Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 03:47 pm GMT

PDB ID	:	6Q9N
Title	:	Crystal structure of PBP2a from MRSA in complex with piperacillin and quinazolinone
Authors	:	Martinez-Caballero, S.; Batuecas, M.T.; Hermoso, J.A.
Deposited on	:	2018-12-18
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

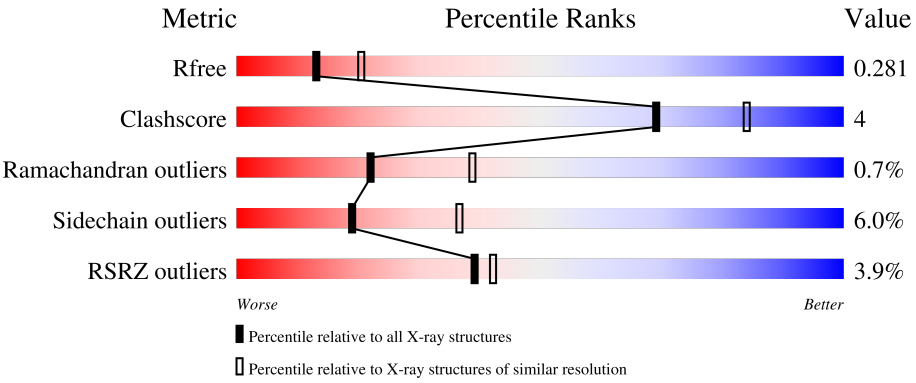
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	642	3% 86% 12%
1	B	642	5% 85% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MUR	A	707	-	-	-	X

2 Entry composition

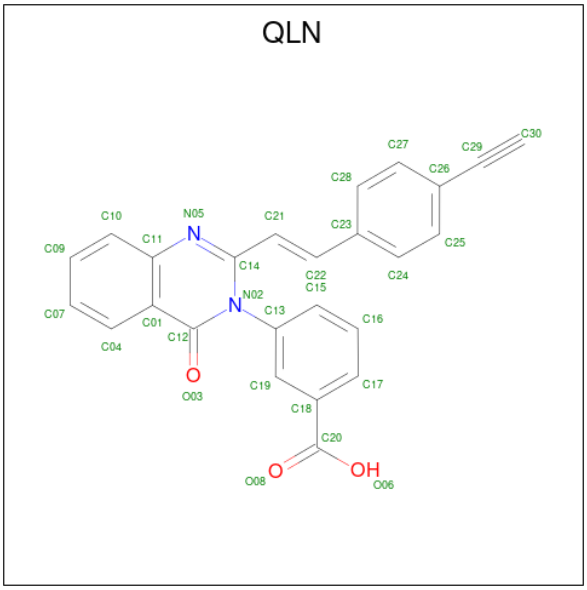
There are 7 unique types of molecules in this entry. The entry contains 10419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin binding protein 2 prime.

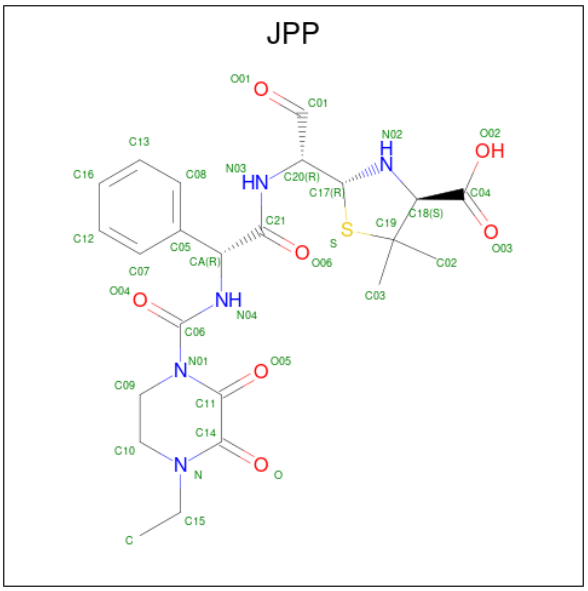
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	1	0
			5127	3231	865	1016	15			
1	B	637	Total	C	N	O	S	0	0	0
			5112	3223	863	1011	15			

- Molecule 2 is 3-[2-[({E})-2-(4-ethynylphenyl)ethenyl]-4-oxidanylidene-quinazolin-3-yl]benzoic acid (three-letter code: QLN) (formula: $C_{25}H_{16}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	25	2	3		

- Molecule 3 is Piperacillin (Open Form) (three-letter code: JPP) (formula: $C_{23}H_{29}N_5O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 36 23 5 7 1	0	0

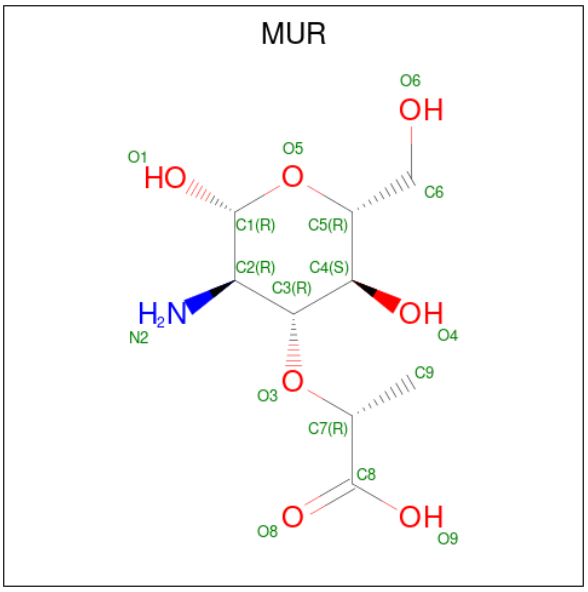
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	2	Total Cl 2 2	0	0

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cd 2 2	0	0
5	B	2	Total Cd 2 2	0	0

- Molecule 6 is beta-muramic acid (three-letter code: MUR) (formula: $C_9H_{17}NO_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 17 9 1 7	0	0

- Molecule 7 is water.

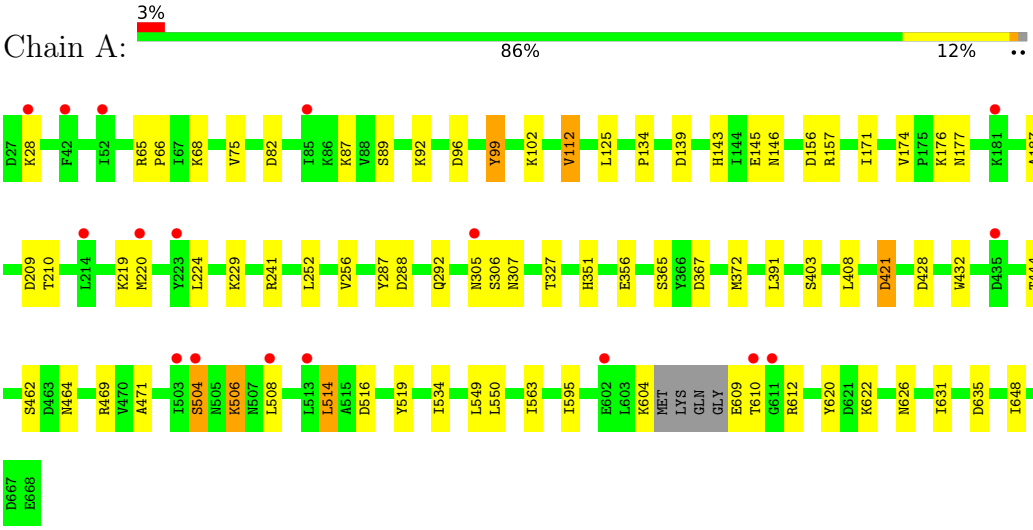
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	59	Total O 59 59	0	0
7	B	30	Total O 30 30	0	0

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.

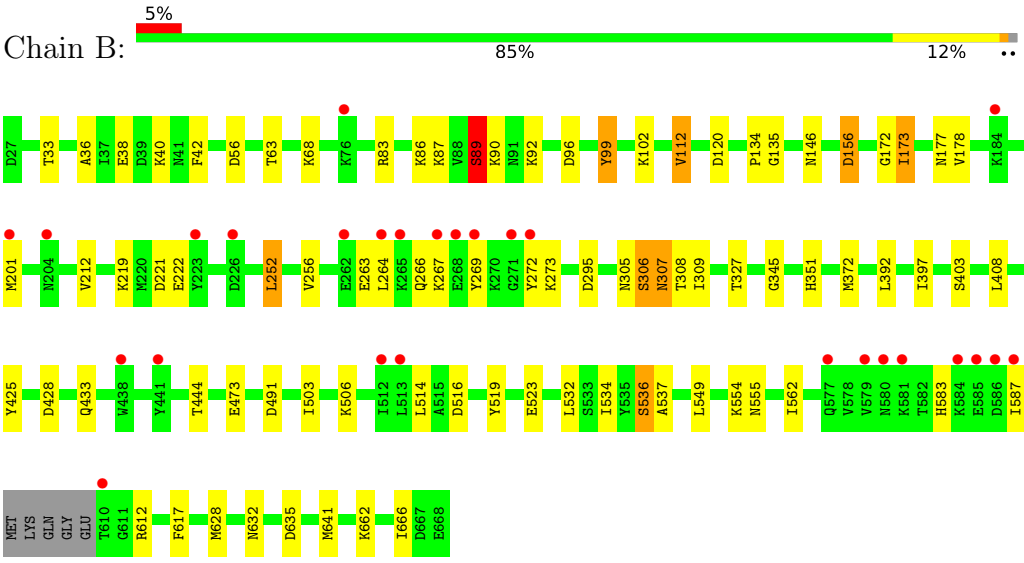
• Molecule 1: Penicillin binding protein 2 prime

Chain A:



• Molecule 1: Penicillin binding protein 2 prime

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.17Å 102.88Å 187.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.50 49.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.55-2.50) 99.9 (49.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.221 , 0.285 0.222 , 0.281	Depositor DCC
R_{free} test set	2763 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10419	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: CL, MUR, CD, JPP, QLN

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	0.64	1/5212 (0.0%)	0.75	2/7008 (0.0%)
1	B	0.64	0/5197	0.75	0/6988
All	All	0.64	1/10409 (0.0%)	0.75	2/13996 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	SER	CB-OG	6.04	1.50	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	403	SER	CA-CB-OG	6.61	129.06	111.20
1	A	403	SER	CB-CA-C	-6.08	98.55	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	SER	Peptide

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	5127	0	5119	39	0
1	B	5112	0	5110	40	0
2	A	30	0	0	1	0
3	A	36	0	27	7	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	17	0	16	2	0
7	A	59	0	0	0	0
7	B	30	0	0	0	0
All	All	10419	0	10272	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (77) 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:A:462:SER:HB3	3:A:702:JPP:C03	1.99	0.93
1:B:403:SER:OG	1:B:599:GLY:HA3	1.79	0.82
1:B:425:TYR:OH	1:B:473:GLU:HG3	1.81	0.80
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.70	0.72
1:B:403:SER:OG	1:B:599:GLY:CA	2.39	0.70
1:A:462:SER:HB3	3:A:702:JPP:H13	1.74	0.69
1:B:583:HIS:O	1:B:587:ILE:HG22	1.97	0.64
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.79	0.63
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.82	0.62
1:B:146:ASN:HD21	1:B:295:ASP:HB3	1.65	0.62
1:B:38:GLU:OE2	1:B:83:ARG:NH2	2.33	0.61
1:B:173:ILE:HG22	1:B:178:VAL:HG21	1.82	0.61
1:B:264:LEU:HD21	1:B:273:LYS:O	2.01	0.60
1:A:241:ARG:HB2	6:A:707:MUR:H1	1.84	0.59
1:A:462:SER:HB3	3:A:702:JPP:H14	1.81	0.57
1:A:256:VAL:O	1:A:372:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ASN:ND2	3:A:702:JPP:O06	2.34	0.56
1:A:612:ARG:NH2	1:A:635:ASP:OD2	2.39	0.54
1:A:471:ALA:HB1	1:A:514:LEU:HD22	1.90	0.53
1:B:351:HIS:CD2	1:B:666:ILE:HD13	2.43	0.53
1:B:408:LEU:HD22	1:B:534:ILE:HG21	1.91	0.53
1:A:516:ASP:HA	1:A:519:TYR:CE1	2.44	0.52
1:A:631:ILE:HD13	1:A:648:ILE:HG22	1.91	0.52
1:A:327:THR:HB	1:A:356:GLU:HB3	1.92	0.51
1:B:306:SER:O	1:B:308:THR:N	2.45	0.50
1:B:269:TYR:HA	1:B:272:TYR:CD1	2.47	0.49
1:B:536:SER:HA	1:B:628:MET:HE3	1.95	0.48
1:A:99:TYR:HD2	1:A:112:VAL:HG11	1.78	0.48
1:A:220:MET:HA	1:A:224:LEU:CD2	2.43	0.48
1:A:462:SER:CB	3:A:702:JPP:C03	2.83	0.48
1:A:65:ARG:HB3	1:A:66:PRO:HD3	1.96	0.47
1:A:305:ASN:HD22	1:B:68:LYS:HB3	1.80	0.47
1:A:462:SER:O	3:A:702:JPP:H14	2.15	0.47
1:A:506:LYS:HE2	1:A:506:LYS:O	2.15	0.47
1:A:143:HIS:HB3	1:A:145:GLU:OE1	2.15	0.47
3:A:702:JPP:H6	3:A:702:JPP:H15	1.56	0.46
1:B:309:ILE:HD12	1:B:309:ILE:N	2.30	0.46
1:B:327:THR:OG1	1:B:549:LEU:HA	2.16	0.46
1:B:89:SER:HB3	1:B:92:LYS:HB2	1.98	0.45
6:A:707:MUR:H7	6:A:707:MUR:H2	1.64	0.45
1:B:89:SER:OG	1:B:90:LYS:N	2.50	0.45
1:A:68:LYS:HB3	1:B:305:ASN:HD22	1.80	0.45
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.52	0.45
1:A:157:ARG:HD3	1:A:666:ILE:O	2.18	0.44
1:B:99:TYR:HD2	1:B:112:VAL:HG11	1.82	0.44
1:A:421:ASP:OD1	1:A:421:ASP:N	2.51	0.44
1:A:351:HIS:HD2	1:A:626:ASN:O	2.00	0.44
1:A:595:ILE:HD11	1:A:620:TYR:OH	2.17	0.43
1:B:173:ILE:CG2	1:B:178:VAL:HG21	2.47	0.43
1:A:171:ILE:HG12	1:A:224:LEU:HD11	2.01	0.43
1:A:432:TRP:CZ2	1:A:469:ARG:HD3	2.53	0.43
1:B:33:THR:O	1:B:36:ALA:HB3	2.19	0.43
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.45	0.43
1:B:603:LEU:HD21	1:B:612:ARG:NE	2.33	0.43
1:B:392:LEU:HD21	1:B:397:ILE:HD13	2.01	0.42
1:B:537:ALA:CB	1:B:562:ILE:HD11	2.48	0.42
1:A:146:ASN:HD22	2:A:701:QLN:C16	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ASP:OD2	1:B:554:LYS:NZ	2.53	0.42
1:B:173:ILE:HG13	1:B:201:MET:CE	2.49	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.90	0.42
1:B:516:ASP:HA	1:B:519:TYR:CE1	2.54	0.42
1:B:173:ILE:HG13	1:B:201:MET:SD	2.59	0.42
1:A:287:TYR:CZ	1:A:550:LEU:HD11	2.55	0.42
1:A:187:ALA:HB1	1:A:192:ILE:O	2.20	0.41
1:A:209:ASP:OD2	1:B:135:GLY:HA2	2.20	0.41
1:B:172:GLY:HA3	1:B:212:VAL:O	2.21	0.41
1:A:408:LEU:HD23	1:A:408:LEU:N	2.36	0.41
1:B:263:GLU:O	1:B:266:GLN:HB2	2.20	0.41
1:B:403:SER:CB	1:B:599:GLY:HA2	2.50	0.41
1:B:587:ILE:HD13	1:B:617:PHE:CE1	2.55	0.41
1:A:220:MET:HA	1:A:224:LEU:HD22	2.03	0.41
1:B:156:ASP:OD1	1:B:156:ASP:C	2.58	0.41
1:A:174:VAL:HA	1:A:210:THR:O	2.22	0.40
1:B:42:PHE:HB3	1:B:63:THR:HA	2.02	0.40
1:A:288:ASP:O	1:A:292:GLN:HG2	2.21	0.40
1:B:256:VAL:O	1:B:372:MET:HG2	2.22	0.40
1:B:345:GLY:HA3	1:B:632:ASN: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	635/642 (99%)	598 (94%)	33 (5%)	4 (1%)	25	43
1	B	633/642 (99%)	599 (95%)	29 (5%)	5 (1%)	19	35
All	All	1268/1284 (99%)	1197 (94%)	62 (5%)	9 (1%)	22	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	306	SER
1	B	307	ASN
1	B	555	ASN
1	A	307	ASN
1	A	504	SER
1	B	89	SER
1	B	221	ASP
1	B	635	ASP

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	570/572 (100%)	534 (94%)	36 (6%)	18	34
1	B	568/572 (99%)	536 (94%)	32 (6%)	21	40
All	All	1138/1144 (100%)	1070 (94%)	68 (6%)	19	37

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	75	VAL
1	A	82	ASP
1	A	87	LYS
1	A	89	SER
1	A	92	LYS
1	A	96	ASP
1	A	99	TYR
1	A	102	LYS
1	A	112	VAL
1	A	125	LEU
1	A	139	ASP
1	A	156	ASP
1	A	177	ASN
1	A	195	ASP

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Mol	Chain	Res	Type
1	A	219	LYS
1	A	229	LYS
1	A	252	LEU
1	A	365	SER
1	A	367	ASP
1	A	391	LEU
1	A	421	ASP
1	A	428	ASP
1	A	444	THR
1	A	447	GLU
1	A	504	SER
1	A	506	LYS
1	A	508	LEU
1	A	514	LEU
1	A	549	LEU
1	A	563	ILE
1	A	604	LYS
1	A	609	GLU
1	A	610	THR
1	A	622	LYS
1	A	662	LYS
1	B	40	LYS
1	B	56	ASP
1	B	86	LYS
1	B	87	LYS
1	B	89	SER
1	B	96	ASP
1	B	99	TYR
1	B	102	LYS
1	B	112	VAL
1	B	120	ASP
1	B	156	ASP
1	B	173	ILE
1	B	177	ASN
1	B	219	LYS
1	B	222	GLU
1	B	252	LEU
1	B	267	LYS
1	B	307	ASN
1	B	419	LEU
1	B	424	SER
1	B	428	ASP

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Mol	Chain	Res	Type
1	B	433	GLN
1	B	444	THR
1	B	491	ASP
1	B	503	ILE
1	B	506	LYS
1	B	514	LEU
1	B	523	GLU
1	B	532	LEU
1	B	536	SER
1	B	641	MET
1	B	662	LYS

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	81	GLN
1	A	91	ASN
1	A	146	ASN
1	A	177	ASN
1	A	203	GLN
1	A	293	HIS
1	A	305	ASN
1	A	442	ASN
1	A	624	ASN
1	A	661	ASN
1	B	107	ASN
1	B	146	ASN
1	B	177	ASN
1	B	305	ASN
1	B	351	HIS
1	B	505	ASN
1	B	624	ASN
1	B	645	ASN
1	B	661	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
3	JPP	A	702	1	31,38,38	4.37	10 (32%)	39,55,55	3.21	18 (46%)
2	QLN	A	701	-	31,33,33	2.02	7 (22%)	33,46,46	1.56	4 (12%)
6	MUR	A	707	-	14,17,17	0.52	0	19,24,24	1.99	6 (31%)

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
3	JPP	A	702	1	-	4/22/64/64	0/3/3/3
2	QLN	A	701	-	-	7/10/15/15	0/4/4/4
6	MUR	A	707	-	-	1/6/30/30	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	JPP	O04-C06	11.12	1.43	1.23
3	A	702	JPP	O-C14	9.99	1.44	1.23
3	A	702	JPP	O05-C11	9.80	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	JPP	O06-C21	9.80	1.42	1.23
3	A	702	JPP	C14-C11	-7.41	1.41	1.53
3	A	702	JPP	C10-N	-7.02	1.34	1.47
3	A	702	JPP	C09-N01	-5.71	1.38	1.48
2	A	701	QLN	C01-C12	5.44	1.51	1.41
2	A	701	QLN	C14-N02	4.49	1.46	1.36
2	A	701	QLN	C18-C20	4.12	1.51	1.47
2	A	701	QLN	C19-C13	4.03	1.43	1.38
3	A	702	JPP	C10-C09	-3.03	1.39	1.51
2	A	701	QLN	C15-C13	2.56	1.43	1.38
2	A	701	QLN	C09-C10	2.15	1.41	1.36
3	A	702	JPP	C06-N01	-2.14	1.37	1.42
2	A	701	QLN	C07-C04	2.11	1.41	1.36
3	A	702	JPP	C17-S	-2.10	1.79	1.84

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	JPP	C19-S-C17	-8.43	75.93	93.99
3	A	702	JPP	C20-N03-C21	-7.92	114.47	123.12
6	A	707	MUR	O5-C1-C2	6.43	117.01	109.51
2	A	701	QLN	C01-C11-N05	-6.25	120.21	123.60
3	A	702	JPP	C18-C19-S	5.70	115.09	103.81
3	A	702	JPP	C03-C19-S	-5.19	100.52	109.21
3	A	702	JPP	C02-C19-S	4.93	117.47	109.21
3	A	702	JPP	N04-C06-N01	4.87	121.12	114.04
3	A	702	JPP	C10-N-C14	4.86	129.99	120.69
3	A	702	JPP	O-C14-N	4.81	128.66	123.66
3	A	702	JPP	CA-N04-C06	-4.28	113.08	121.17
3	A	702	JPP	C02-C19-C18	-4.25	98.23	112.33
2	A	701	QLN	C15-C13-C19	-4.07	116.92	121.74
3	A	702	JPP	C05-CA-C21	-3.42	100.47	108.16
3	A	702	JPP	C15-N-C14	-3.14	115.88	119.64
3	A	702	JPP	O04-C06-N01	2.70	122.81	119.78
3	A	702	JPP	C10-C09-N01	2.62	113.72	108.78
6	A	707	MUR	C9-C7-C8	-2.58	110.02	113.35
6	A	707	MUR	C3-C4-C5	2.57	115.13	109.66
6	A	707	MUR	C1-C2-C3	2.55	114.80	110.14
3	A	702	JPP	C17-C20-N03	-2.54	104.44	109.98
3	A	702	JPP	O06-C21-CA	2.53	125.04	120.64
3	A	702	JPP	O04-C06-N04	-2.49	116.07	123.05
6	A	707	MUR	O1-C1-O5	-2.30	103.48	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	707	MUR	C4-C3-C2	2.22	115.75	111.37
2	A	701	QLN	C16-C15-C13	2.03	121.26	118.63
2	A	701	QLN	C15-C13-N02	2.01	121.10	119.24
3	A	702	JPP	C05-CA-N04	-2.00	107.69	112.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	QLN	C15-C13-N02-C12
2	A	701	QLN	C19-C13-N02-C12
2	A	701	QLN	C15-C13-N02-C14
2	A	701	QLN	C19-C13-N02-C14
2	A	701	QLN	N05-C14-C21-C22
3	A	702	JPP	C-C15-N-C10
6	A	707	MUR	C2-C3-O3-C7
2	A	701	QLN	C21-C22-C23-C24
2	A	701	QLN	C21-C22-C23-C28
3	A	702	JPP	C21-CA-N04-C06
3	A	702	JPP	C-C15-N-C14
3	A	702	JPP	C01-C20-N03-C21

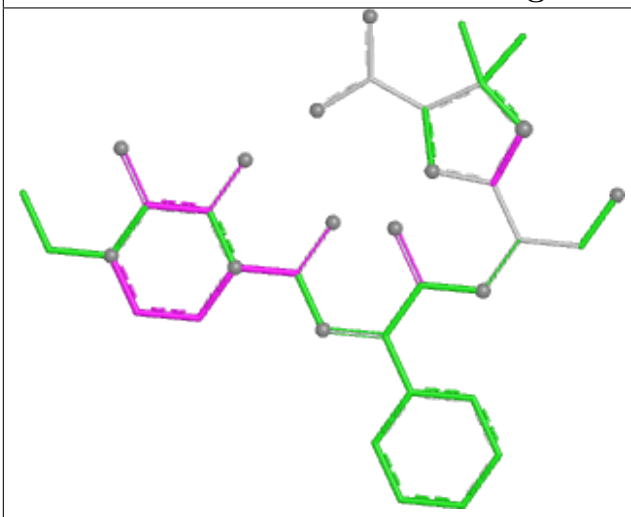
There are no ring outliers.

3 monomers are involved in 10 short contacts:

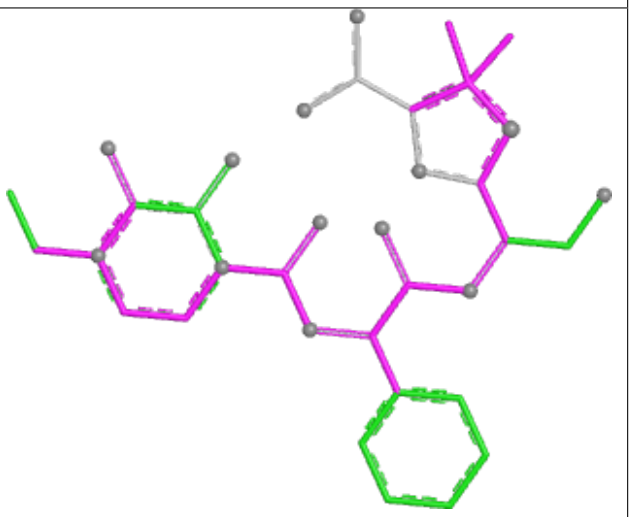
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	JPP	7	0
2	A	701	QLN	1	0
6	A	707	MUR	2	0

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.

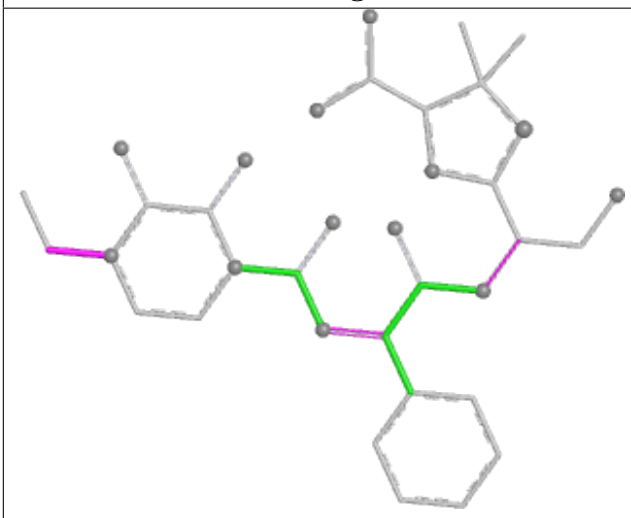
Ligand JPP A 702



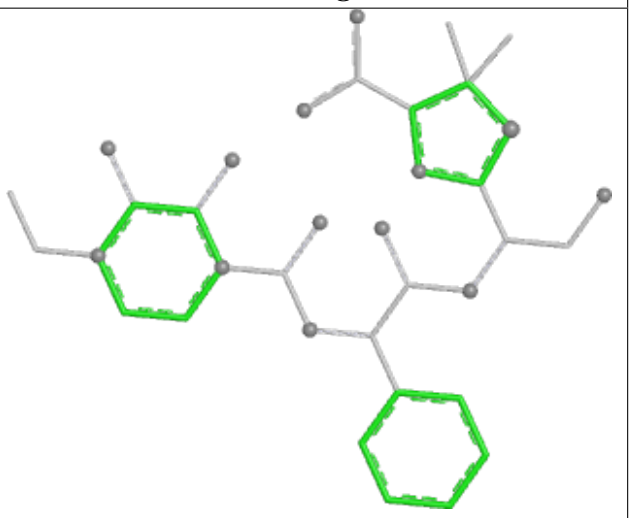
Bond lengths



Bond angles

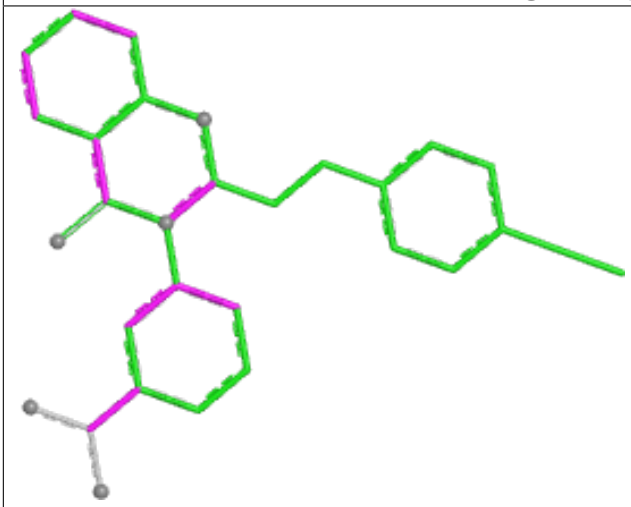


Torsions

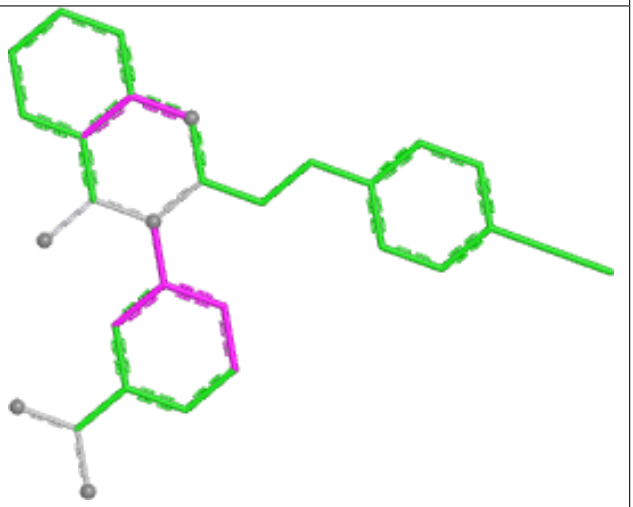


Rings

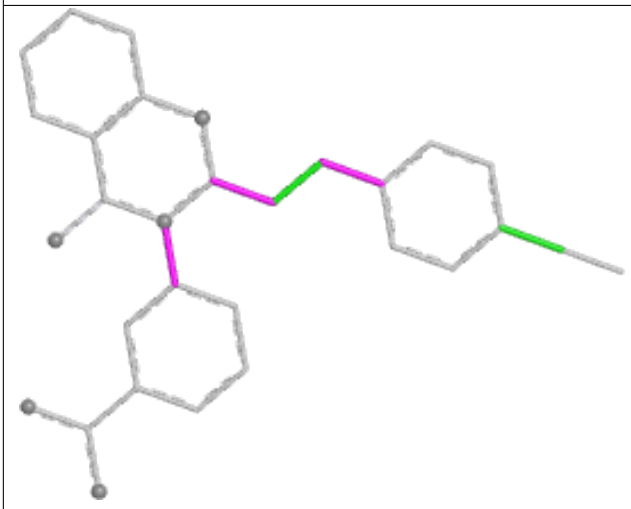
Ligand QLN A 701



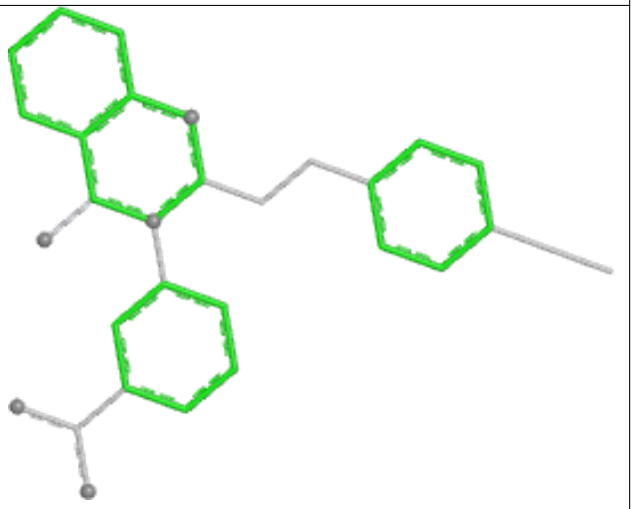
Bond lengths



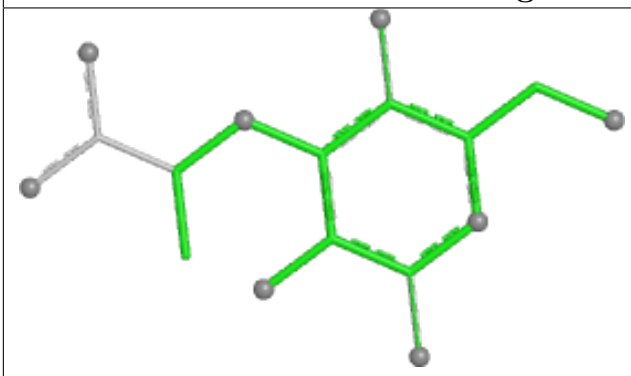
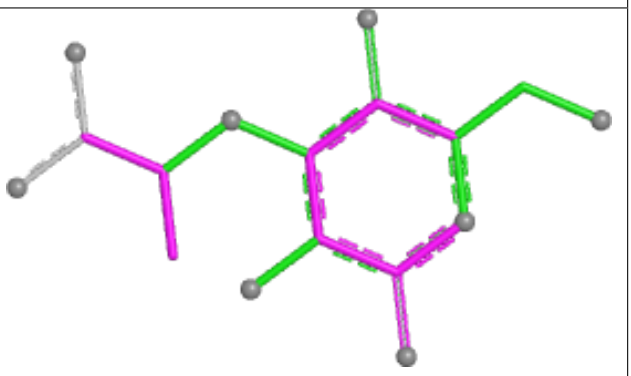
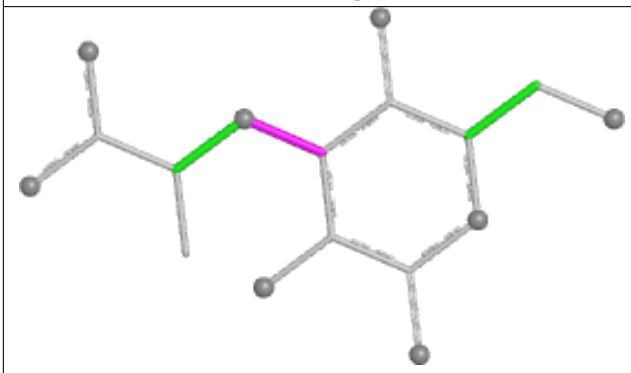
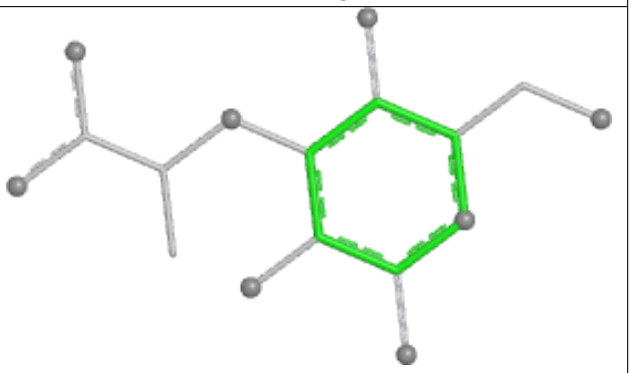
Bond angles



Torsions



Rings

Ligand MUR A 707	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	638/642 (99%)	0.29	18 (2%)	53	56	42, 71, 108, 150	0
1	B	637/642 (99%)	0.39	32 (5%)	28	30	47, 74, 117, 145	0
All	All	1275/1284 (99%)	0.34	50 (3%)	39	42	42, 73, 111, 150	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	585	GLU	5.2
1	A	504	SER	4.6
1	B	587	ILE	4.4
1	B	579	VAL	4.3
1	B	610	THR	4.3
1	B	580	ASN	4.0
1	B	223	TYR	3.8
1	B	581	LYS	3.6
1	A	503	ILE	3.5
1	A	181	LYS	3.5
1	A	508	LEU	3.4
1	B	441	TYR	3.3
1	B	265	LYS	3.3
1	B	603	LEU	3.2
1	B	512	ILE	3.1
1	A	610	THR	3.1
1	A	513	LEU	3.1
1	A	223	TYR	3.0
1	B	272	TYR	3.0
1	A	305	ASN	3.0
1	B	264	LEU	2.9
1	B	269	TYR	2.9
1	B	577	GLN	2.8
1	A	214	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	422	LYS	2.7
1	A	611	GLY	2.7
1	B	198	LYS	2.7
1	B	513	LEU	2.7
1	B	267	LYS	2.6
1	B	196	TYR	2.6
1	B	438	TRP	2.5
1	B	204	ASN	2.5
1	B	268	GLU	2.5
1	B	184	LYS	2.3
1	B	586	ASP	2.3
1	A	52	ILE	2.3
1	A	42	PHE	2.3
1	A	459	ILE	2.3
1	A	220	MET	2.2
1	A	435	ASP	2.2
1	B	271	GLY	2.2
1	B	201	MET	2.2
1	B	584	LYS	2.2
1	A	602	GLU	2.2
1	A	85	ILE	2.1
1	A	28	LYS	2.1
1	B	199	GLN	2.1
1	B	226	ASP	2.1
1	B	76	LYS	2.0
1	B	262	GLU	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)

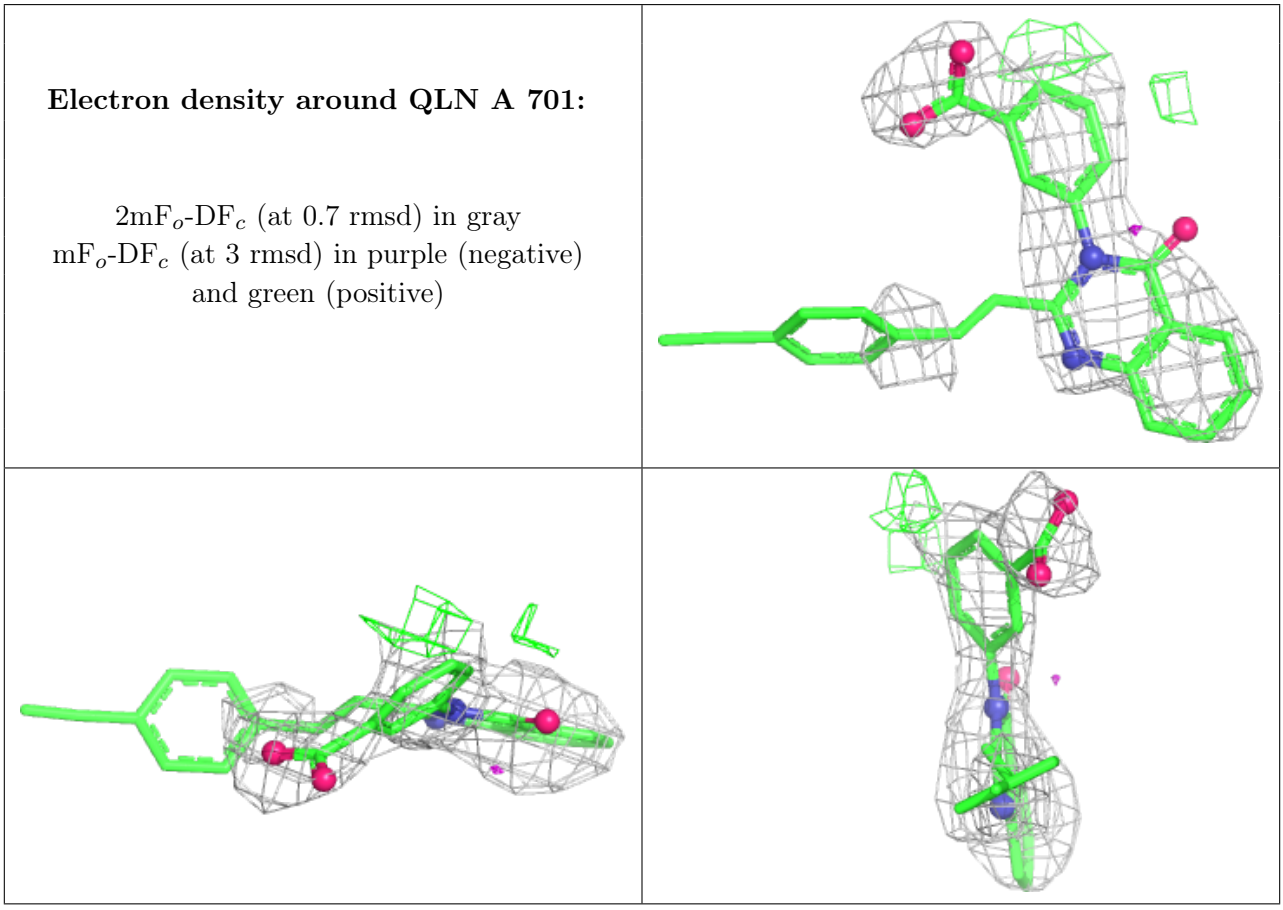
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	QLN	A	701	30/30	0.70	0.36	106,135,141,142	0
6	MUR	A	707	17/17	0.77	0.46	76,83,99,101	0
3	JPP	A	702	36/36	0.90	0.22	68,77,84,86	0
5	CD	A	705	1/1	0.98	0.12	73,73,73,73	0
5	CD	A	706	1/1	0.98	0.15	58,58,58,58	0
5	CD	B	703	1/1	0.98	0.17	58,58,58,58	0
4	CL	B	702	1/1	0.98	0.09	50,50,50,50	0
4	CL	A	704	1/1	0.99	0.09	50,50,50,50	0
5	CD	B	704	1/1	0.99	0.16	60,60,60,60	0
4	CL	A	703	1/1	0.99	0.15	74,74,74,74	0
4	CL	B	701	1/1	1.00	0.15	54,54,54,54	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.

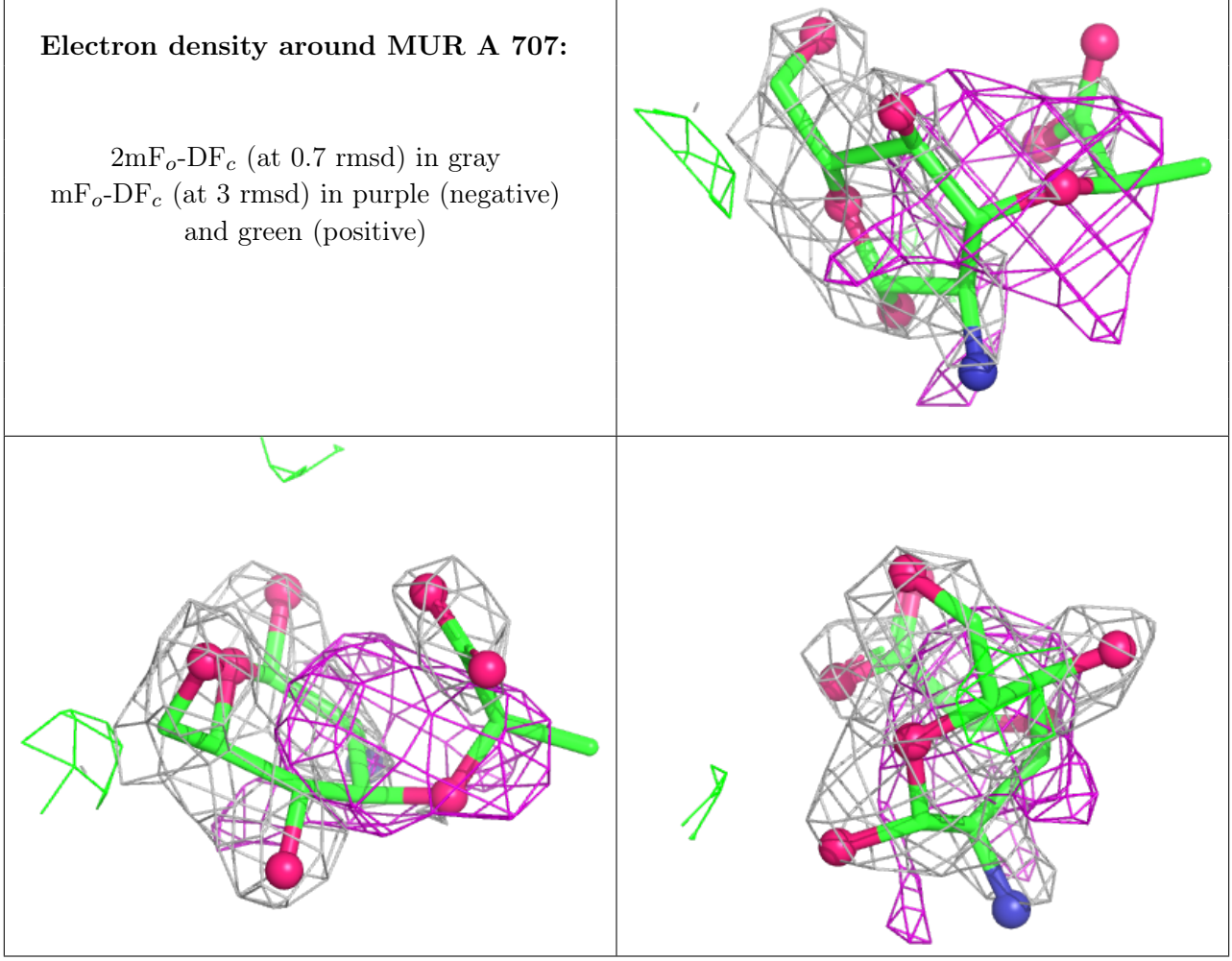
Electron density around QLN A 701:

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



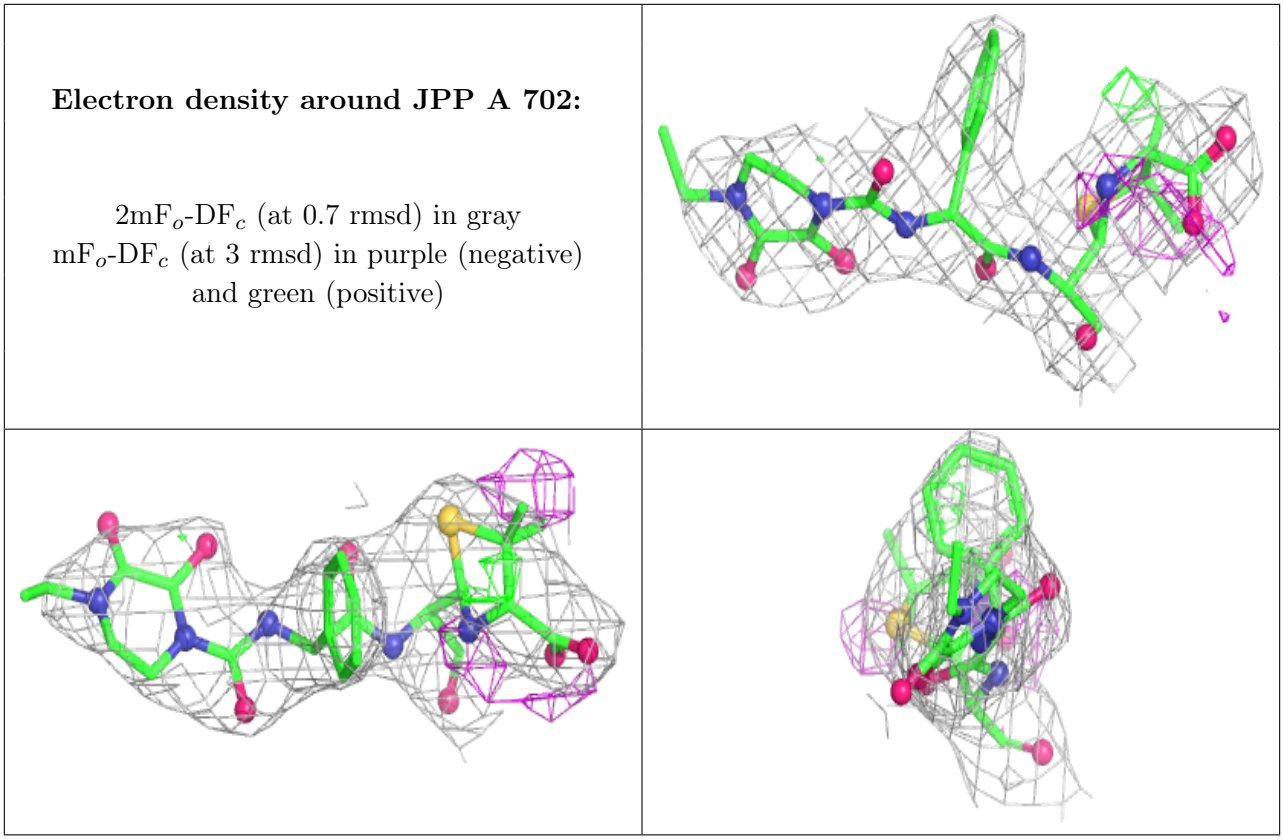
Electron density around MUR A 707:

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



Electron density around JPP A 702:

$2mF_o$-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.