



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:51 am BST

PDB ID : 5BK7
Title : The structure of MppP E15A mutant soaked with the substrate L-arginine
Authors : Han, L.; Silvaggi, N.R.
Deposited on : 2018-01-27
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 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 : 2.11
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) : 2.11

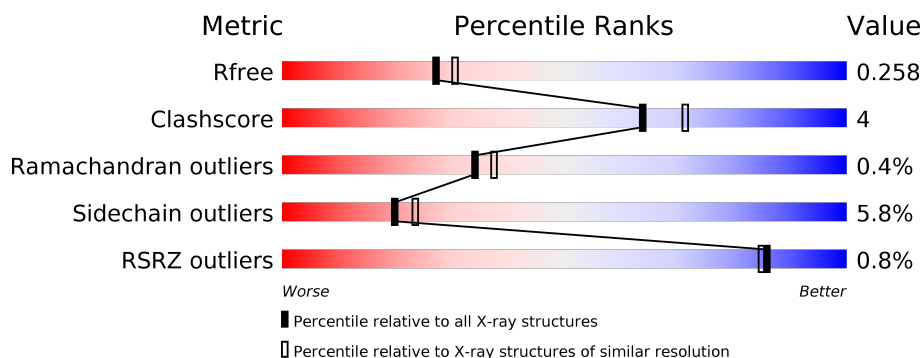
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	<div> <div style="width: 87%;"></div> <div style="width: 10%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>87% 10% ..</div>
1	B	376	<div> <div style="width: 83%;"></div> <div style="width: 13%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>83% 13% ..</div>
1	C	376	<div> <div style="width: 82%;"></div> <div style="width: 14%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>82% 14% ..</div>
1	D	376	<div> <div style="width: 87%;"></div> <div style="width: 9%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>87% 9% ..</div>
1	E	376	<div> <div style="width: 84%;"></div> <div style="width: 11%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>84% 11% ..</div>
1	F	376	<div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>81% 15% ..</div>

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Mol	Chain	Length	Quality of chain
1	G	376	
1	H	376	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46508 atoms, of which 22598 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.

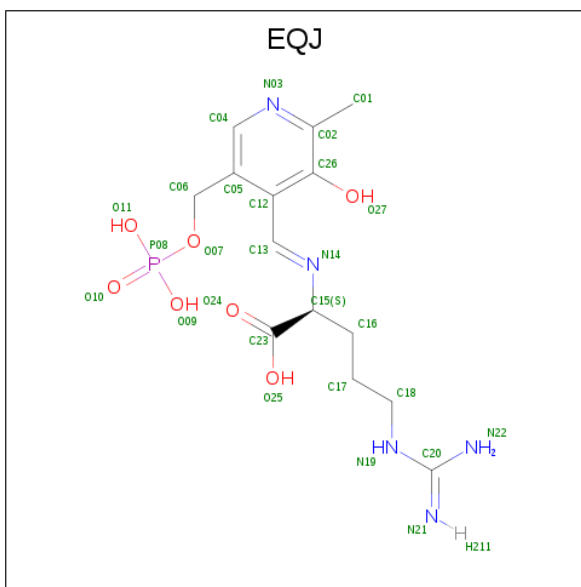
- Molecule 1 is a protein called PLP-Dependent L-Arginine Hydroxylase MppP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	S	6	0	0
			5662	1798	2807	506	544	7			
1	B	368	Total	C	H	N	O	S	6	0	0
			5660	1798	2805	506	544	7			
1	C	368	Total	C	H	N	O	S	6	0	0
			5657	1798	2802	506	544	7			
1	D	368	Total	C	H	N	O	S	6	0	0
			5661	1798	2806	506	544	7			
1	E	368	Total	C	H	N	O	S	6	0	0
			5662	1798	2807	506	544	7			
1	F	368	Total	C	H	N	O	S	6	0	0
			5660	1798	2805	506	544	7			
1	G	368	Total	C	H	N	O	S	6	0	0
			5660	1798	2805	506	544	7			
1	H	369	Total	C	H	N	O	S	6	0	0
			5680	1804	2817	507	545	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
B	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
C	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
D	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
E	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
F	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
G	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5
H	15	ALA	GLU	engineered mutation	UNP A0A0X1KHF5

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	C	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	D	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	E	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	F	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	G	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		
2	H	1	Total	C	H	N	O	P	0	0
			45	14	18	5	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total	O	0	0
			184	184		
3	B	53	Total	O	0	0
			53	53		
3	C	70	Total	O	0	0
			70	70		
3	D	142	Total	O	0	0
			142	142		

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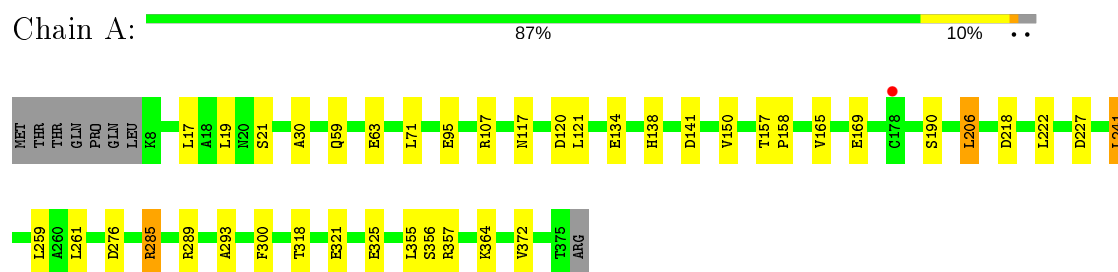
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	156	Total 156	O 156	0	0
3	F	41	Total 41	O 41	0	0
3	G	42	Total 42	O 42	0	0
3	H	158	Total 158	O 158	0	0

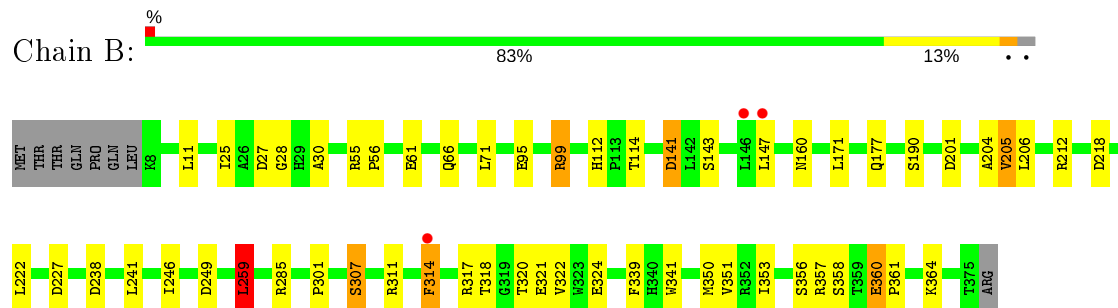
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

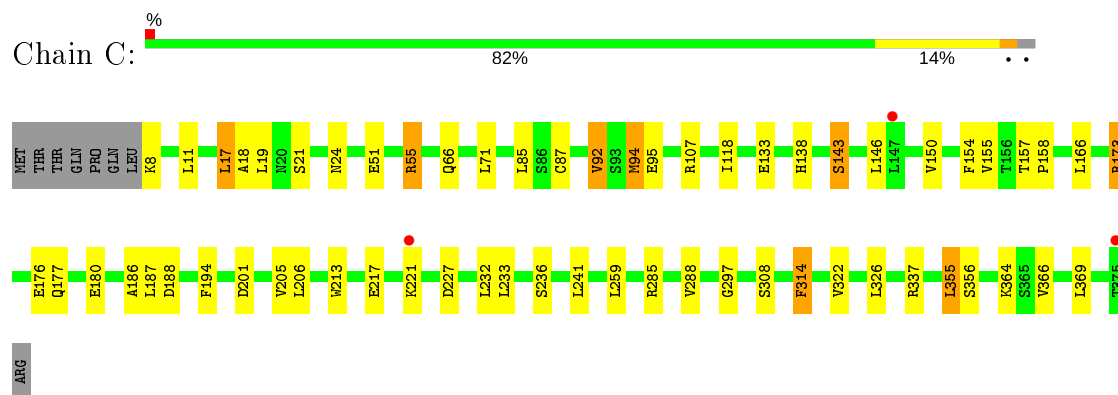
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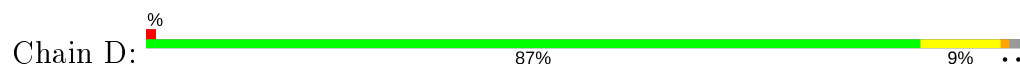
• Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



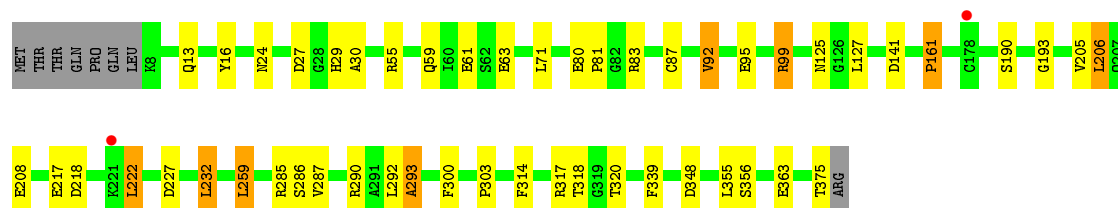
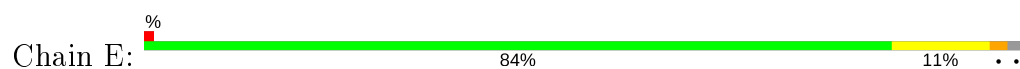
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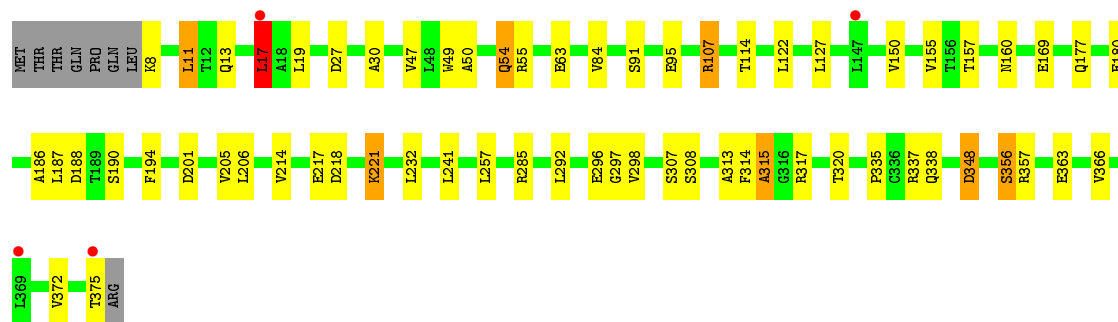
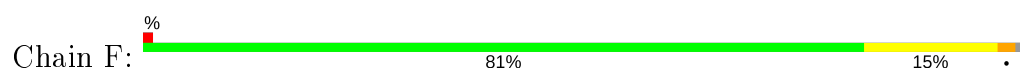
• Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



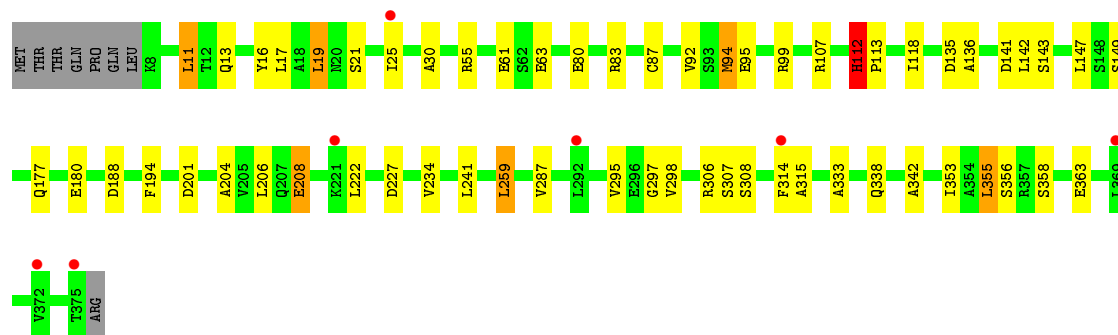
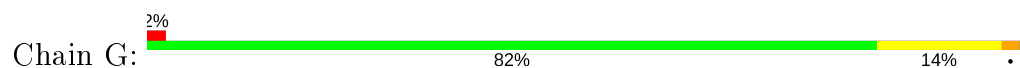
- Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



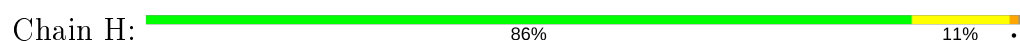
- Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP

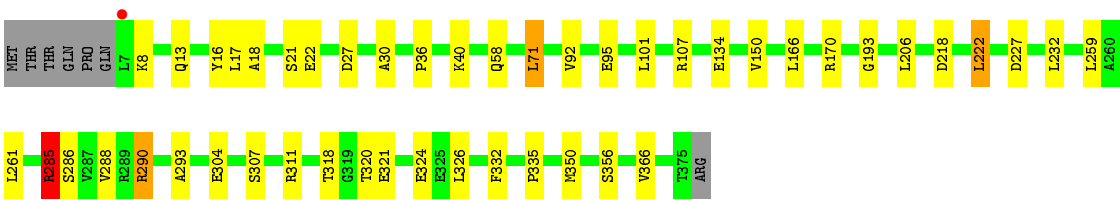


- Molecule 1: PLP-Dependent L-Arginine Hydroxylase MppP



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.44Å 200.51Å 139.93Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	45.40 – 2.20 45.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (45.40-2.20) 89.0 (45.40-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.201 , 0.258 0.201 , 0.258	Depositor DCC
R_{free} test set	2001 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.156 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	46508	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8376e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	0/2916	0.84	8/3971 (0.2%)
1	B	0.56	0/2916	0.70	2/3971 (0.1%)
1	C	0.55	0/2916	0.72	3/3971 (0.1%)
1	D	0.71	1/2916 (0.0%)	0.81	2/3971 (0.1%)
1	E	0.67	0/2916	0.81	6/3971 (0.2%)
1	F	0.54	0/2916	0.68	1/3971 (0.0%)
1	G	0.55	0/2916	0.71	2/3971 (0.1%)
1	H	0.70	2/2924 (0.1%)	0.79	5/3982 (0.1%)
All	All	0.62	3/23336 (0.0%)	0.76	29/31779 (0.1%)

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	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	304	GLU	CB-CG	6.21	1.64	1.52
1	H	134	GLU	CB-CG	5.46	1.62	1.52
1	D	336	CYS	CB-SG	-5.32	1.73	1.81

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	112	HIS	C-N-CD	-11.60	95.08	120.60
1	A	285	ARG	NE-CZ-NH2	-11.35	114.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	E	285	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	285	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	E	55	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	H	285	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	141	ASP	CB-CG-OD1	6.68	124.31	118.30
1	E	141	ASP	CB-CG-OD1	6.62	124.25	118.30
1	G	94	MET	CG-SD-CE	-6.51	89.78	100.20
1	H	71	LEU	CA-CB-CG	6.34	129.88	115.30
1	B	55	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	94	MET	CG-SD-CE	-6.10	90.44	100.20
1	D	71	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	141	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	C	55	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	120	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	285	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	241	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	357	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	17	LEU	CB-CG-CD1	5.46	120.28	111.00
1	H	27	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	B	259	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	206	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	259	LEU	CA-CB-CG	5.25	127.38	115.30
1	H	222	LEU	CA-CB-CG	5.20	127.25	115.30
1	E	206	LEU	CA-CB-CG	5.12	127.08	115.30
1	E	127	LEU	CA-CB-CG	-5.10	103.57	115.30
1	H	285	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	112	HIS	Peptide

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	2855	2807	2805	15	0
1	B	2855	2805	2805	30	0
1	C	2855	2802	2805	31	0
1	D	2855	2806	2805	21	0
1	E	2855	2807	2805	23	0
1	F	2855	2805	2805	31	0
1	G	2855	2805	2805	27	0
1	H	2863	2817	2816	20	0
2	A	27	18	0	0	0
2	B	27	18	0	1	0
2	C	27	18	0	2	0
2	D	27	18	0	0	0
2	E	27	18	0	0	0
2	F	27	18	0	1	0
2	G	27	18	0	0	0
2	H	27	18	0	0	0
3	A	184	0	0	2	0
3	B	53	0	0	1	0
3	C	70	0	0	6	0
3	D	142	0	0	2	0
3	E	156	0	0	2	0
3	F	41	0	0	4	0
3	G	42	0	0	3	0
3	H	158	0	0	3	0
All	All	23910	22598	22451	192	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 (192) 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:H:324:GLU:OE1	3:H:501:HOH:O	1.95	0.83
1:H:335:PRO:O	3:H:502:HOH:O	1.99	0.81
1:D:55:ARG:O	3:D:501:HOH:O	2.00	0.78
1:C:51:GLU:OE1	3:C:501:HOH:O	2.02	0.77
1:H:218:ASP:O	3:H:503:HOH:O	2.03	0.77
1:G:94:MET:HE3	1:G:118:ILE:HG23	1.66	0.76
1:C:94:MET:HE1	1:C:118:ILE:HG23	1.67	0.75
1:B:30:ALA:HA	1:B:356:SER:HB3	1.68	0.73
1:F:335:PRO:O	3:F:501:HOH:O	2.07	0.72
1:G:204:ALA:O	1:G:208:GLU:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:ASP:OD2	1:F:221:LYS:NZ	2.20	0.70
1:C:133:GLU:OE1	3:C:502:HOH:O	2.08	0.69
1:B:249:ASP:OD1	3:B:501:HOH:O	2.09	0.69
1:G:135:ASP:OD1	1:G:136:ALA:N	2.25	0.69
1:G:194:PHE:O	3:G:501:HOH:O	2.13	0.67
1:G:25:ILE:O	1:G:25:ILE:HG22	1.96	0.65
1:D:218:ASP:O	3:D:502:HOH:O	2.16	0.63
1:G:30:ALA:HA	1:G:356:SER:HB3	1.80	0.62
1:F:50:ALA:O	1:F:54:GLN:HG2	2.01	0.60
1:G:141:ASP:O	3:G:502:HOH:O	2.17	0.60
1:A:276:ASP:OD2	3:A:501:HOH:O	2.17	0.59
1:B:320:THR:O	1:B:324:GLU:HG3	2.03	0.59
1:F:30:ALA:HA	1:F:356:SER:HB2	1.84	0.58
1:D:30:ALA:HA	1:D:356:SER:HB3	1.84	0.58
1:H:30:ALA:HA	1:H:356:SER:HB3	1.85	0.58
1:C:173:ARG:NH1	1:C:176:GLU:OE2	2.37	0.58
1:C:297:GLY:O	1:C:314:PHE:HA	2.04	0.57
1:F:297:GLY:HA3	1:F:315:ALA:HB2	1.85	0.57
1:A:59:GLN:O	1:A:63:GLU:HG3	2.04	0.56
1:C:288:VAL:HG22	1:C:366:VAL:HG11	1.87	0.55
1:G:87:CYS:HB3	1:G:92:VAL:CG2	2.37	0.55
1:E:30:ALA:HA	1:E:356:SER:HB3	1.89	0.55
1:H:286:SER:O	1:H:290:ARG:CG	2.55	0.55
1:A:318:THR:CG2	1:A:321:GLU:H	2.20	0.54
1:H:318:THR:HG22	1:H:320:THR:N	2.21	0.54
1:A:30:ALA:HA	1:A:356:SER:HB3	1.88	0.54
1:B:171:LEU:HG	1:B:205:VAL:HG21	1.90	0.53
1:E:99:ARG:CG	1:E:125:ASN:OD1	2.56	0.53
1:F:177:GLN:O	1:F:180:GLU:HG2	2.08	0.53
1:A:169:GLU:OE1	1:E:290:ARG:HD2	2.08	0.53
1:E:99:ARG:HG3	1:E:125:ASN:OD1	2.09	0.53
1:A:325:GLU:HG2	1:A:372:VAL:HG13	1.89	0.53
1:B:147:LEU:HD21	1:B:177:GLN:HB3	1.91	0.52
1:H:286:SER:O	1:H:290:ARG:HG3	2.09	0.52
1:B:318:THR:HG23	1:B:321:GLU:H	1.74	0.52
1:G:94:MET:CE	1:G:118:ILE:HG12	2.40	0.52
1:H:285:ARG:NH2	1:H:307:SER:O	2.34	0.52
1:C:138:HIS:CD2	1:C:166:LEU:HD12	2.45	0.51
1:C:95:GLU:OE2	1:D:95:GLU:OE2	2.28	0.51
1:B:285:ARG:NH2	1:B:307:SER:O	2.43	0.51
1:E:217:GLU:OE2	3:E:501:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:HD2	3:F:504:HOH:O	2.11	0.51
1:H:318:THR:HG22	1:H:320:THR:H	1.76	0.50
1:B:114:THR:HA	1:B:160:ASN:O	2.12	0.50
1:B:318:THR:CG2	1:B:321:GLU:H	2.25	0.50
1:D:87:CYS:HB3	1:D:92:VAL:CG2	2.42	0.50
1:F:122:LEU:HD22	1:F:127:LEU:HD12	1.94	0.49
1:G:147:LEU:HD21	1:G:177:GLN:HB3	1.94	0.49
1:G:142:LEU:HB2	1:G:147:LEU:HD11	1.94	0.49
1:F:188:ASP:OD2	2:F:401:EQJ:N03	2.45	0.49
1:C:180:GLU:OE2	3:C:503:HOH:O	2.19	0.49
1:F:363:GLU:O	1:F:366:VAL:HG22	2.13	0.49
1:E:193:GLY:HA3	1:E:222:LEU:HD11	1.95	0.48
1:B:61:GLU:HA	1:B:259:LEU:HG	1.95	0.48
1:E:161:PRO:HD3	1:E:339:PHE:CD1	2.49	0.48
1:B:212:ARG:HG2	1:B:238:ASP:OD2	2.14	0.48
1:F:292:LEU:O	1:F:298:VAL:HG21	2.14	0.48
1:B:190:SER:HA	1:B:218:ASP:HB3	1.95	0.48
1:E:59:GLN:O	1:E:63:GLU:HG3	2.13	0.48
1:B:314:PHE:CZ	1:B:322:VAL:HG21	2.48	0.48
1:A:134:GLU:O	1:A:138:HIS:HD2	1.96	0.48
1:F:186:ALA:HA	1:F:214:VAL:O	2.13	0.48
1:H:36:PRO:O	1:H:40:LYS:HG2	2.13	0.48
1:G:95:GLU:OE2	1:H:95:GLU:OE2	2.31	0.48
1:A:95:GLU:OE1	1:B:95:GLU:OE2	2.31	0.48
1:D:101:LEU:HD12	1:D:241:LEU:HD13	1.96	0.48
1:F:47:VAL:HG13	3:F:508:HOH:O	2.14	0.47
1:B:314:PHE:HZ	1:B:351:VAL:HG13	1.78	0.47
1:C:337:ARG:HG3	3:C:555:HOH:O	2.15	0.47
1:C:157:THR:HA	1:C:158:PRO:C	2.35	0.47
1:D:169:GLU:OE1	1:H:290:ARG:HD3	2.14	0.47
1:F:17:LEU:HD13	1:F:17:LEU:O	2.15	0.47
1:F:11:LEU:HD13	1:F:338:GLN:HB2	1.96	0.47
1:C:17:LEU:HD13	1:C:17:LEU:O	2.14	0.46
1:E:318:THR:HG22	1:E:320:THR:N	2.30	0.46
1:E:87:CYS:HB3	1:E:92:VAL:CG2	2.45	0.46
1:A:117:ASN:O	1:A:121:LEU:HG	2.15	0.46
1:C:194:PHE:O	3:C:504:HOH:O	2.21	0.46
1:E:13:GLN:HA	1:E:16:TYR:CD2	2.51	0.46
1:C:155:VAL:HG22	1:C:187:LEU:HD22	1.97	0.46
1:H:193:GLY:HA3	1:H:222:LEU:HD11	1.97	0.46
1:F:298:VAL:HA	1:F:313:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:HIS:CD2	1:G:342:ALA:H	2.33	0.46
1:G:25:ILE:CG2	1:G:353:ILE:HG23	2.46	0.46
1:H:286:SER:O	1:H:290:ARG:HG2	2.16	0.46
1:E:61:GLU:HA	1:E:259:LEU:HG	1.98	0.46
1:A:289:ARG:HG2	1:A:300:PHE:CE1	2.50	0.45
1:A:318:THR:HG23	1:A:321:GLU:H	1.80	0.45
1:G:25:ILE:O	1:G:333:ALA:HA	2.16	0.45
1:B:27:ASP:O	1:B:357:ARG:NH2	2.40	0.45
1:H:288:VAL:HG22	1:H:366:VAL:HG11	1.97	0.45
1:B:318:THR:HG22	1:B:321:GLU:CG	2.47	0.45
1:B:318:THR:HG22	1:B:321:GLU:HG3	1.98	0.45
1:D:80:GLU:HG2	1:D:83:ARG:HG3	1.98	0.45
1:B:314:PHE:CE2	1:B:322:VAL:HG21	2.51	0.45
1:B:360:GLU:HB3	1:B:361:PRO:CD	2.47	0.44
1:F:292:LEU:O	1:F:298:VAL:CG2	2.65	0.44
1:B:11:LEU:HD13	1:B:339:PHE:CZ	2.52	0.44
1:H:13:GLN:HA	1:H:16:TYR:CD2	2.53	0.44
1:H:18:ALA:HB2	1:H:332:PHE:HB3	2.00	0.44
1:C:143:SER:HB2	1:C:146:LEU:H	1.82	0.44
1:H:166:LEU:HD11	1:H:170:ARG:HG3	1.98	0.44
1:G:61:GLU:HA	1:G:259:LEU:HG	1.99	0.44
1:G:188:ASP:OD1	1:G:188:ASP:C	2.56	0.44
1:C:314:PHE:CE1	1:C:322:VAL:HG21	2.53	0.43
1:B:301:PRO:HG3	1:B:350:MET:CE	2.49	0.43
1:G:107:ARG:NH2	1:G:149:SER:OG	2.50	0.43
1:C:155:VAL:HG22	1:C:187:LEU:CD2	2.48	0.43
1:F:194:PHE:CE1	1:F:308:SER:HB3	2.53	0.43
3:E:507:HOH:O	1:F:91:SER:HB2	2.18	0.43
1:C:18:ALA:O	1:C:24:ASN:HB2	2.19	0.43
1:D:157:THR:HG23	1:D:157:THR:O	2.18	0.43
1:C:55:ARG:HD2	3:C:521:HOH:O	2.19	0.43
1:E:300:PHE:O	1:E:303:PRO:HD3	2.18	0.43
1:E:287:VAL:HG11	1:E:363:GLU:HG3	2.01	0.43
1:A:190:SER:HA	1:A:218:ASP:HB3	2.00	0.43
1:C:155:VAL:CG2	1:C:187:LEU:HD22	2.49	0.43
1:C:314:PHE:CZ	1:C:322:VAL:HG21	2.53	0.43
1:C:213:TRP:CD1	1:C:236:SER:HB3	2.54	0.43
1:C:85:LEU:HD12	1:C:233:LEU:HD23	2.00	0.43
1:F:217:GLU:HB2	1:F:232:LEU:HB2	2.01	0.43
1:B:99:ARG:HG2	1:B:246:ILE:HD13	2.00	0.42
1:C:217:GLU:HB2	1:C:232:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:SER:HA	1:D:218:ASP:HB3	2.00	0.42
1:E:24:ASN:C	1:E:24:ASN:OD1	2.57	0.42
1:F:169:GLU:HA	1:F:169:GLU:OE2	2.19	0.42
1:C:308:SER:O	1:C:355:LEU:HB2	2.19	0.42
1:E:95:GLU:OE2	1:F:95:GLU:OE2	2.36	0.42
1:C:326:LEU:HD11	1:C:369:LEU:HD13	2.01	0.42
1:F:27:ASP:O	1:F:357:ARG:NH2	2.45	0.42
1:D:24:ASN:C	1:D:24:ASN:OD1	2.56	0.42
1:A:157:THR:HG23	1:A:157:THR:O	2.19	0.42
1:A:158:PRO:HG3	1:A:165:VAL:HG22	2.02	0.42
1:D:157:THR:HA	1:D:158:PRO:C	2.39	0.42
1:F:372:VAL:O	1:F:375:THR:HG22	2.20	0.42
1:D:213:TRP:CD1	1:D:236:SER:HB3	2.55	0.41
1:E:80:GLU:HG2	1:E:83:ARG:HG3	2.02	0.41
1:A:19:LEU:O	3:A:502:HOH:O	2.22	0.41
1:G:16:TYR:HA	1:G:19:LEU:CD2	2.50	0.41
1:G:55:ARG:NH2	1:G:63:GLU:OE2	2.38	0.41
1:C:154:PHE:HA	1:C:186:ALA:O	2.20	0.41
1:C:221:LYS:NZ	2:C:401:EQJ:C13	2.83	0.41
1:E:190:SER:HA	1:E:218:ASP:HB3	2.02	0.41
1:E:27:ASP:OD1	1:E:29:HIS:HB2	2.21	0.41
1:F:190:SER:HA	1:F:218:ASP:HB3	2.02	0.41
1:G:177:GLN:O	1:G:180:GLU:HG2	2.20	0.41
1:C:188:ASP:OD2	2:C:401:EQJ:N03	2.54	0.41
1:D:14:TRP:HE1	1:D:338:GLN:HE22	1.69	0.41
1:D:61:GLU:HA	1:D:259:LEU:HG	2.01	0.41
1:B:301:PRO:HG3	1:B:350:MET:HE3	2.03	0.41
1:D:292:LEU:O	1:D:293:ALA:C	2.59	0.41
1:D:87:CYS:HB3	1:D:92:VAL:HG22	2.03	0.41
1:E:217:GLU:HB2	1:E:232:LEU:HB2	2.03	0.41
1:B:311:ARG:HB3	1:B:350:MET:HE2	2.02	0.41
1:B:311:ARG:HD2	1:B:350:MET:HE2	2.02	0.41
1:G:11:LEU:HD13	1:G:338:GLN:HB2	2.03	0.41
1:B:112:HIS:HB2	1:B:341:TRP:CZ2	2.56	0.41
1:B:201:ASP:O	1:B:204:ALA:HB3	2.20	0.41
1:B:28:GLY:N	2:B:401:EQJ:O24	2.54	0.41
1:C:87:CYS:HB3	1:C:92:VAL:HG22	2.03	0.41
1:F:114:THR:HA	1:F:160:ASN:O	2.21	0.41
1:G:295:VAL:HB	1:G:298:VAL:HG21	2.03	0.41
1:G:308:SER:O	1:G:355:LEU:HB2	2.21	0.41
1:B:25:ILE:HD12	1:B:353:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:THR:HG22	1:H:321:GLU:H	1.85	0.41
1:D:109:ALA:HA	1:D:130:VAL:HG23	2.03	0.40
1:F:107:ARG:HB2	1:F:107:ARG:HH21	1.86	0.40
1:G:297:GLY:HA2	1:G:315:ALA:HB2	2.02	0.40
1:D:193:GLY:HA3	1:D:222:LEU:HD11	2.03	0.40
1:F:337:ARG:NH1	1:F:348:ASP:OD2	2.54	0.40
1:E:87:CYS:HB3	1:E:92:VAL:HG22	2.04	0.40
1:C:177:GLN:O	1:C:180:GLU:HG2	2.22	0.40
1:F:155:VAL:O	1:F:187:LEU:HA	2.22	0.40
1:F:49:TRP:HA	1:F:257:LEU:HD13	2.03	0.40
1:F:55:ARG:HH22	1:F:63:GLU:CD	2.23	0.40
1:G:83:ARG:HB2	3:G:504:HOH:O	2.22	0.40
1:D:109:ALA:HA	1:D:130:VAL:CG2	2.51	0.40
1:D:217:GLU:HB2	1:D:232:LEU:HB2	2.03	0.40
1:E:292:LEU:O	1:E:293:ALA:C	2.59	0.40
1:F:84:VAL:HG23	3:F:511:HOH:O	2.21	0.40
1:G:287:VAL:CG1	1:G:363:GLU:HG2	2.52	0.40
1:H:311:ARG:HD2	1:H:350:MET:HE3	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	366/376 (97%)	358 (98%)	7 (2%)	1 (0%)	41	46
1	B	366/376 (97%)	351 (96%)	13 (4%)	2 (0%)	29	31
1	C	366/376 (97%)	352 (96%)	13 (4%)	1 (0%)	41	46
1	D	366/376 (97%)	356 (97%)	9 (2%)	1 (0%)	41	46
1	E	366/376 (97%)	358 (98%)	7 (2%)	1 (0%)	41	46
1	F	366/376 (97%)	351 (96%)	12 (3%)	3 (1%)	19	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	366/376 (97%)	349 (95%)	15 (4%)	2 (0%)	29	31
1	H	367/376 (98%)	358 (98%)	8 (2%)	1 (0%)	41	46
All	All	2929/3008 (97%)	2833 (97%)	84 (3%)	12 (0%)	34	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ASP
1	E	293	ALA
1	F	201	ASP
1	G	201	ASP
1	H	293	ALA
1	A	293	ALA
1	C	201	ASP
1	D	293	ALA
1	F	315	ALA
1	G	113	PRO
1	F	296	GLU
1	B	360	GLU

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	306/314 (98%)	292 (95%)	14 (5%)	27	34
1	B	306/314 (98%)	289 (94%)	17 (6%)	21	25
1	C	306/314 (98%)	284 (93%)	22 (7%)	14	15
1	D	306/314 (98%)	292 (95%)	14 (5%)	27	34
1	E	306/314 (98%)	288 (94%)	18 (6%)	19	23
1	F	306/314 (98%)	286 (94%)	20 (6%)	17	19
1	G	306/314 (98%)	286 (94%)	20 (6%)	17	19
1	H	307/314 (98%)	289 (94%)	18 (6%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2449/2512 (98%)	2306 (94%)	143 (6%)	20	23

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	21	SER
1	A	71	LEU
1	A	107	ARG
1	A	150	VAL
1	A	206	LEU
1	A	222	LEU
1	A	227	ASP
1	A	241	LEU
1	A	259	LEU
1	A	261	LEU
1	A	285	ARG
1	A	355	LEU
1	A	364	LYS
1	B	56	PRO
1	B	66	GLN
1	B	71	LEU
1	B	99	ARG
1	B	141	ASP
1	B	143	SER
1	B	205	VAL
1	B	206	LEU
1	B	222	LEU
1	B	227	ASP
1	B	241	LEU
1	B	259	LEU
1	B	307	SER
1	B	314	PHE
1	B	317	ARG
1	B	358	SER
1	B	364	LYS
1	C	8	LYS
1	C	11	LEU
1	C	17	LEU
1	C	19	LEU
1	C	21	SER
1	C	66	GLN

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Mol	Chain	Res	Type
1	C	71	LEU
1	C	92	VAL
1	C	107	ARG
1	C	143	SER
1	C	150	VAL
1	C	173	ARG
1	C	205	VAL
1	C	206	LEU
1	C	227	ASP
1	C	241	LEU
1	C	259	LEU
1	C	285	ARG
1	C	314	PHE
1	C	355	LEU
1	C	356	SER
1	C	364	LYS
1	D	8	LYS
1	D	21	SER
1	D	48	LEU
1	D	71	LEU
1	D	80	GLU
1	D	164	ARG
1	D	206	LEU
1	D	222	LEU
1	D	227	ASP
1	D	232	LEU
1	D	259	LEU
1	D	261	LEU
1	D	321	GLU
1	D	327	GLN
1	E	71	LEU
1	E	81	PRO
1	E	92	VAL
1	E	99	ARG
1	E	161	PRO
1	E	205	VAL
1	E	206	LEU
1	E	208	GLU
1	E	222	LEU
1	E	227	ASP
1	E	232	LEU
1	E	259	LEU

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Mol	Chain	Res	Type
1	E	286	SER
1	E	314	PHE
1	E	317	ARG
1	E	348	ASP
1	E	355	LEU
1	E	375	THR
1	F	8	LYS
1	F	11	LEU
1	F	13	GLN
1	F	17	LEU
1	F	19	LEU
1	F	54	GLN
1	F	107	ARG
1	F	150	VAL
1	F	157	THR
1	F	205	VAL
1	F	206	LEU
1	F	221	LYS
1	F	241	LEU
1	F	285	ARG
1	F	307	SER
1	F	314	PHE
1	F	317	ARG
1	F	320	THR
1	F	348	ASP
1	F	356	SER
1	G	11	LEU
1	G	13	GLN
1	G	17	LEU
1	G	19	LEU
1	G	21	SER
1	G	80	GLU
1	G	99	ARG
1	G	143	SER
1	G	206	LEU
1	G	208	GLU
1	G	222	LEU
1	G	227	ASP
1	G	234	VAL
1	G	241	LEU
1	G	259	LEU
1	G	306	ARG

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Mol	Chain	Res	Type
1	G	307	SER
1	G	314	PHE
1	G	355	LEU
1	G	358	SER
1	H	8	LYS
1	H	17	LEU
1	H	21	SER
1	H	22	GLU
1	H	58	GLN
1	H	71	LEU
1	H	92	VAL
1	H	101	LEU
1	H	107	ARG
1	H	150	VAL
1	H	206	LEU
1	H	227	ASP
1	H	232	LEU
1	H	259	LEU
1	H	261	LEU
1	H	285	ARG
1	H	290	ARG
1	H	326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	B	29	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EQJ	H	401	-	24,27,27	2.16	7 (29%)	28,37,37	2.08	7 (25%)
2	EQJ	G	401	-	24,27,27	2.11	5 (20%)	28,37,37	1.70	3 (10%)
2	EQJ	D	401	-	24,27,27	2.14	4 (16%)	28,37,37	1.52	3 (10%)
2	EQJ	E	401	-	24,27,27	2.39	6 (25%)	28,37,37	1.31	6 (21%)
2	EQJ	C	401	-	24,27,27	2.16	6 (25%)	28,37,37	1.88	6 (21%)
2	EQJ	F	401	-	24,27,27	2.23	7 (29%)	28,37,37	1.27	4 (14%)
2	EQJ	B	401	-	24,27,27	2.19	4 (16%)	28,37,37	1.19	2 (7%)
2	EQJ	A	400	-	24,27,27	2.19	5 (20%)	28,37,37	1.79	3 (10%)

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	EQJ	H	401	-	-	2/18/22/22	0/1/1/1
2	EQJ	G	401	-	-	3/18/22/22	0/1/1/1
2	EQJ	D	401	-	-	1/18/22/22	0/1/1/1
2	EQJ	E	401	-	-	5/18/22/22	0/1/1/1
2	EQJ	C	401	-	-	3/18/22/22	0/1/1/1
2	EQJ	F	401	-	-	7/18/22/22	0/1/1/1
2	EQJ	B	401	-	-	5/18/22/22	0/1/1/1
2	EQJ	A	400	-	-	5/18/22/22	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	EQJ	C20-N19	8.84	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	EQJ	C20-N19	8.32	1.49	1.33
2	F	401	EQJ	C20-N19	8.29	1.49	1.33
2	D	401	EQJ	C20-N19	8.03	1.49	1.33
2	C	401	EQJ	C20-N19	7.89	1.48	1.33
2	A	400	EQJ	C20-N19	7.86	1.48	1.33
2	G	401	EQJ	C20-N19	7.77	1.48	1.33
2	H	401	EQJ	C20-N19	6.94	1.46	1.33
2	D	401	EQJ	C12-C13	3.92	1.54	1.46
2	A	400	EQJ	C12-C13	3.70	1.53	1.46
2	H	401	EQJ	P08-O09	-3.54	1.41	1.54
2	A	400	EQJ	C20-N21	3.39	1.45	1.32
2	E	401	EQJ	C20-N21	3.27	1.45	1.32
2	G	401	EQJ	C20-N21	3.22	1.45	1.32
2	B	401	EQJ	C12-C13	3.15	1.52	1.46
2	E	401	EQJ	C12-C13	3.10	1.52	1.46
2	F	401	EQJ	C20-N21	3.07	1.44	1.32
2	C	401	EQJ	C20-N21	3.03	1.44	1.32
2	G	401	EQJ	C12-C13	2.97	1.52	1.46
2	H	401	EQJ	C12-C13	2.94	1.52	1.46
2	H	401	EQJ	P08-O11	-2.90	1.43	1.54
2	C	401	EQJ	C26-C02	-2.88	1.38	1.40
2	E	401	EQJ	P08-O09	-2.88	1.43	1.54
2	D	401	EQJ	C20-N21	2.88	1.43	1.32
2	B	401	EQJ	C20-N21	2.87	1.43	1.32
2	F	401	EQJ	C26-C02	-2.77	1.38	1.40
2	E	401	EQJ	C26-C02	-2.67	1.38	1.40
2	C	401	EQJ	C12-C13	2.66	1.51	1.46
2	H	401	EQJ	C20-N21	2.63	1.42	1.32
2	B	401	EQJ	C06-C05	2.59	1.57	1.50
2	D	401	EQJ	C06-C05	2.53	1.57	1.50
2	A	400	EQJ	C26-C02	-2.48	1.38	1.40
2	H	401	EQJ	C13-N14	2.46	1.31	1.27
2	F	401	EQJ	C12-C13	2.44	1.51	1.46
2	C	401	EQJ	C06-C05	2.42	1.57	1.50
2	F	401	EQJ	C06-C05	2.39	1.57	1.50
2	A	400	EQJ	C13-N14	2.34	1.31	1.27
2	G	401	EQJ	C13-N14	2.23	1.31	1.27
2	C	401	EQJ	P08-O07	2.13	1.67	1.60
2	F	401	EQJ	C13-N14	2.10	1.31	1.27
2	F	401	EQJ	C12-C26	-2.08	1.37	1.40
2	H	401	EQJ	C16-C15	2.04	1.55	1.53
2	E	401	EQJ	C01-C02	2.04	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	EQJ	C26-C02	-2.03	1.38	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	EQJ	C12-C26-C02	-6.01	116.47	120.19
2	H	401	EQJ	C15-N14-C13	5.93	125.43	117.40
2	C	401	EQJ	C15-N14-C13	5.89	125.39	117.40
2	G	401	EQJ	C15-N14-C13	5.89	125.39	117.40
2	D	401	EQJ	C15-N14-C13	5.43	124.76	117.40
2	H	401	EQJ	O07-P08-O10	4.14	118.09	106.47
2	H	401	EQJ	C12-C26-C02	-4.02	117.70	120.19
2	C	401	EQJ	C12-C26-C02	-3.89	117.78	120.19
2	H	401	EQJ	O11-P08-O09	-3.87	92.85	107.64
2	A	400	EQJ	C05-C04-N03	-3.85	117.41	123.82
2	G	401	EQJ	C12-C26-C02	-3.08	118.28	120.19
2	H	401	EQJ	C05-C04-N03	-3.06	118.72	123.82
2	C	401	EQJ	C05-C04-N03	-2.99	118.84	123.82
2	F	401	EQJ	C05-C04-N03	-2.78	119.18	123.82
2	A	400	EQJ	C04-N03-C02	2.75	124.26	119.17
2	F	401	EQJ	C12-C26-C02	-2.72	118.50	120.19
2	G	401	EQJ	C05-C04-N03	-2.68	119.36	123.82
2	B	401	EQJ	C12-C26-C02	-2.55	118.61	120.19
2	B	401	EQJ	C05-C04-N03	-2.45	119.74	123.82
2	D	401	EQJ	C05-C04-N03	-2.43	119.77	123.82
2	F	401	EQJ	C04-N03-C02	2.34	123.49	119.17
2	H	401	EQJ	C04-C05-C12	2.33	122.44	118.15
2	E	401	EQJ	C05-C04-N03	-2.28	120.01	123.82
2	C	401	EQJ	C12-C13-N14	-2.27	117.97	123.01
2	E	401	EQJ	C04-N03-C02	2.24	123.32	119.17
2	E	401	EQJ	C16-C17-C18	-2.21	105.44	112.05
2	F	401	EQJ	C16-C17-C18	-2.17	105.56	112.05
2	C	401	EQJ	C04-N03-C02	2.16	123.17	119.17
2	E	401	EQJ	C01-C02-N03	2.15	121.87	117.67
2	E	401	EQJ	C01-C02-C26	-2.09	118.31	120.89
2	H	401	EQJ	O11-P08-O07	2.08	112.28	106.73
2	C	401	EQJ	C26-C12-C05	2.08	119.86	118.26
2	D	401	EQJ	C17-C18-N19	-2.05	106.35	112.21
2	E	401	EQJ	O07-P08-O10	2.03	112.17	106.47

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	401	EQJ	C16-C15-N14-C13
2	H	401	EQJ	C06-O07-P08-O11
2	G	401	EQJ	C16-C15-N14-C13
2	D	401	EQJ	C16-C15-N14-C13
2	E	401	EQJ	C23-C15-C16-C17
2	E	401	EQJ	N14-C15-C16-C17
2	E	401	EQJ	C16-C15-N14-C13
2	E	401	EQJ	C23-C15-N14-C13
2	C	401	EQJ	C16-C15-N14-C13
2	C	401	EQJ	C06-O07-P08-O09
2	C	401	EQJ	C06-O07-P08-O11
2	F	401	EQJ	C16-C15-N14-C13
2	F	401	EQJ	C23-C15-N14-C13
2	F	401	EQJ	C06-O07-P08-O09
2	F	401	EQJ	C06-O07-P08-O11
2	B	401	EQJ	C23-C15-C16-C17
2	B	401	EQJ	N14-C15-C16-C17
2	B	401	EQJ	C16-C15-N14-C13
2	B	401	EQJ	C23-C15-N14-C13
2	A	400	EQJ	C16-C15-N14-C13
2	A	400	EQJ	C23-C15-N14-C13
2	A	400	EQJ	C06-O07-P08-O09
2	A	400	EQJ	C06-O07-P08-O10
2	B	401	EQJ	C15-C16-C17-C18
2	F	401	EQJ	C06-O07-P08-O10
2	E	401	EQJ	C15-C16-C17-C18
2	G	401	EQJ	C06-O07-P08-O10
2	F	401	EQJ	C15-C16-C17-C18
2	F	401	EQJ	C17-C18-N19-C20
2	G	401	EQJ	C06-O07-P08-O09
2	A	400	EQJ	C06-O07-P08-O11

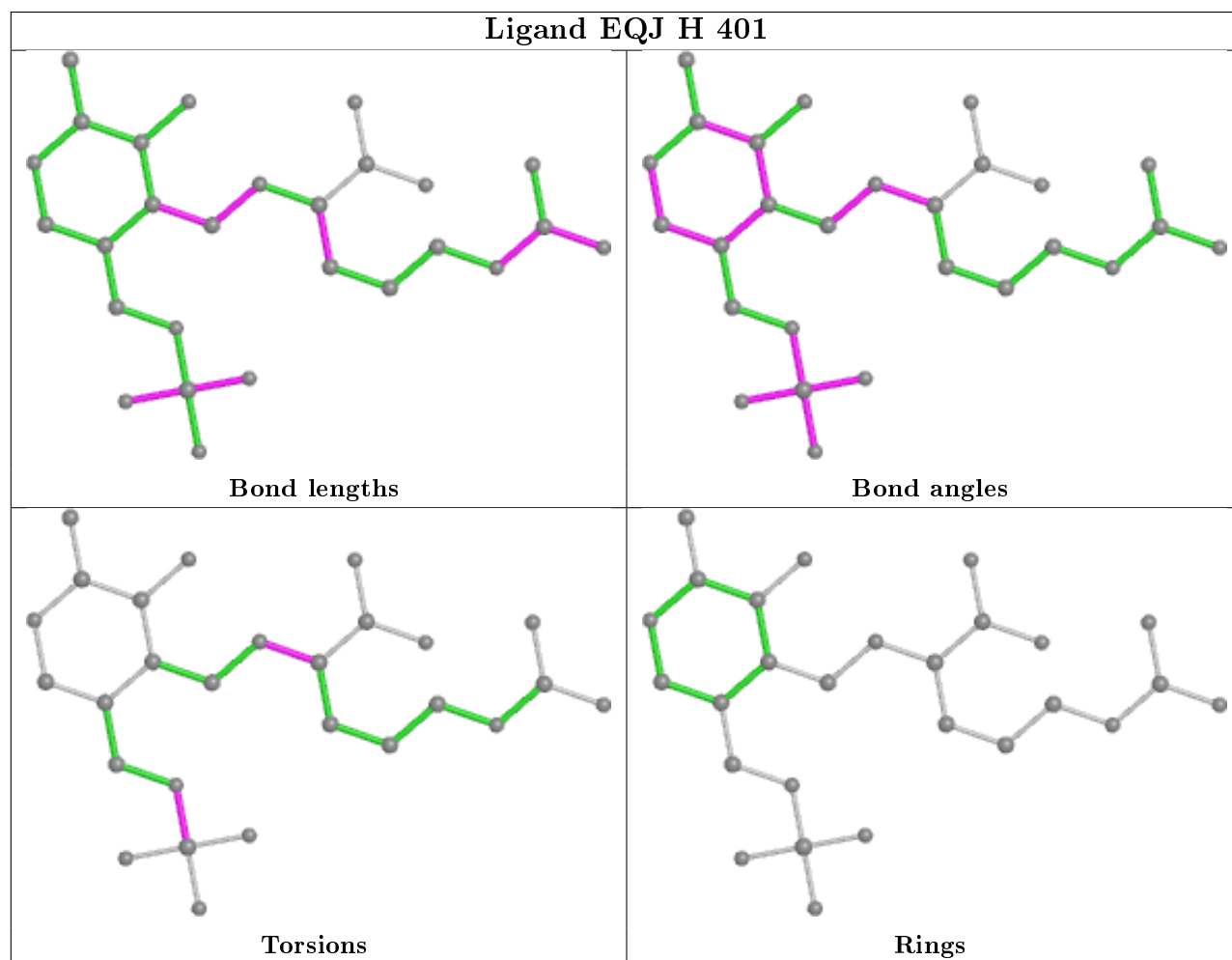
There are no ring outliers.

3 monomers are involved in 4 short contacts:

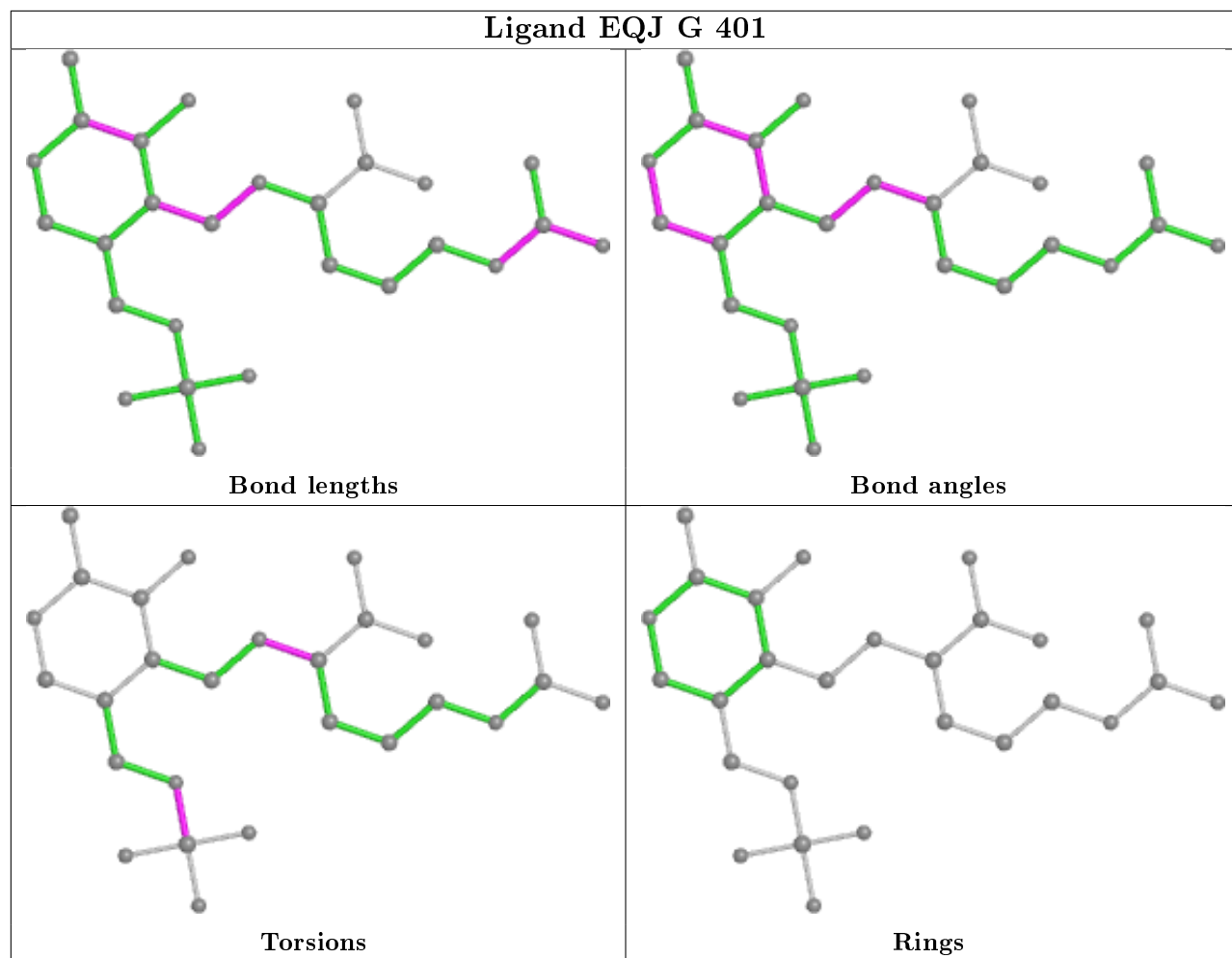
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	EQJ	2	0
2	F	401	EQJ	1	0
2	B	401	EQJ	1	0

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

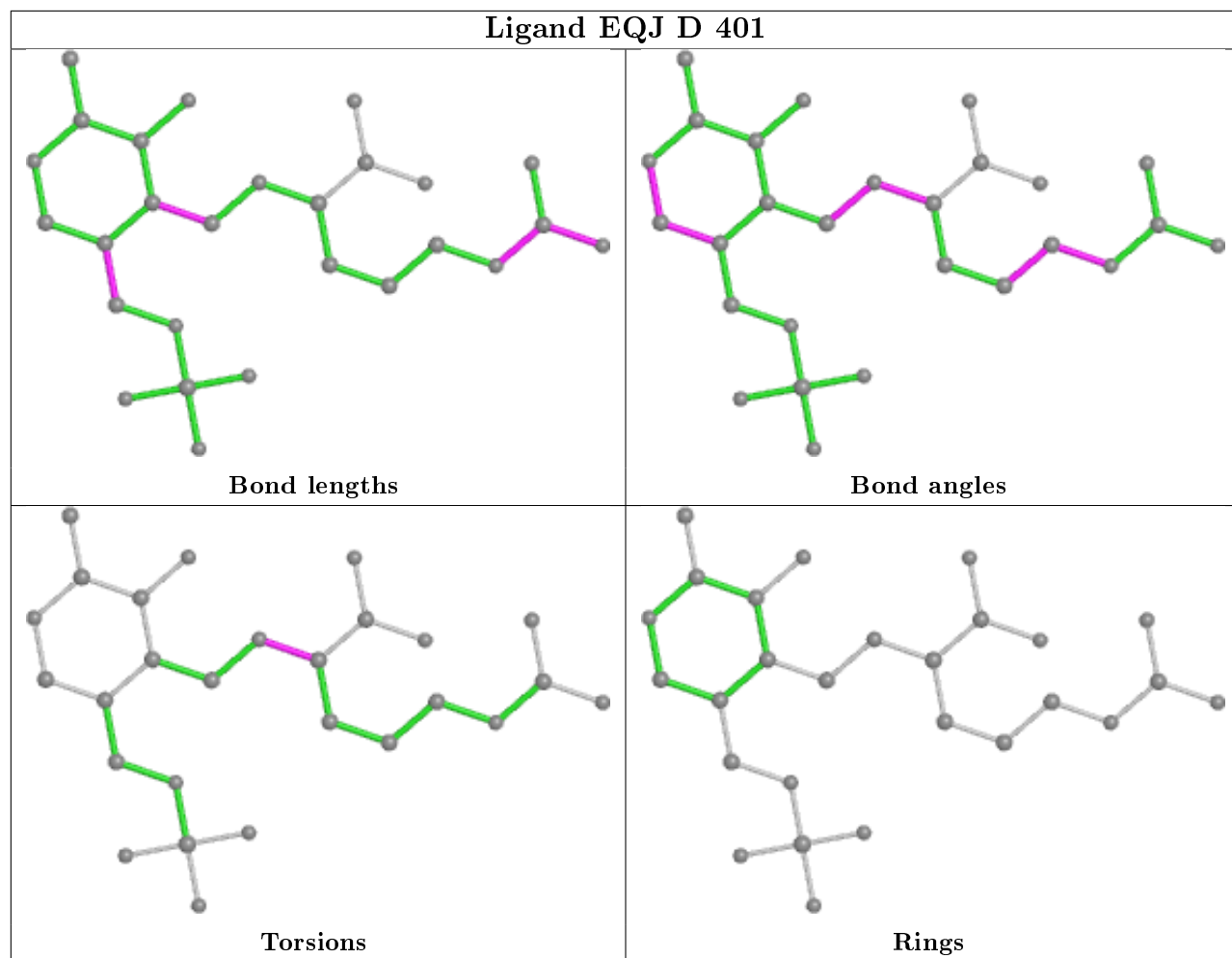
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



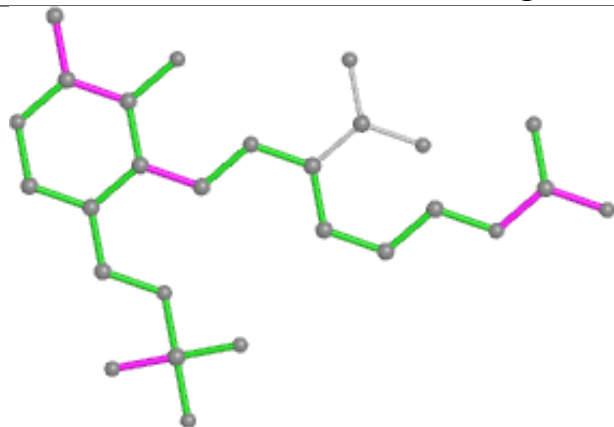
Ligand EQJ G 401



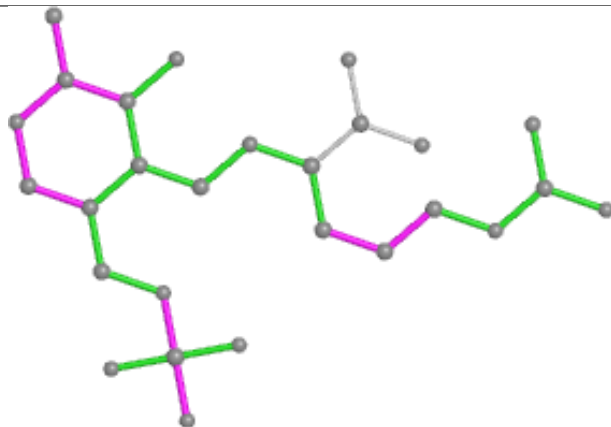
Ligand EQJ D 401



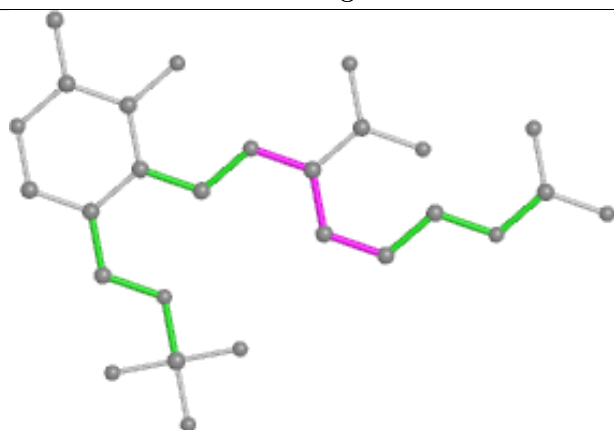
Ligand EQJ E 401



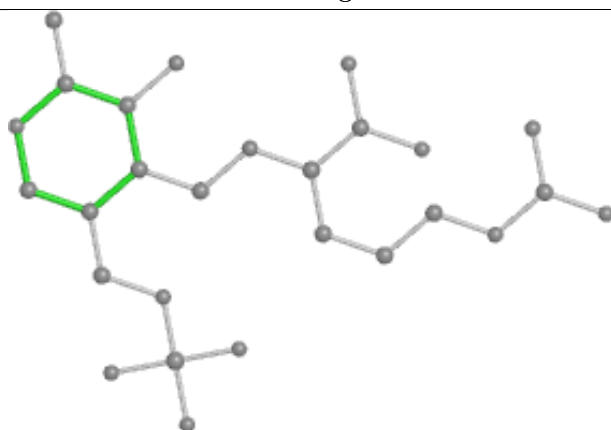
Bond lengths



Bond angles

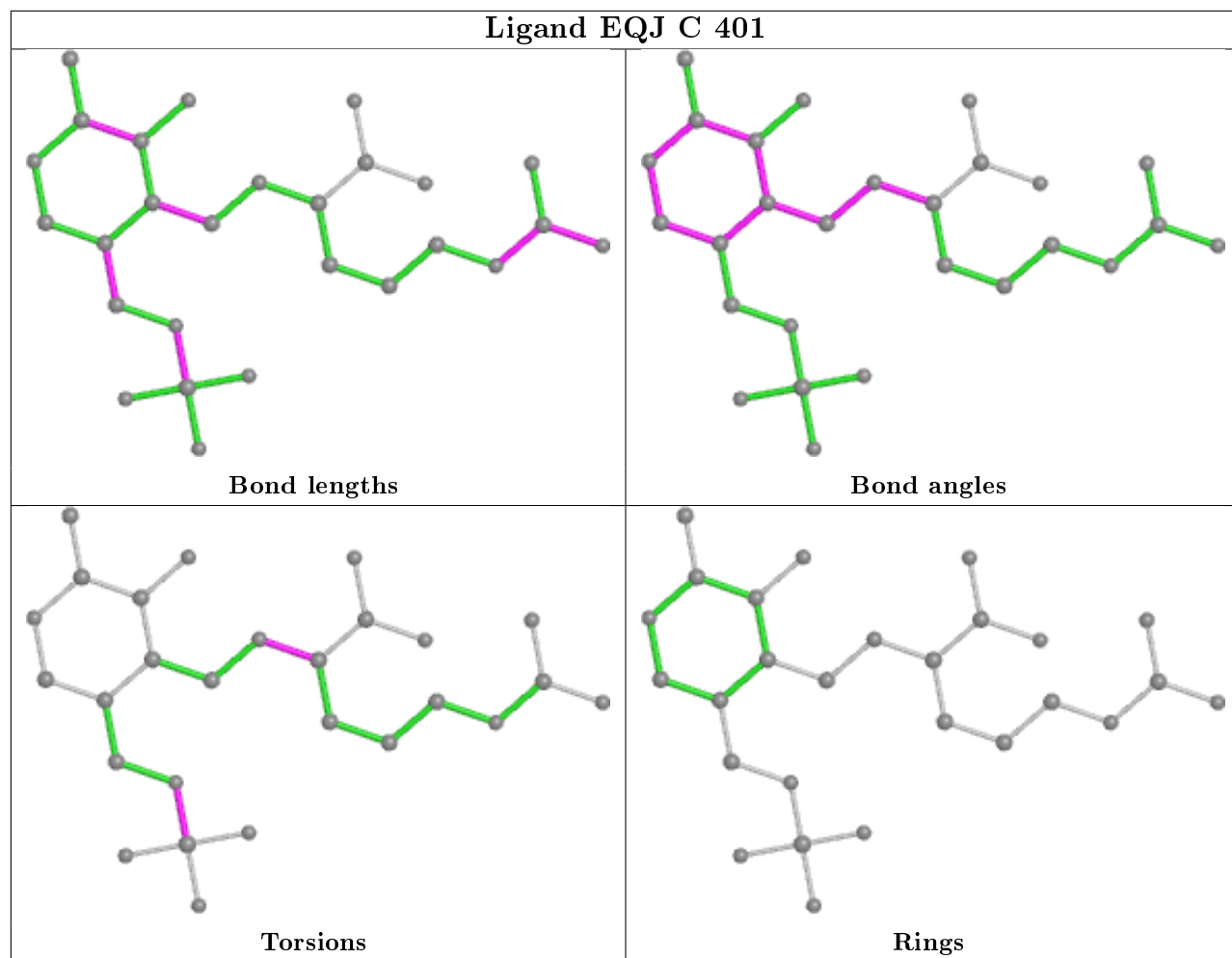


Torsions

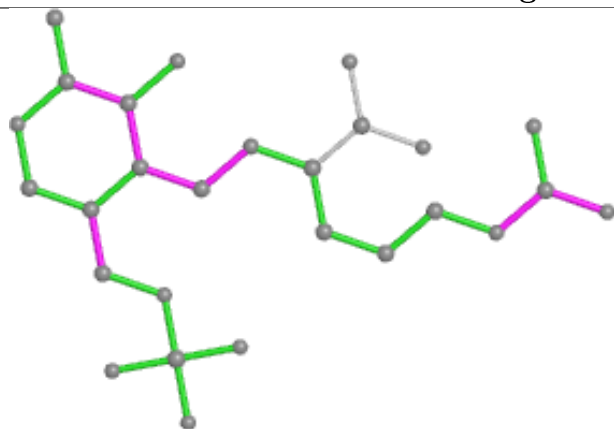


Rings

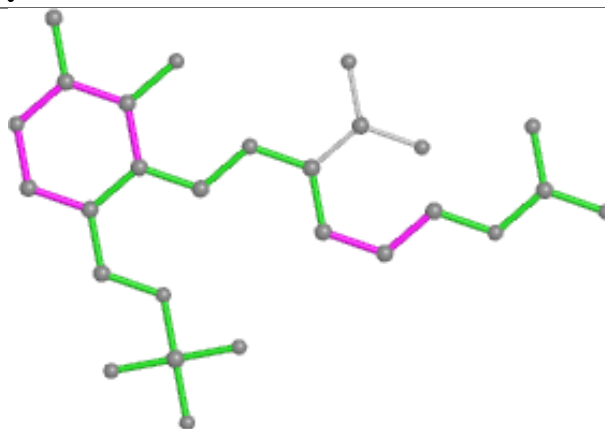
Ligand EQJ C 401



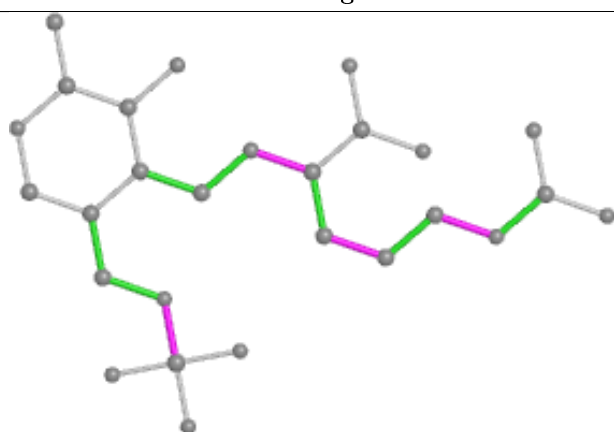
Ligand EQJ F 401



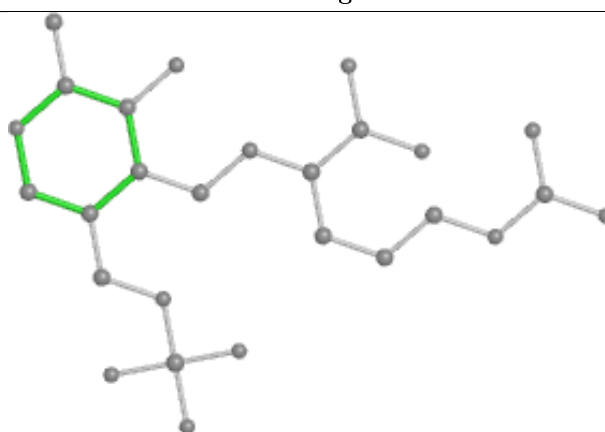
Bond lengths



Bond angles

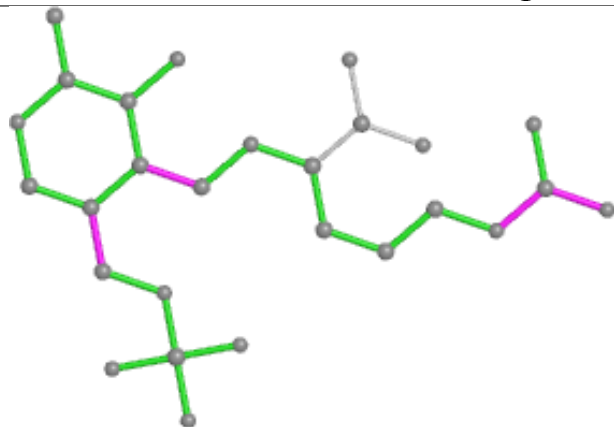


Torsions

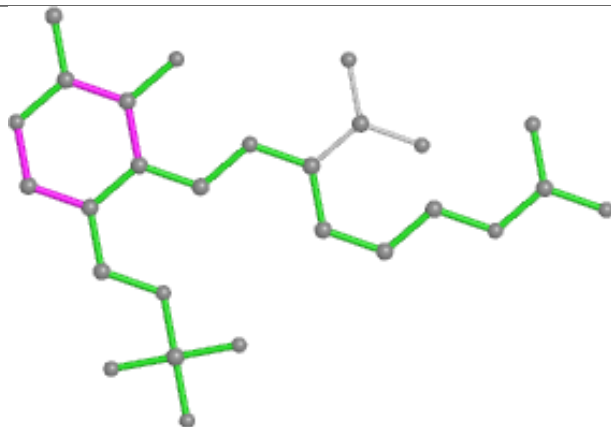


Rings

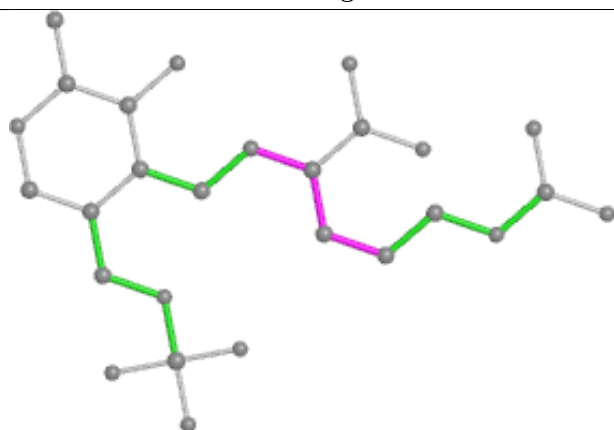
Ligand EQJ B 401



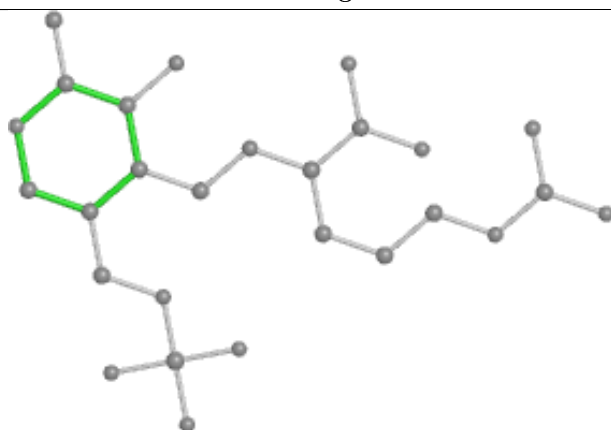
Bond lengths



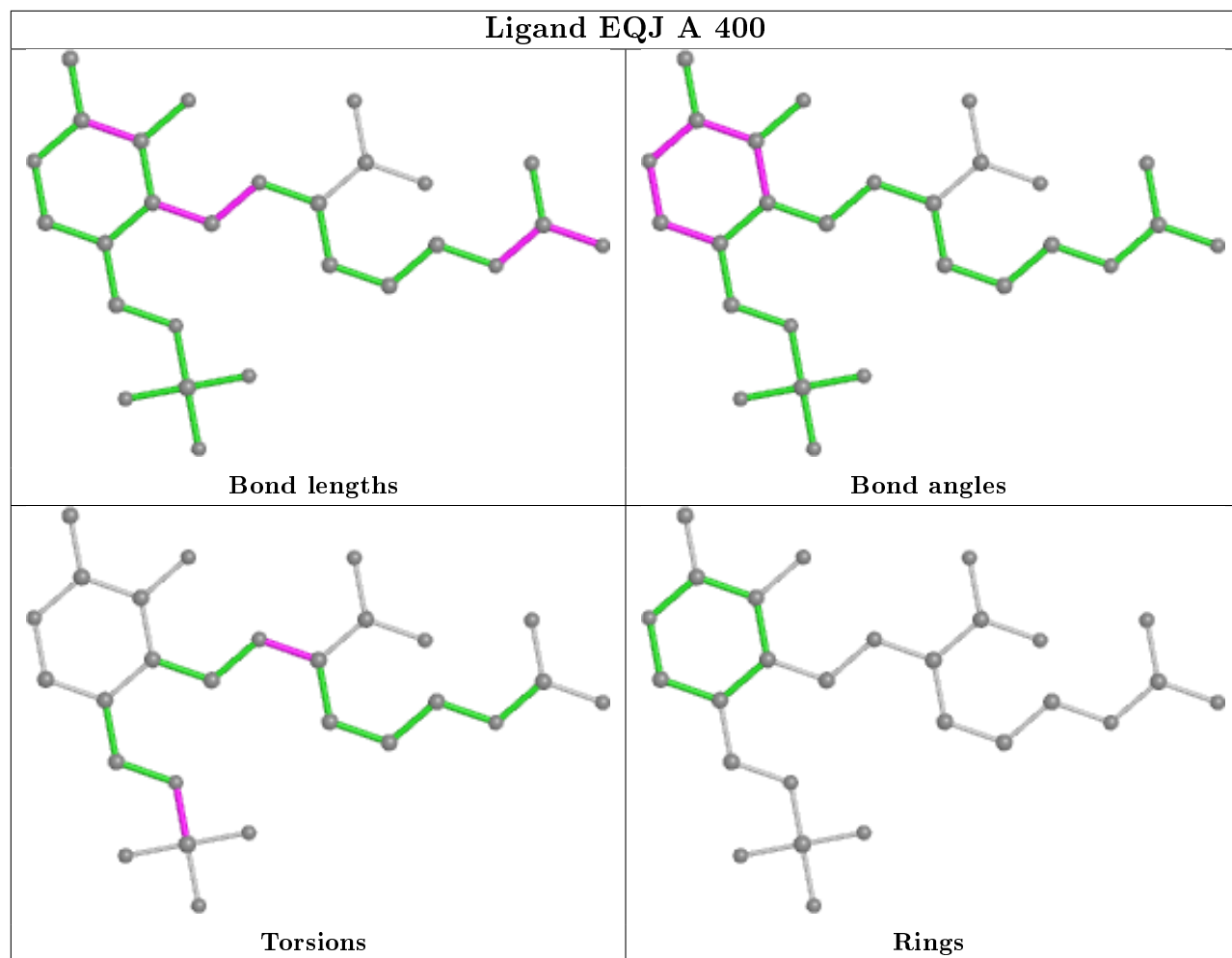
Bond angles



Torsions



Rings



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%)	-0.40	1 (0%) 94 93	19, 28, 59, 166	1 (0%)
1	B	368/376 (97%)	-0.07	3 (0%) 86 85	24, 45, 82, 156	1 (0%)
1	C	368/376 (97%)	-0.03	3 (0%) 86 85	23, 47, 88, 185	1 (0%)
1	D	368/376 (97%)	-0.41	2 (0%) 91 90	19, 28, 56, 131	1 (0%)
1	E	368/376 (97%)	-0.37	2 (0%) 91 90	20, 30, 62, 134	1 (0%)
1	F	368/376 (97%)	0.05	4 (1%) 80 79	26, 48, 92, 132	1 (0%)
1	G	368/376 (97%)	0.07	7 (1%) 66 65	25, 49, 84, 137	1 (0%)
1	H	369/376 (98%)	-0.38	1 (0%) 94 93	18, 28, 60, 154	1 (0%)
All	All	2945/3008 (97%)	-0.19	23 (0%) 86 85	18, 37, 79, 185	8 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	375	THR	4.5
1	E	178	CYS	3.9
1	G	25	ILE	3.3
1	A	178	CYS	3.0
1	B	147	LEU	3.0
1	F	369	LEU	3.0
1	C	221	LYS	3.0
1	E	221	LYS	2.9
1	D	94	MET	2.7
1	G	372	VAL	2.5
1	C	375	THR	2.4
1	F	147	LEU	2.3
1	G	314	PHE	2.2
1	G	221	LYS	2.2
1	B	146	LEU	2.2
1	C	147	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	369	LEU	2.1
1	B	314	PHE	2.1
1	F	17	LEU	2.1
1	F	375	THR	2.1
1	H	7	LEU	2.0
1	D	367	GLN	2.0
1	G	292	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

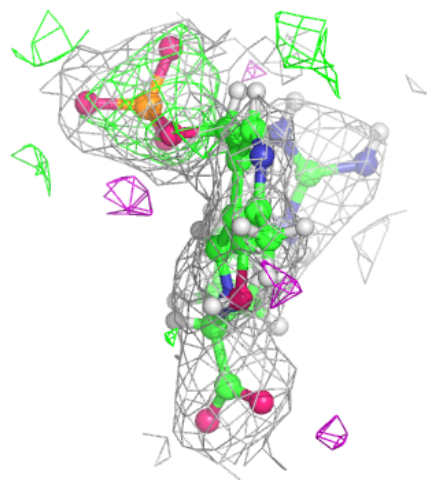
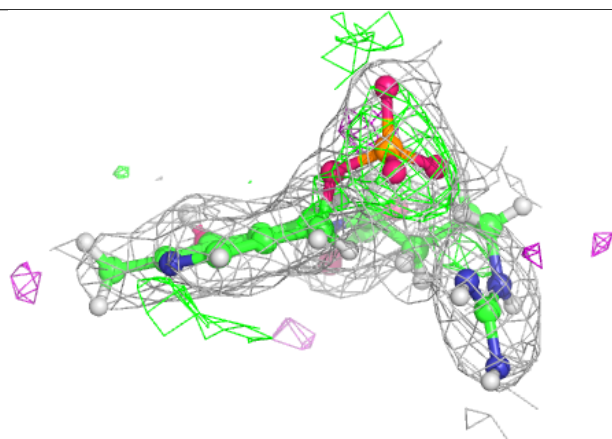
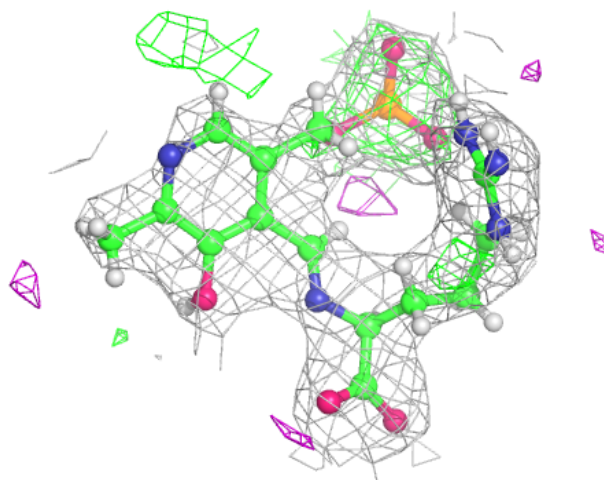
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EQJ	B	401	27/27	0.79	0.24	46,98,174,179	0
2	EQJ	E	401	27/27	0.86	0.17	27,42,101,184	0
2	EQJ	H	401	27/27	0.93	0.14	20,37,74,118	0
2	EQJ	G	401	27/27	0.94	0.16	35,72,127,158	0
2	EQJ	F	401	27/27	0.96	0.17	36,82,168,170	0
2	EQJ	C	401	27/27	0.96	0.13	32,64,125,129	0
2	EQJ	D	401	27/27	0.98	0.11	23,33,40,43	0
2	EQJ	A	400	27/27	0.98	0.10	21,29,36,41	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.

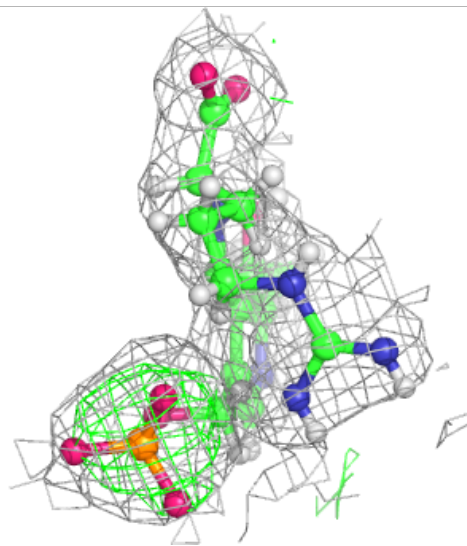
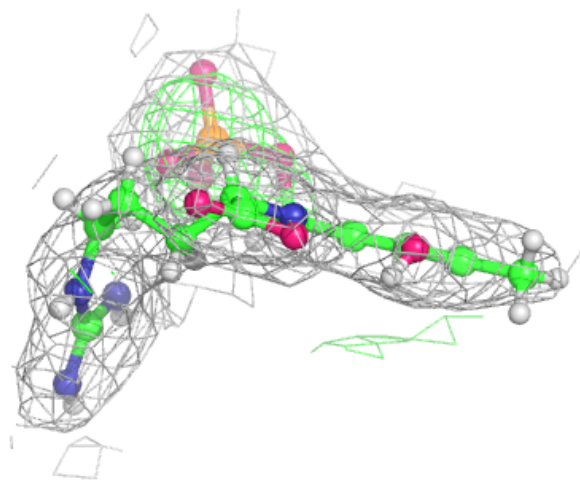
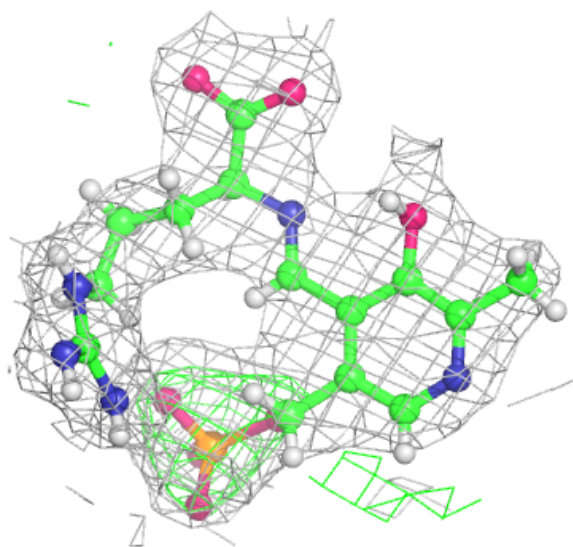
Electron density around EQJ B 401:

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



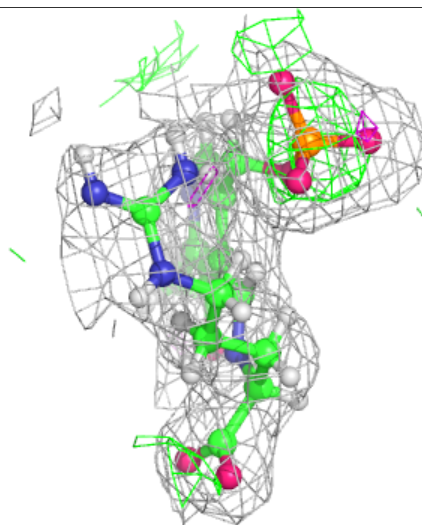
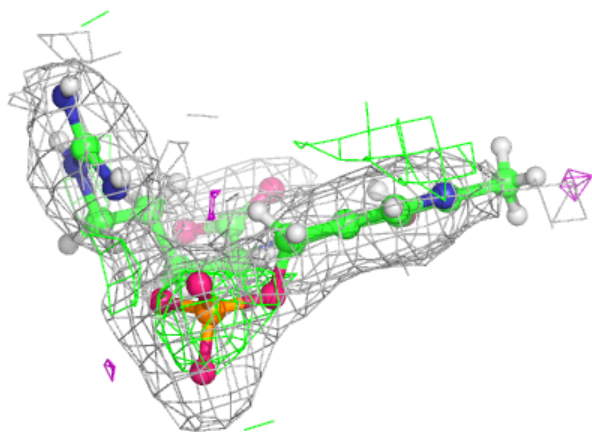
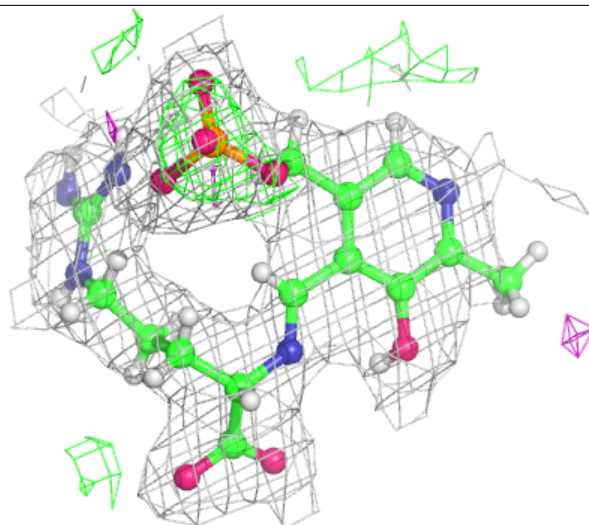
Electron density around EQJ E 401:

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



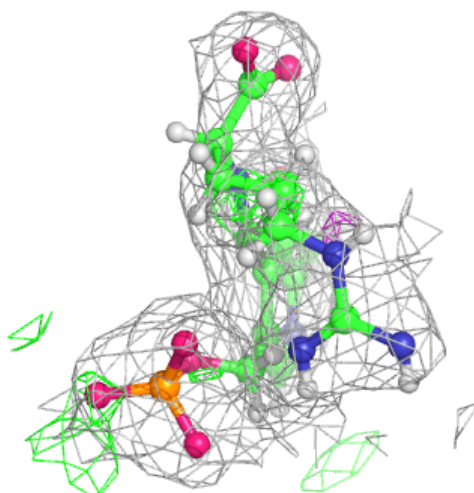
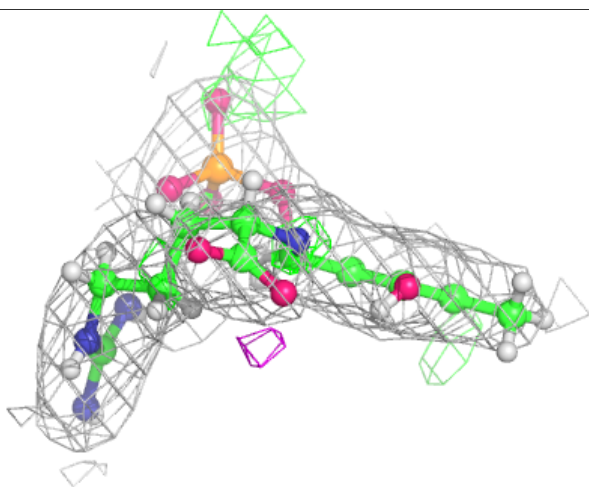
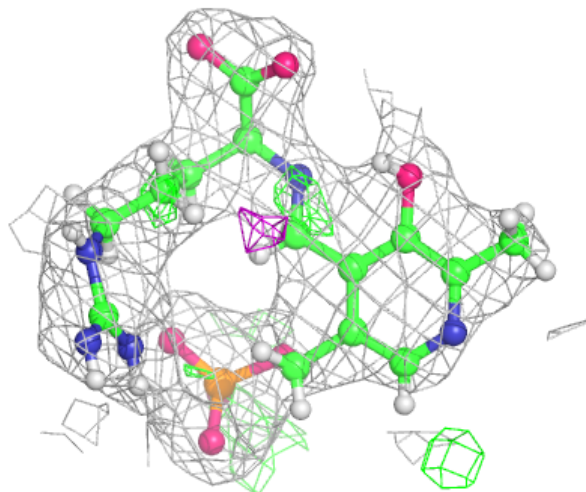
Electron density around EQJ H 401:

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



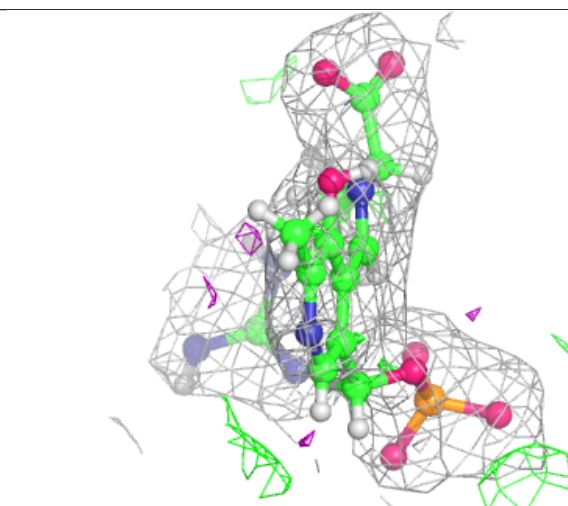
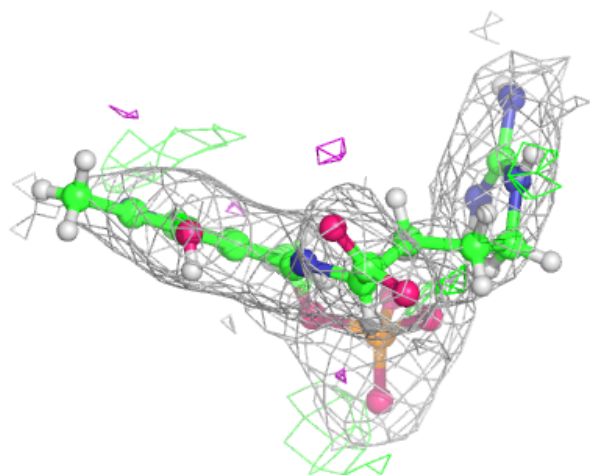
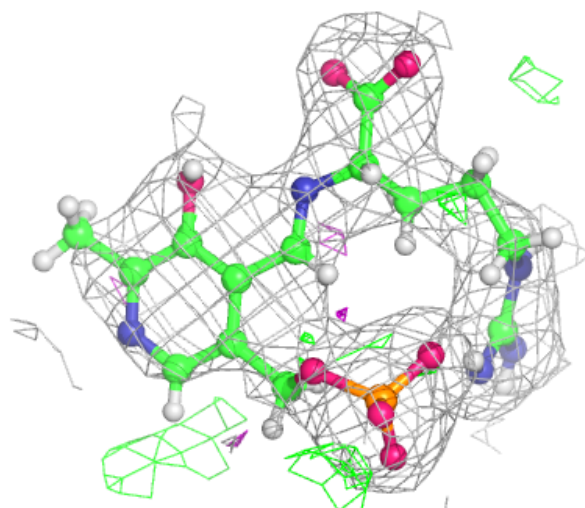
Electron density around EQJ G 401:

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



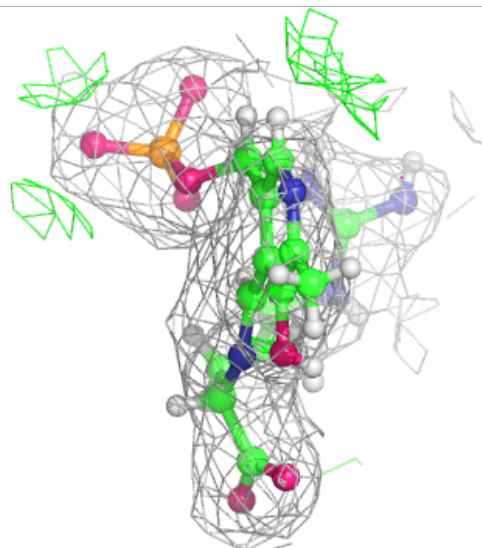
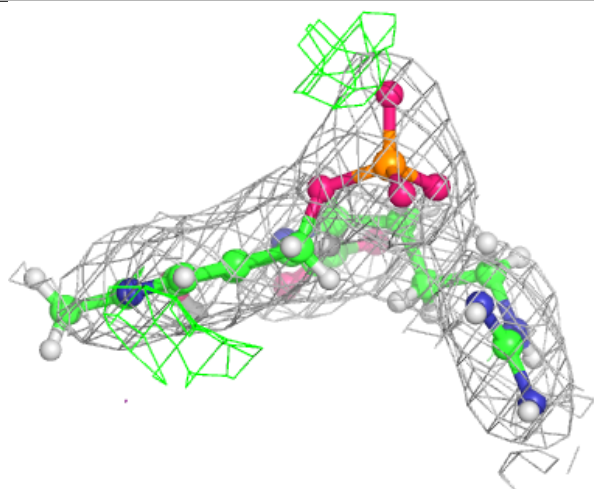
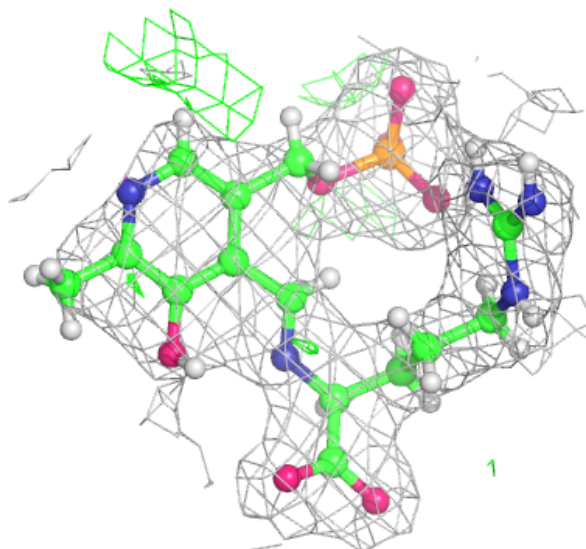
Electron density around EQJ F 401:

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



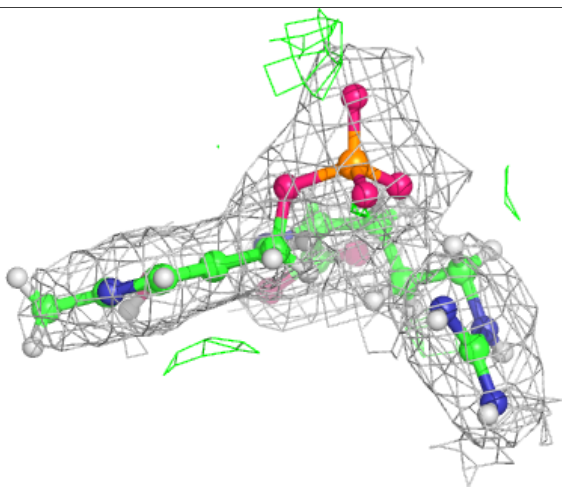
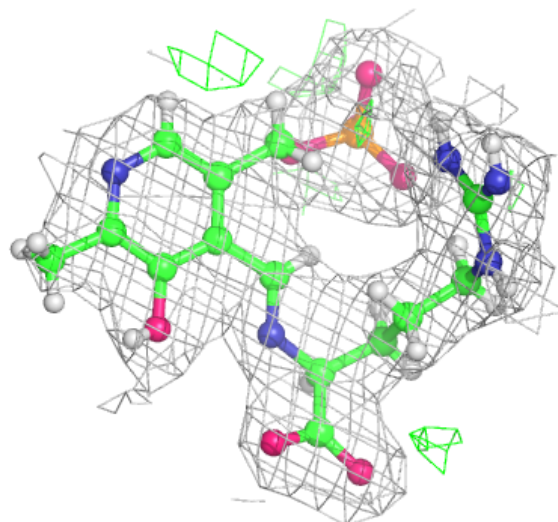
Electron density around EQJ C 401:

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



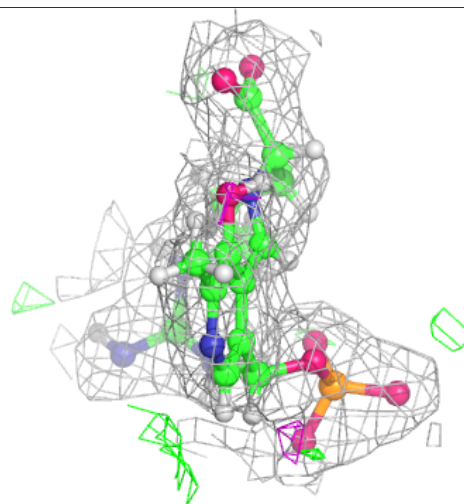
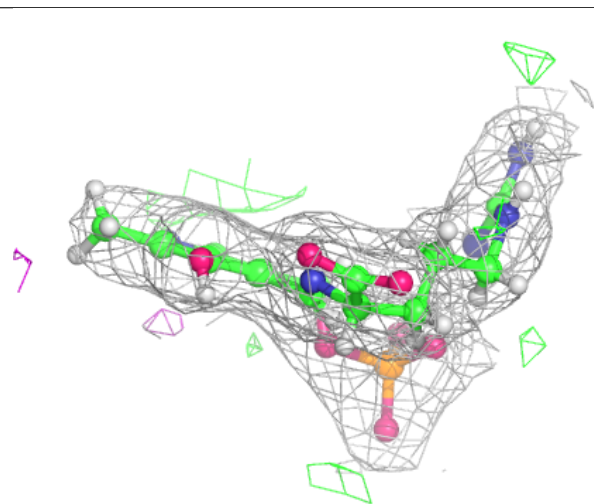
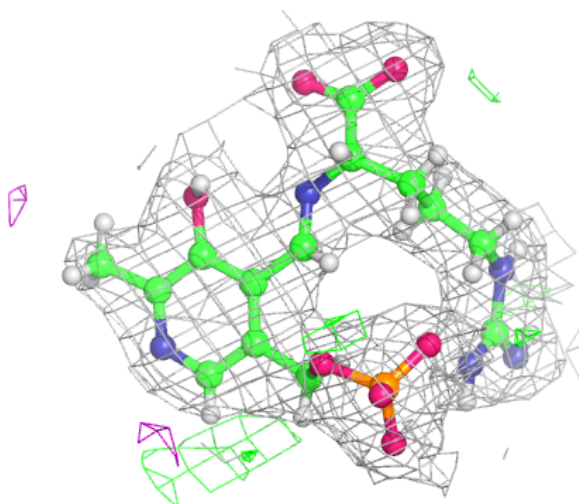
Electron density around EQJ D 401:

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



Electron density around EQJ A 400:

$2mF_o-DF_c$ (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.