



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 04:23 PM EST

PDB ID : 5PZY
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-(2-chlorophenyl)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 : 2.21 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.16
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)	:	2.16

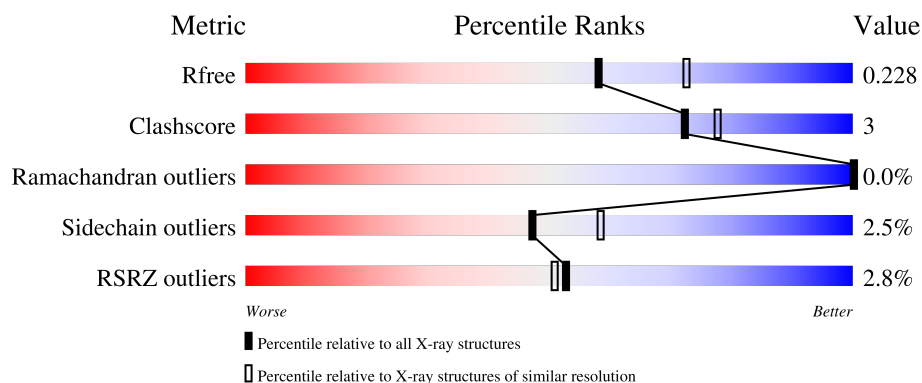
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	338	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	338	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	338	<div> <div>0%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	338	<div> <div>0%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	E	338	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	338	<div><div></div><div>6%</div><div>84%</div><div>10%</div><div>6%</div></div>
1	G	338	<div><div></div><div>%</div><div>85%</div><div>9%</div><div>6%</div></div>
1	H	338	<div><div></div><div>%</div><div>86%</div><div>8%</div><div>6%</div></div>

2 Entry composition

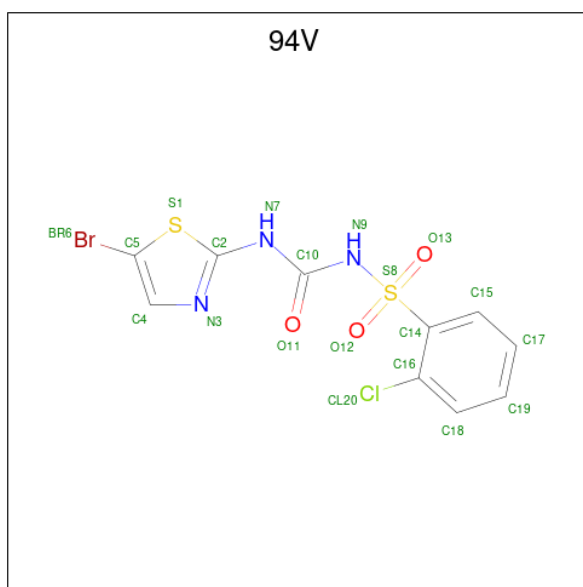
There are 3 unique types of molecules in this entry. The entry contains 20552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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]-2-chlorobenzene-1-sulfonamide (three-letter code: 94V) (formula: C₁₀H₇BrClN₃O₃S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	B	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	C	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	D	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	E	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	F	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	G	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		
2	H	1	Total	Br	C	Cl	N	O	S	0	1
			20	1	10	1	3	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	86	Total	O	0	0
			86	86		
3	C	137	Total	O	0	0
			137	137		
3	D	150	Total	O	0	0
			150	150		

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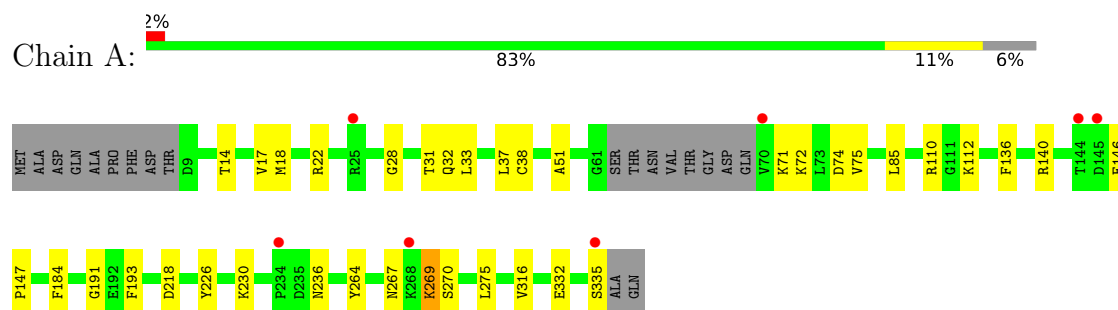
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	78	Total 78	O 78	0	0
3	F	74	Total 74	O 74	0	0
3	G	149	Total 149	O 149	0	0
3	H	125	Total 125	O 125	0	0

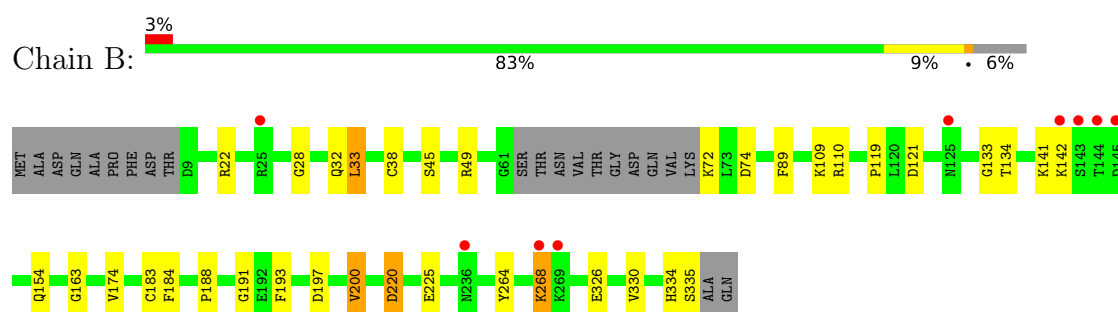
3 Residue-property plots [i](#)

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.

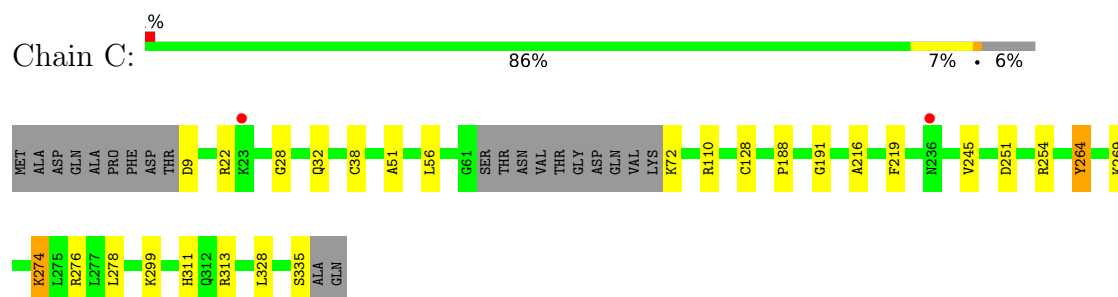
• Molecule 1: Fructose-1,6-bisphosphatase 1



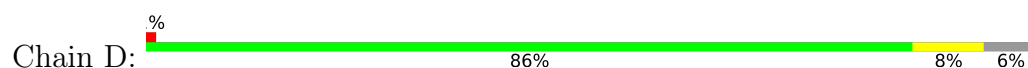
• Molecule 1: Fructose-1,6-bisphosphatase 1

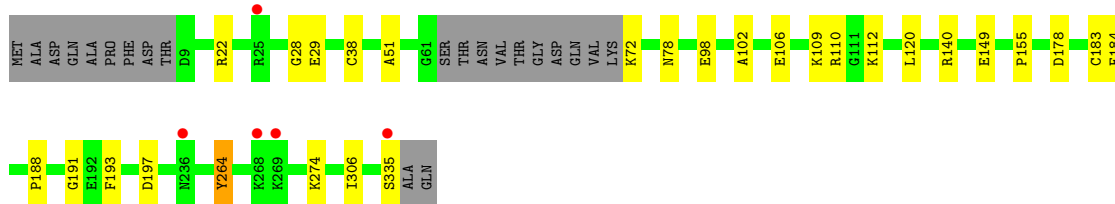


• Molecule 1: Fructose-1,6-bisphosphatase 1

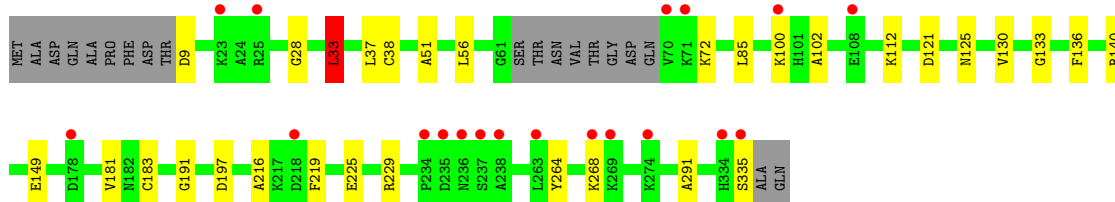
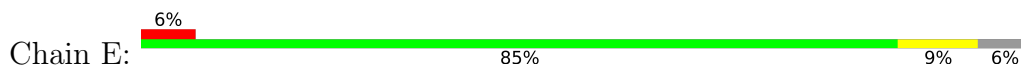


• Molecule 1: Fructose-1,6-bisphosphatase 1

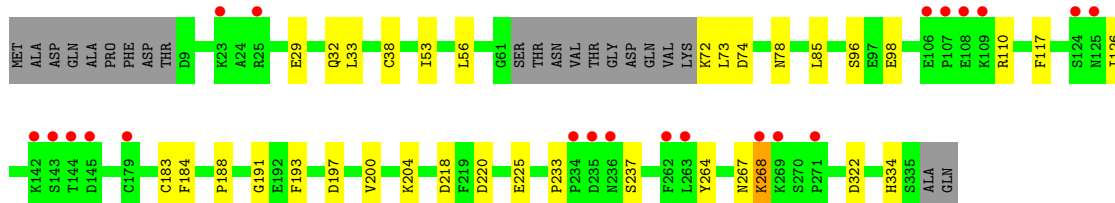
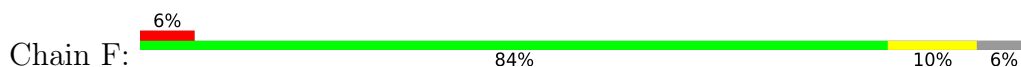




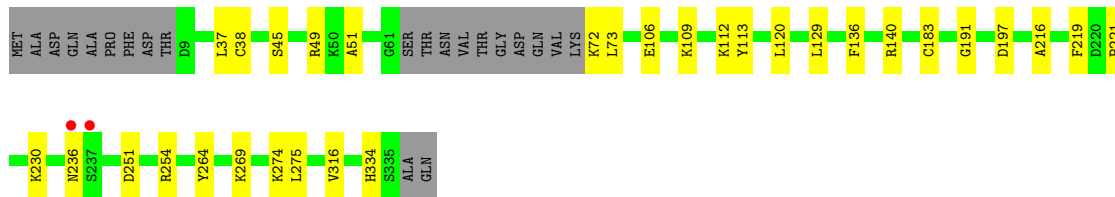
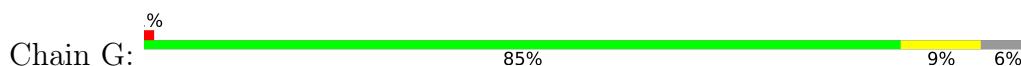
• Molecule 1: Fructose-1,6-bisphosphatase 1



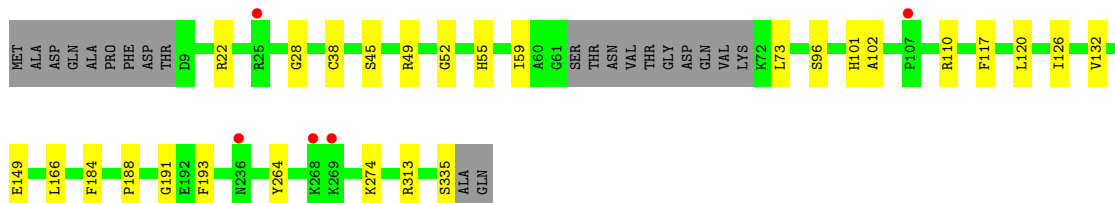
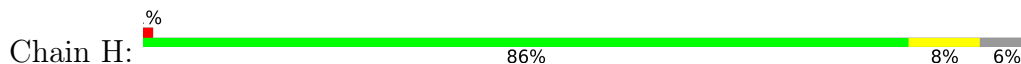
• Molecule 1: Fructose-1,6-bisphosphatase 1



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.21Å 283.78Å 83.37Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	24.25 – 2.21 24.26 – 2.21	Depositor EDS
% Data completeness (in resolution range)	93.0 (24.25-2.21) 93.0 (24.26-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.173 , 0.228 0.173 , 0.228	Depositor DCC
R_{free} test set	7106 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20552	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 94V

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	0.41	0/2495	0.59	0/3368
1	B	0.38	0/2479	0.59	1/3347 (0.0%)
1	C	0.43	0/2468	0.61	0/3333
1	D	0.45	0/2479	0.63	0/3347
1	E	0.37	0/2495	0.57	1/3368 (0.0%)
1	F	0.36	0/2479	0.57	0/3347
1	G	0.44	0/2479	0.60	0/3347
1	H	0.43	0/2468	0.60	0/3333
All	All	0.41	0/19842	0.60	2/26790 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	33	LEU	CA-CB-CG	6.10	129.33	115.30

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	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2431	0	2478	21	0
1	C	2425	0	2469	18	0
1	D	2431	0	2478	18	0
1	E	2447	0	2500	16	0
1	F	2430	0	2474	20	0
1	G	2430	0	2474	17	0
1	H	2425	0	2469	16	0
2	A	20	0	0	2	0
2	B	20	0	0	3	0
2	C	20	0	0	2	0
2	D	20	0	0	2	0
2	E	20	0	0	2	0
2	F	20	0	0	0	0
2	G	20	0	0	0	0
2	H	20	0	0	1	0
3	A	128	0	0	0	0
3	B	86	0	0	0	0
3	C	137	0	0	4	0
3	D	150	0	0	0	0
3	E	78	0	0	3	0
3	F	74	0	0	0	0
3	G	149	0	0	4	0
3	H	125	0	0	1	0
All	All	20552	0	19838	135	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 (135) 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:142:LYS:HE2	1:B:154:GLN:HG2	1.56	0.85
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.64	0.80
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.65	0.77
1:E:102:ALA:HB3	1:E:149:GLU:HG2	1.67	0.77
1:G:113:TYR:OH	1:G:140[B]:ARG:NH2	2.25	0.69
1:C:264:TYR:CZ	1:C:274:LYS:HG2	2.27	0.69
1:C:9:ASP:N	3:C:502:HOH:O	2.26	0.69
1:B:32:GLN:OE1	1:D:22:ARG:NH1	2.24	0.68
1:F:191:GLY:HA3	1:H:191:GLY:HA3	1.76	0.67
1:C:128:CYS:O	3:C:501:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.75	0.66
1:C:274:LYS:NZ	3:C:505:HOH:O	2.29	0.66
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.82	0.61
1:F:96:SER:HB2	1:F:117:PHE:CZ	2.36	0.61
1:H:274:LYS:O	1:H:313:ARG:NH1	2.32	0.61
1:F:204:LYS:NZ	1:F:322:ASP:OD2	2.31	0.61
1:F:29:GLU:HG2	1:H:22:ARG:HH12	1.64	0.60
1:F:32:GLN:OE1	1:H:22:ARG:NH1	2.34	0.60
1:C:299:LYS:NZ	3:C:508:HOH:O	2.35	0.59
1:C:274:LYS:O	1:C:313:ARG:NH1	2.36	0.58
1:G:274:LYS:NZ	3:G:503:HOH:O	2.36	0.57
1:G:112:LYS:NZ	3:G:501:HOH:O	2.38	0.56
1:A:236:ASN:O	1:A:236:ASN:ND2	2.39	0.56
1:E:183:CYS:HB2	1:E:197:ASP:HB2	1.88	0.55
1:H:126:ILE:HD13	1:H:132:VAL:HG11	1.88	0.55
1:D:155:PRO:HB3	1:D:306:ILE:HD13	1.89	0.55
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.38	0.54
1:E:9:ASP:N	3:E:504:HOH:O	2.40	0.54
1:H:55:HIS:HA	1:H:59:ILE:HG22	1.90	0.53
1:B:142:LYS:HE2	1:B:154:GLN:CG	2.36	0.51
1:G:51:ALA:HA	1:H:188:PRO:HD2	1.92	0.51
1:D:106:GLU:OE2	1:D:109:LYS:HE2	2.11	0.51
1:F:225:GLU:OE1	1:F:334:HIS:NE2	2.39	0.50
1:A:17:VAL:HG12	1:A:31:THR:OG1	2.11	0.50
1:A:71:LYS:HD3	1:A:75:VAL:HG12	1.92	0.50
1:A:112:LYS:HE3	1:A:140[A]:ARG:HH21	1.77	0.50
1:B:22:ARG:HG2	2:B:401[A]:94V:C4	2.41	0.50
1:C:51:ALA:HA	1:D:188:PRO:HD2	1.94	0.50
1:E:225:GLU:O	1:E:229:ARG:HG3	2.13	0.49
1:A:14:THR:HG22	1:A:18:MET:HE3	1.94	0.49
1:C:276:ARG:NH1	1:C:311:HIS:O	2.46	0.49
1:D:78:ASN:HB2	1:D:98:GLU:HG3	1.95	0.49
1:A:51:ALA:HA	1:B:188:PRO:HD2	1.95	0.48
1:E:51:ALA:HA	1:F:188:PRO:HD2	1.94	0.48
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.28	0.48
1:E:216:ALA:HA	1:E:219:PHE:CD2	2.49	0.48
1:A:32:GLN:OE1	1:C:22:ARG:NH1	2.39	0.48
1:B:119:PRO:HA	1:B:134:THR:HG23	1.95	0.48
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.94	0.48
1:D:264:TYR:CE1	1:D:274:LYS:HB2	2.49	0.47
1:D:28:GLY:HA2	2:D:401[A]:94V:C10	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:GLU:OE2	1:G:109:LYS:HE2	2.14	0.47
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.50	0.47
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.44	0.47
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.96	0.47
1:E:33:LEU:HD13	1:E:85:LEU:HD22	1.96	0.47
1:F:33:LEU:HD11	1:F:85:LEU:HD22	1.97	0.46
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.97	0.46
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.97	0.46
1:G:216:ALA:HA	1:G:219:PHE:CD2	2.51	0.46
1:G:120:LEU:HA	1:G:120:LEU:HD12	1.79	0.46
1:A:146:GLU:HG3	1:A:147:PRO:HD2	1.98	0.46
1:D:28:GLY:HA2	2:D:401[A]:94V:O11	2.15	0.46
1:D:72:LYS:HZ3	1:D:72:LYS:HG3	1.56	0.46
1:F:191:GLY:HA2	3:H:609:HOH:O	2.16	0.46
1:H:45:SER:O	1:H:49:ARG:HD3	2.16	0.46
1:F:184:PHE:HB3	1:F:193:PHE:HB3	1.98	0.45
1:F:218:ASP:O	1:F:267:ASN:HB2	2.16	0.45
1:B:45:SER:O	1:B:49:ARG:HD3	2.17	0.45
1:H:28:GLY:HA2	2:H:401[A]:94V:O11	2.16	0.45
1:A:28:GLY:HA2	2:A:401[A]:94V:O11	2.17	0.45
1:E:100:LYS:N	3:E:510:HOH:O	2.48	0.45
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.98	0.45
1:A:275:LEU:HD12	1:A:316:VAL:HG11	1.97	0.45
1:B:183:CYS:SG	1:B:200:VAL:HG21	2.57	0.45
1:B:163:GLY:HA3	1:B:174:VAL:O	2.17	0.45
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.99	0.45
1:A:33:LEU:HD11	1:A:85:LEU:HD22	1.99	0.44
1:A:146:GLU:CG	1:A:147:PRO:HD2	2.47	0.44
1:F:56:LEU:HD23	1:F:56:LEU:HA	1.78	0.44
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.53	0.44
1:E:100:LYS:NZ	3:E:516:HOH:O	2.50	0.44
1:A:218:ASP:OD2	1:A:269:LYS:HE3	2.18	0.44
1:F:53:ILE:HD12	1:F:56:LEU:HD12	1.99	0.44
1:G:45:SER:O	1:G:49:ARG:HD3	2.17	0.44
1:B:183:CYS:HB2	1:B:197:ASP:HB2	2.00	0.44
1:B:121:ASP:N	1:B:133:GLY:O	2.48	0.43
1:B:89:PHE:HA	1:B:109:LYS:O	2.18	0.43
1:G:230:LYS:NZ	3:G:519:HOH:O	2.51	0.43
3:G:579:HOH:O	1:H:52:GLY:HA2	2.18	0.43
1:D:112:LYS:HB2	1:D:140[B]:ARG:NH1	2.33	0.43
1:G:275:LEU:HD12	1:G:316:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLU:O	1:B:330:VAL:HG23	2.19	0.43
1:E:125:ASN:O	1:E:130:VAL:HG12	2.18	0.43
2:A:401[A]:94V:O11	2:A:401[A]:94V:S1	2.77	0.43
1:E:37:LEU:HD21	1:E:136:PHE:CG	2.54	0.43
1:A:184:PHE:HB3	1:A:193:PHE:HB3	2.00	0.43
1:E:28:GLY:HA2	2:E:401[A]:94V:C10	2.49	0.43
1:F:78:ASN:HB2	1:F:98:GLU:HG3	2.01	0.43
1:G:221:PRO:HB2	1:G:334:HIS:ND1	2.34	0.43
1:D:183:CYS:HB2	1:D:197:ASP:HB2	2.00	0.43
1:E:181:VAL:HG21	1:E:291:ALA:HB2	2.01	0.43
2:C:401[A]:94V:O11	2:C:401[A]:94V:S1	2.76	0.42
1:B:28:GLY:HA2	2:B:401[A]:94V:C10	2.49	0.42
1:B:74:ASP:OD1	1:B:74:ASP:N	2.51	0.42
1:B:22:ARG:HH12	1:D:29:GLU:HG2	1.83	0.42
1:C:28:GLY:HA2	2:C:401[A]:94V:C10	2.49	0.42
2:B:401[A]:94V:O11	2:B:401[A]:94V:S1	2.77	0.42
1:C:56:LEU:HD13	1:C:56:LEU:HA	1.89	0.42
1:B:220:ASP:HB2	1:B:268:LYS:NZ	2.34	0.41
1:G:129:LEU:HD12	1:H:166:LEU:HD23	2.01	0.41
1:A:22:ARG:NH1	1:C:32:GLN:OE1	2.51	0.41
1:F:33:LEU:HD12	1:F:33:LEU:HA	1.82	0.41
1:F:74:ASP:N	1:F:74:ASP:OD1	2.54	0.41
1:A:33:LEU:CD1	1:A:85:LEU:HD22	2.51	0.41
1:A:74:ASP:N	1:A:74:ASP:OD1	2.53	0.41
1:D:184:PHE:HB3	1:D:193:PHE:HB3	2.03	0.41
1:H:120:LEU:HD12	1:H:120:LEU:HA	1.91	0.41
1:H:73:LEU:HD12	1:H:73:LEU:HA	1.83	0.41
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.91	0.41
1:E:121:ASP:N	1:E:133:GLY:O	2.48	0.41
2:E:401[A]:94V:S1	2:E:401[A]:94V:O11	2.79	0.41
1:F:220:ASP:HA	1:F:268:LYS:NZ	2.35	0.41
1:A:226:TYR:CE1	1:A:230:LYS:HE3	2.56	0.41
1:E:112:LYS:HD2	1:E:140[B]:ARG:NE	2.36	0.41
1:F:73:LEU:HD23	1:F:126:ILE:HD13	2.02	0.41
1:B:225:GLU:OE1	1:B:334:HIS:NE2	2.32	0.41
1:C:245:VAL:HG23	1:C:254:ARG:HH21	1.85	0.41
1:D:120:LEU:HA	1:D:120:LEU:HD12	1.91	0.41
1:G:37:LEU:HD21	1:G:136:PHE:CG	2.56	0.41
1:A:267:ASN:OD1	1:A:270:SER:N	2.53	0.40
1:H:96:SER:HB2	1:H:117:PHE:CZ	2.57	0.40
1:A:37:LEU:HD21	1:A:136:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PRO:HD2	1:D:51:ALA:HA	2.04	0.40
1:F:233:PRO:HG2	1:F:237:SER:O	2.21	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	316/338 (94%)	311 (98%)	5 (2%)	0	100	100
1	B	314/338 (93%)	306 (98%)	7 (2%)	1 (0%)	41	45
1	C	313/338 (93%)	304 (97%)	9 (3%)	0	100	100
1	D	314/338 (93%)	307 (98%)	7 (2%)	0	100	100
1	E	316/338 (94%)	309 (98%)	7 (2%)	0	100	100
1	F	314/338 (93%)	306 (98%)	8 (2%)	0	100	100
1	G	314/338 (93%)	307 (98%)	7 (2%)	0	100	100
1	H	313/338 (93%)	307 (98%)	6 (2%)	0	100	100
All	All	2514/2704 (93%)	2457 (98%)	56 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	LYS

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	267/281 (95%)	260 (97%)	7 (3%)	46	57
1	B	265/281 (94%)	256 (97%)	9 (3%)	37	46
1	C	264/281 (94%)	256 (97%)	8 (3%)	41	51
1	D	265/281 (94%)	260 (98%)	5 (2%)	57	69
1	E	267/281 (95%)	260 (97%)	7 (3%)	46	57
1	F	265/281 (94%)	259 (98%)	6 (2%)	50	62
1	G	265/281 (94%)	259 (98%)	6 (2%)	50	62
1	H	264/281 (94%)	259 (98%)	5 (2%)	57	69
All	All	2122/2248 (94%)	2069 (98%)	53 (2%)	47	58

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	CYS
1	A	72	LYS
1	A	110	ARG
1	A	264	TYR
1	A	269	LYS
1	A	332	GLU
1	A	335	SER
1	B	33	LEU
1	B	38	CYS
1	B	72	LYS
1	B	110	ARG
1	B	200	VAL
1	B	220	ASP
1	B	264	TYR
1	B	268	LYS
1	B	335	SER
1	C	38	CYS
1	C	72	LYS
1	C	110	ARG
1	C	264	TYR
1	C	269	LYS
1	C	274	LYS
1	C	278	LEU
1	C	335	SER

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Mol	Chain	Res	Type
1	D	38	CYS
1	D	110	ARG
1	D	178	ASP
1	D	264	TYR
1	D	335	SER
1	E	33	LEU
1	E	38	CYS
1	E	56	LEU
1	E	72	LYS
1	E	264	TYR
1	E	268	LYS
1	E	335	SER
1	F	38	CYS
1	F	72	LYS
1	F	110	ARG
1	F	200	VAL
1	F	264	TYR
1	F	268	LYS
1	G	38	CYS
1	G	72	LYS
1	G	73	LEU
1	G	236	ASN
1	G	264	TYR
1	G	269	LYS
1	H	38	CYS
1	H	101	HIS
1	H	110	ARG
1	H	264	TYR
1	H	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	94V	D	401[A]	-	18,21,21	0.75	0	21,30,30	0.77	1 (4%)
2	94V	G	401[A]	-	18,21,21	0.76	1 (5%)	21,30,30	0.82	1 (4%)
2	94V	F	401[A]	-	18,21,21	0.64	0	21,30,30	0.76	1 (4%)
2	94V	H	401[A]	-	18,21,21	0.75	0	21,30,30	0.75	1 (4%)
2	94V	A	401[A]	-	18,21,21	0.52	0	21,30,30	0.81	1 (4%)
2	94V	C	401[A]	-	18,21,21	0.96	0	21,30,30	0.90	1 (4%)
2	94V	B	401[A]	-	18,21,21	0.65	0	21,30,30	0.75	1 (4%)
2	94V	E	401[A]	-	18,21,21	0.89	1 (5%)	21,30,30	0.83	1 (4%)

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	94V	D	401[A]	-	-	3/13/15/15	0/2/2/2
2	94V	G	401[A]	-	-	1/13/15/15	0/2/2/2
2	94V	F	401[A]	-	-	2/13/15/15	0/2/2/2
2	94V	H	401[A]	-	-	4/13/15/15	0/2/2/2
2	94V	A	401[A]	-	-	4/13/15/15	0/2/2/2
2	94V	C	401[A]	-	-	3/13/15/15	0/2/2/2
2	94V	B	401[A]	-	-	3/13/15/15	0/2/2/2
2	94V	E	401[A]	-	-	1/13/15/15	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401[A]	94V	C10-N7	2.45	1.42	1.37
2	G	401[A]	94V	C2-N7	2.05	1.40	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401[A]	94V	BR6-C5-C4	2.47	128.40	124.51
2	A	401[A]	94V	BR6-C5-C4	2.41	128.31	124.51
2	C	401[A]	94V	BR6-C5-C4	2.40	128.29	124.51
2	D	401[A]	94V	BR6-C5-C4	2.31	128.15	124.51
2	G	401[A]	94V	BR6-C5-C4	2.28	128.10	124.51
2	H	401[A]	94V	BR6-C5-C4	2.27	128.08	124.51
2	B	401[A]	94V	BR6-C5-C4	2.27	128.07	124.51
2	F	401[A]	94V	BR6-C5-C4	2.20	127.97	124.51

There are no chirality outliers.

All (21) torsion outliers are listed below:

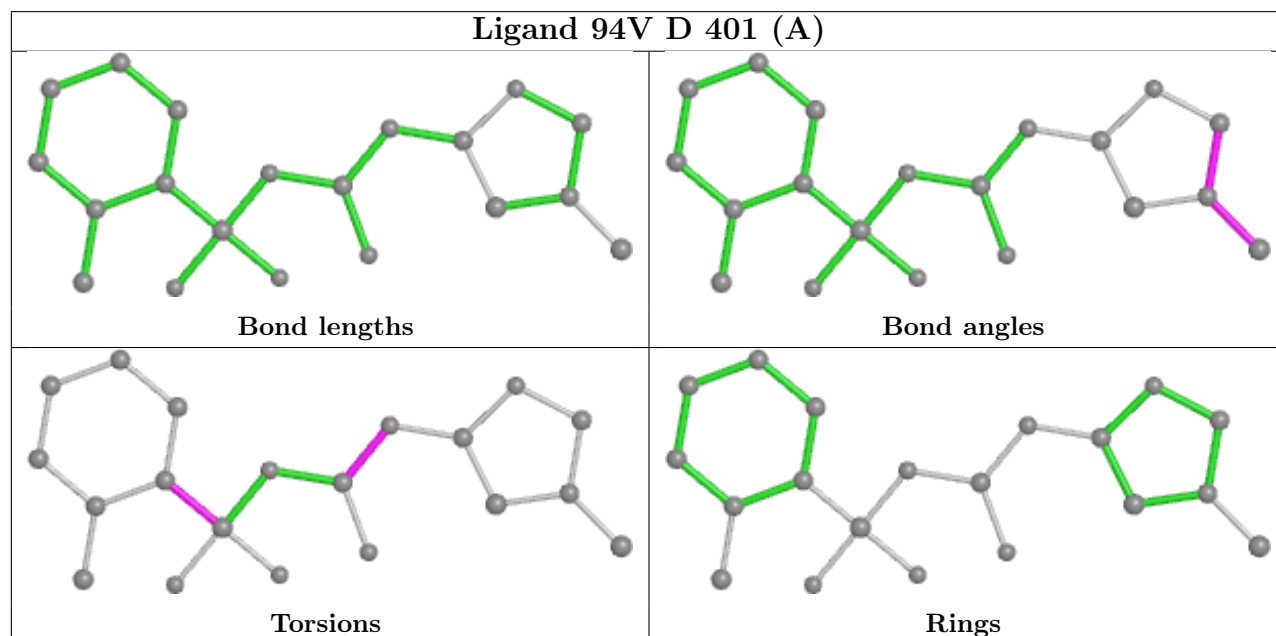
Mol	Chain	Res	Type	Atoms
2	D	401[A]	94V	N9-C10-N7-C2
2	G	401[A]	94V	N9-C10-N7-C2
2	F	401[A]	94V	N9-C10-N7-C2
2	H	401[A]	94V	N9-C10-N7-C2
2	A	401[A]	94V	N9-C10-N7-C2
2	C	401[A]	94V	N9-C10-N7-C2
2	B	401[A]	94V	N9-C10-N7-C2
2	E	401[A]	94V	N9-C10-N7-C2
2	B	401[A]	94V	C16-C14-S8-O13
2	C	401[A]	94V	C16-C14-S8-N9
2	A	401[A]	94V	C10-N9-S8-O13
2	H	401[A]	94V	C16-C14-S8-O13
2	C	401[A]	94V	C16-C14-S8-O13
2	B	401[A]	94V	C16-C14-S8-N9
2	H	401[A]	94V	C10-N9-S8-O13
2	H	401[A]	94V	C10-N9-S8-O12
2	A	401[A]	94V	C10-N9-S8-O12
2	D	401[A]	94V	C16-C14-S8-N9
2	F	401[A]	94V	C16-C14-S8-N9
2	D	401[A]	94V	C16-C14-S8-O13
2	A	401[A]	94V	C16-C14-S8-O13

There are no ring outliers.

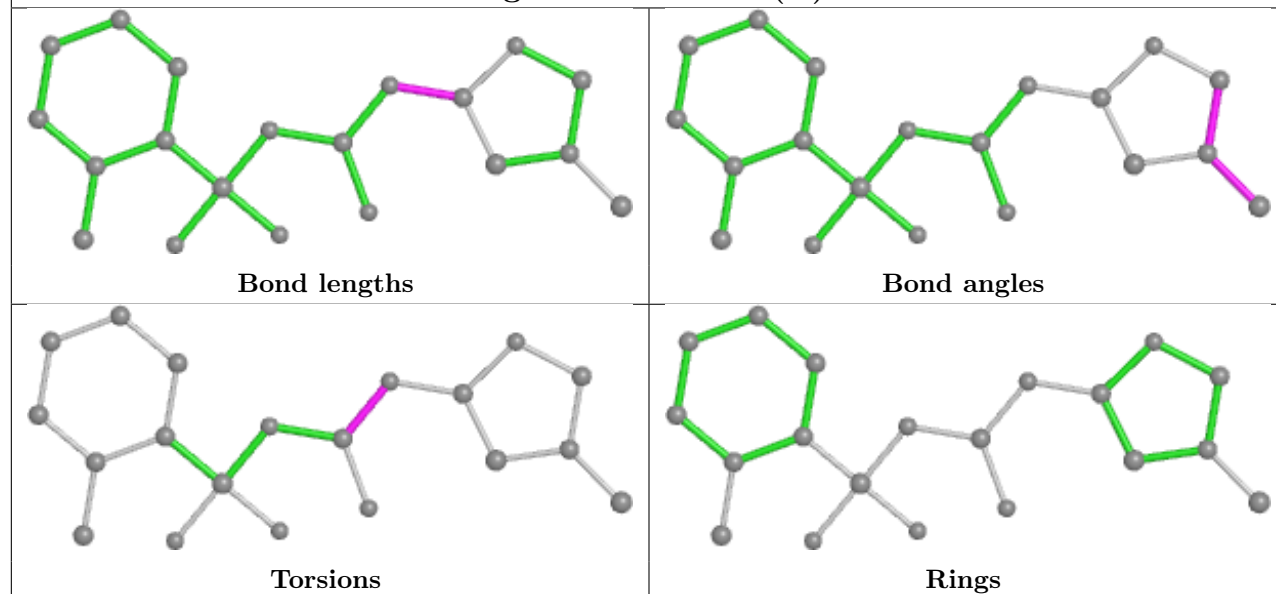
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401[A]	94V	2	0
2	H	401[A]	94V	1	0
2	A	401[A]	94V	2	0
2	C	401[A]	94V	2	0
2	B	401[A]	94V	3	0
2	E	401[A]	94V	2	0

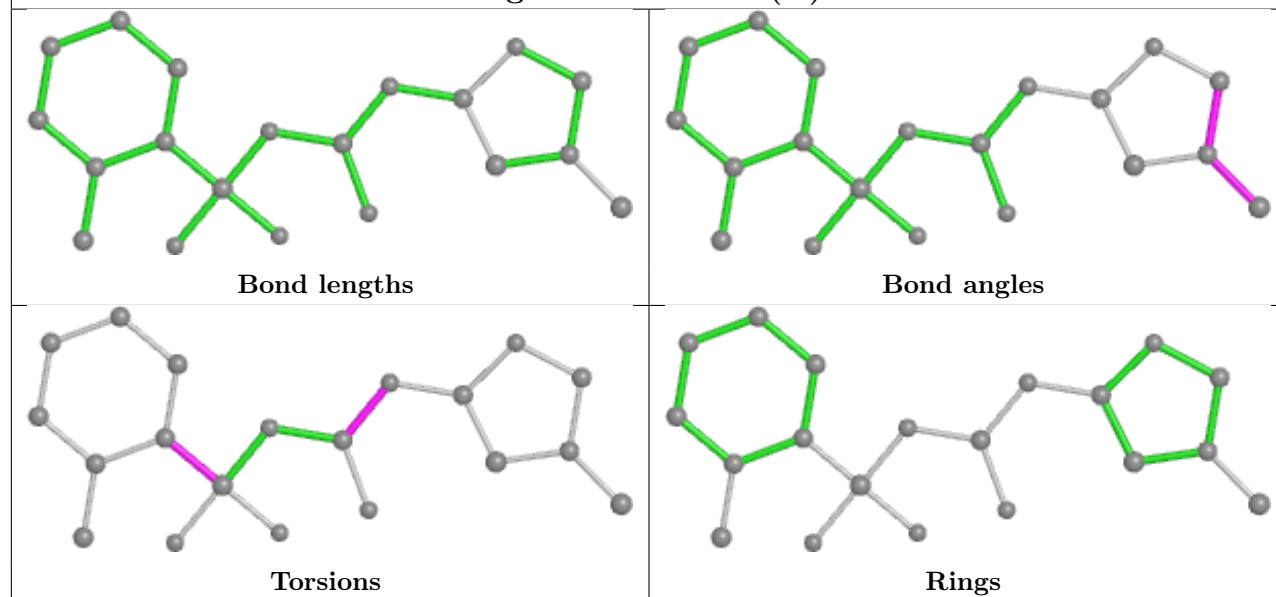
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



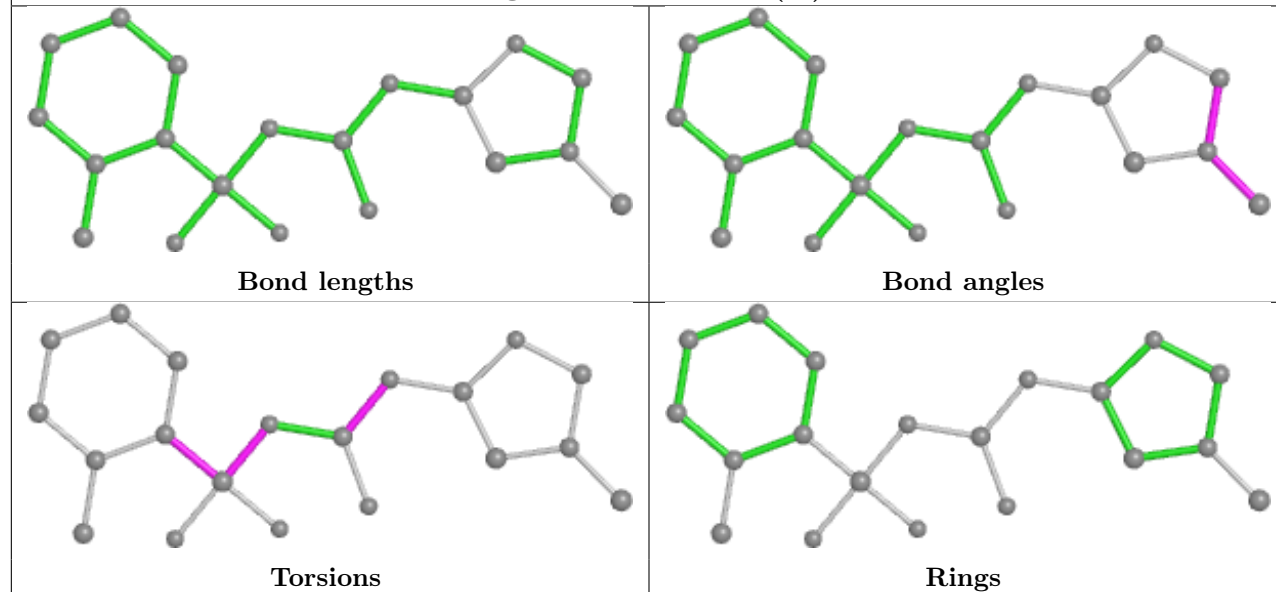
Ligand 94V G 401 (A)



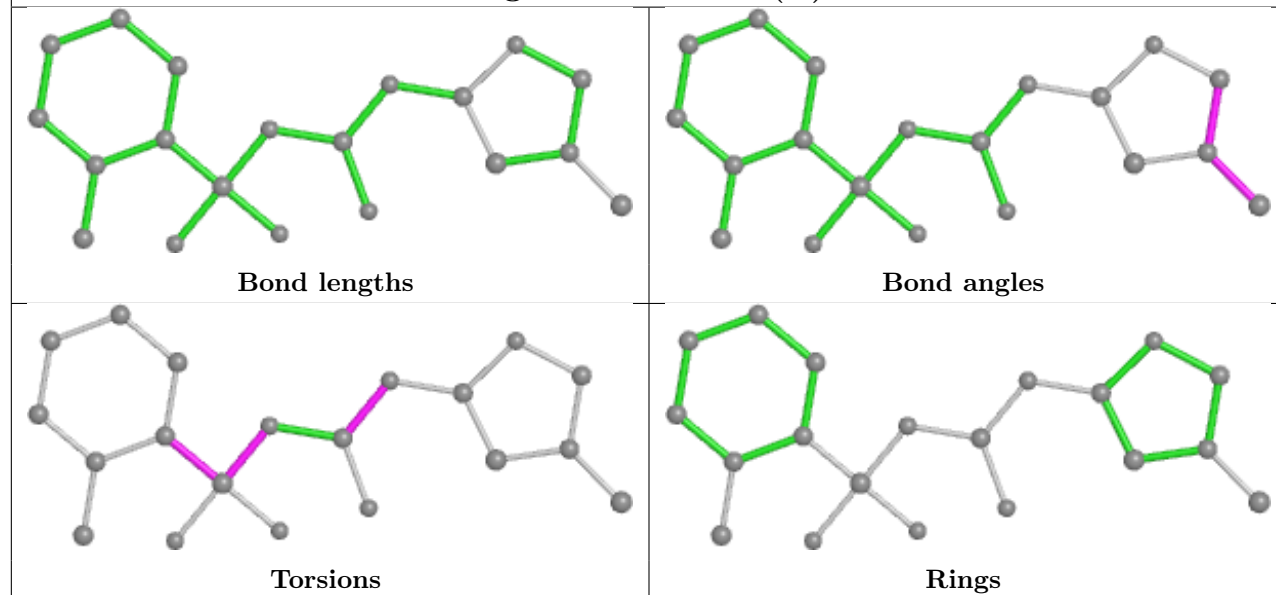
Ligand 94V F 401 (A)



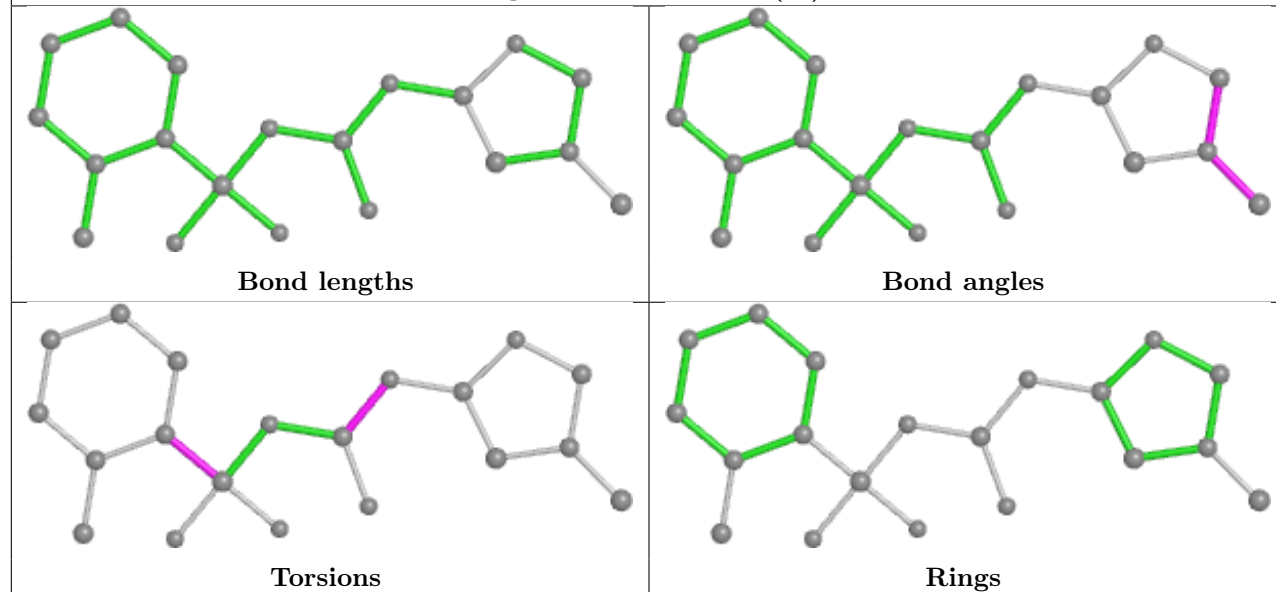
Ligand 94V H 401 (A)



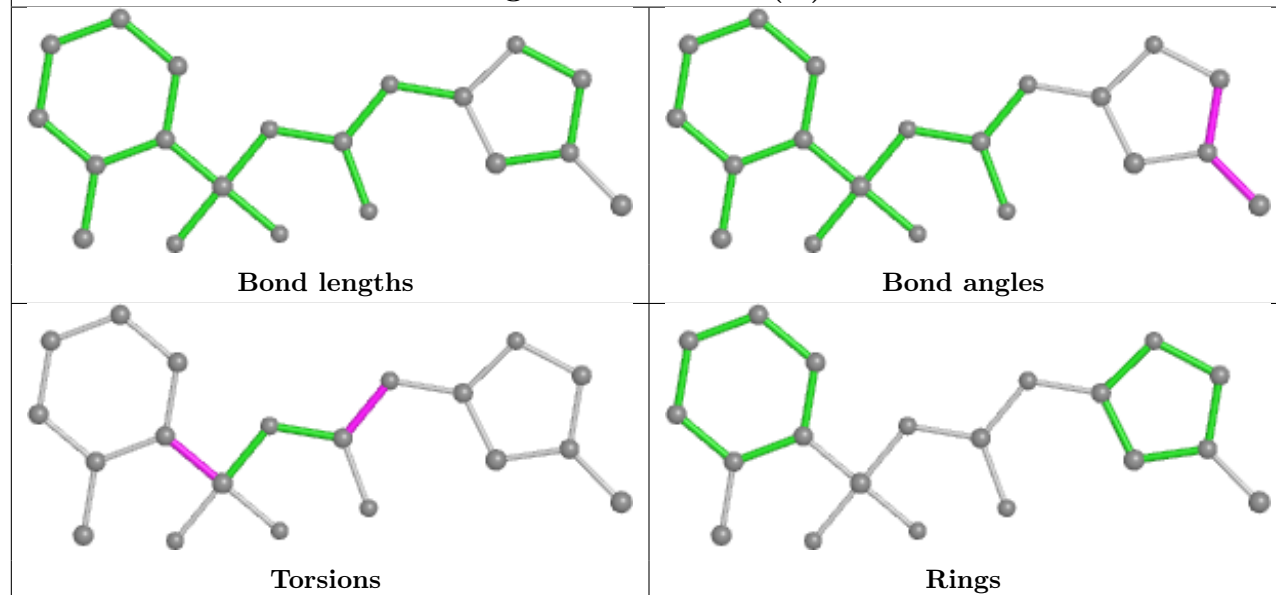
Ligand 94V A 401 (A)

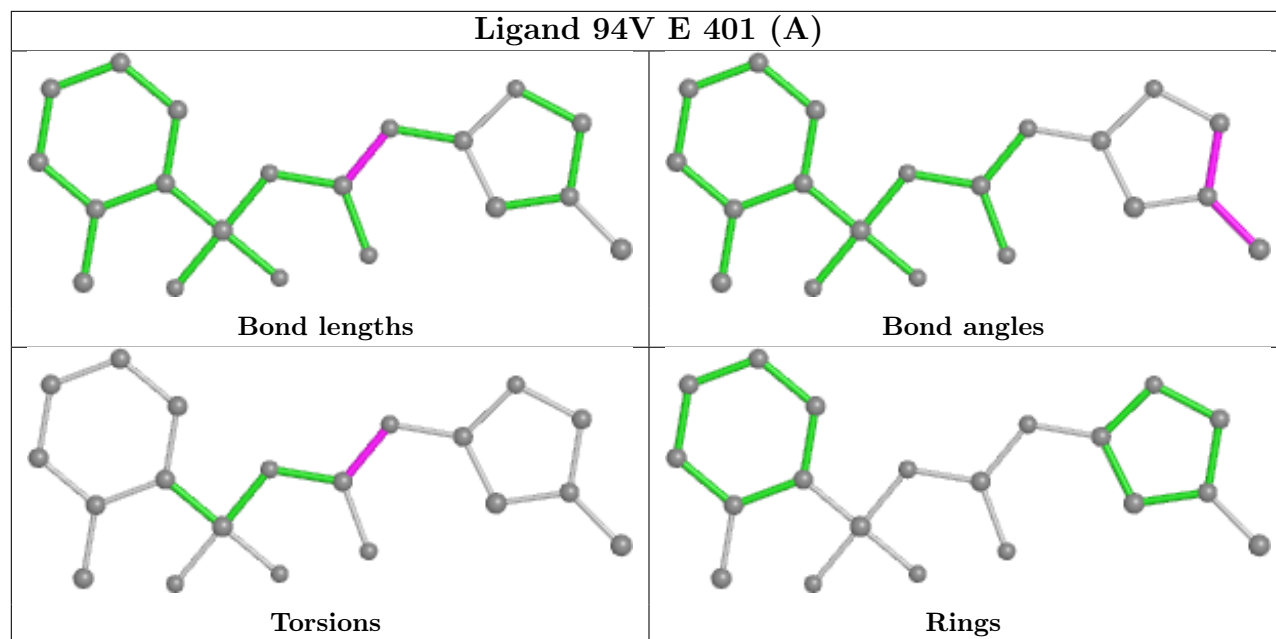


Ligand 94V C 401 (A)



Ligand 94V B 401 (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 ⓘ

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%)	-0.18	7 (2%) 62 60	21, 37, 68, 113	0
1	B	317/338 (93%)	-0.11	9 (2%) 53 51	22, 40, 78, 127	0
1	C	317/338 (93%)	-0.36	2 (0%) 89 88	20, 32, 60, 88	0
1	D	317/338 (93%)	-0.36	5 (1%) 72 70	17, 31, 57, 96	0
1	E	319/338 (94%)	0.01	19 (5%) 21 20	26, 45, 83, 121	0
1	F	317/338 (93%)	-0.02	21 (6%) 18 17	26, 46, 88, 115	0
1	G	317/338 (93%)	-0.33	2 (0%) 89 88	22, 34, 66, 88	0
1	H	317/338 (93%)	-0.22	5 (1%) 72 70	22, 38, 64, 88	0
All	All	2540/2704 (93%)	-0.19	70 (2%) 53 51	17, 38, 72, 127	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	7.7
1	A	70	VAL	6.5
1	E	268	LYS	4.8
1	E	235	ASP	4.6
1	B	144	THR	4.4
1	A	268	LYS	4.4
1	A	144	THR	4.4
1	F	144	THR	4.3
1	E	237	SER	4.2
1	B	236	ASN	4.0
1	H	236	ASN	3.8
1	F	234	PRO	3.7
1	F	25	ARG	3.7
1	E	269	LYS	3.6
1	B	142	LYS	3.6
1	E	236	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	335	SER	3.5
1	C	236	ASN	3.4
1	B	269	LYS	3.3
1	D	236	ASN	3.2
1	F	269	LYS	3.1
1	F	268	LYS	3.0
1	G	236	ASN	3.0
1	E	334	HIS	3.0
1	H	269	LYS	2.9
1	E	335	SER	2.9
1	A	335	SER	2.9
1	F	125	ASN	2.8
1	F	236	ASN	2.8
1	G	237	SER	2.8
1	B	268	LYS	2.8
1	B	125	ASN	2.6
1	F	109	LYS	2.6
1	D	269	LYS	2.6
1	F	108	GLU	2.6
1	E	234	PRO	2.6
1	E	238	ALA	2.5
1	F	271	PRO	2.5
1	H	268	LYS	2.5
1	F	23	LYS	2.5
1	F	142	LYS	2.5
1	B	25	ARG	2.4
1	A	25	ARG	2.4
1	F	143	SER	2.4
1	E	25	ARG	2.4
1	E	218	ASP	2.4
1	E	274	LYS	2.4
1	F	263	LEU	2.4
1	D	25	ARG	2.3
1	A	234	PRO	2.2
1	F	145	ASP	2.2
1	E	100	LYS	2.2
1	H	107	PRO	2.2
1	E	108	GLU	2.2
1	F	106	GLU	2.2
1	F	262	PHE	2.1
1	E	178	ASP	2.1
1	B	143	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	263	LEU	2.1
1	F	107	PRO	2.1
1	F	124	SER	2.1
1	H	25	ARG	2.1
1	D	268	LYS	2.1
1	E	23	LYS	2.1
1	B	145	ASP	2.1
1	E	71	LYS	2.0
1	A	145	ASP	2.0
1	F	235	ASP	2.0
1	C	23	LYS	2.0
1	F	179	CYS	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.

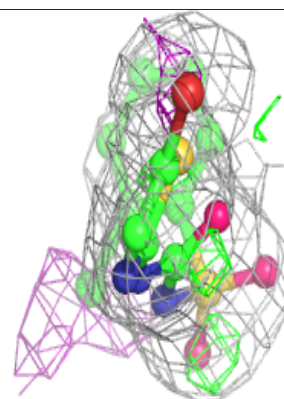
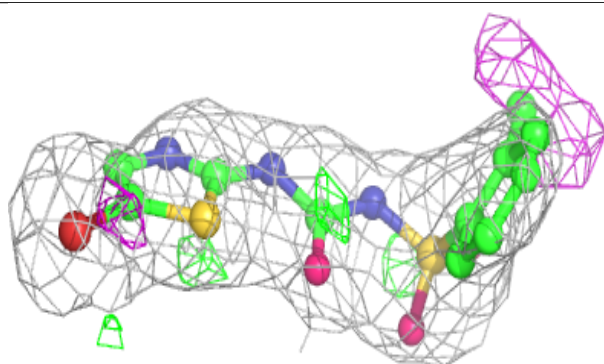
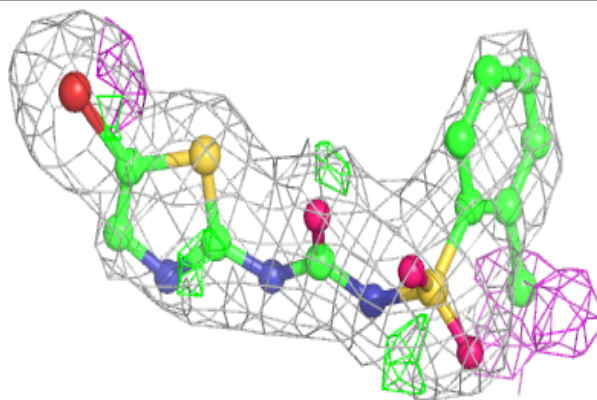
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	94V	F	401[A]	20/20	0.93	0.15	46,59,76,102	20
2	94V	G	401[A]	20/20	0.95	0.12	28,33,52,73	20
2	94V	A	401[A]	20/20	0.95	0.12	20,36,62,86	0
2	94V	B	401[A]	20/20	0.95	0.13	29,37,63,75	20
2	94V	E	401[A]	20/20	0.95	0.13	27,42,63,101	0
2	94V	H	401[A]	20/20	0.96	0.12	44,57,81,97	0
2	94V	D	401[A]	20/20	0.96	0.11	31,47,73,95	0
2	94V	C	401[A]	20/20	0.97	0.10	24,36,50,73	20

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.

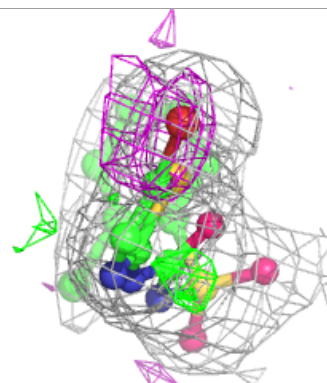
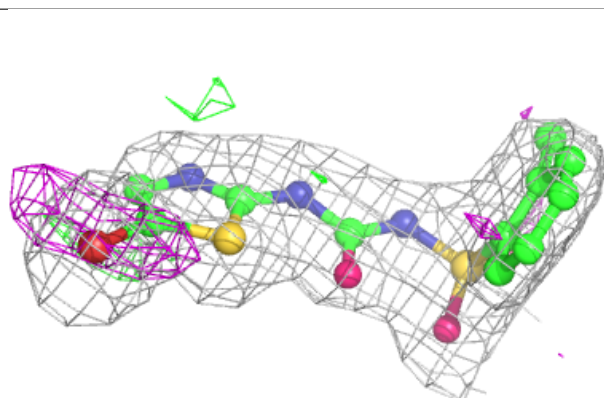
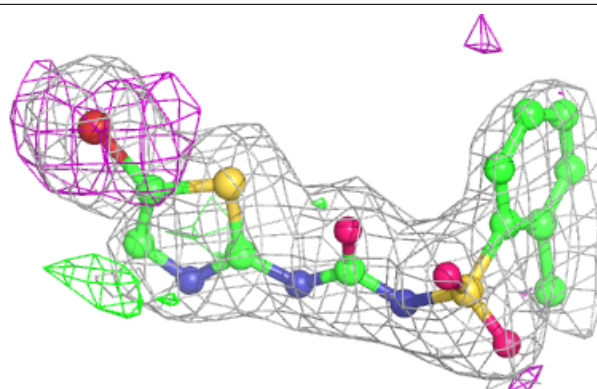
Electron density around 94V F 401 (A):

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



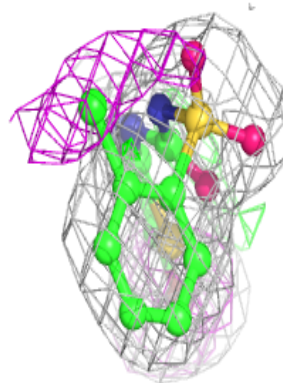
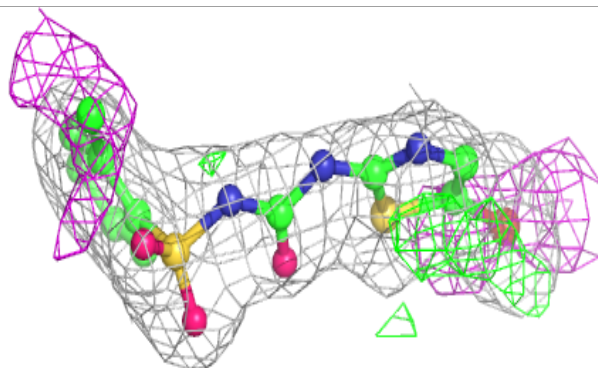
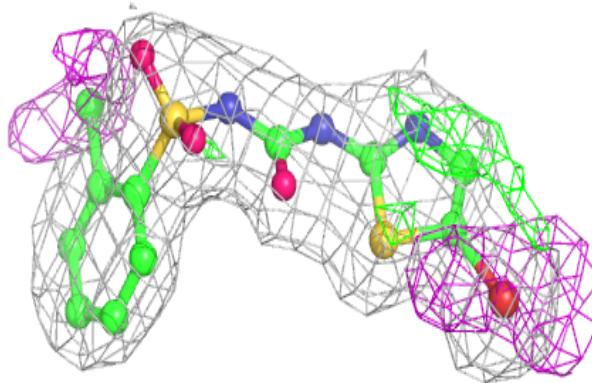
Electron density around 94V G 401 (A):

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

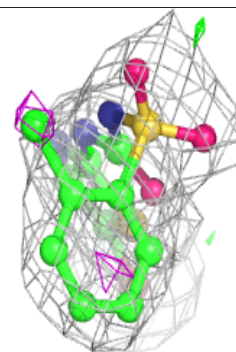
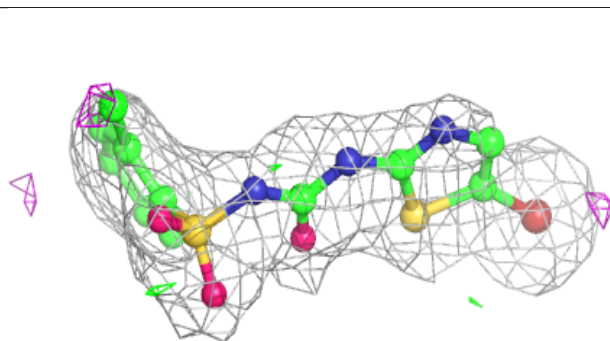
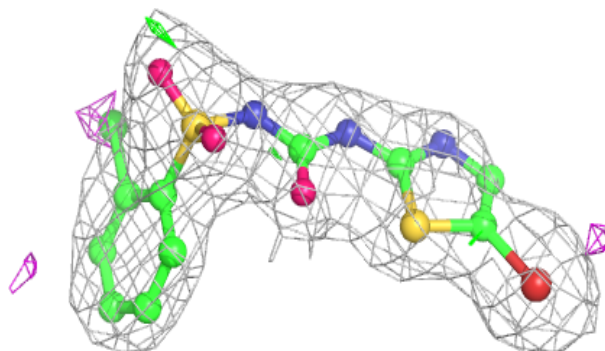


Electron density around 94V A 401 (A):

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

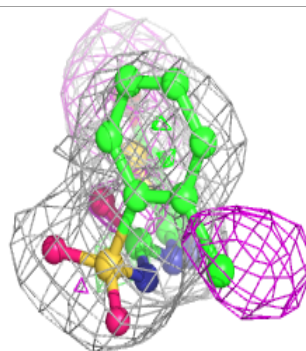
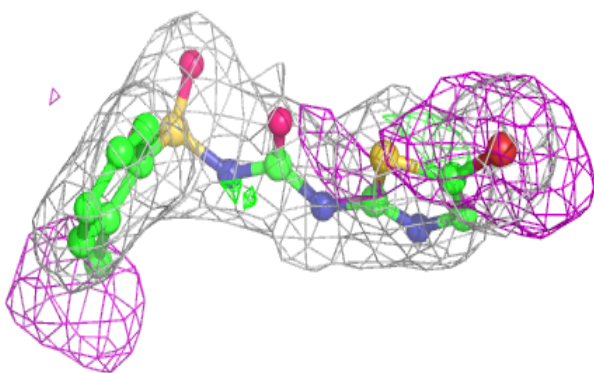
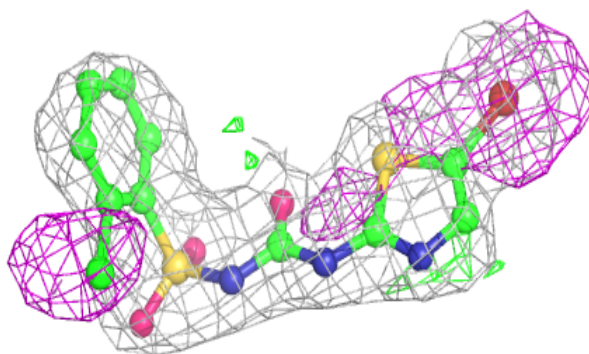
**Electron density around 94V B 401 (A):**

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

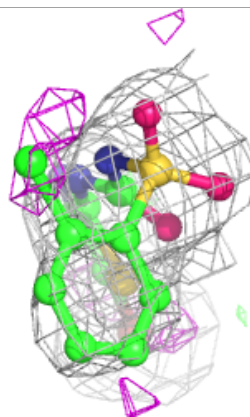
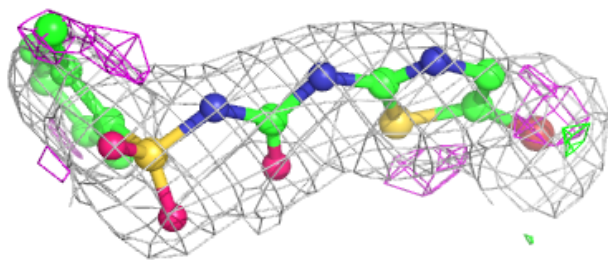
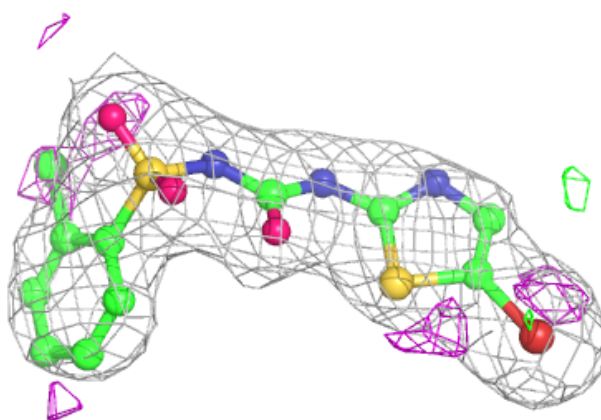


Electron density around 94V E 401 (A):

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

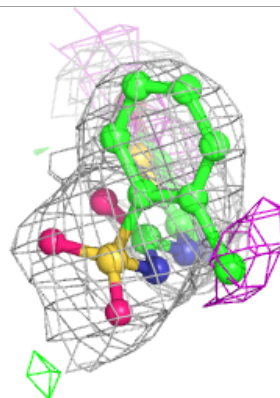
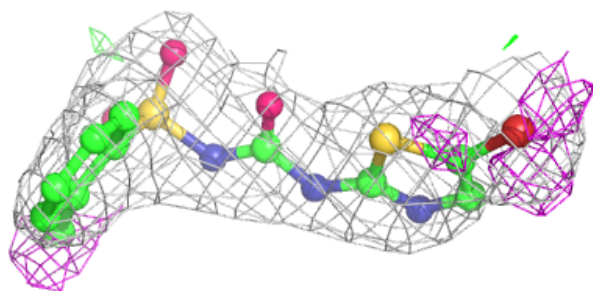
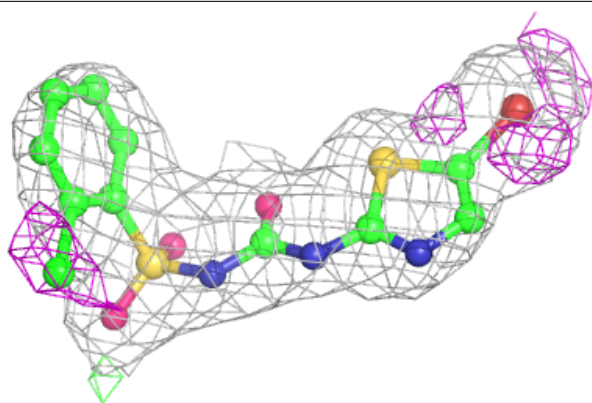
**Electron density around 94V H 401 (A):**

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

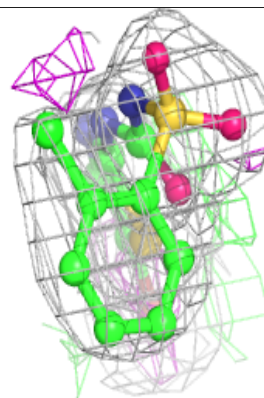
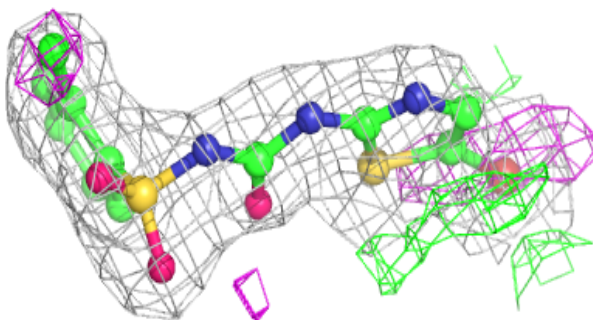
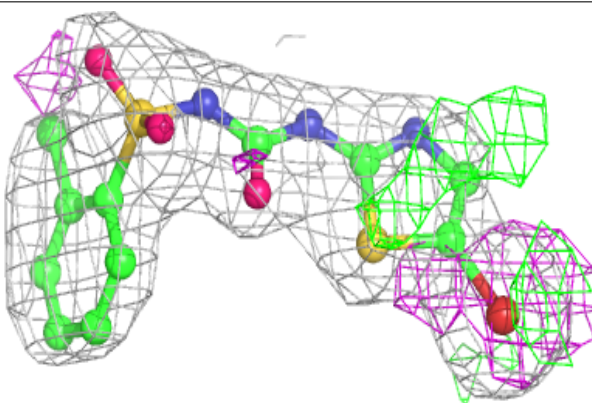


Electron density around 94V D 401 (A):

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

**Electron density around 94V C 401 (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.