



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 02:01 PM EST

PDB ID : 6C92
Title : The structure of MppP soaked with the product 2-ketoarginine
Authors : Han, L.; Silvaggi, N.R.
Deposited on : 2018-01-25
Resolution : 1.83 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

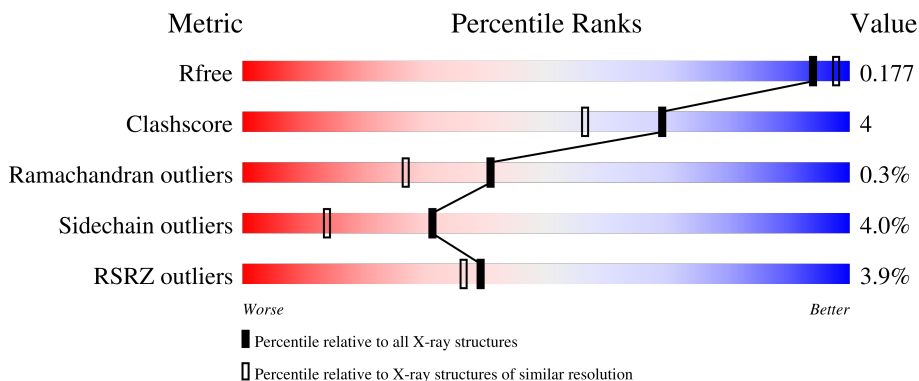
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


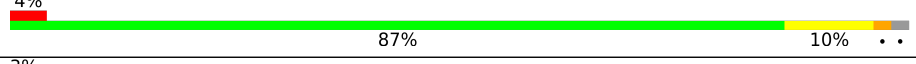


The reported resolution of this entry is 1.83 Å.

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	376	 3% 86% 9% ••
2	B	376	 4% 87% 10% ••
2	C	376	 3% 84% 10% • 6%
2	D	376	 5% 83% 10% • 6%

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
4	EGV	C	401	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23471 atoms, of which 11103 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.

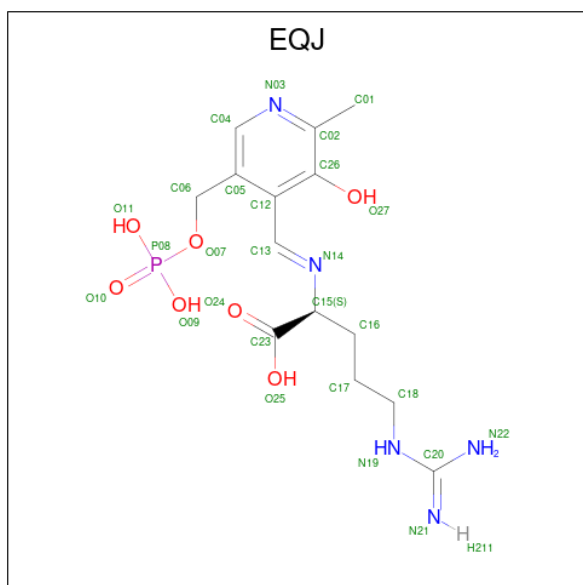
- Molecule 1 is a protein called PLP-Dependent L-Arginine Hydroxylase MppP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	367	5643	1794	2793	504	545	7	0	0	0

- Molecule 2 is a protein called PLP-Dependent L-Arginine Hydroxylase MppP.

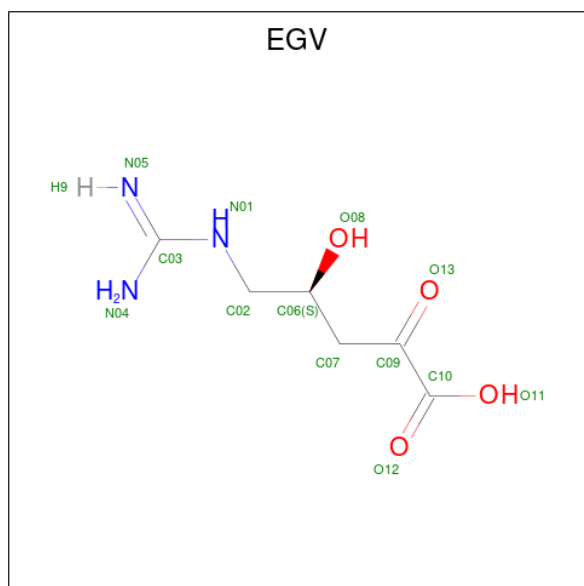
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace	
			Total	C	H	N	O	P				S
2	B	369	5732	1822	2837	510	555	1	7	0	4	0
2	C	355	5486	1740	2715	493	530	1	7	0	2	0
2	D	353	5491	1740	2722	493	528	1	7	0	6	0

- Molecule 3 is (E)-N 2 -({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)-L-arginine (three-letter code: EQJ) (formula: C₁₄H₂₂N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	A	1	45	14	18	5	7	1	0	0

- Molecule 4 is (4S)-5-carbamimidamido-4-hydroxy-2-oxopentanoic acid (three-letter code: EGV) (formula: C₆H₁₁N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	B	1	21	6	9	3	3	0	0
4	C	1	21	6	9	3	3	0	0

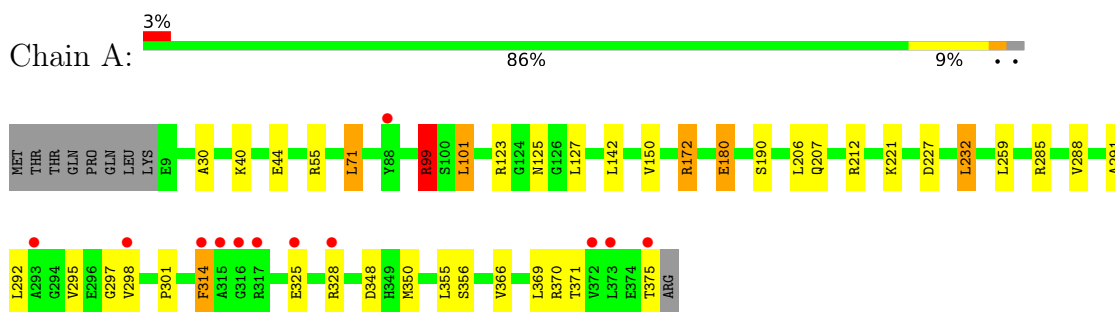
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	264	Total	O	0	0
			264	264		
5	C	261	Total	O	0	0
			261	261		
5	D	255	Total	O	0	0
			255	255		

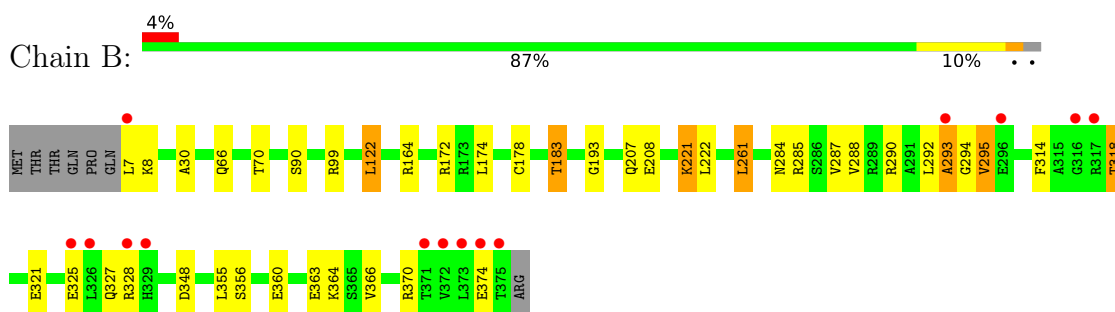
3 Residue-property plots [i](#)

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.

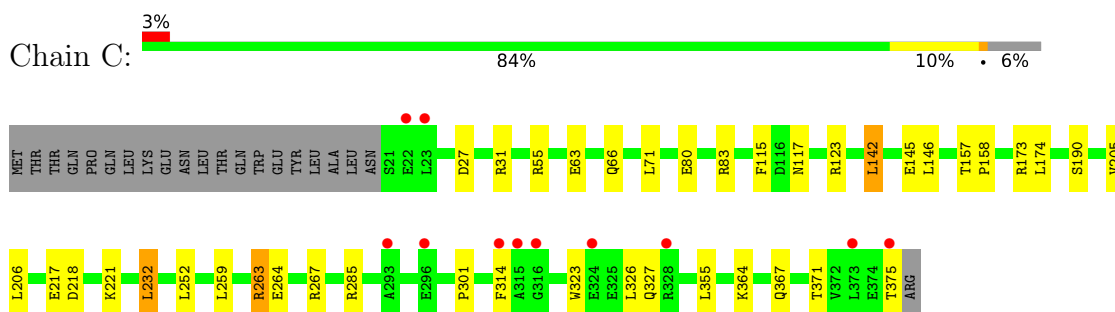
- Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



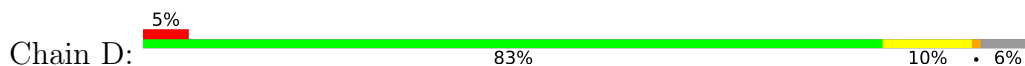
- Molecule 2: PLP-Dependent L-Arginine Hydroxylase MppP

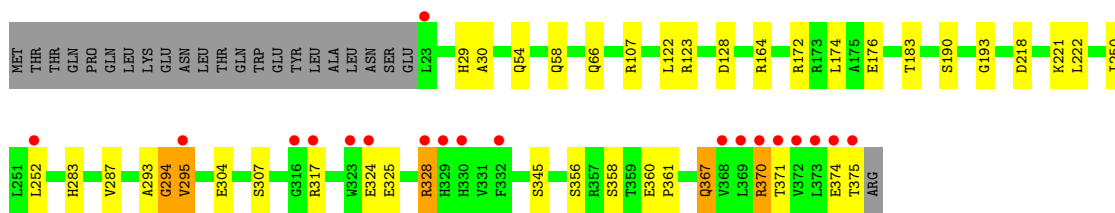


- Molecule 2: PLP-Dependent L-Arginine Hydroxylase MppP



- Molecule 2: PLP-Dependent L-Arginine Hydroxylase MppP





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.86Å 108.78Å 195.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.59 – 1.83 44.59 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.59-1.83) 99.9 (44.59-1.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.83Å)	Xtrriage
Refinement program	PHENIX (1.10_2148: ???)	Depositor
R, R_{free}	0.151 , 0.175 0.152 , 0.177	Depositor DCC
R_{free} test set	2000 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23471	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% 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: LLP, EQJ, EGV

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	0.47	1/2911 (0.0%)	0.74	11/3965 (0.3%)
2	B	0.46	0/2949	0.64	4/4015 (0.1%)
2	C	0.50	0/2808	0.76	5/3821 (0.1%)
2	D	0.47	0/2824	0.66	0/3843
All	All	0.47	1/11492 (0.0%)	0.70	20/15644 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CB-CG	-5.13	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	285	ARG	NE-CZ-NH2	-14.54	113.03	120.30
2	C	285	ARG	NE-CZ-NH1	12.33	126.46	120.30
1	A	285	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	55	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	55	ARG	NE-CZ-NH1	8.61	124.60	120.30
2	C	263	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	99	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	285	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	C	263	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	71	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	101	LEU	CA-CB-CG	5.76	128.54	115.30
2	C	55	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	261	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	127	LEU	CA-CB-CG	-5.53	102.58	115.30
1	A	172	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	99	ARG	NE-CZ-NH1	-5.31	117.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	232	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	212	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	B	285	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	2850	2793	2793	18	0
2	B	2895	2837	2823	19	0
2	C	2771	2715	2712	26	0
2	D	2769	2722	2702	20	0
3	A	27	18	0	0	0
4	B	12	9	0	1	0
4	C	12	9	0	1	0
5	A	252	0	0	5	0
5	B	264	0	0	4	1
5	C	261	0	0	11	2
5	D	255	0	0	5	1
All	All	12368	11103	11030	82	2

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

All (82) 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)
2:D:176:GLU:OE1	5:D:401:HOH:O	1.82	0.98
2:C:263:ARG:NH1	2:C:264:GLU:OE2	2.08	0.86
2:C:83:ARG:O	5:C:502:HOH:O	1.98	0.81
2:C:145:GLU:OE2	5:C:503:HOH:O	2.00	0.79
2:D:172:ARG:NH2	5:D:402:HOH:O	1.91	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:ARG:NH1	5:C:501:HOH:O	1.95	0.71
2:D:370:ARG:NH1	2:D:374:GLU:OE1	2.24	0.71
2:D:304:GLU:OE2	5:D:403:HOH:O	2.08	0.70
2:C:66:GLN:HG2	5:C:547:HOH:O	1.94	0.68
2:B:370:ARG:NH1	2:B:374:GLU:OE2	2.25	0.68
2:D:317:ARG:NH2	2:D:375:THR:OG1	2.31	0.62
1:A:123:ARG:NH1	5:A:502:HOH:O	1.98	0.61
2:C:142:LEU:HG	2:C:146:LEU:HD23	1.84	0.59
1:A:301:PRO:HG2	1:A:350:MET:CE	2.33	0.59
1:A:99:ARG:HG2	1:A:125:ASN:OD1	2.04	0.58
2:C:263:ARG:HD2	2:C:267:ARG:CZ	2.33	0.57
4:C:401:EGV:N05	2:D:250:ILE:O	2.39	0.56
1:A:291:ALA:O	1:A:370:ARG:HD2	2.06	0.55
2:C:27:ASP:HB3	5:C:504:HOH:O	2.07	0.55
2:B:318:THR:HG22	2:B:321:GLU:H	1.72	0.54
2:C:252:LEU:HD22	5:C:569:HOH:O	2.06	0.53
1:A:325:GLU:OE1	1:A:328:ARG:NH1	2.42	0.53
2:B:172:ARG:NH1	5:B:506:HOH:O	2.34	0.52
1:A:30:ALA:HA	1:A:356:SER:HB3	1.92	0.52
2:B:294:GLY:O	2:B:295:VAL:O	2.29	0.50
2:C:66:GLN:CG	5:C:547:HOH:O	2.57	0.50
2:D:325:GLU:OE2	2:D:328:ARG:NH1	2.41	0.50
2:C:263:ARG:HG2	2:C:263:ARG:HH11	1.75	0.50
2:B:90:SER:HB3	2:B:221:LLP:H5'2	1.93	0.50
2:B:30:ALA:HA	2:B:356:SER:HB3	1.93	0.50
1:A:190:SER:OG	1:A:221:LYS:CD	2.60	0.50
2:B:207:GLN:NE2	5:B:502:HOH:O	2.27	0.49
2:D:367:GLN:O	2:D:371:THR:HG23	2.13	0.48
2:D:283:HIS:O	2:D:287:VAL:HG13	2.13	0.48
1:A:295:VAL:O	1:A:298:VAL:HG22	2.14	0.47
2:B:284:ASN:HA	2:B:287:VAL:HG13	1.95	0.47
2:B:221:LLP:C4'	4:B:401:EGV:O13	2.63	0.47
2:D:358:SER:O	2:D:361:PRO:HD2	2.15	0.47
2:B:193:GLY:HA3	2:B:222:LEU:HD21	1.95	0.47
2:D:190:SER:HA	2:D:218:ASP:HB3	1.98	0.46
2:D:370:ARG:NH1	2:D:371:THR:HA	2.31	0.46
2:B:288:VAL:HG22	2:B:366:VAL:HG21	1.97	0.46
2:C:63:GLU:HB3	2:C:263:ARG:HD3	1.98	0.46
1:A:288:VAL:HG22	1:A:366:VAL:HG21	1.98	0.46
2:C:31:ARG:NH1	5:C:508:HOH:O	2.49	0.45
1:A:123:ARG:NH2	5:A:502:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:LYS:O	2:C:367:GLN:HB3	2.15	0.45
2:C:190:SER:HA	2:C:218:ASP:HB3	1.98	0.45
2:D:107:ARG:HG2	2:D:128:ASP:HB2	1.98	0.45
1:A:297:GLY:O	1:A:314:PHE:HA	2.16	0.45
1:A:142:LEU:HD13	5:A:564:HOH:O	2.15	0.45
2:D:345:SER:OG	5:D:404:HOH:O	2.21	0.45
2:B:178:CYS:HA	2:B:183:THR:HG23	1.99	0.45
2:B:325:GLU:OE2	2:B:328:ARG:NH2	2.42	0.45
2:C:80:GLU:HG2	2:C:83:ARG:HG2	1.99	0.44
1:A:172:ARG:NE	5:A:501:HOH:O	1.97	0.44
2:C:371:THR:O	2:C:375:THR:HG22	2.18	0.44
2:D:294:GLY:O	2:D:295:VAL:O	2.35	0.43
2:C:123[A]:ARG:NH1	5:C:505:HOH:O	2.24	0.43
1:A:207:GLN:NE2	5:A:507:HOH:O	2.41	0.43
2:B:290:ARG:O	2:B:293:ALA:HB2	2.17	0.43
2:C:142:LEU:HD22	2:C:174:LEU:CD1	2.48	0.43
1:A:40:LYS:NZ	1:A:44:GLU:OE2	2.51	0.43
2:B:360:GLU:H	2:B:360:GLU:CD	2.22	0.43
2:D:193:GLY:HA3	2:D:222:LEU:HD21	2.00	0.43
1:A:371:THR:O	1:A:375:THR:HG22	2.19	0.43
2:D:58:GLN:OE1	5:D:405:HOH:O	2.21	0.43
2:B:7:LEU:N	5:B:514:HOH:O	2.52	0.42
2:C:31:ARG:CZ	5:C:501:HOH:O	2.57	0.42
2:C:217:GLU:HB2	2:C:232:LEU:HB2	2.01	0.42
1:A:180:GLU:HB2	2:D:123[B]:ARG:NH1	2.35	0.42
2:B:208:GLU:OE1	5:B:501:HOH:O	2.22	0.42
2:B:360:GLU:O	2:B:364:LYS:HG2	2.20	0.42
2:C:80:GLU:HG2	2:C:83:ARG:CG	2.50	0.41
2:C:157:THR:HA	2:C:158:PRO:C	2.39	0.41
1:A:292:LEU:HD11	1:A:369:LEU:HD23	2.01	0.41
2:C:323:TRP:CZ2	2:C:327:GLN:OE1	2.73	0.41
2:D:30:ALA:HA	2:D:356:SER:HB3	2.01	0.41
2:B:66:GLN:O	2:B:70:THR:HG23	2.20	0.41
2:C:123[A]:ARG:HD2	5:C:505:HOH:O	2.20	0.41
2:D:360:GLU:HB3	2:D:361:PRO:HD3	2.02	0.40
2:C:115:PHE:CE2	2:C:117:ASN:HB3	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:745:HOH:O	5:D:651:HOH:O[4_555]	2.11	0.09
5:B:746:HOH:O	5:C:754:HOH:O[4_555]	2.18	0.02

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	365/376 (97%)	357 (98%)	8 (2%)	0	100	100
2	B	370/376 (98%)	357 (96%)	11 (3%)	2 (0%)	29	15
2	C	354/376 (94%)	347 (98%)	7 (2%)	0	100	100
2	D	356/376 (95%)	350 (98%)	3 (1%)	3 (1%)	19	7
All	All	1445/1504 (96%)	1411 (98%)	29 (2%)	5 (0%)	41	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	293	ALA
2	B	295	VAL
2	D	293	ALA
2	D	294	GLY
2	D	295	VAL

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	306/315 (97%)	295 (96%)	11 (4%)	35	17
2	B	311/314 (99%)	298 (96%)	13 (4%)	30	12
2	C	295/314 (94%)	284 (96%)	11 (4%)	34	16
2	D	297/314 (95%)	284 (96%)	13 (4%)	28	11
All	All	1209/1257 (96%)	1161 (96%)	48 (4%)	31	14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	99	ARG
1	A	101	LEU
1	A	150	VAL
1	A	206	LEU
1	A	227	ASP
1	A	232	LEU
1	A	259	LEU
1	A	314	PHE
1	A	348	ASP
1	A	355	LEU
2	B	8	LYS
2	B	122	LEU
2	B	164	ARG
2	B	174	LEU
2	B	183	THR
2	B	261	LEU
2	B	292	LEU
2	B	314	PHE
2	B	318	THR
2	B	327	GLN
2	B	348	ASP
2	B	355	LEU
2	B	363	GLU
2	C	71	LEU
2	C	142	LEU
2	C	173	ARG
2	C	205	VAL
2	C	206	LEU
2	C	232	LEU
2	C	259	LEU
2	C	301	PRO
2	C	314	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	326	LEU
2	C	355	LEU
2	D	29	HIS
2	D	54	GLN
2	D	66	GLN
2	D	122	LEU
2	D	164	ARG
2	D	174	LEU
2	D	183	THR
2	D	252	LEU
2	D	307	SER
2	D	324	GLU
2	D	328	ARG
2	D	367	GLN
2	D	370	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	LLP	C	221	2	23,24,25	0.97	1 (4%)	25,32,34	1.38	3 (12%)
2	LLP	B	221	2	23,24,25	1.31	3 (13%)	25,32,34	1.45	3 (12%)
2	LLP	D	221	2	23,24,25	1.25	3 (13%)	25,32,34	1.48	4 (16%)

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	LLP	C	221	2	-	4/16/17/19	0/1/1/1
2	LLP	B	221	2	-	6/16/17/19	0/1/1/1
2	LLP	D	221	2	-	6/16/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	221	LLP	O-C	4.21	1.36	1.19
2	B	221	LLP	O-C	3.50	1.33	1.19
2	B	221	LLP	C3-C2	3.31	1.44	1.40
2	C	221	LLP	C3-C2	2.77	1.43	1.40
2	B	221	LLP	OP4-C5'	-2.46	1.35	1.45
2	D	221	LLP	OP4-C5'	-2.28	1.36	1.45
2	D	221	LLP	C3-C2	2.07	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	221	LLP	OP2-P-OP4	-4.01	96.06	106.73
2	D	221	LLP	OP2-P-OP4	-3.75	96.76	106.73
2	B	221	LLP	OP2-P-OP4	-3.65	97.02	106.73
2	B	221	LLP	C5'-C5-C6	-3.53	113.56	119.37
2	D	221	LLP	OP4-P-OP1	3.09	115.14	106.47
2	C	221	LLP	OP2-P-OP1	2.47	120.35	110.68
2	B	221	LLP	C3-C4-C5	-2.38	116.43	118.26
2	D	221	LLP	OP4-C5'-C5	2.28	113.70	109.35
2	D	221	LLP	C5'-C5-C6	-2.05	115.99	119.37
2	C	221	LLP	C5'-C5-C6	-2.02	116.04	119.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	221	LLP	C4-C5-C5'-OP4
2	B	221	LLP	C6-C5-C5'-OP4
2	B	221	LLP	C5'-OP4-P-OP2
2	C	221	LLP	C4-C5-C5'-OP4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	221	LLP	C6-C5-C5'-OP4
2	D	221	LLP	C-CA-CB-CG
2	D	221	LLP	CA-CB-CG-CD
2	C	221	LLP	C4-C4'-NZ-CE
2	B	221	LLP	CA-CB-CG-CD
2	B	221	LLP	C5'-OP4-P-OP1
2	D	221	LLP	CD-CE-NZ-C4'
2	D	221	LLP	C6-C5-C5'-OP4
2	D	221	LLP	C4-C5-C5'-OP4
2	C	221	LLP	CA-CB-CG-CD
2	B	221	LLP	C5'-OP4-P-OP3
2	D	221	LLP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	221	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	EQJ	A	401	-	27,27,27	2.10	6 (22%)	32,37,37	1.75	6 (18%)
4	EGV	B	401	-	11,11,12	2.39	4 (36%)	12,13,15	1.48	1 (8%)
4	EGV	C	401	-	11,11,12	2.56	5 (45%)	12,13,15	2.25	5 (41%)

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	EQJ	A	401	-	-	3/22/22/22	0/1/1/1
4	EGV	B	401	-	-	3/11/11/13	-
4	EGV	C	401	-	-	5/11/11/13	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	EQJ	C20-N19	7.65	1.48	1.33
4	C	401	EGV	C03-N01	5.98	1.45	1.33
4	B	401	EGV	C03-N01	5.81	1.44	1.33
3	A	401	EQJ	C12-C13	3.90	1.54	1.46
4	C	401	EGV	C07-C09	3.14	1.54	1.51
4	B	401	EGV	O11-C10	-3.07	1.21	1.30
4	B	401	EGV	C03-N05	3.04	1.44	1.32
4	C	401	EGV	C03-N05	3.02	1.44	1.32
3	A	401	EQJ	C13-N14	2.74	1.32	1.27
4	C	401	EGV	O13-C09	-2.64	1.17	1.23
3	A	401	EQJ	C20-N21	2.62	1.42	1.32
3	A	401	EQJ	C16-C15	2.33	1.56	1.53
3	A	401	EQJ	C06-C05	2.28	1.57	1.50
4	B	401	EGV	C03-N04	-2.11	1.26	1.34
4	C	401	EGV	O11-C10	-2.08	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	EQJ	C15-N14-C13	6.57	126.79	117.31
4	C	401	EGV	C07-C09-C10	4.32	123.99	115.97
4	B	401	EGV	C06-C07-C09	-4.29	104.79	113.63
4	C	401	EGV	N01-C03-N05	-3.75	114.10	120.70
4	C	401	EGV	O11-C10-C09	3.12	122.52	113.97
3	A	401	EQJ	C17-C16-C15	2.97	119.95	114.31
3	A	401	EQJ	C05-C04-N03	-2.68	119.36	123.82
3	A	401	EQJ	O25-C23-O24	-2.56	118.28	124.09
4	C	401	EGV	O11-C10-O12	-2.52	117.83	123.61
3	A	401	EQJ	N19-C20-N21	-2.37	116.53	120.70
3	A	401	EQJ	C12-C26-C02	-2.26	118.79	120.19
4	C	401	EGV	N04-C03-N01	2.07	123.97	119.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

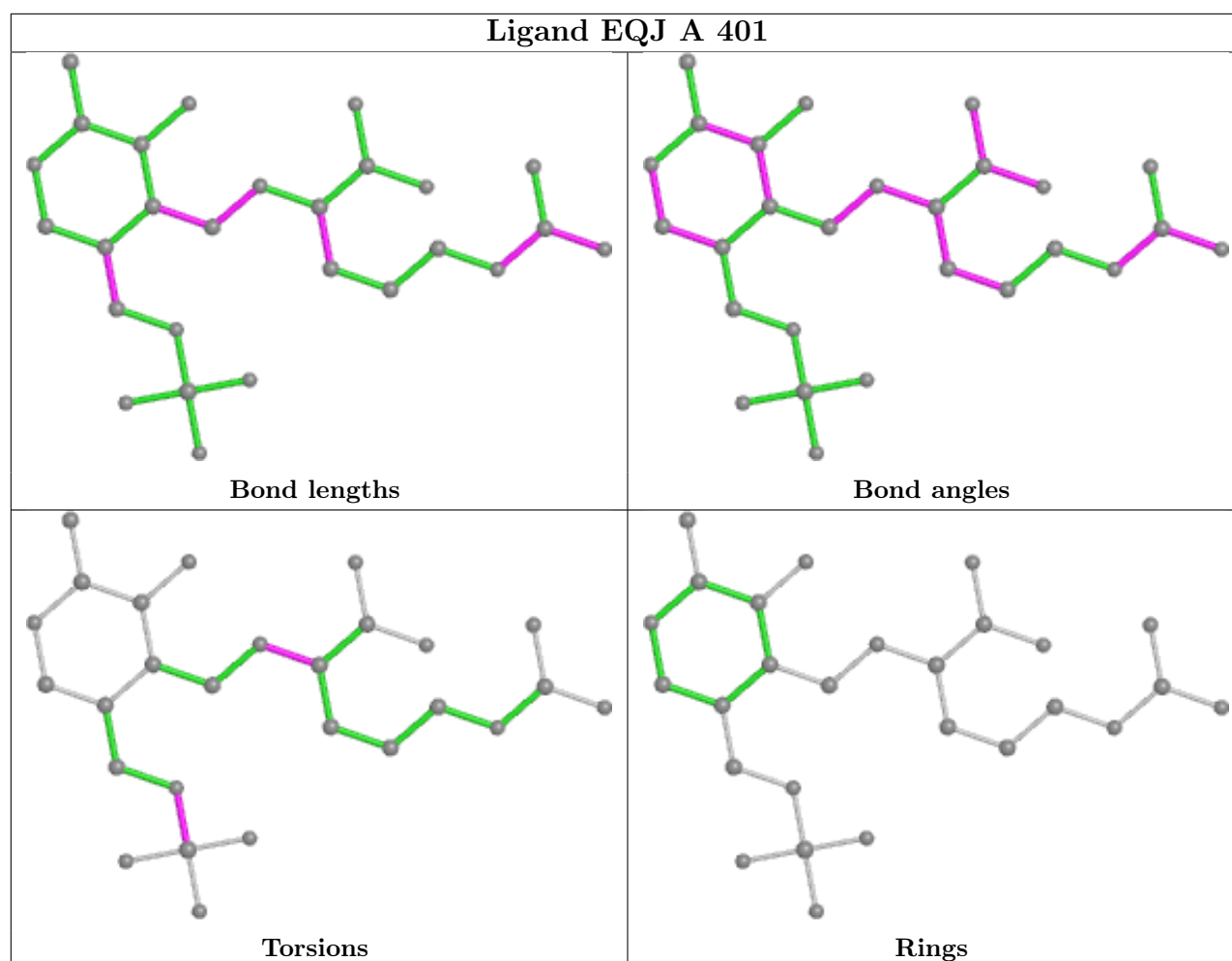
Mol	Chain	Res	Type	Atoms
3	A	401	EQJ	C16-C15-N14-C13
4	C	401	EGV	C07-C09-C10-O11
4	C	401	EGV	O13-C09-C10-O11
4	C	401	EGV	C07-C09-C10-O12
4	C	401	EGV	O13-C09-C10-O12
4	C	401	EGV	N01-C02-C06-C07
4	B	401	EGV	C06-C07-C09-C10
3	A	401	EQJ	C06-O07-P08-O10
4	B	401	EGV	N01-C02-C06-C07
3	A	401	EQJ	C06-O07-P08-O11
4	B	401	EGV	C02-C06-C07-C09

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	EGV	1	0
4	C	401	EGV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	367/376 (97%)	-0.05	12 (3%) 46 43	15, 28, 59, 79	0
2	B	368/376 (97%)	-0.16	14 (3%) 40 37	16, 26, 62, 95	0
2	C	354/376 (94%)	-0.18	11 (3%) 49 46	13, 27, 60, 98	0
2	D	352/376 (93%)	-0.15	19 (5%) 25 23	13, 26, 62, 90	0
All	All	1441/1504 (95%)	-0.13	56 (3%) 39 36	13, 27, 61, 98	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	375	THR	7.4
2	B	375	THR	7.1
1	A	293	ALA	6.1
2	C	316	GLY	5.2
2	D	373	LEU	4.9
1	A	375	THR	4.8
1	A	316	GLY	4.8
2	C	315	ALA	4.6
2	B	7	LEU	4.5
1	A	315	ALA	4.3
2	D	328	ARG	4.2
2	B	372	VAL	4.2
2	C	375	THR	3.9
2	D	372	VAL	3.8
2	D	370	ARG	3.6
2	D	330	HIS	3.6
2	D	371	THR	3.6
2	B	328	ARG	3.5
2	C	22	GLU	3.4
2	B	371	THR	3.2
2	D	316	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	328	ARG	3.0
2	B	373	LEU	3.0
2	D	329	HIS	3.0
2	B	316	GLY	2.9
2	C	296	GLU	2.8
2	D	323	TRP	2.8
2	B	296	GLU	2.8
2	C	314	PHE	2.7
1	A	314	PHE	2.6
2	C	23	LEU	2.6
2	D	368	VAL	2.6
2	D	324	GLU	2.6
2	D	374	GLU	2.6
2	D	332	PHE	2.5
2	D	23	LEU	2.5
2	D	317	ARG	2.5
1	A	325	GLU	2.5
2	B	317	ARG	2.4
2	B	325	GLU	2.4
2	C	293	ALA	2.4
1	A	298	VAL	2.4
2	B	326	LEU	2.4
2	B	374	GLU	2.4
2	B	329	HIS	2.3
1	A	372	VAL	2.3
2	D	252	LEU	2.3
2	C	328	ARG	2.2
2	C	324	GLU	2.2
2	B	293	ALA	2.2
2	D	295	VAL	2.1
1	A	88	TYR	2.1
1	A	373	LEU	2.1
2	C	373	LEU	2.1
2	D	369	LEU	2.1
1	A	317	ARG	2.0

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

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	LLP	B	221	24/25	0.97	0.14	18,26,68,72	0
2	LLP	C	221	24/25	0.98	0.15	15,29,47,47	0
2	LLP	D	221	24/25	0.98	0.13	18,24,42,48	0

6.3 Carbohydrates [i](#)

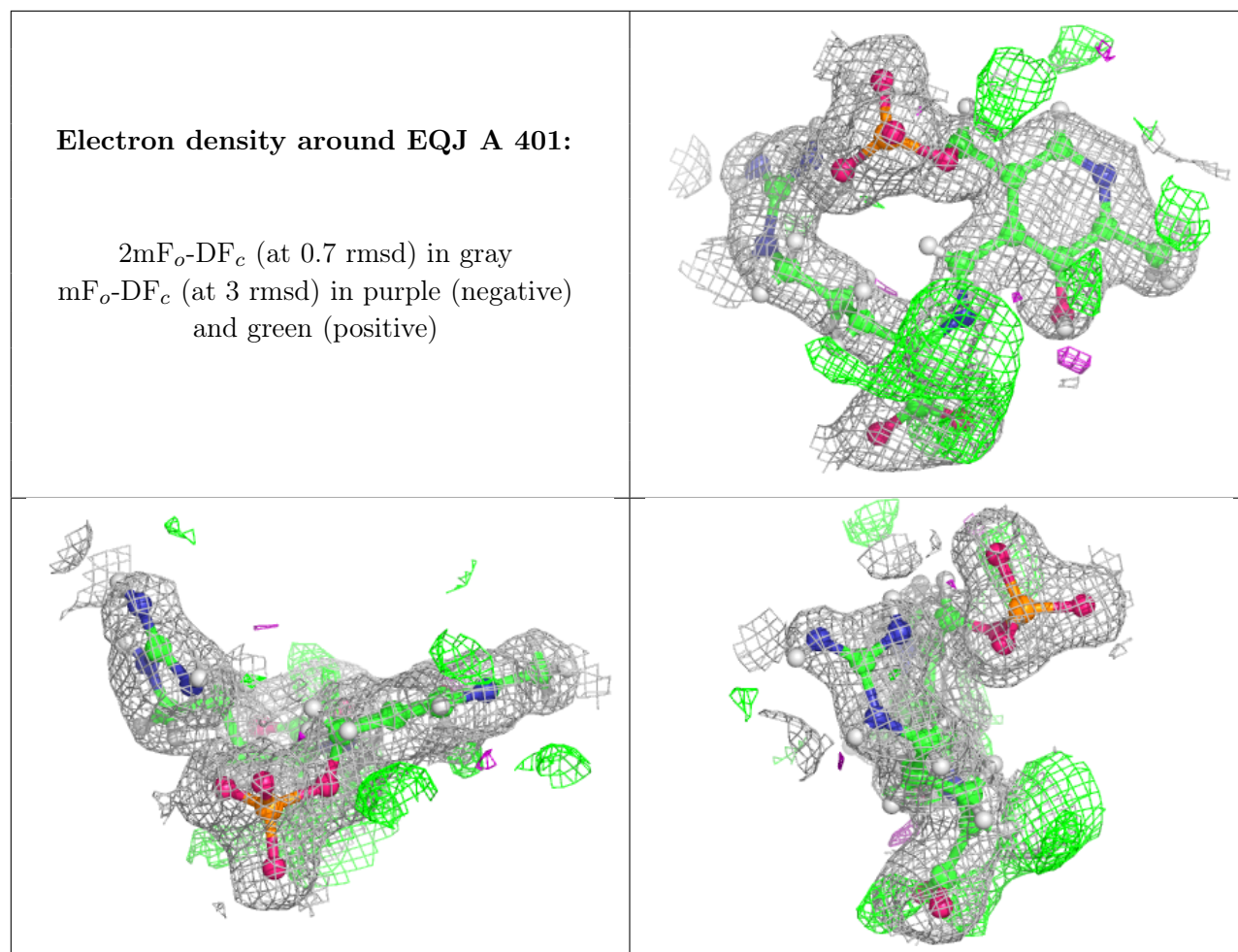
There are no monosaccharides in this entry.

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
4	EGV	C	401	12/13	0.92	0.24	23,43,81,108	0
4	EGV	B	401	12/13	0.95	0.15	20,39,53,56	0
3	EQJ	A	401	27/27	0.97	0.19	17,35,56,76	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.