Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 01:55 AM UTC

PDB ID	:	5F91 / pdb_00005f91
Title	:	Fumarate hydratase of Mycobacterium tuberculosis in complex with formate and allosteric modulator (N-(5-(azepan-1-ylsulfonyl)-2-methoxyphenyl)-2-(4-oxo-3,4-dihydrophthalazin-1-yl)acetamide)
Authors	:	Kasbekar, M.; Fischer, G.; Mott, B.T.; Yasgar, A.; Hyvonen, M.; Boshoff, H.I.; Abell, C.; Barry, C.E.; Thomas, C.J.
Deposited on	:	2015-12-09
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

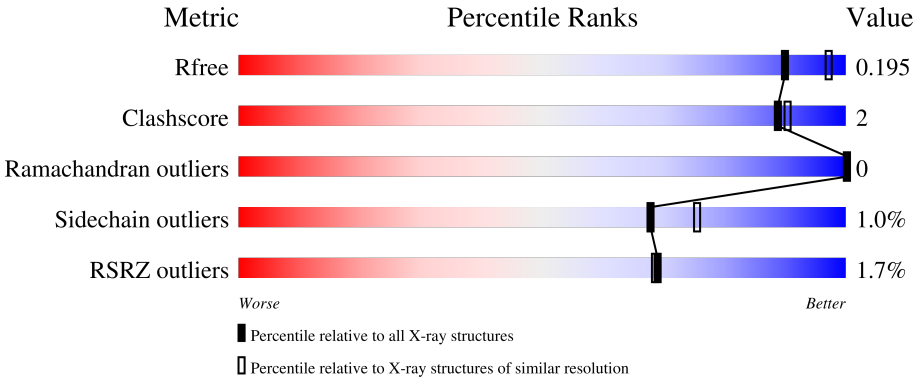
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 <=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	495	2% 86% · 10%
1	B	495	2% 87% · 9%
1	C	495	% 86% · 9%
1	D	495	% 85% · 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14886 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 Fumarate hydratase class II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	30	1	0
			3313	2064	604	635	10			
1	B	452	Total	C	N	O	S	55	1	0
			3351	2087	610	643	11			
1	C	448	Total	C	N	O	S	15	1	0
			3341	2081	609	640	11			
1	D	440	Total	C	N	O	S	35	1	0
			3258	2031	593	624	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WN92
A	-19	HIS	-	expression tag	UNP P9WN92
A	-18	HIS	-	expression tag	UNP P9WN92
A	-17	HIS	-	expression tag	UNP P9WN92
A	-16	HIS	-	expression tag	UNP P9WN92
A	-15	HIS	-	expression tag	UNP P9WN92
A	-14	HIS	-	expression tag	UNP P9WN92
A	-13	SER	-	expression tag	UNP P9WN92
A	-12	SER	-	expression tag	UNP P9WN92
A	-11	GLY	-	expression tag	UNP P9WN92
A	-10	VAL	-	expression tag	UNP P9WN92
A	-9	ASP	-	expression tag	UNP P9WN92
A	-8	LEU	-	expression tag	UNP P9WN92
A	-7	GLY	-	expression tag	UNP P9WN92
A	-6	THR	-	expression tag	UNP P9WN92
A	-5	GLU	-	expression tag	UNP P9WN92
A	-4	ASN	-	expression tag	UNP P9WN92
A	-3	LEU	-	expression tag	UNP P9WN92
A	-2	TYR	-	expression tag	UNP P9WN92
A	-1	PHE	-	expression tag	UNP P9WN92
A	0	GLN	-	expression tag	UNP P9WN92

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P9WN92
B	-20	MET	-	initiating methionine	UNP P9WN92
B	-19	HIS	-	expression tag	UNP P9WN92
B	-18	HIS	-	expression tag	UNP P9WN92
B	-17	HIS	-	expression tag	UNP P9WN92
B	-16	HIS	-	expression tag	UNP P9WN92
B	-15	HIS	-	expression tag	UNP P9WN92
B	-14	HIS	-	expression tag	UNP P9WN92
B	-13	SER	-	expression tag	UNP P9WN92
B	-12	SER	-	expression tag	UNP P9WN92
B	-11	GLY	-	expression tag	UNP P9WN92
B	-10	VAL	-	expression tag	UNP P9WN92
B	-9	ASP	-	expression tag	UNP P9WN92
B	-8	LEU	-	expression tag	UNP P9WN92
B	-7	GLY	-	expression tag	UNP P9WN92
B	-6	THR	-	expression tag	UNP P9WN92
B	-5	GLU	-	expression tag	UNP P9WN92
B	-4	ASN	-	expression tag	UNP P9WN92
B	-3	LEU	-	expression tag	UNP P9WN92
B	-2	TYR	-	expression tag	UNP P9WN92
B	-1	PHE	-	expression tag	UNP P9WN92
B	0	GLN	-	expression tag	UNP P9WN92
B	1	SER	-	expression tag	UNP P9WN92
C	-20	MET	-	initiating methionine	UNP P9WN92
C	-19	HIS	-	expression tag	UNP P9WN92
C	-18	HIS	-	expression tag	UNP P9WN92
C	-17	HIS	-	expression tag	UNP P9WN92
C	-16	HIS	-	expression tag	UNP P9WN92
C	-15	HIS	-	expression tag	UNP P9WN92
C	-14	HIS	-	expression tag	UNP P9WN92
C	-13	SER	-	expression tag	UNP P9WN92
C	-12	SER	-	expression tag	UNP P9WN92
C	-11	GLY	-	expression tag	UNP P9WN92
C	-10	VAL	-	expression tag	UNP P9WN92
C	-9	ASP	-	expression tag	UNP P9WN92
C	-8	LEU	-	expression tag	UNP P9WN92
C	-7	GLY	-	expression tag	UNP P9WN92
C	-6	THR	-	expression tag	UNP P9WN92
C	-5	GLU	-	expression tag	UNP P9WN92
C	-4	ASN	-	expression tag	UNP P9WN92
C	-3	LEU	-	expression tag	UNP P9WN92
C	-2	TYR	-	expression tag	UNP P9WN92

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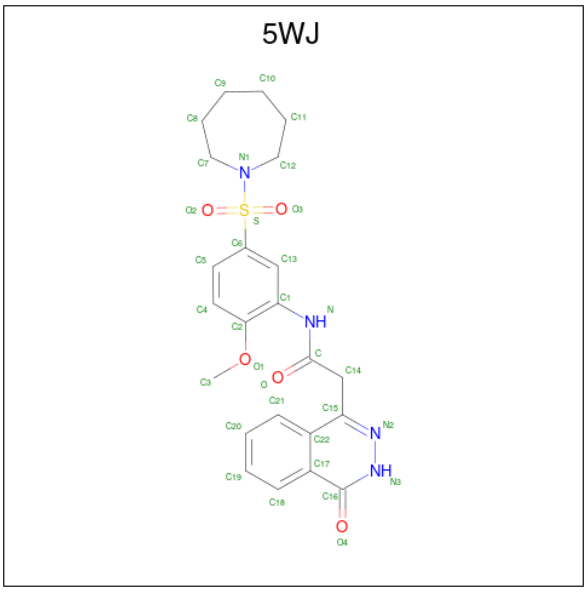
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PHE	-	expression tag	UNP P9WN92
C	0	GLN	-	expression tag	UNP P9WN92
C	1	SER	-	expression tag	UNP P9WN92
D	-20	MET	-	initiating methionine	UNP P9WN92
D	-19	HIS	-	expression tag	UNP P9WN92
D	-18	HIS	-	expression tag	UNP P9WN92
D	-17	HIS	-	expression tag	UNP P9WN92
D	-16	HIS	-	expression tag	UNP P9WN92
D	-15	HIS	-	expression tag	UNP P9WN92
D	-14	HIS	-	expression tag	UNP P9WN92
D	-13	SER	-	expression tag	UNP P9WN92
D	-12	SER	-	expression tag	UNP P9WN92
D	-11	GLY	-	expression tag	UNP P9WN92
D	-10	VAL	-	expression tag	UNP P9WN92
D	-9	ASP	-	expression tag	UNP P9WN92
D	-8	LEU	-	expression tag	UNP P9WN92
D	-7	GLY	-	expression tag	UNP P9WN92
D	-6	THR	-	expression tag	UNP P9WN92
D	-5	GLU	-	expression tag	UNP P9WN92
D	-4	ASN	-	expression tag	UNP P9WN92
D	-3	LEU	-	expression tag	UNP P9WN92
D	-2	TYR	-	expression tag	UNP P9WN92
D	-1	PHE	-	expression tag	UNP P9WN92
D	0	GLN	-	expression tag	UNP P9WN92
D	1	SER	-	expression tag	UNP P9WN92

- Molecule 2 is {N}-[5-(azepan-1-ylsulfonyl)-2-methoxy-phenyl]-2-(4-oxidanylidene-3 {H}-phthalazin-1-yl)ethanamide (CCD ID: 5WJ) (formula: $C_{23}H_{26}N_4O_5S$).

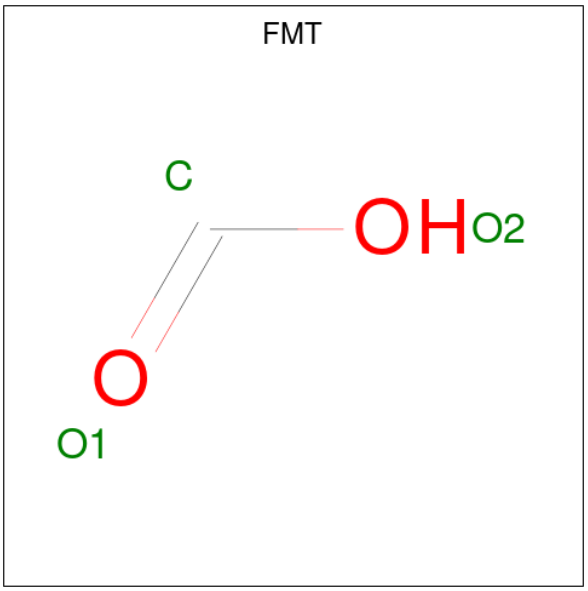


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 33 23 4 5 1	0	0
2	C	1	Total C N O S 33 23 4 5 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	3	Total Cl 3 3	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

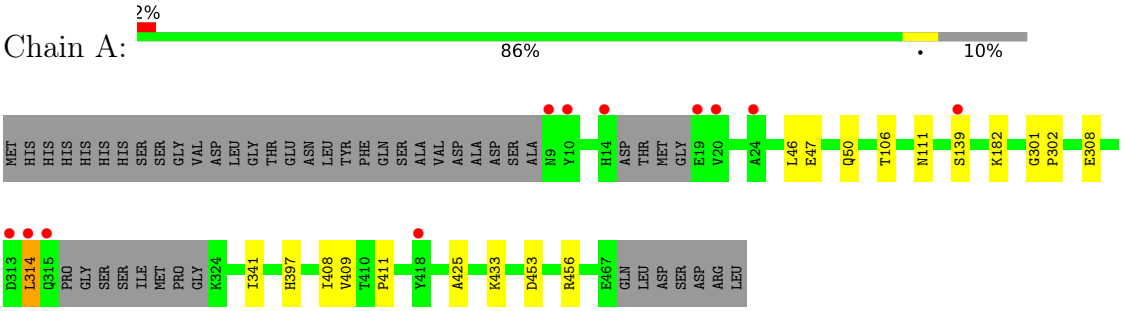
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	440	Total O 440 440	0	0
5	B	384	Total O 384 384	0	0
5	C	380	Total O 380 380	0	0
5	D	345	Total O 345 345	0	0

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.

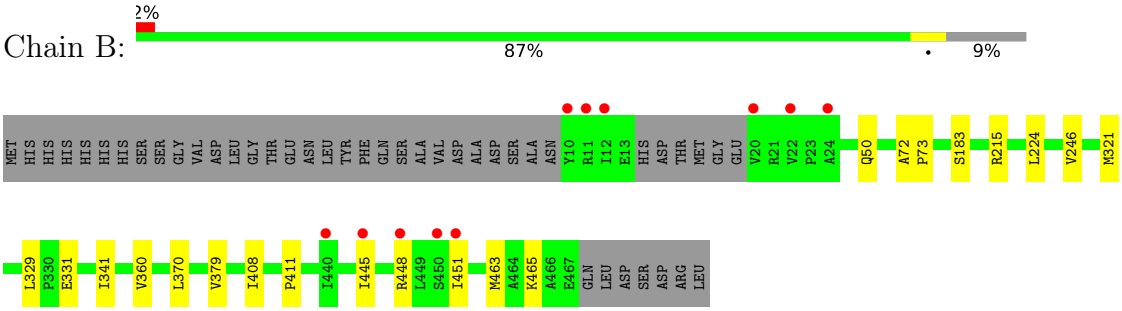
• Molecule 1: Fumarate hydratase class II

Chain A:



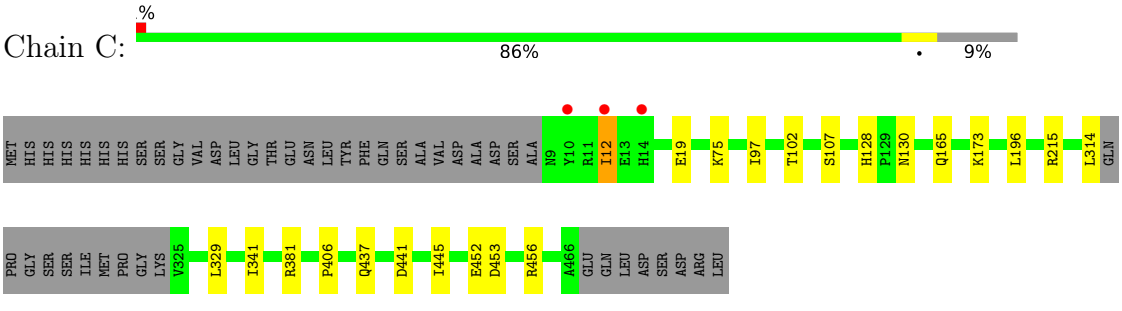
• Molecule 1: Fumarate hydratase class II

Chain B:



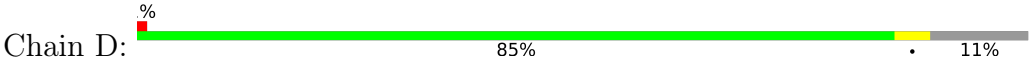
• Molecule 1: Fumarate hydratase class II

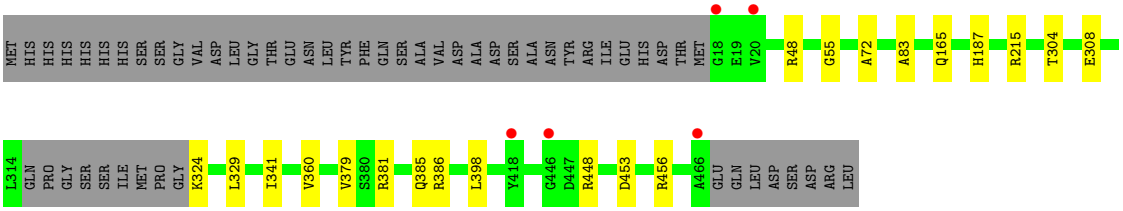
Chain C:



• Molecule 1: Fumarate hydratase class II

Chain D:




MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER ALA VAL ASP ALA ASP SER ALA ASN TYR ARG ILE GLU HIS ASP THR MET G18 E19 V20 R48 G55 A72 A83 Q165 H187 R215 T304 E308
L314 GLN PRO GLY SER SER ILE MET PRO GLY K324 L329 I341 V360 V379 S380 R381 Q385 R386 L398 Y418 G446 D447 R448 D453 R456 A466 GLU GLN LEU ASP SER ASP ARG LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.21Å 96.50Å 124.38Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	48.81 – 2.00 48.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.81-2.00) 95.1 (48.81-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.194 0.153 , 0.195	Depositor DCC
R_{free} test set	6505 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14886	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5WJ, FMT, CL

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	0.48	0/3359	0.75	0/4564
1	B	0.51	0/3397	0.78	2/4617 (0.0%)
1	C	0.47	0/3390	0.77	0/4607
1	D	0.48	0/3302	0.76	2/4490 (0.0%)
All	All	0.49	0/13448	0.76	4/18278 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	MET	CA-C-N	6.67	126.92	119.32
1	B	321	MET	C-N-CA	6.67	126.92	119.32
1	D	72	ALA	CA-C-N	5.07	125.10	119.32
1	D	72	ALA	C-N-CA	5.07	125.10	119.32

There are no chirality outliers.

There are no planarity outliers.

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	3313	0	3345	12	0
1	B	3351	0	3389	11	0
1	C	3341	0	3382	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3258	0	3296	14	0
2	A	33	0	0	0	0
2	C	33	0	0	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
4	B	3	0	1	0	0
5	A	440	0	0	3	0
5	B	384	0	0	4	0
5	C	380	0	0	5	0
5	D	345	0	0	7	0
All	All	14886	0	13413	50	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 2.

All (50) 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:165:GLN:OE1	1:D:381:ARG:NH2	2.14	0.79
1:B:445:ILE:HD13	1:B:451:ILE:HG12	1.66	0.77
5:B:834:HOH:O	1:C:102:THR:HG21	1.87	0.72
1:B:465:LYS:NZ	5:B:601:HOH:O	2.23	0.71
1:D:453:ASP:OD1	1:D:456:ARG:NH1	2.26	0.66
1:C:165:GLN:OE1	1:C:381:ARG:NH1	2.29	0.66
1:A:46:LEU:HD22	1:A:50:GLN:HG2	1.79	0.64
1:C:453:ASP:OD1	1:C:456:ARG:NH2	2.30	0.63
1:B:408:ILE:HB	1:B:463:MET:HE1	1.82	0.61
1:B:360:VAL:HG22	5:B:814:HOH:O	2.02	0.60
1:C:75:LYS:NZ	5:C:609:HOH:O	2.38	0.55
1:B:411:PRO:HG2	1:B:463:MET:HE2	1.89	0.55
1:D:48:ARG:HG2	5:D:627:HOH:O	2.07	0.54
1:C:128:HIS:CE1	1:C:130:ASN:HB2	2.45	0.52
1:A:47:GLU:HG3	5:A:919:HOH:O	2.09	0.51
1:D:360:VAL:HG22	5:D:761:HOH:O	2.12	0.50
1:C:97:ILE:HD13	1:C:107:SER:HB3	1.94	0.49
1:C:452:GLU:OE1	5:C:601:HOH:O	2.17	0.49
1:C:12:ILE:HD11	1:C:19:GLU:HB3	1.95	0.48
1:D:308:GLU:HB3	1:D:398:LEU:HD21	1.94	0.48
1:A:409:VAL:HG11	1:A:425:ALA:HB2	1.96	0.48
1:D:385:GLN:NE2	5:D:612:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:HIS:NE2	5:A:607:HOH:O	2.30	0.47
1:D:381:ARG:NH1	5:D:605:HOH:O	2.32	0.47
1:C:406:PRO:HD2	5:C:653:HOH:O	2.15	0.46
1:C:215[A]:ARG:NH1	5:C:605:HOH:O	2.32	0.46
1:B:215[B]:ARG:NH1	5:B:603:HOH:O	2.35	0.45
1:A:111:ASN:HD22	1:A:111:ASN:C	2.25	0.45
1:D:324:LYS:N	5:D:619:HOH:O	2.50	0.44
1:D:386:ARG:NH2	5:D:620:HOH:O	2.51	0.44
1:C:445:ILE:O	5:C:602:HOH:O	2.21	0.44
1:D:215:ARG:NH1	5:D:606:HOH:O	2.36	0.43
1:C:437:GLN:NE2	1:C:441:ASP:OD1	2.48	0.42
1:A:408:ILE:O	1:A:411:PRO:HD2	2.19	0.42
1:A:433:LYS:NZ	5:A:624:HOH:O	2.51	0.42
1:B:50:GLN:HG2	1:B:370:LEU:CD1	2.50	0.42
1:B:331:GLU:OE2	1:D:187:HIS:ND1	2.38	0.42
1:C:128:HIS:HE1	1:C:130:ASN:HB2	1.83	0.42
1:A:182:LYS:NZ	1:A:308:GLU:OE1	2.50	0.42
1:A:453:ASP:OD1	1:A:456:ARG:NH2	2.46	0.42
1:C:173:LYS:HD3	1:C:173:LYS:HA	1.93	0.42
1:B:183:SER:HB2	1:D:304:THR:HG21	2.00	0.41
1:C:329:LEU:HD23	1:C:329:LEU:HA	1.78	0.41
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.94	0.41
1:D:55:GLY:O	1:D:83:ALA:HB1	2.21	0.41
1:D:329:LEU:HD23	1:D:329:LEU:HA	1.80	0.41
1:B:72:ALA:HA	1:B:73:PRO:HD3	1.93	0.41
1:A:301:GLY:HA3	1:A:302:PRO:HA	1.88	0.41
1:B:224:LEU:HD12	1:B:246:VAL:HG22	2.02	0.41
1:A:106:THR:HB	1:A:139:SER:HB2	2.02	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	442/495 (89%)	433 (98%)	9 (2%)	0	100	100
1	B	449/495 (91%)	439 (98%)	10 (2%)	0	100	100
1	C	445/495 (90%)	435 (98%)	10 (2%)	0	100	100
1	D	437/495 (88%)	427 (98%)	10 (2%)	0	100	100
All	All	1773/1980 (90%)	1734 (98%)	39 (2%)	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	338/383 (88%)	336 (99%)	2 (1%)	78	85
1	B	344/383 (90%)	340 (99%)	4 (1%)	63	70
1	C	344/383 (90%)	340 (99%)	4 (1%)	63	70
1	D	333/383 (87%)	330 (99%)	3 (1%)	70	78
All	All	1359/1532 (89%)	1346 (99%)	13 (1%)	68	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	LEU
1	A	341	ILE
1	B	329	LEU
1	B	341	ILE
1	B	379	VAL
1	B	448	ARG
1	C	12	ILE
1	C	196	LEU
1	C	314	LEU
1	C	341	ILE
1	D	341	ILE
1	D	379	VAL
1	D	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	178	HIS
1	A	268	GLN
1	A	339	GLN
1	A	368	ASN
1	A	437	GLN
1	B	158	HIS
1	B	236	ASN
1	B	339	GLN
1	B	368	ASN
1	B	385	GLN
1	C	63	GLN
1	C	339	GLN
1	C	368	ASN
1	D	63	GLN
1	D	339	GLN
1	D	343	ASN
1	D	368	ASN
1	D	397	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)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5WJ	A	501	-	36,36,36	1.53	3 (8%)	44,51,51	1.54	9 (20%)
4	FMT	B	501	-	2,2,2	0.75	0	1,1,1	0.27	0
2	5WJ	C	501	-	36,36,36	1.57	3 (8%)	44,51,51	1.55	10 (22%)

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	5WJ	A	501	-	-	7/22/31/31	0/4/4/4
2	5WJ	C	501	-	-	7/22/31/31	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	5WJ	C6-S	-5.33	1.69	1.76
2	A	501	5WJ	C6-S	-5.30	1.69	1.76
2	C	501	5WJ	C16-N3	4.51	1.42	1.35
2	C	501	5WJ	C15-N2	4.29	1.32	1.29
2	A	501	5WJ	C15-N2	4.25	1.32	1.29
2	A	501	5WJ	C16-N3	3.87	1.41	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	5WJ	O2-S-N1	4.34	110.77	106.69
2	A	501	5WJ	O2-S-N1	4.24	110.68	106.69
2	C	501	5WJ	C6-S-N1	-4.05	102.38	107.28
2	A	501	5WJ	C4-C5-C6	3.16	122.51	119.44
2	A	501	5WJ	C5-C6-C13	-2.94	117.05	120.68
2	A	501	5WJ	C2-C1-N	2.77	121.88	116.73
2	C	501	5WJ	C5-C6-C13	-2.63	117.43	120.68
2	A	501	5WJ	O4-C16-N3	-2.59	117.57	120.88
2	C	501	5WJ	O4-C16-N3	-2.54	117.62	120.88
2	A	501	5WJ	C6-S-N1	-2.52	104.24	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	5WJ	C2-C1-N	2.44	121.27	116.73
2	C	501	5WJ	C5-C6-S	2.32	122.04	119.73
2	C	501	5WJ	C16-N3-N2	-2.28	125.44	127.98
2	A	501	5WJ	C14-C-N	2.26	117.64	115.06
2	A	501	5WJ	O4-C16-C17	2.22	127.24	123.27
2	A	501	5WJ	C5-C6-S	2.18	121.90	119.73
2	C	501	5WJ	O4-C16-C17	2.12	127.06	123.27
2	C	501	5WJ	C14-C-N	2.10	117.46	115.06
2	C	501	5WJ	C4-C5-C6	2.04	121.43	119.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	5WJ	C12-N1-S-O2
2	A	501	5WJ	C12-N1-S-O3
2	C	501	5WJ	C12-N1-S-O3
2	C	501	5WJ	C12-N1-S-O2
2	C	501	5WJ	C5-C6-S-O3
2	C	501	5WJ	C5-C6-S-N1
2	A	501	5WJ	C5-C6-S-O3
2	C	501	5WJ	C13-C6-S-O3
2	A	501	5WJ	C5-C6-S-N1
2	A	501	5WJ	C12-N1-S-C6
2	A	501	5WJ	C13-C6-S-O3
2	C	501	5WJ	C13-C6-S-N1
2	A	501	5WJ	C13-C6-S-N1
2	C	501	5WJ	C12-N1-S-C6

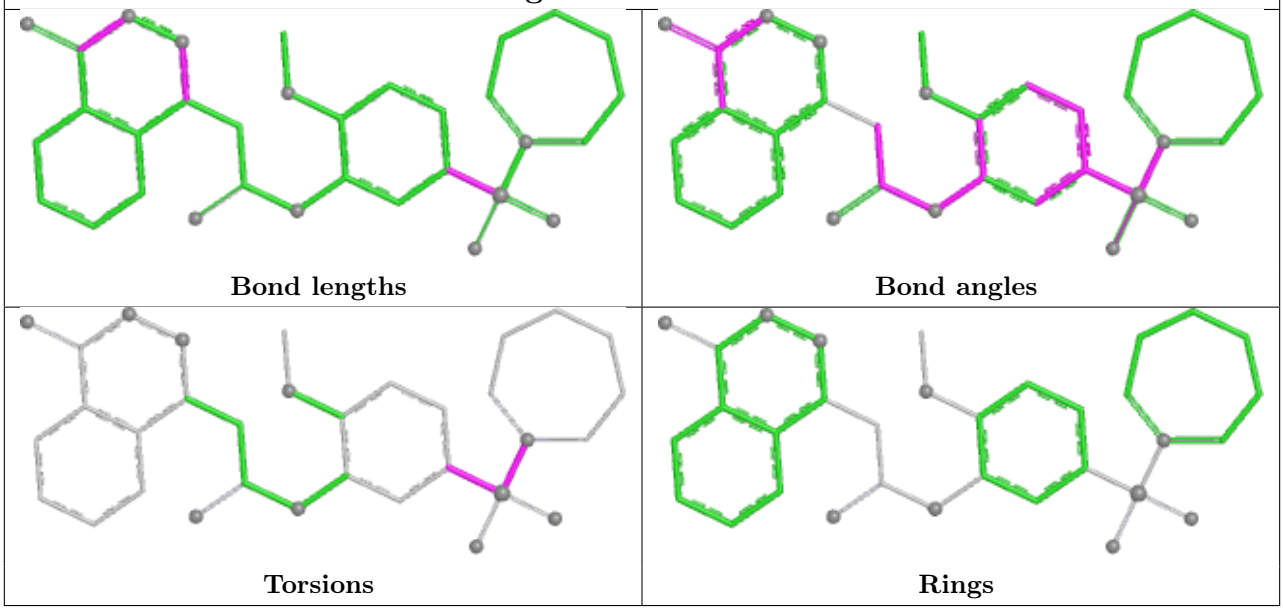
There are no ring outliers.

No monomer is involved in short contacts.

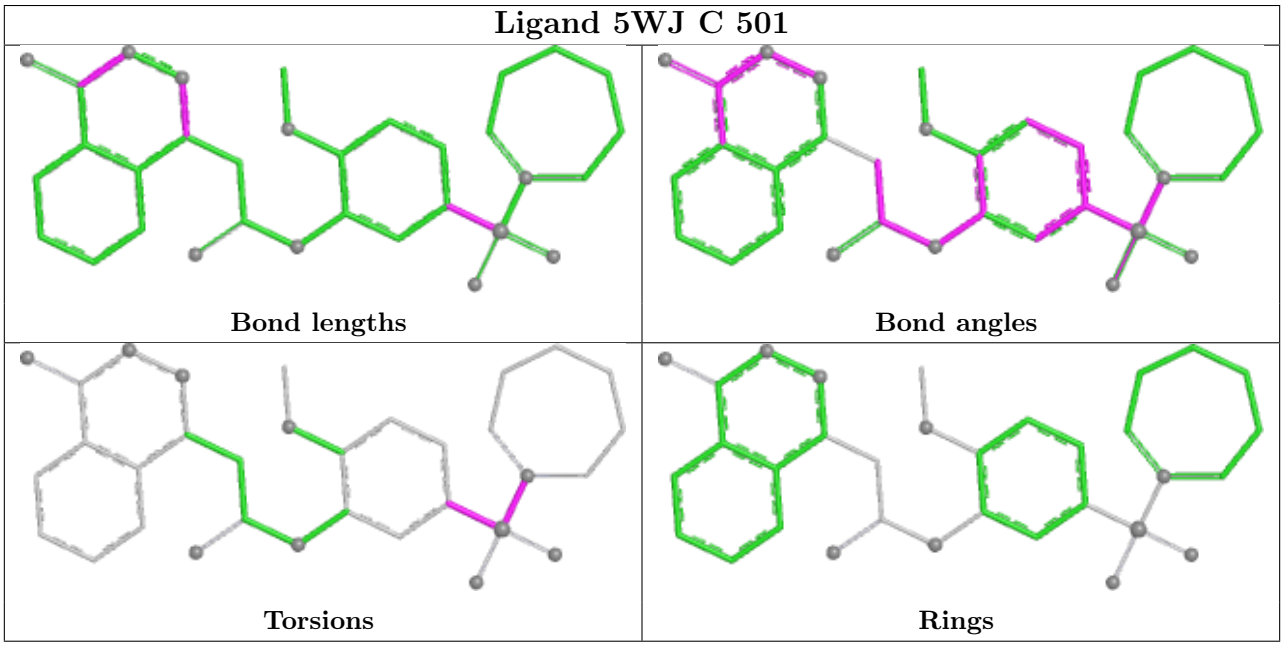
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5WJ A 501



Ligand 5WJ C 501



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, 95^{th} 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	447/495 (90%)	-0.46	11 (2%)	58	58	11, 21, 42, 70	8 (1%)
1	B	452/495 (91%)	-0.35	11 (2%)	59	59	9, 22, 49, 66	13 (2%)
1	C	448/495 (90%)	-0.37	3 (0%)	84	84	12, 22, 45, 78	5 (1%)
1	D	440/495 (88%)	-0.34	5 (1%)	78	77	13, 21, 48, 72	10 (2%)
All	All	1787/1980 (90%)	-0.38	30 (1%)	69	68	9, 21, 46, 78	36 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	TYR	3.9
1	D	18	GLY	3.9
1	A	14	HIS	3.8
1	B	12	ILE	3.6
1	C	10	TYR	3.5
1	B	450	SER	3.3
1	A	314	LEU	3.0
1	A	10	TYR	2.9
1	A	9	ASN	2.9
1	A	313	ASP	2.9
1	C	14	HIS	2.7
1	A	315	GLN	2.6
1	A	20	VAL	2.6
1	B	22	VAL	2.6
1	B	24	ALA	2.6
1	B	451	ILE	2.5
1	B	20	VAL	2.5
1	D	466	ALA	2.4
1	A	24	ALA	2.4
1	D	418	TYR	2.3
1	C	12	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	448	ARG	2.3
1	D	446	GLY	2.3
1	A	139	SER	2.3
1	B	445	ILE	2.2
1	B	11	ARG	2.2
1	A	19	GLU	2.1
1	A	418	TYR	2.1
1	D	20	VAL	2.0
1	B	440	ILE	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)

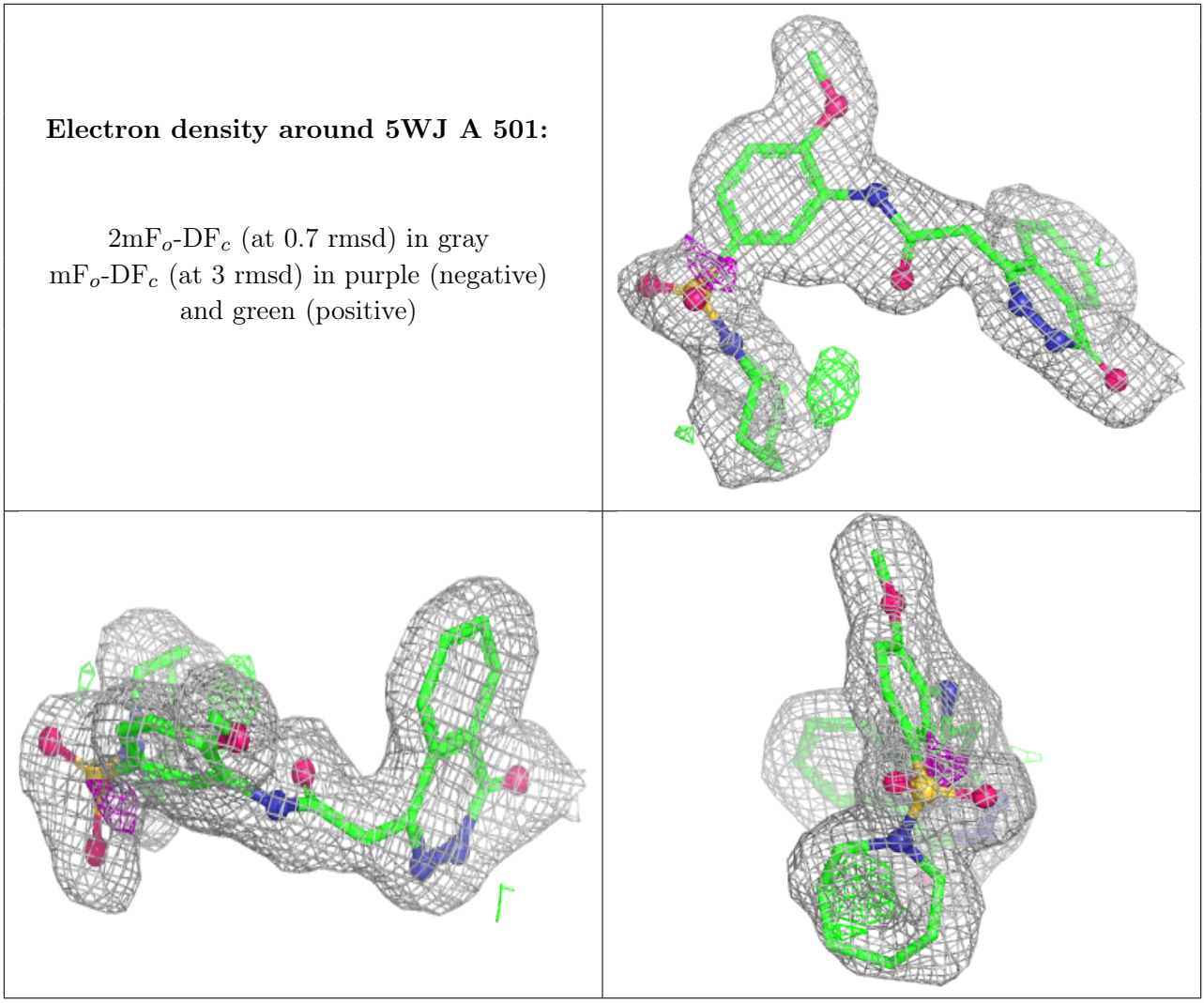
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	CL	B	503	1/1	0.91	0.17	71,71,71,71	0
3	CL	A	502	1/1	0.92	0.11	66,66,66,66	0
3	CL	B	502	1/1	0.94	0.10	68,68,68,68	0
3	CL	B	504	1/1	0.95	0.10	58,58,58,58	0
3	CL	D	501	1/1	0.95	0.09	63,63,63,63	0
2	5WJ	A	501	33/33	0.96	0.07	21,25,38,50	0
4	FMT	B	501	3/3	0.96	0.06	24,24,29,31	0
2	5WJ	C	501	33/33	0.97	0.06	18,24,37,55	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.

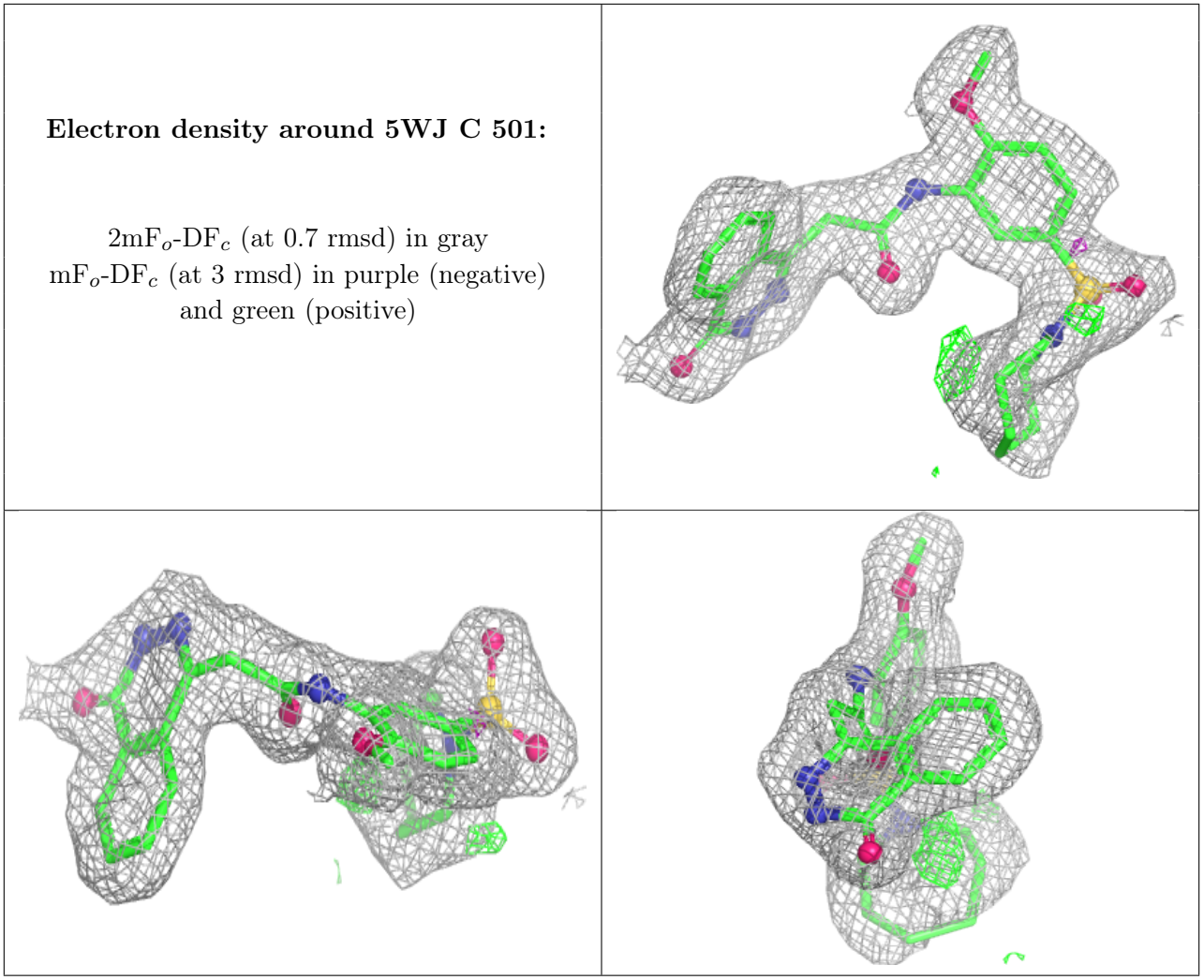
Electron density around 5WJ A 501:

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



Electron density around 5WJ C 501:

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



6.5 Other polymers

There are no such residues in this entry.