	G	28	0	0	1	0
2	H	28	0	0	0	0
3	A	42	0	0	4	0
3	B	32	0	0	2	0
3	C	54	0	0	3	0
3	D	75	0	0	4	0
3	E	27	0	0	1	0
3	F	15	0	0	3	0
3	G	73	0	0	14	0
3	H	65	0	0	9	0
All	All	20072	0	19838	236	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 236 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:B:102:ALA:HB3	1:B:149:GLU:HG2	1.59	0.84
1:B:38:CYS:SG	3:B:529:HOH:O	2.36	0.83
1:A:154:GLN:HB3	1:A:158:ASN:HD22	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:TYR:O	3:H:502:HOH:O	2.01	0.79
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.70	0.73

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:O	1:F:329:LYS:NZ[1_655]	2.16	0.04
1:D:332:GLU:OE2	1:G:313:ARG:NE[2_646]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	316/338 (94%)	310 (98%)	6 (2%)	0	100	100
1	B	314/338 (93%)	306 (98%)	8 (2%)	0	100	100
1	C	313/338 (93%)	304 (97%)	9 (3%)	0	100	100
1	D	314/338 (93%)	305 (97%)	9 (3%)	0	100	100
1	E	316/338 (94%)	308 (98%)	8 (2%)	0	100	100
1	F	314/338 (93%)	306 (98%)	8 (2%)	0	100	100
1	G	314/338 (93%)	305 (97%)	9 (3%)	0	100	100
1	H	313/338 (93%)	305 (97%)	8 (3%)	0	100	100
All	All	2514/2704 (93%)	2449 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	267/281 (95%)	258 (97%)	9 (3%)	37	63
1	B	265/281 (94%)	258 (97%)	7 (3%)	46	72
1	C	264/281 (94%)	258 (98%)	6 (2%)	50	75
1	D	265/281 (94%)	260 (98%)	5 (2%)	57	79
1	E	267/281 (95%)	258 (97%)	9 (3%)	37	63
1	F	265/281 (94%)	258 (97%)	7 (3%)	46	72
1	G	265/281 (94%)	257 (97%)	8 (3%)	41	67
1	H	264/281 (94%)	261 (99%)	3 (1%)	73	88
All	All	2122/2248 (94%)	2068 (98%)	54 (2%)	49	73

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	38	CYS
1	E	278	LEU
1	G	264	TYR
1	E	140[A]	ARG
1	E	232	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	95G	B	401	-	25,30,30	0.86	0	24,44,44	1.25	2 (8%)
2	95G	G	401	-	25,30,30	0.94	1 (4%)	24,44,44	1.31	2 (8%)
2	95G	C	401	-	25,30,30	1.18	2 (8%)	24,44,44	1.06	2 (8%)
2	95G	D	401	-	25,30,30	0.94	1 (4%)	24,44,44	1.39	2 (8%)
2	95G	A	401	-	25,30,30	0.94	2 (8%)	24,44,44	1.02	2 (8%)
2	95G	E	401	-	25,30,30	0.92	2 (8%)	24,44,44	1.36	2 (8%)
2	95G	F	401	-	25,30,30	0.87	2 (8%)	24,44,44	0.82	2 (8%)
2	95G	H	401	-	25,30,30	0.99	1 (4%)	24,44,44	0.95	2 (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	95G	B	401	-	-	3/15/19/19	0/3/3/3
2	95G	G	401	-	-	1/15/19/19	0/3/3/3
2	95G	C	401	-	-	1/15/19/19	0/3/3/3
2	95G	D	401	-	-	4/15/19/19	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	95G	A	401	-	-	3/15/19/19	0/3/3/3
2	95G	E	401	-	-	1/15/19/19	0/3/3/3
2	95G	F	401	-	-	1/15/19/19	0/3/3/3
2	95G	H	401	-	-	1/15/19/19	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	95G	C24-N26	3.31	1.42	1.36
2	C	401	95G	C24-N26	3.23	1.42	1.36
2	H	401	95G	C24-N26	2.85	1.41	1.36
2	C	401	95G	C6-N8	2.84	1.38	1.34
2	E	401	95G	C24-N26	2.49	1.41	1.36

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	95G	C1-C3-CL7	-5.51	124.12	127.69
2	G	401	95G	C1-C3-CL7	-5.32	124.25	127.69
2	E	401	95G	C1-C3-CL7	-5.30	124.26	127.69
2	B	401	95G	C1-C3-CL7	-4.86	124.54	127.69
2	C	401	95G	C1-C3-CL7	-3.32	125.54	127.69

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	95G	N19-C27-N26-C24
2	B	401	95G	N19-C27-N26-C24
2	C	401	95G	N19-C27-N26-C24
2	D	401	95G	N19-C27-N26-C24
2	E	401	95G	N19-C27-N26-C24

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	95G	1	0
2	G	401	95G	1	0
2	C	401	95G	2	0
2	D	401	95G	2	0

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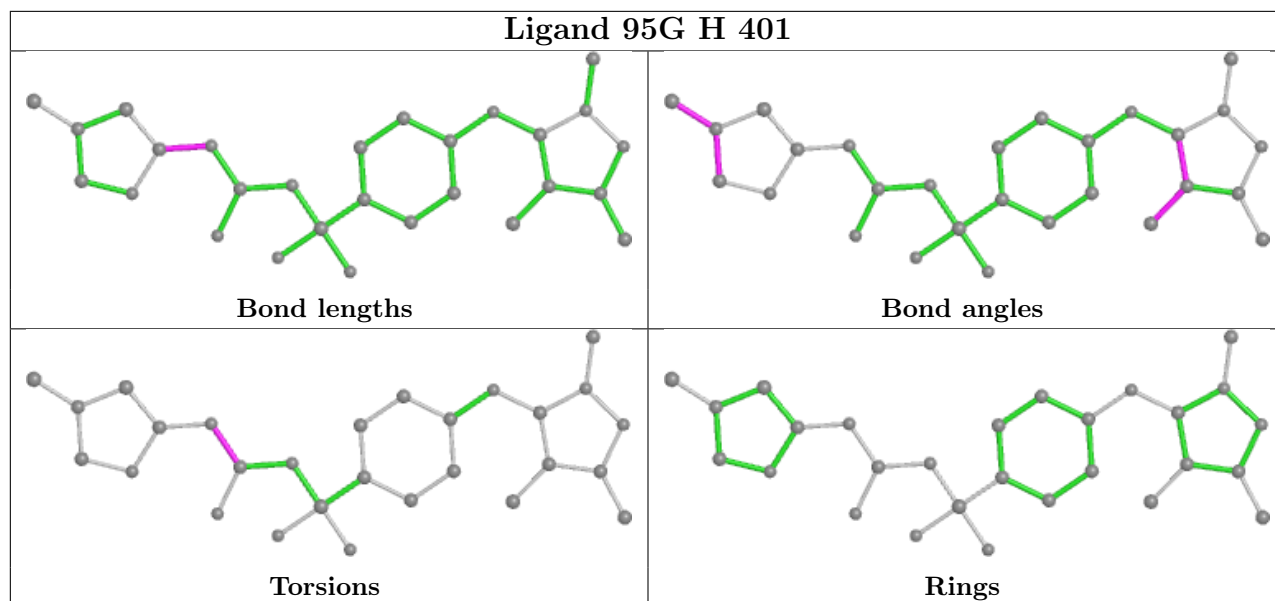| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	95G	3	0
2	F	401	95G	2	0

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 95G B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 95G H 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	153:LEU	C	154:GLN	N	1.20

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	319/338 (94%)	-0.16	12 (3%)	40	33	21, 47, 79, 118	0
1	B	317/338 (93%)	-0.00	8 (2%)	57	51	22, 52, 93, 130	0
1	C	317/338 (93%)	-0.19	3 (0%)	84	82	24, 40, 69, 123	0
1	D	317/338 (93%)	-0.34	5 (1%)	72	68	20, 35, 65, 101	0
1	E	319/338 (94%)	0.05	13 (4%)	37	30	24, 55, 90, 111	0
1	F	317/338 (93%)	0.04	16 (5%)	28	23	29, 55, 98, 144	0
1	G	317/338 (93%)	-0.20	6 (1%)	66	62	24, 41, 71, 111	0
1	H	317/338 (93%)	-0.16	8 (2%)	57	51	28, 45, 76, 116	0
All	All	2540/2704 (93%)	-0.12	71 (2%)	53	46	20, 46, 84, 144	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	4.7
1	F	144	THR	4.7
1	A	144	THR	4.6
1	F	236	ASN	4.0
1	B	268	LYS	3.9

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	95G	A	401	28/28	0.96	0.12	15,50,65,69	0
2	95G	B	401	28/28	0.96	0.13	42,57,68,75	1
2	95G	C	401	28/28	0.96	0.10	28,50,60,62	1
2	95G	F	401	28/28	0.96	0.12	20,57,68,76	0
2	95G	E	401	28/28	0.97	0.12	15,50,60,70	0
2	95G	D	401	28/28	0.97	0.12	29,50,62,67	1
2	95G	G	401	28/28	0.97	0.14	32,43,59,65	1
2	95G	H	401	28/28	0.97	0.11	40,57,63,77	1

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 95G A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
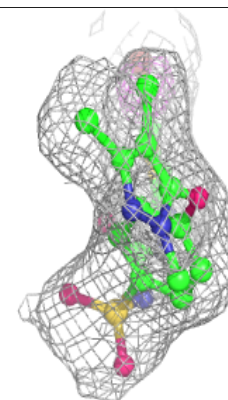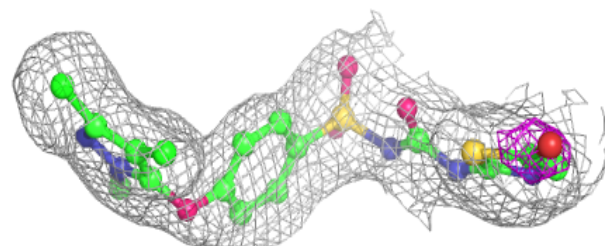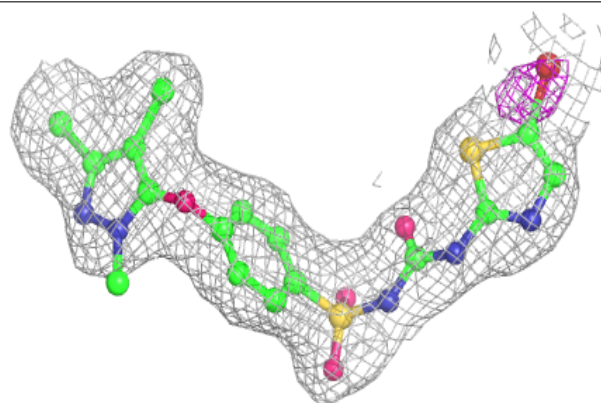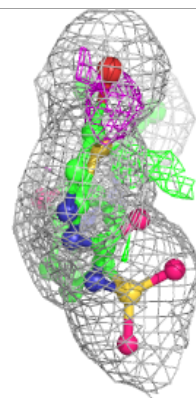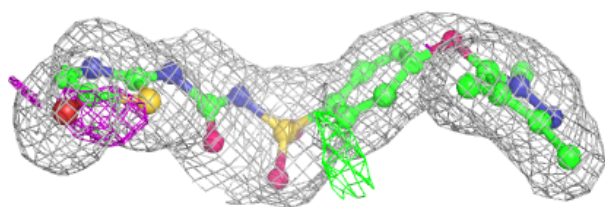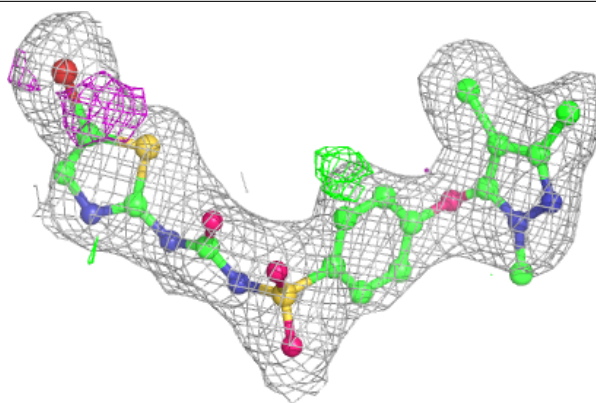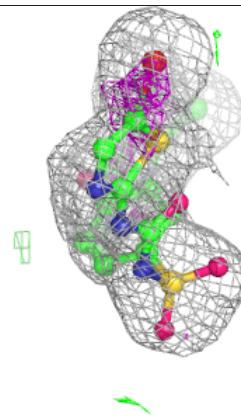mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
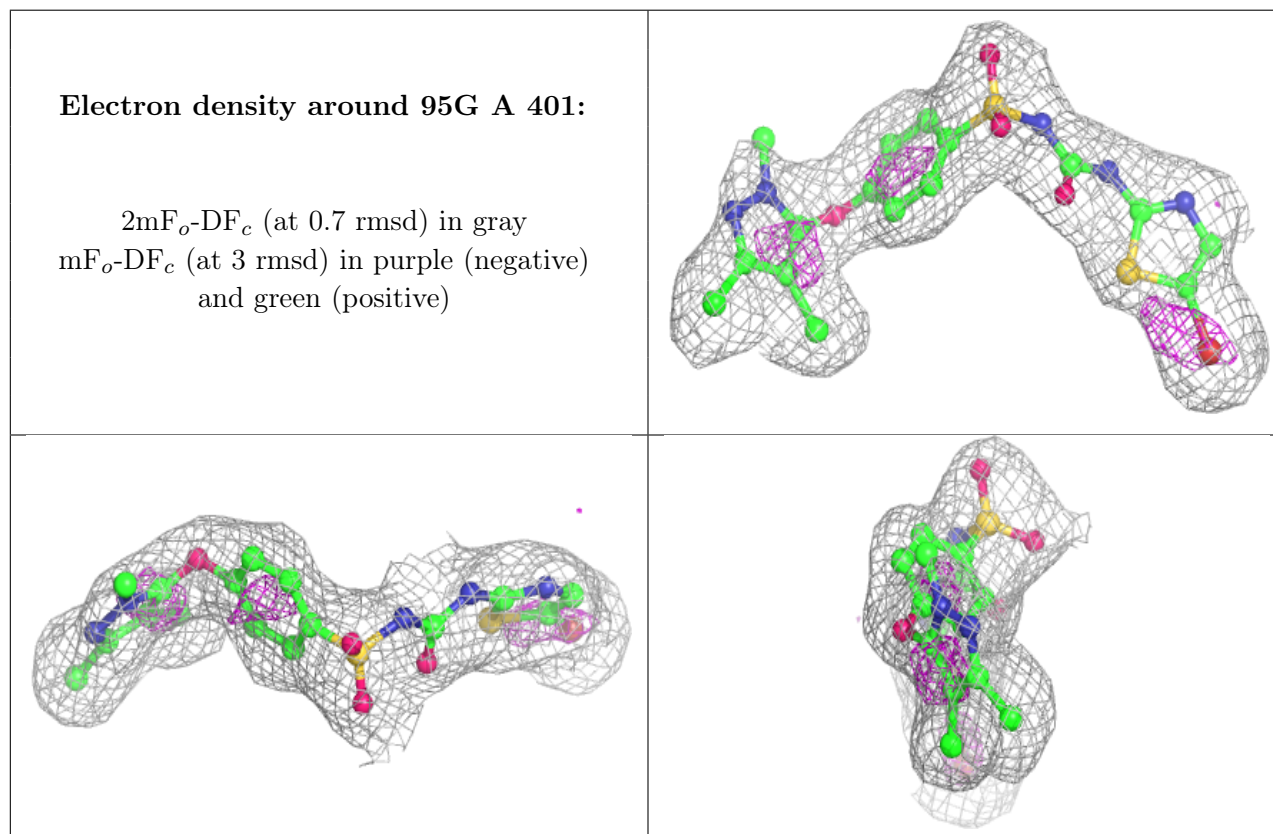
Electron density around 95G B 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
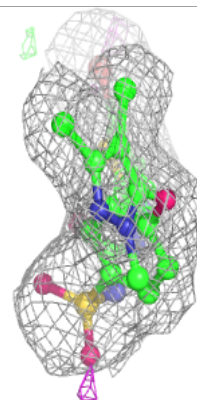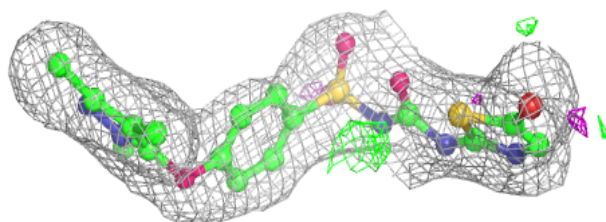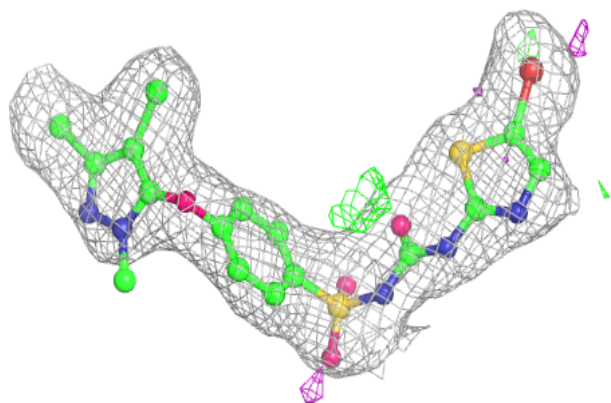
Electron density around 95G C 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
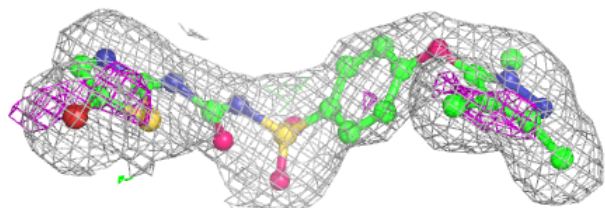$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
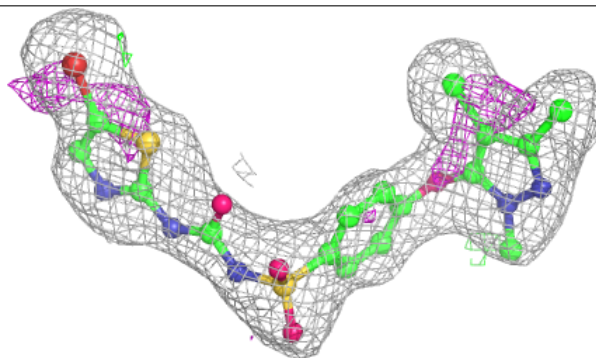and green (positive)
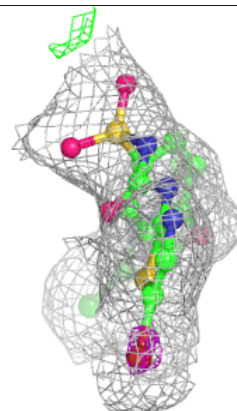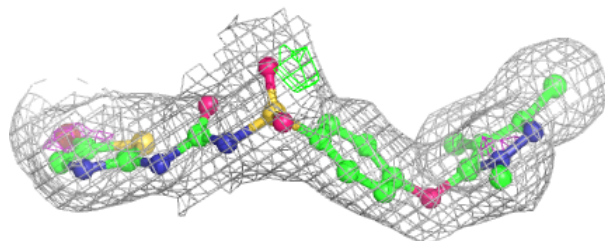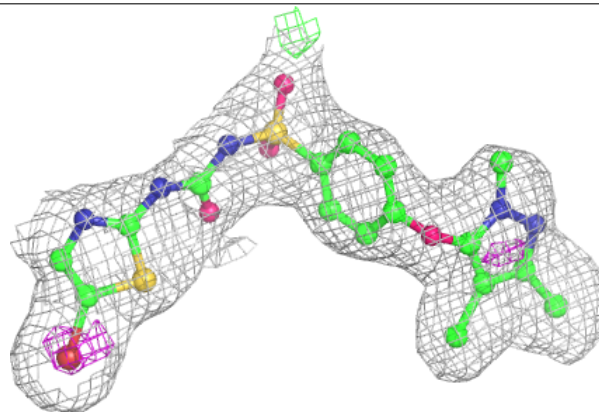
Electron density around 95G F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
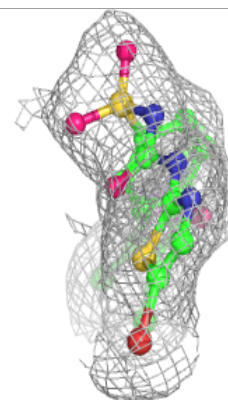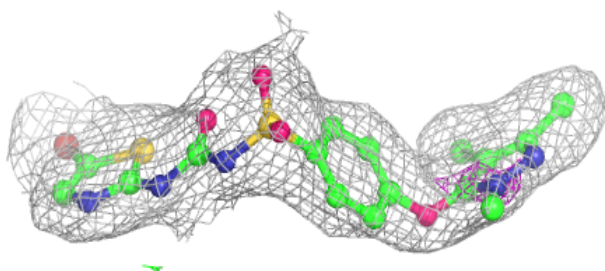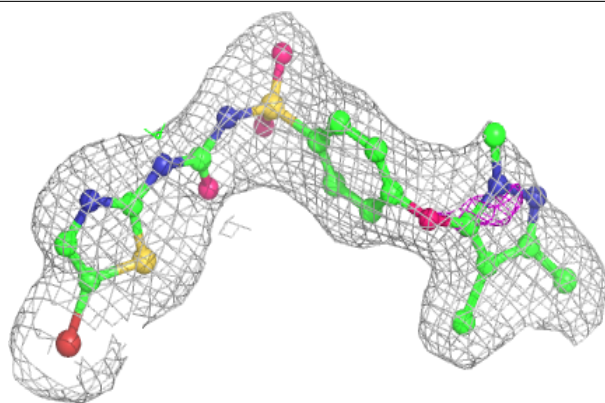
Electron density around 95G E 401:

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

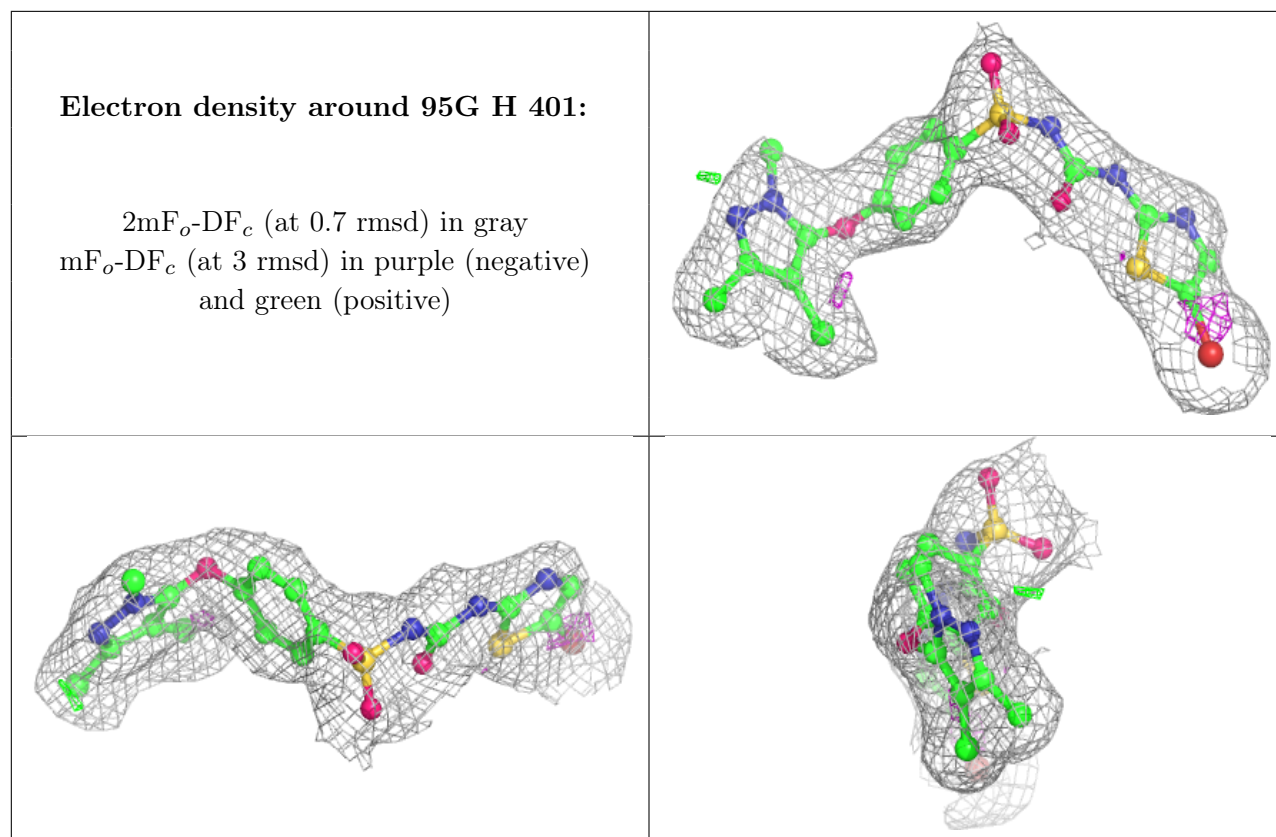**Electron density around 95G D 401:**

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

Electron density around 95G G 401:

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

Electron density around 95G H 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.