



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:49 AM UTC

PDB ID : 6C8T / pdb_00006c8t
Title : The structure of MppP soaked with the substrate L-Arg
Authors : Han, L.; Silvaggi, N.R.
Deposited on : 2018-01-25
Resolution : 2.20 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 : 4-5-2 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

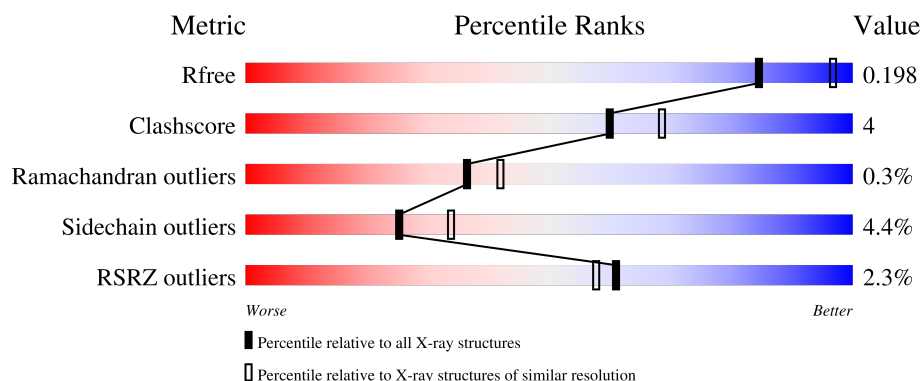
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	376	2% 90% 8% ..
1	B	376	2% 84% 12% ..
1	C	376	2% 85% 11% ..
2	D	376	2% 85% 8% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23402 atoms, of which 11215 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.

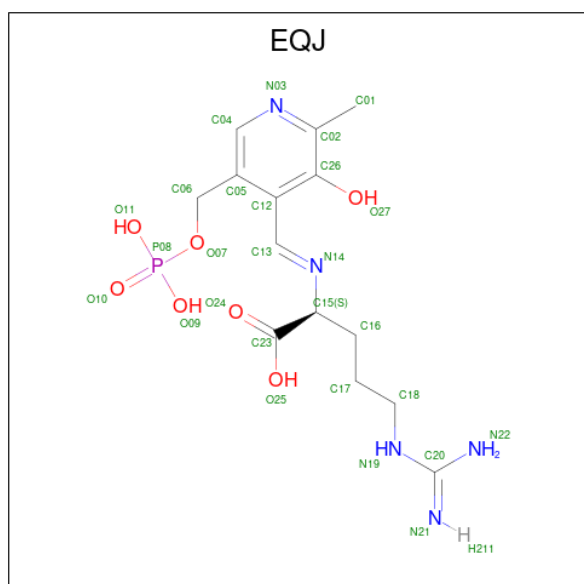
- Molecule 1 is a protein called PLP-Dependent L-Arginine Hydroxylase MppP.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	S		6	0	0
			5665	1800	2806	506	546	7				
1	B	368	Total	C	H	N	O	S		6	5	0
			5706	1811	2828	509	551	7				
1	C	368	Total	C	H	N	O	S		6	2	0
			5677	1803	2812	507	548	7				

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	D	354	Total	C	H	N	O	P	S	0	5	0
			5490	1743	2715	491	533	1	7			

- Molecule 3 is (E)-N 2 -({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-arginine (CCD ID: EQJ) (formula: C₁₄H₂₂N₅O₇P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

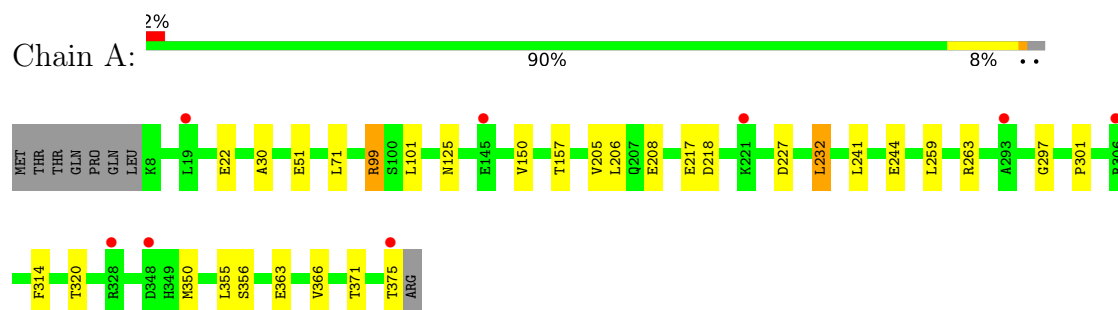
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	187	Total	O	0	0
			187	187		
5	C	169	Total	O	0	0
			169	169		
5	D	175	Total	O	0	0
			175	175		

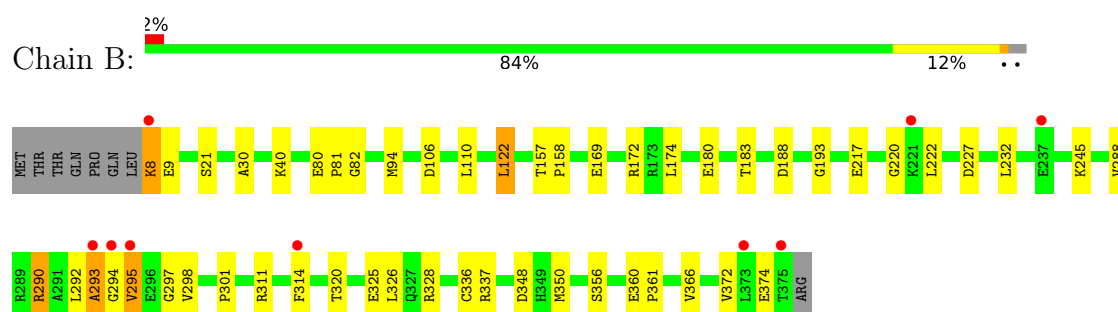
3 Residue-property plots [i](#)

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.

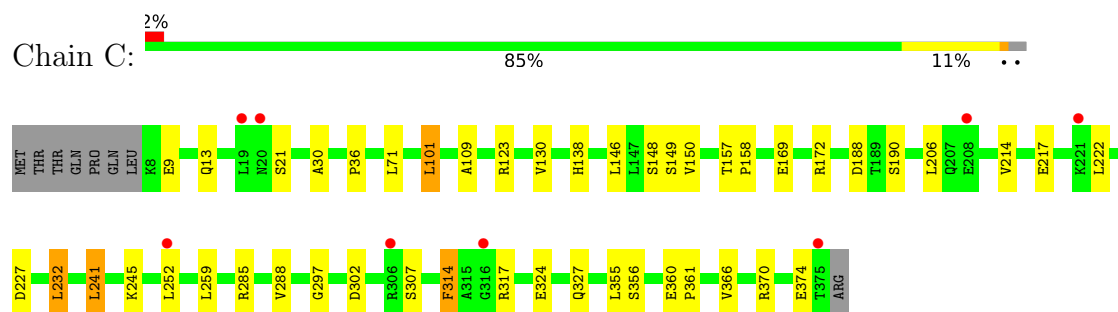
• Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



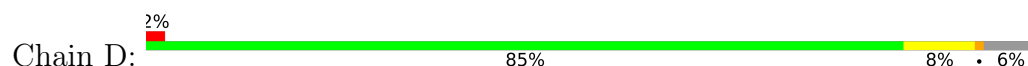
• Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP

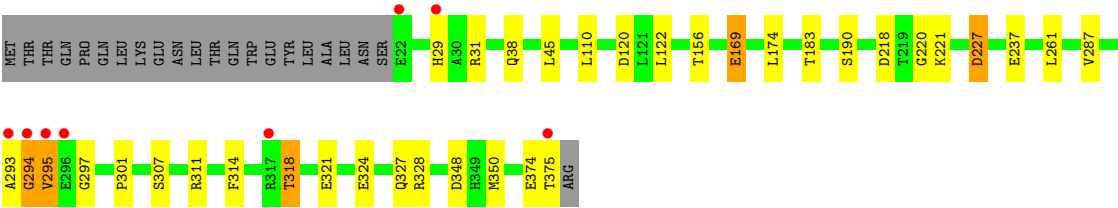


• Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



• 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	85.79Å 108.42Å 196.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.20 49.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.6 (49.05-2.20) 91.6 (49.05-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.78 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.146 , 0.195 0.148 , 0.198	Depositor DCC
R_{free} test set	2000 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23402	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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: CL, LLP, EQJ

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	0.44	0/2920	0.61	0/3976
1	B	0.44	0/2957	0.61	0/4026
1	C	0.46	0/2932	0.62	0/3992
2	D	0.46	0/2826	0.62	0/3847
All	All	0.45	0/11635	0.62	0/15841

There are no bond length outliers.

There are no bond angle outliers.

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	2859	2806	2806	14	0
1	B	2878	2828	2812	37	0
1	C	2865	2812	2806	27	0
2	D	2775	2715	2702	21	0
3	A	27	18	0	0	0
3	B	27	18	0	1	0
3	C	27	18	0	1	0
4	D	1	0	0	0	0
5	A	197	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	187	0	0	12	1
5	C	169	0	0	10	1
5	D	175	0	0	6	2
All	All	12187	11215	11126	98	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 (98) 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:C:370:ARG:NH1	1:C:374:GLU:OE2	1.99	0.95
2:D:220:GLY:O	5:D:501:HOH:O	1.90	0.88
1:B:180:GLU:OE1	5:B:501:HOH:O	1.92	0.86
1:B:220:GLY:O	5:B:502:HOH:O	1.94	0.84
1:B:180:GLU:OE1	5:B:503:HOH:O	1.97	0.81
1:B:8:LYS:N	5:B:508:HOH:O	2.12	0.81
1:C:302:ASP:OD1	5:C:501:HOH:O	2.00	0.80
1:C:227:ASP:OD2	5:C:502:HOH:O	2.02	0.77
2:D:237:GLU:OE2	5:D:502:HOH:O	2.06	0.72
1:B:169:GLU:OE1	5:B:504:HOH:O	2.08	0.71
1:B:180:GLU:OE1	5:B:506:HOH:O	2.10	0.69
1:B:80:GLU:OE1	5:B:505:HOH:O	2.10	0.69
1:B:106:ASP:OD2	5:B:507:HOH:O	2.11	0.67
2:D:120:ASP:OD2	5:D:503:HOH:O	2.15	0.65
1:B:172:ARG:NH1	5:B:511:HOH:O	2.29	0.64
1:C:360:GLU:HG2	1:C:361:PRO:HD3	1.82	0.61
1:C:148:SER:OG	5:C:504:HOH:O	2.16	0.60
1:A:301:PRO:HG2	1:A:350:MET:CE	2.34	0.58
1:B:311:ARG:HB3	1:B:350:MET:CE	2.34	0.58
1:B:325:GLU:OE1	1:B:328:ARG:NH2	2.37	0.57
1:A:244:GLU:OE2	5:A:501:HOH:O	2.18	0.56
2:D:227:ASP:CG	5:D:507:HOH:O	2.48	0.56
1:B:301:PRO:HG3	1:B:350:MET:HE3	1.88	0.55
1:C:285:ARG:NH2	1:C:307:SER:O	2.39	0.55
1:A:371:THR:O	1:A:375:THR:HG22	2.06	0.55
1:B:294:GLY:O	1:B:295:VAL:C	2.50	0.55
1:A:218:ASP:O	5:A:502:HOH:O	2.18	0.54
1:A:301:PRO:HG2	1:A:350:MET:HE3	1.90	0.53
2:D:301:PRO:CG	2:D:350:MET:HE3	2.39	0.52
1:B:169:GLU:H	1:B:169:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ARG:HD2	2:D:350:MET:CE	2.41	0.51
1:B:30:ALA:HA	1:B:356:SER:HB3	1.91	0.51
1:B:360:GLU:HB2	1:B:361:PRO:HD3	1.93	0.50
1:A:208:GLU:OE1	2:D:324:GLU:OE1	2.29	0.50
1:B:311:ARG:HD2	1:B:350:MET:CE	2.40	0.50
1:B:245:LYS:HE2	5:B:548:HOH:O	2.12	0.50
1:C:252:LEU:CD2	5:C:645:HOH:O	2.59	0.50
1:A:30:ALA:HA	1:A:356:SER:HB3	1.94	0.49
1:C:109:ALA:HA	1:C:130:VAL:HG22	1.93	0.49
1:B:40:LYS:NZ	5:B:512:HOH:O	2.32	0.49
1:B:320:THR:HG23	5:B:631:HOH:O	2.12	0.49
1:C:36:PRO:HD2	5:C:590:HOH:O	2.12	0.49
1:C:217:GLU:HB2	1:C:232:LEU:HB2	1.94	0.49
1:C:9:GLU:HB2	1:C:13:GLN:OE1	2.13	0.48
1:C:101:LEU:HD13	1:C:241:LEU:HD21	1.94	0.48
1:B:301:PRO:CG	1:B:350:MET:HE3	2.44	0.48
1:C:297:GLY:O	1:C:314:PHE:HA	2.14	0.48
1:A:99:ARG:HG2	1:A:125:ASN:OD1	2.14	0.48
1:C:123:ARG:HD3	5:C:553:HOH:O	2.14	0.47
1:B:372:VAL:C	1:B:374:GLU:H	2.23	0.47
2:D:311:ARG:HD2	2:D:350:MET:HE1	1.97	0.47
1:C:190:SER:HB2	5:C:556:HOH:O	2.15	0.47
1:B:80:GLU:H	1:B:80:GLU:CD	2.23	0.47
2:D:297:GLY:O	2:D:314:PHE:HA	2.15	0.47
1:B:360:GLU:H	1:B:360:GLU:CD	2.22	0.46
1:B:311:ARG:HD2	1:B:350:MET:HE1	1.96	0.46
2:D:318:THR:HG22	2:D:321:GLU:H	1.80	0.46
1:B:94:MET:CE	1:B:122:LEU:HD13	2.46	0.46
1:A:217:GLU:HB2	1:A:232:LEU:HB2	1.96	0.46
2:D:301:PRO:HG3	2:D:350:MET:HE3	1.98	0.46
2:D:301:PRO:HG2	2:D:350:MET:HE3	1.98	0.46
2:D:237:GLU:CD	5:D:502:HOH:O	2.56	0.45
1:B:157:THR:HA	1:B:158:PRO:C	2.40	0.45
1:C:360:GLU:HG2	1:C:361:PRO:CD	2.46	0.45
1:B:94:MET:HE3	1:B:122:LEU:HD13	1.99	0.45
1:B:81:PRO:HA	1:B:82:GLY:HA2	1.83	0.45
1:B:188:ASP:OD2	3:B:401:EQJ:N03	2.50	0.45
2:D:294:GLY:O	2:D:295:VAL:O	2.35	0.45
1:B:295:VAL:HG23	1:B:298:VAL:HB	1.99	0.45
1:C:252:LEU:HD23	5:C:645:HOH:O	2.16	0.45
1:C:188:ASP:OD1	1:C:188:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:HA	1:A:366:VAL:HG12	2.00	0.44
1:C:30:ALA:HA	1:C:356:SER:HB3	2.00	0.44
2:D:45:LEU:HD21	2:D:261:LEU:HD13	2.00	0.43
1:A:157:THR:HG23	1:A:157:THR:O	2.19	0.43
1:B:193:GLY:HA3	1:B:222:LEU:HD11	2.00	0.43
1:C:288:VAL:HG22	1:C:366:VAL:HG21	2.00	0.43
2:D:190:SER:HA	2:D:218:ASP:HB3	2.01	0.43
2:D:29:HIS:HB2	2:D:31:ARG:NH1	2.33	0.43
1:C:157:THR:HA	1:C:158:PRO:C	2.44	0.43
1:B:336:CYS:O	1:B:337:ARG:C	2.62	0.42
2:D:169:GLU:H	2:D:169:GLU:CD	2.27	0.42
1:C:245:LYS:NZ	5:C:509:HOH:O	2.35	0.42
1:C:324:GLU:O	1:C:327:GLN:HG3	2.19	0.42
2:D:311:ARG:HB3	2:D:350:MET:CE	2.49	0.42
1:A:51:GLU:OE2	1:A:263:ARG:NH2	2.41	0.42
1:C:130:VAL:HG21	1:C:146:LEU:HD11	2.01	0.41
1:C:188:ASP:OD2	3:C:401:EQJ:N03	2.52	0.41
1:B:217:GLU:HB2	1:B:232:LEU:HB2	2.03	0.41
2:D:374:GLU:O	2:D:375:THR:C	2.63	0.41
1:C:130:VAL:O	1:C:130:VAL:HG23	2.19	0.41
1:A:301:PRO:HG2	1:A:350:MET:HE1	2.03	0.41
1:B:297:GLY:O	1:B:314:PHE:HA	2.21	0.41
1:B:288:VAL:HG22	1:B:366:VAL:HG11	2.02	0.41
1:C:138:HIS:NE2	5:C:503:HOH:O	2.06	0.40
2:D:38:GLN:NE2	5:D:508:HOH:O	2.37	0.40
1:B:290:ARG:O	1:B:293:ALA:HB2	2.21	0.40
1:A:297:GLY:O	1:A:314:PHE:HA	2.22	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:B:681:HOH:O	5:D:664:HOH:O[1_455]	1.98	0.22
5:C:506:HOH:O	5:D:625:HOH:O[4_497]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/376 (97%)	360 (98%)	6 (2%)	0	100	100
1	B	371/376 (99%)	359 (97%)	10 (3%)	2 (0%)	24	27
1	C	368/376 (98%)	360 (98%)	8 (2%)	0	100	100
2	D	356/376 (95%)	347 (98%)	6 (2%)	3 (1%)	16	16
All	All	1461/1504 (97%)	1426 (98%)	30 (2%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/315 (98%)	294 (96%)	13 (4%)	26	36
1	B	312/315 (99%)	300 (96%)	12 (4%)	29	40
1	C	309/315 (98%)	293 (95%)	16 (5%)	21	26
2	D	298/314 (95%)	285 (96%)	13 (4%)	25	34
All	All	1226/1259 (97%)	1172 (96%)	54 (4%)	25	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	71	LEU
1	A	99	ARG
1	A	101	LEU
1	A	150	VAL
1	A	205	VAL
1	A	206	LEU
1	A	227	ASP
1	A	232	LEU
1	A	241	LEU
1	A	259	LEU
1	A	320	THR
1	A	355	LEU
1	B	8	LYS
1	B	9	GLU
1	B	21	SER
1	B	110	LEU
1	B	122	LEU
1	B	174	LEU
1	B	183	THR
1	B	227	ASP
1	B	290	ARG
1	B	292	LEU
1	B	326	LEU
1	B	348	ASP
1	C	21	SER
1	C	71	LEU
1	C	101	LEU
1	C	149	SER
1	C	150	VAL
1	C	169	GLU
1	C	172	ARG
1	C	206	LEU
1	C	214	VAL
1	C	222	LEU
1	C	232	LEU
1	C	241	LEU
1	C	259	LEU
1	C	314	PHE
1	C	317	ARG
1	C	355	LEU
2	D	110	LEU

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Mol	Chain	Res	Type
2	D	122	LEU
2	D	156	THR
2	D	169	GLU
2	D	174	LEU
2	D	183	THR
2	D	227	ASP
2	D	287	VAL
2	D	307	SER
2	D	318	THR
2	D	327	GLN
2	D	328	ARG
2	D	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	329	HIS
1	B	29	HIS
1	B	125	ASN
1	C	29	HIS
1	C	58	GLN
1	C	59	GLN
1	C	75	HIS
2	D	58	GLN
2	D	75	HIS
2	D	283	HIS
2	D	330	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	D	221	2	23,24,25	1.29	3 (13%)	25,32,34	1.68	5 (20%)

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	D	221	2	-	4/16/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	221	LLP	O-C	4.08	1.35	1.20
2	D	221	LLP	C3-C2	2.98	1.44	1.41
2	D	221	LLP	C6-C5	2.10	1.41	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	221	LLP	OP2-P-OP4	-4.49	94.95	106.67
2	D	221	LLP	OP4-C5'-C5	3.27	115.49	109.36
2	D	221	LLP	OP4-P-OP1	3.15	114.96	106.44
2	D	221	LLP	OP2-P-OP1	2.67	121.23	110.83
2	D	221	LLP	C2'-C2-C3	-2.50	117.87	120.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	221	LLP	C4-C5-C5'-OP4
2	D	221	LLP	C6-C5-C5'-OP4
2	D	221	LLP	CG-CD-CE-NZ
2	D	221	LLP	C4-C4'-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is 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	EQJ	C	401	-	27,27,27	2.29	7 (25%)	32,37,37	1.65	5 (15%)
3	EQJ	B	401	-	27,27,27	2.14	6 (22%)	32,37,37	1.18	3 (9%)
3	EQJ	A	401	-	27,27,27	2.10	7 (25%)	32,37,37	1.80	4 (12%)

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	C	401	-	-	3/22/22/22	0/1/1/1
3	EQJ	B	401	-	-	4/22/22/22	0/1/1/1
3	EQJ	A	401	-	-	3/22/22/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	EQJ	C20-N19	8.31	1.49	1.33
3	B	401	EQJ	C20-N19	8.23	1.49	1.33
3	A	401	EQJ	C20-N19	7.50	1.47	1.33
3	B	401	EQJ	C12-C13	3.60	1.54	1.46
3	C	401	EQJ	C20-N21	3.35	1.44	1.32
3	C	401	EQJ	C12-C13	3.34	1.53	1.46
3	A	401	EQJ	C12-C13	3.34	1.53	1.46
3	A	401	EQJ	C20-N21	3.27	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	EQJ	C16-C15	3.21	1.57	1.53
3	B	401	EQJ	C13-N14	3.05	1.32	1.27
3	C	401	EQJ	C16-C15	2.98	1.56	1.53
3	C	401	EQJ	C13-N14	2.91	1.32	1.27
3	B	401	EQJ	C20-N21	2.88	1.42	1.32
3	A	401	EQJ	C13-N14	2.72	1.32	1.27
3	C	401	EQJ	C06-C05	2.63	1.57	1.50
3	B	401	EQJ	C06-C05	2.45	1.57	1.50
3	C	401	EQJ	C26-C02	-2.29	1.38	1.41
3	B	401	EQJ	C26-C02	-2.25	1.38	1.41
3	A	401	EQJ	C06-C05	2.07	1.56	1.50
3	A	401	EQJ	C01-C02	2.03	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	EQJ	C15-N14-C13	7.16	127.40	116.77
3	C	401	EQJ	C15-N14-C13	6.47	126.38	116.77
3	A	401	EQJ	O07-P08-O10	3.03	114.64	106.44
3	C	401	EQJ	O25-C23-O24	-2.63	118.11	124.08
3	B	401	EQJ	C05-C04-N03	-2.55	119.68	123.83
3	C	401	EQJ	C05-C04-N03	-2.48	119.80	123.83
3	A	401	EQJ	C05-C04-N03	-2.46	119.82	123.83
3	A	401	EQJ	O25-C23-O24	-2.29	118.89	124.08
3	C	401	EQJ	C04-N03-C02	2.18	123.16	119.20
3	B	401	EQJ	C12-C26-C02	-2.15	118.93	120.14
3	B	401	EQJ	C01-C02-C26	-2.15	118.28	120.80
3	C	401	EQJ	O07-P08-O10	2.15	112.25	106.44

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	EQJ	C16-C15-N14-C13
3	B	401	EQJ	C06-O07-P08-O09
3	C	401	EQJ	C16-C15-N14-C13
3	C	401	EQJ	C06-O07-P08-O10
3	C	401	EQJ	C06-O07-P08-O11
3	B	401	EQJ	C16-C17-C18-N19
3	A	401	EQJ	C06-O07-P08-O10
3	B	401	EQJ	C06-O07-P08-O11
3	A	401	EQJ	C06-O07-P08-O09

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Mol	Chain	Res	Type	Atoms
3	B	401	EQJ	C26-C12-C13-N14

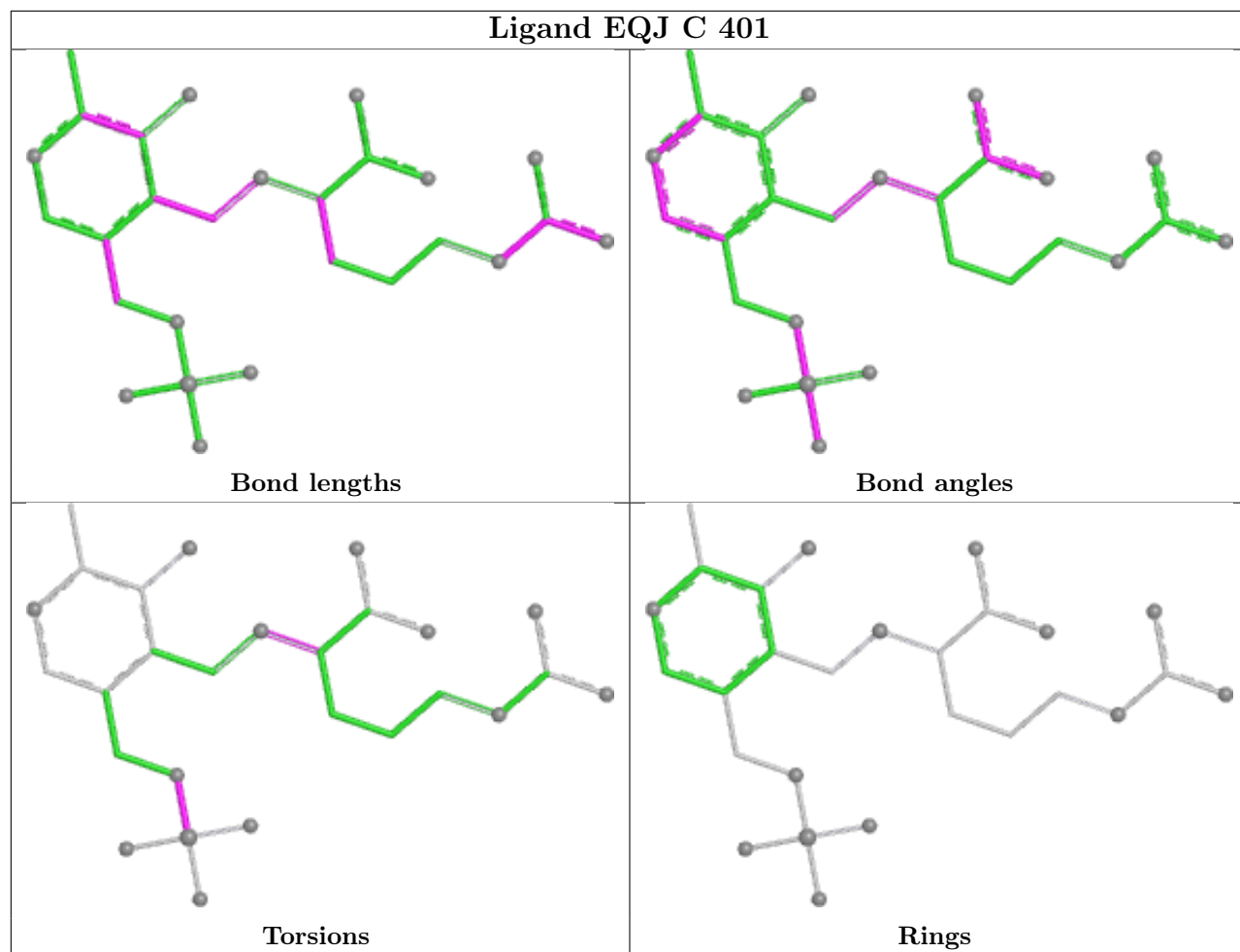
There are no ring outliers.

2 monomers are involved in 2 short contacts:

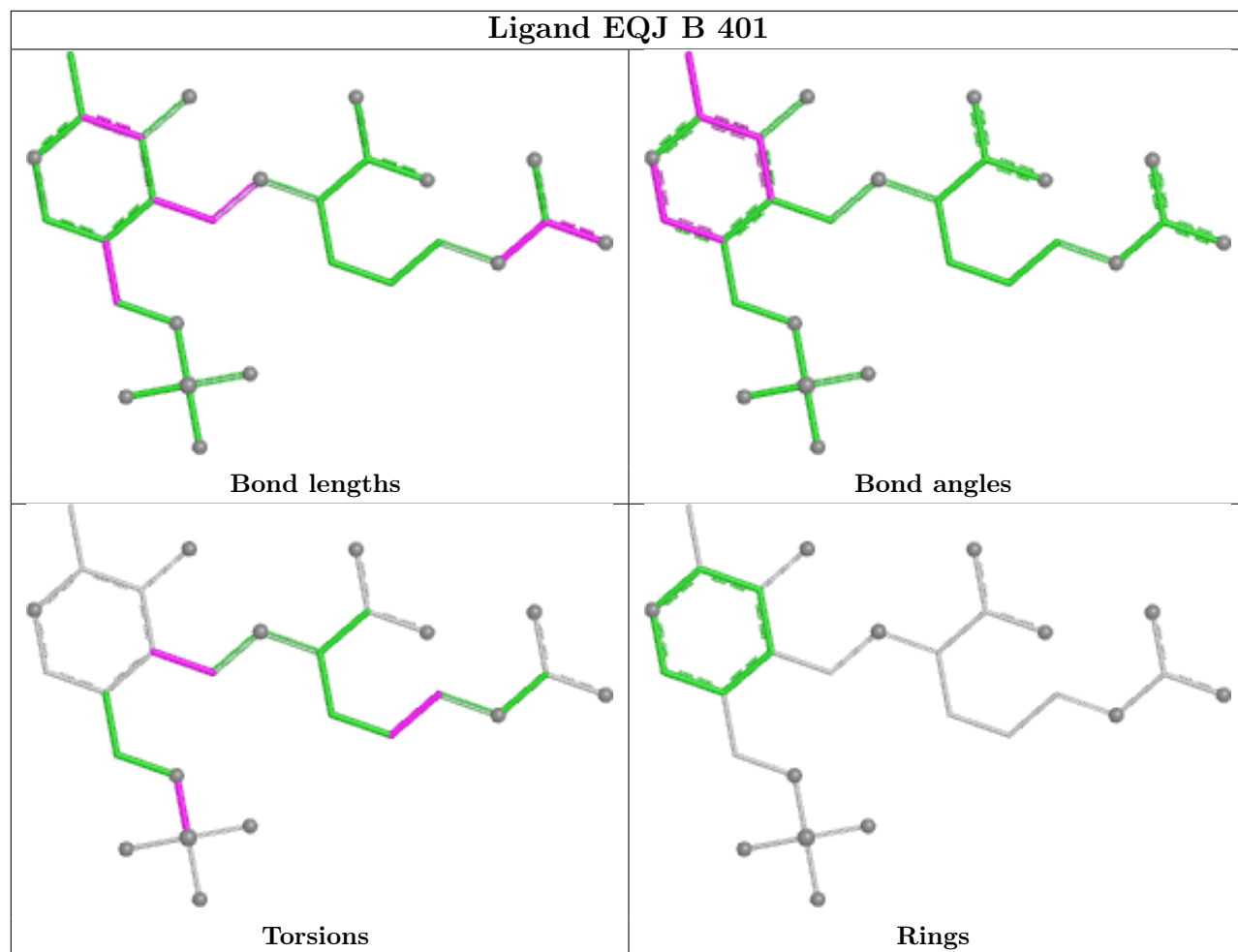
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	EQJ	1	0
3	B	401	EQJ	1	0

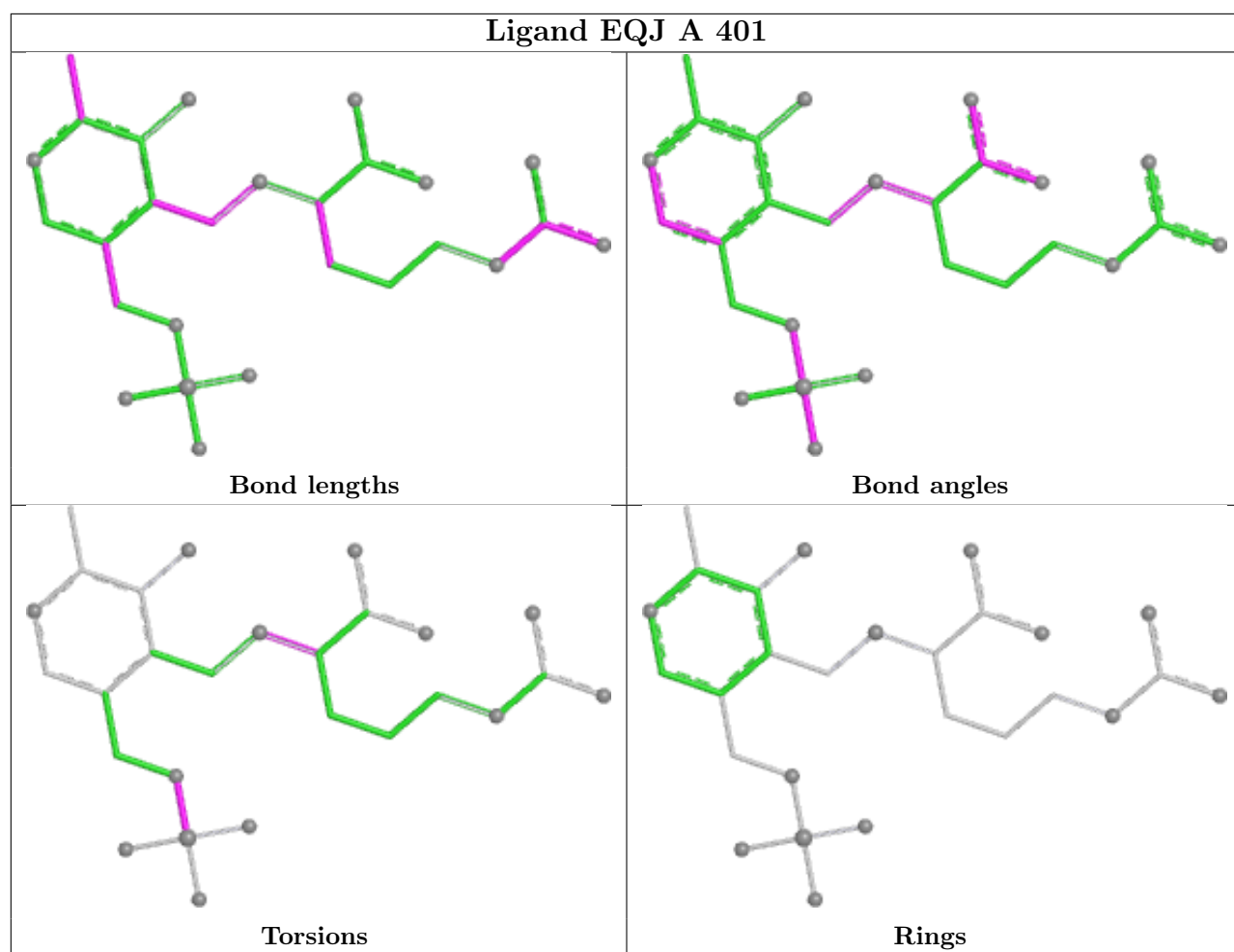
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand EQJ C 401



Ligand EQJ B 401





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	368/376 (97%)	-0.64	8 (2%) 62 59	15, 31, 73, 117	1 (0%)
1	B	368/376 (97%)	-0.60	9 (2%) 59 56	8, 30, 76, 138	4 (1%)
1	C	368/376 (97%)	-0.58	8 (2%) 62 59	9, 31, 72, 108	2 (0%)
2	D	353/376 (93%)	-0.57	8 (2%) 61 58	11, 29, 79, 140	3 (0%)
All	All	1457/1504 (96%)	-0.60	33 (2%) 61 58	8, 30, 76, 140	10 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	LYS	6.1
1	B	375	THR	4.4
1	B	293	ALA	4.3
1	B	221	LYS	3.9
1	A	221	LYS	3.6
2	D	22	GLU	3.5
2	D	29	HIS	3.4
2	D	293	ALA	3.4
1	B	294	GLY	3.3
1	C	19	LEU	3.2
2	D	294	GLY	2.9
2	D	296	GLU	2.7
2	D	317	ARG	2.7
1	B	295	VAL	2.7
1	A	19	LEU	2.6
1	A	375	THR	2.6
1	C	375	THR	2.5
1	B	373	LEU	2.4
1	C	306	ARG	2.4
1	C	316	GLY	2.4
1	A	293	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	314	PHE	2.4
1	A	306	ARG	2.3
1	B	237	GLU	2.3
1	A	348	ASP	2.3
1	C	20	ASN	2.3
1	A	145	GLU	2.2
2	D	375	THR	2.2
2	D	295	VAL	2.1
1	C	208	GLU	2.1
1	C	252	LEU	2.1
1	A	328	ARG	2.1
1	B	8	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	LLP	D	221	24/25	0.99	0.04	12,24,32,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

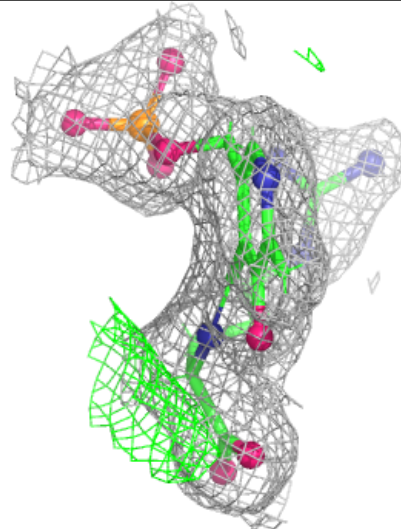
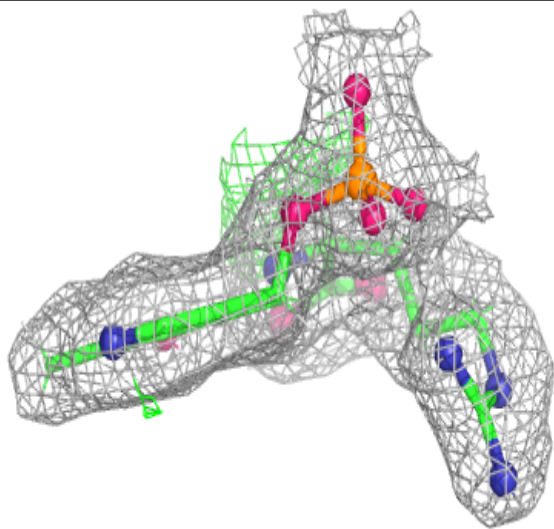
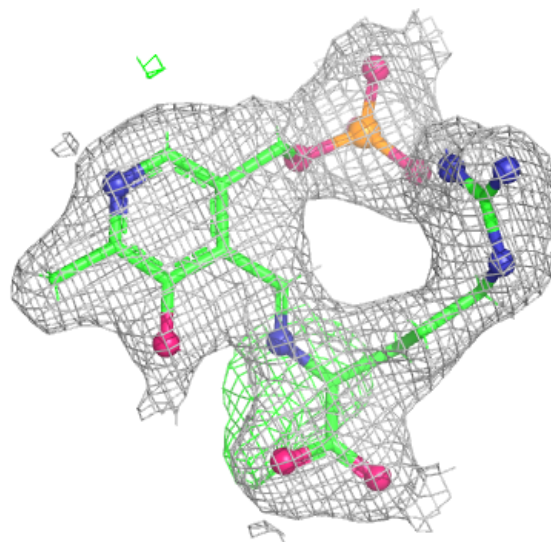
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EQJ	A	401	27/27	0.98	0.06	17,30,46,54	0
3	EQJ	B	401	27/27	0.98	0.06	14,29,43,50	0
3	EQJ	C	401	27/27	0.98	0.06	17,29,49,59	0
4	CL	D	401	1/1	0.99	0.04	35,35,35,35	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.

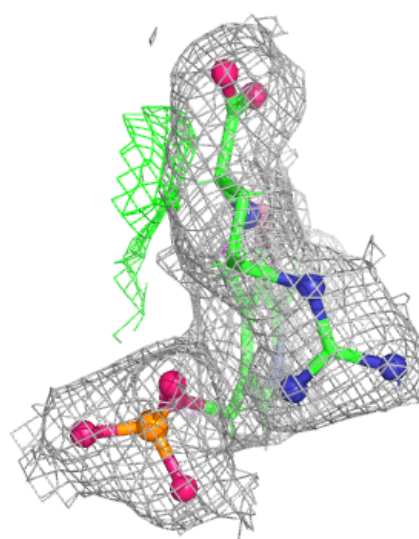
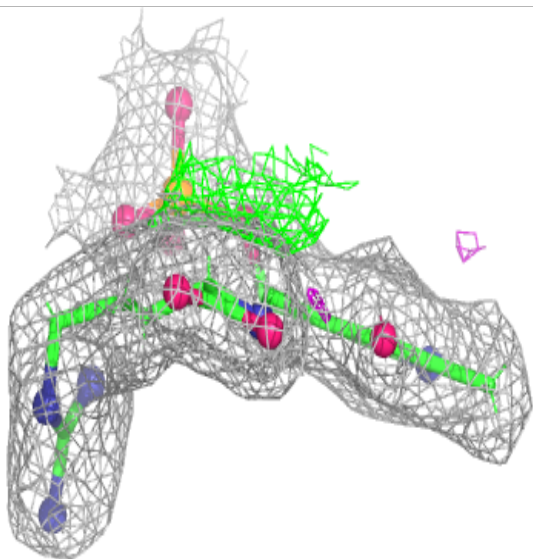
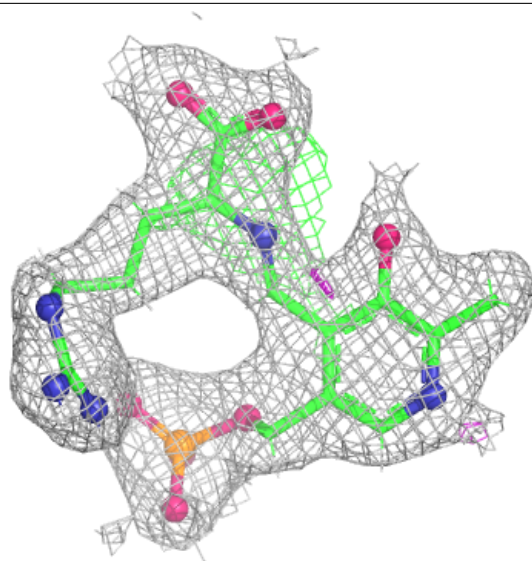
Electron density around EQJ A 401:

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



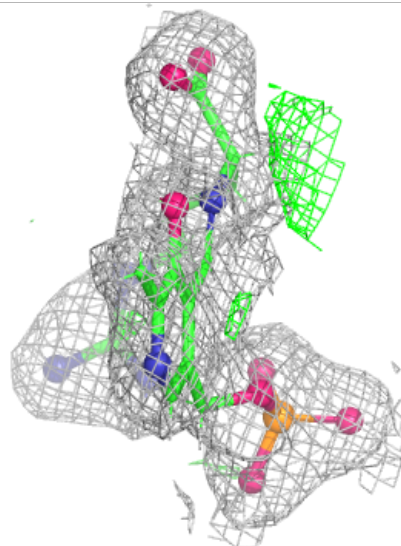
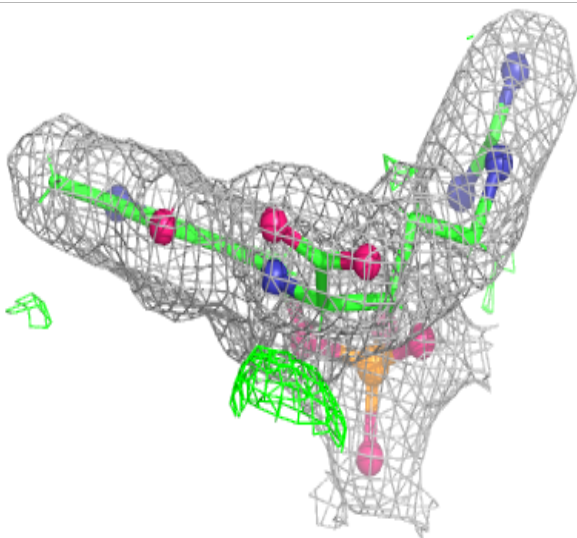
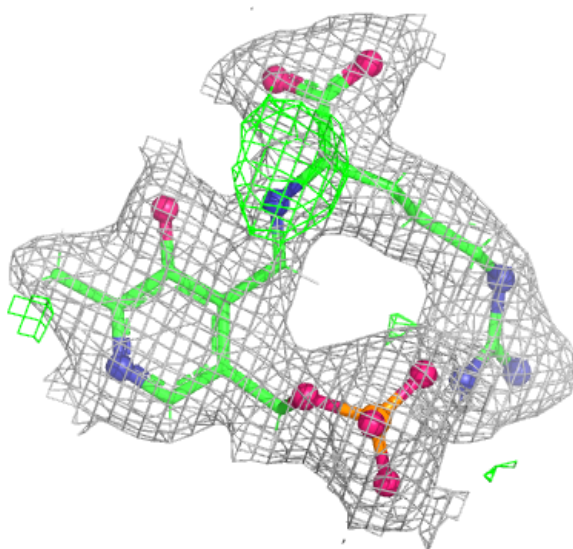
Electron density around EQJ B 401:

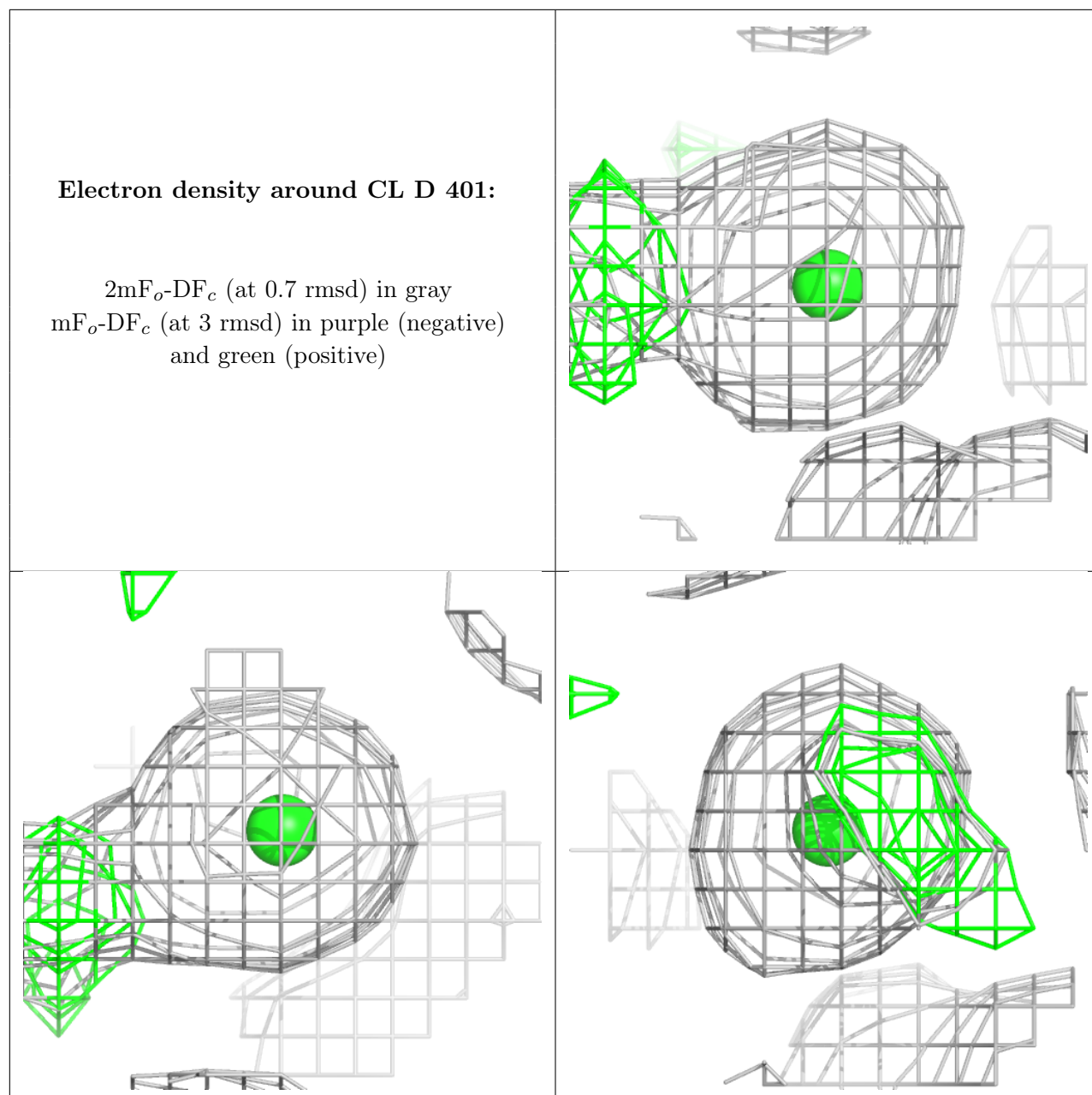
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EQJ C 401:

$2mF_o-DF_c$ (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.