



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:01 pm BST

PDB ID : 6P3H  
Title : Crystal structure of LigU(K66M) bound to substrate  
Authors : Cory, S.A.; Hogancamp, T.N.; Raushel, F.M.; Barondeau, D.P.  
Deposited on : 2019-05-23  
Resolution : 1.62 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](mailto: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.

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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

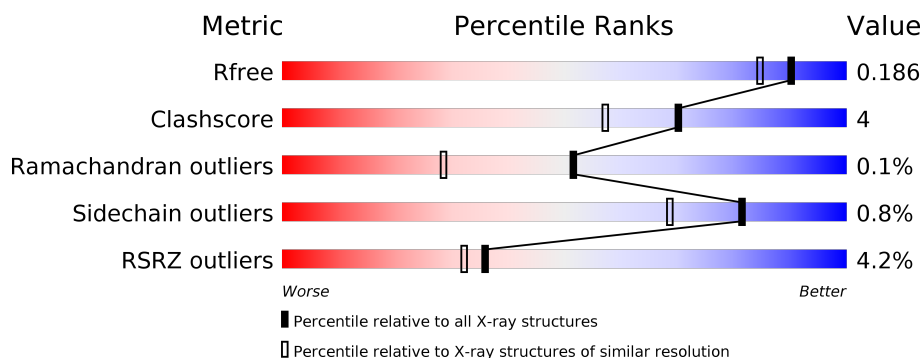
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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  $\geq 3$ , 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	365	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div></div> </div> </div>
1	B	365	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> </div>
1	C	365	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	D	365	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12083 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called (4E)-oxalomesaconate Delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	7	0
			2577	1605	447	502	23			
1	D	351	Total	C	N	O	S	0	13	0
			2630	1633	459	514	24			
1	C	352	Total	C	N	O	S	0	14	0
			2642	1639	459	520	24			
1	B	351	Total	C	N	O	S	0	17	0
			2656	1647	460	526	23			

There are 36 discrepancies between the modelled and reference sequences:

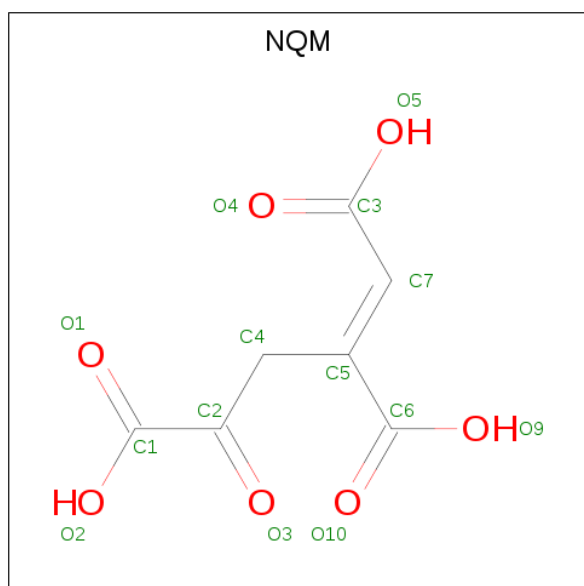
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	MET	LYS	engineered mutation	UNP Q0KJL4
A	358	LEU	-	expression tag	UNP Q0KJL4
A	359	GLU	-	expression tag	UNP Q0KJL4
A	360	HIS	-	expression tag	UNP Q0KJL4
A	361	HIS	-	expression tag	UNP Q0KJL4
A	362	HIS	-	expression tag	UNP Q0KJL4
A	363	HIS	-	expression tag	UNP Q0KJL4
A	364	HIS	-	expression tag	UNP Q0KJL4
A	365	HIS	-	expression tag	UNP Q0KJL4
D	66	MET	LYS	engineered mutation	UNP Q0KJL4
D	358	LEU	-	expression tag	UNP Q0KJL4
D	359	GLU	-	expression tag	UNP Q0KJL4
D	360	HIS	-	expression tag	UNP Q0KJL4
D	361	HIS	-	expression tag	UNP Q0KJL4
D	362	HIS	-	expression tag	UNP Q0KJL4
D	363	HIS	-	expression tag	UNP Q0KJL4
D	364	HIS	-	expression tag	UNP Q0KJL4
D	365	HIS	-	expression tag	UNP Q0KJL4
C	66	MET	LYS	engineered mutation	UNP Q0KJL4
C	358	LEU	-	expression tag	UNP Q0KJL4
C	359	GLU	-	expression tag	UNP Q0KJL4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	360	HIS	-	expression tag	UNP Q0KJL4
C	361	HIS	-	expression tag	UNP Q0KJL4
C	362	HIS	-	expression tag	UNP Q0KJL4
C	363	HIS	-	expression tag	UNP Q0KJL4
C	364	HIS	-	expression tag	UNP Q0KJL4
C	365	HIS	-	expression tag	UNP Q0KJL4
B	66	MET	LYS	engineered mutation	UNP Q0KJL4
B	358	LEU	-	expression tag	UNP Q0KJL4
B	359	GLU	-	expression tag	UNP Q0KJL4
B	360	HIS	-	expression tag	UNP Q0KJL4
B	361	HIS	-	expression tag	UNP Q0KJL4
B	362	HIS	-	expression tag	UNP Q0KJL4
B	363	HIS	-	expression tag	UNP Q0KJL4
B	364	HIS	-	expression tag	UNP Q0KJL4
B	365	HIS	-	expression tag	UNP Q0KJL4

- Molecule 2 is (1E)-4-oxobut-1-ene-1,2,4-tricarboxylic acid (three-letter code: NQM) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	7	7		
2	D	1	Total	C	O	0	0
			14	7	7		
2	C	1	Total	C	O	0	0
			14	7	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			14	7	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

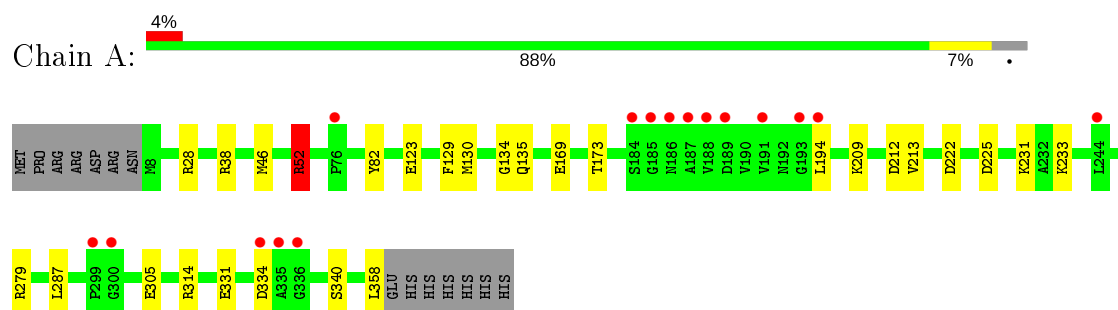
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	306	Total	O	0	0
			306	306		
4	D	293	Total	O	0	0
			293	293		
4	C	441	Total	O	0	0
			441	441		
4	B	476	Total	O	0	0
			476	476		

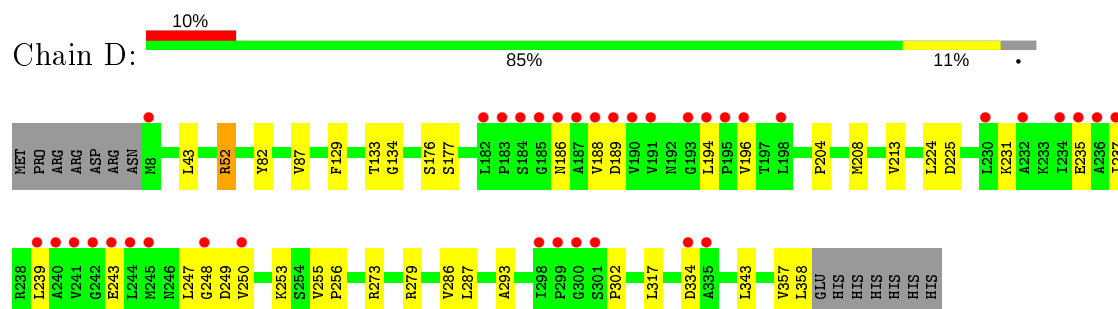
### 3 Residue-property plots [i](#)

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.

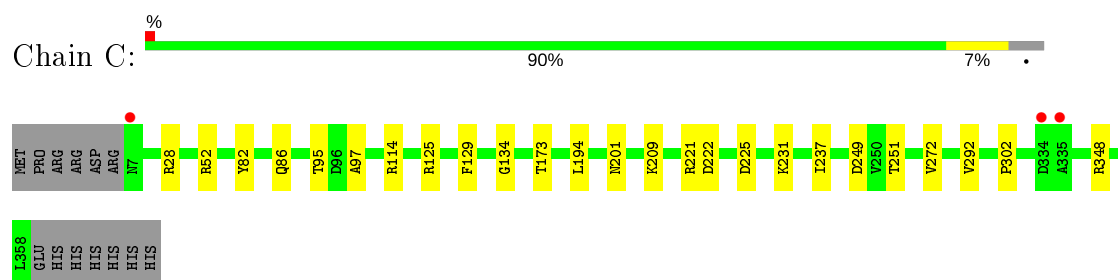
- Molecule 1: (4E)-oxalomesaconate Delta-isomerase



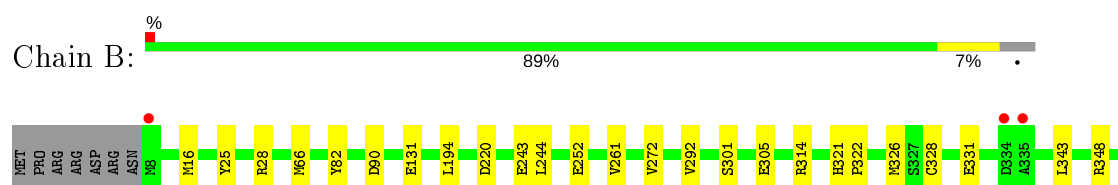
- Molecule 1: (4E)-oxalomesaconate Delta-isomerase



- Molecule 1: (4E)-oxalomesaconate Delta-isomerase



- Molecule 1: (4E)-oxalomesaconate Delta-isomerase



1358
GLU
HIS
HIS
HIS
HIS
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.88Å 134.00Å 168.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 1.62 39.46 – 1.62	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.46-1.62) 97.2 (39.46-1.62)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.15.2 _3472	Depositor
R, $R_{free}$	0.157 , 0.187 0.156 , 0.186	Depositor DCC
$R_{free}$ test set	2000 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 40.70 % 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 2.6329e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.67	0/2617	0.82	8/3561 (0.2%)
1	B	0.85	4/2696 (0.1%)	0.87	2/3670 (0.1%)
1	C	0.78	0/2682	0.85	1/3649 (0.0%)
1	D	0.69	1/2670 (0.0%)	0.78	3/3631 (0.1%)
All	All	0.75	5/10665 (0.0%)	0.83	14/14511 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	357	VAL	CB-CG2	-5.33	1.41	1.52
1	B	66[A]	MET	CB-CG	5.28	1.68	1.51
1	B	66[B]	MET	CB-CG	5.28	1.68	1.51
1	B	301[A]	SER	CB-OG	5.14	1.49	1.42
1	B	301[B]	SER	CB-OG	5.14	1.49	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52[A]	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	52[B]	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	D	52[A]	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	D	52[B]	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	38	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	52[A]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	52[B]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	287	LEU	CA-CB-CG	-5.74	102.10	115.30
1	A	279	ARG	CG-CD-NE	-5.42	100.43	111.80
1	A	287	LEU	CA-CB-CG	-5.34	103.03	115.30
1	C	114	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	46	MET	CG-SD-CE	-5.16	91.94	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	B	326	MET	CG-SD-CE	-5.03	92.15	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2577	0	2582	18	0
1	B	2656	0	2631	18	0
1	C	2642	0	2627	18	0
1	D	2630	0	2621	25	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	306	0	0	4	0
4	B	476	0	0	11	0
4	C	441	0	0	8	1
4	D	293	0	0	2	0
All	All	12083	0	10461	76	1

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 (76) 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:B:220[B]:ASP:OD2	4:B:501:HOH:O	1.81	0.97
1:A:135:GLN:HE22	1:A:173:THR:HA	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90[B]:ASP:OD1	4:B:502:HOH:O	1.96	0.83
1:D:176:SER:OG	4:D:501:HOH:O	2.01	0.74
1:B:28[B]:ARG:NH1	4:B:506:HOH:O	2.22	0.72
1:C:249:ASP:OD1	1:C:251:THR:HG23	1.91	0.70
1:B:252:GLU:OE2	4:B:503:HOH:O	2.10	0.70
1:D:255:VAL:HG22	1:D:256:PRO:HA	1.74	0.69
1:A:135:GLN:NE2	1:A:173:THR:HA	2.02	0.69
1:B:90[B]:ASP:OD1	4:B:504:HOH:O	2.12	0.68
1:C:222[A]:ASP:OD1	4:C:501:HOH:O	2.12	0.66
1:C:225:ASP:HA	1:C:231:LYS:HE3	1.76	0.66
1:D:186:ASN:HB2	1:D:189:ASP:OD2	1.98	0.62
1:A:213:VAL:HG12	1:A:233:LYS:HD3	1.83	0.61
1:B:131:GLU:OE2	4:B:505:HOH:O	2.16	0.60
1:B:243[B]:GLU:HG2	4:B:515:HOH:O	2.01	0.60
1:A:194:LEU:HD22	1:A:212:ASP:HB3	1.83	0.60
1:B:244:LEU:HG	4:B:515:HOH:O	2.02	0.60
1:A:331:GLU:HG2	1:A:340:SER:OG	2.02	0.60
1:B:305[A]:GLU:HG2	4:B:718:HOH:O	2.01	0.59
1:C:173[B]:THR:HG23	1:C:201:ASN:OD1	2.02	0.59
1:D:194:LEU:HD12	1:D:237:ILE:HD11	1.86	0.58
1:D:243:GLU:OE2	1:D:248:GLY:HA2	2.04	0.57
1:B:272[A]:VAL:HG21	1:B:292:VAL:HG11	1.86	0.57
1:C:97:ALA:HB3	4:C:584:HOH:O	2.05	0.56
1:B:28[A]:ARG:NH1	4:B:518:HOH:O	2.39	0.56
1:B:261:VAL:HG12	1:B:272[A]:VAL:HG22	1.90	0.54
1:A:52[A]:ARG:HA	1:A:52[A]:ARG:HE	1.72	0.54
1:C:52[B]:ARG:NH1	4:C:505:HOH:O	2.40	0.54
1:D:208:MET:HE1	1:D:213:VAL:HG11	1.89	0.54
1:D:247:LEU:HD13	1:D:255:VAL:HG13	1.89	0.53
1:A:222[B]:ASP:OD2	4:A:501:HOH:O	2.19	0.52
1:B:28[B]:ARG:HD2	4:B:506:HOH:O	2.10	0.52
1:D:293:ALA:HB1	1:D:317:LEU:HD12	1.92	0.51
1:D:250:VAL:HA	1:D:253:LYS:HD2	1.92	0.50
1:A:169[B]:GLU:HG3	4:A:777:HOH:O	2.12	0.50
1:C:125[A]:ARG:NH1	4:C:503:HOH:O	2.35	0.49
1:D:225:ASP:O	1:D:231:LYS:HE2	2.12	0.49
1:D:247:LEU:O	1:D:253:LYS:NZ	2.42	0.49
1:D:286:VAL:HG13	1:D:343:LEU:HD22	1.95	0.49
1:D:235:GLU:OE2	1:D:239:LEU:HG	2.12	0.49
1:D:334:ASP:OD1	1:D:334:ASP:N	2.44	0.49
1:A:225:ASP:HA	1:A:231:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328[A]:CYS:SG	1:B:343:LEU:HD21	2.54	0.48
1:D:188:VAL:HG22	1:D:302:PRO:HD3	1.95	0.48
1:A:209:LYS:NZ	1:A:305:GLU:OE2	2.44	0.47
1:A:28:ARG:NH1	4:A:506:HOH:O	2.38	0.47
1:C:173[B]:THR:HG22	4:C:632:HOH:O	2.15	0.46
1:C:97:ALA:HB2	4:C:741:HOH:O	2.16	0.46
1:D:52[B]:ARG:CZ	4:D:596:HOH:O	2.63	0.46
1:C:125[A]:ARG:HD3	4:C:874:HOH:O	2.16	0.45
1:C:272:VAL:HG21	1:C:292:VAL:HG11	1.98	0.45
1:B:314[B]:ARG:HD2	1:B:331:GLU:OE2	2.16	0.45
1:D:358:LEU:HA	1:D:358:LEU:HD23	1.70	0.45
1:C:86:GLN:HB3	1:C:95:THR:HG22	1.99	0.45
1:B:16:MET:HB2	1:B:25:TYR:CE1	2.52	0.44
1:A:130:MET:CE	1:A:135:GLN:HG3	2.47	0.44
1:D:358:LEU:HG	1:B:348:ARG:HD2	1.98	0.44
1:D:177:SER:HB2	1:D:204:PRO:HG3	2.00	0.44
1:A:358:LEU:HG	1:C:348:ARG:HD2	1.99	0.44
1:A:52[A]:ARG:NH1	1:C:221:ARG:HH21	2.15	0.43
1:D:189:ASP:O	1:D:196:VAL:HG22	2.18	0.43
1:C:28:ARG:NH1	4:C:520:HOH:O	2.52	0.42
1:A:123:GLU:O	4:A:502:HOH:O	2.22	0.42
1:C:194:LEU:HD21	1:C:237:ILE:HD11	2.02	0.42
1:D:224:LEU:HD11	1:D:273:ARG:HG3	2.02	0.42
1:D:133:THR:HB	1:D:176:SER:HB2	2.01	0.41
1:D:129:PHE:CZ	1:D:134:GLY:HA2	2.56	0.41
1:D:43:LEU:HD23	1:D:87:VAL:HG13	2.03	0.41
1:C:129:PHE:CZ	1:C:134:GLY:HA2	2.56	0.41
1:B:321:HIS:HB2	1:B:322:PRO:CD	2.50	0.41
1:A:130:MET:HE3	1:A:135:GLN:HG3	2.03	0.40
1:D:52[A]:ARG:HE	1:D:52[A]:ARG:HA	1.85	0.40
1:A:129:PHE:CZ	1:A:134:GLY:HA2	2.56	0.40
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.90	0.40
1:C:209:LYS:HG3	1:C:302:PRO:HB3	2.02	0.40

All (1) 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)
4:C:885:HOH:O	4:C:915:HOH:O[2_555]	2.16	0.04

## 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	356/365 (98%)	348 (98%)	7 (2%)	1 (0%)	41	21
1	B	366/365 (100%)	358 (98%)	8 (2%)	0	100	100
1	C	364/365 (100%)	357 (98%)	7 (2%)	0	100	100
1	D	362/365 (99%)	355 (98%)	7 (2%)	0	100	100
All	All	1448/1460 (99%)	1418 (98%)	29 (2%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	ASP

### 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	273/280 (98%)	268 (98%)	5 (2%)	59	34
1	B	283/280 (101%)	282 (100%)	1 (0%)	91	84
1	C	281/280 (100%)	280 (100%)	1 (0%)	91	84
1	D	279/280 (100%)	274 (98%)	5 (2%)	59	34
All	All	1116/1120 (100%)	1104 (99%)	12 (1%)	81	56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52[A]	ARG
1	A	52[B]	ARG
1	A	82	TYR
1	A	314[A]	ARG
1	A	314[B]	ARG
1	D	82	TYR
1	D	249[A]	ASP
1	D	249[B]	ASP
1	D	279[A]	ARG
1	D	279[B]	ARG
1	C	82	TYR
1	B	82	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	135	GLN
1	D	337	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NQM	B	401	-	4,13,13	1.83	2 (50%)	2,17,17	3.42	1 (50%)
2	NQM	C	401	-	4,13,13	1.48	1 (25%)	2,17,17	3.64	1 (50%)
2	NQM	A	401	-	4,13,13	1.81	2 (50%)	2,17,17	4.06	2 (100%)
2	NQM	D	401	-	4,13,13	1.65	1 (25%)	2,17,17	5.10	2 (100%)

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	NQM	B	401	-	-	2/6/16/16	-
2	NQM	C	401	-	-	2/6/16/16	-
2	NQM	A	401	-	-	2/6/16/16	-
2	NQM	D	401	-	-	2/6/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NQM	O3-C2	2.96	1.27	1.22
2	A	401	NQM	C7-C5	2.58	1.37	1.34
2	D	401	NQM	O3-C2	2.57	1.26	1.22
2	A	401	NQM	O3-C2	2.45	1.26	1.22
2	C	401	NQM	C7-C5	2.11	1.36	1.34
2	B	401	NQM	C7-C5	2.09	1.36	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NQM	O3-C2-C4	6.85	128.29	120.56
2	A	401	NQM	O3-C2-C4	5.15	126.37	120.56
2	C	401	NQM	O3-C2-C4	5.00	126.20	120.56
2	B	401	NQM	O3-C2-C4	4.58	125.72	120.56
2	A	401	NQM	C3-C7-C5	-2.54	121.76	127.06
2	D	401	NQM	C3-C7-C5	-2.24	122.40	127.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

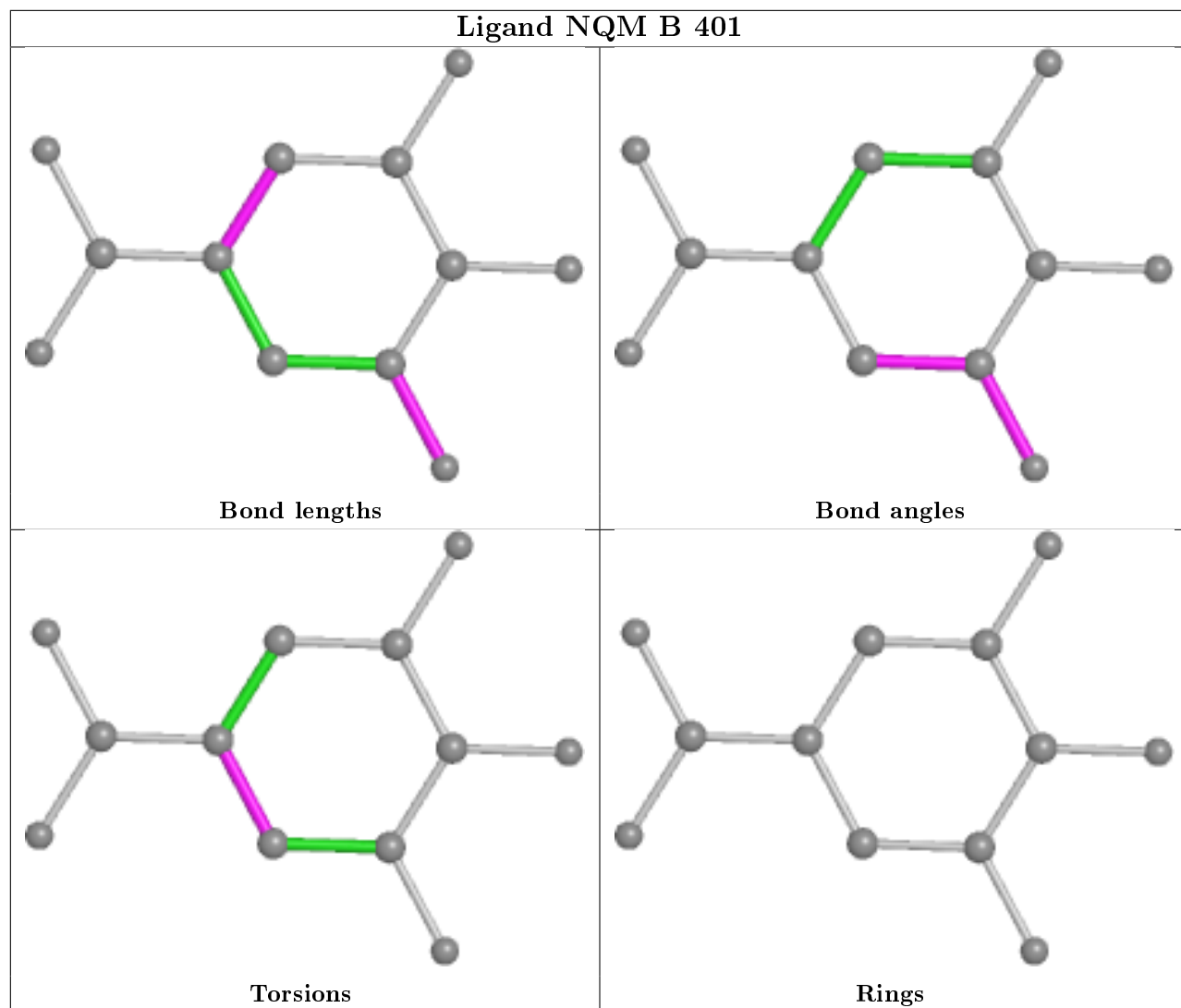
Mol	Chain	Res	Type	Atoms
2	B	401	NQM	C2-C4-C5-C7
2	B	401	NQM	C2-C4-C5-C6
2	C	401	NQM	C2-C4-C5-C7
2	C	401	NQM	C2-C4-C5-C6
2	A	401	NQM	C2-C4-C5-C7
2	A	401	NQM	C2-C4-C5-C6
2	D	401	NQM	C2-C4-C5-C7
2	D	401	NQM	C2-C4-C5-C6

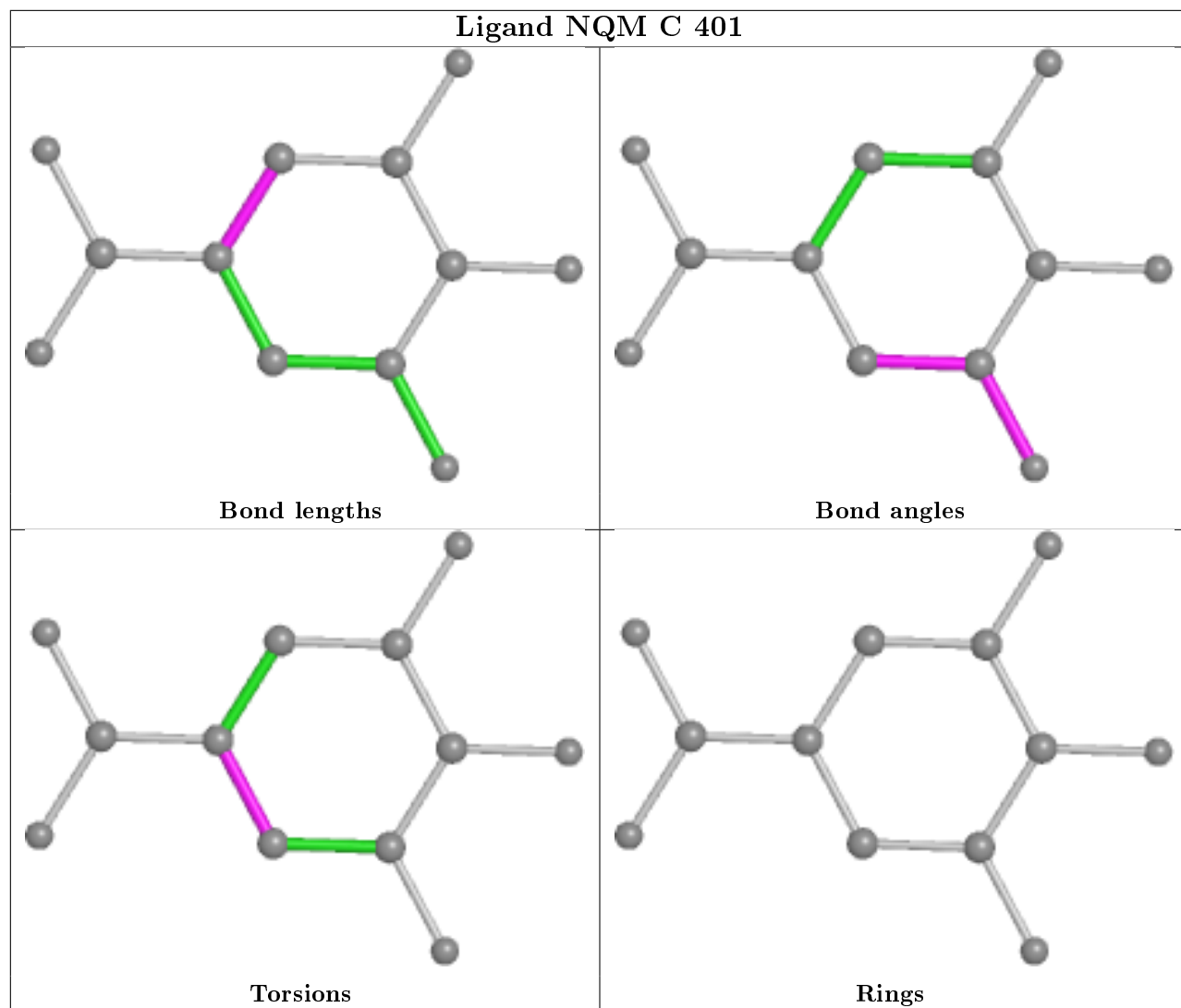
There are no ring outliers.

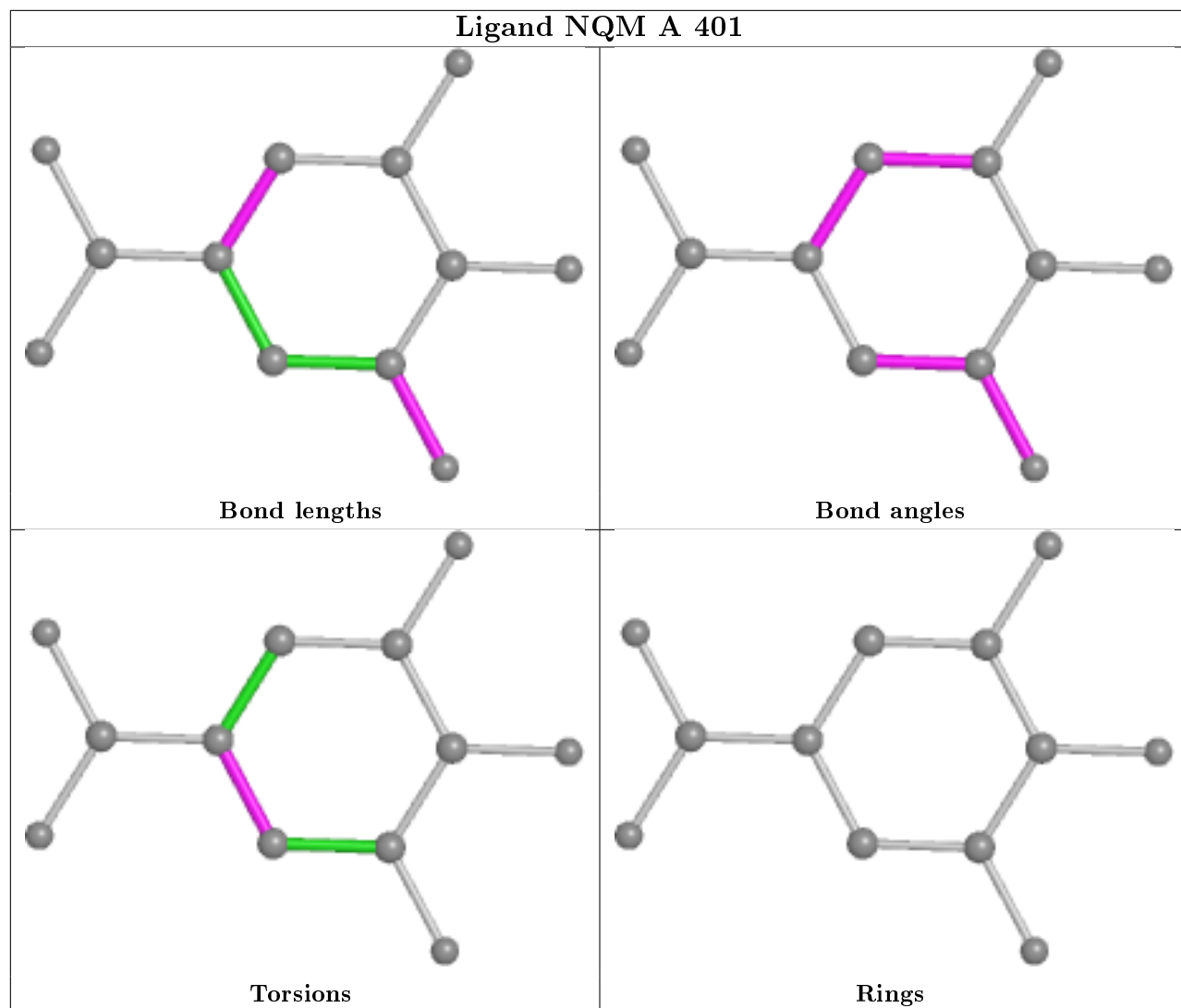
No monomer is involved in short contacts.

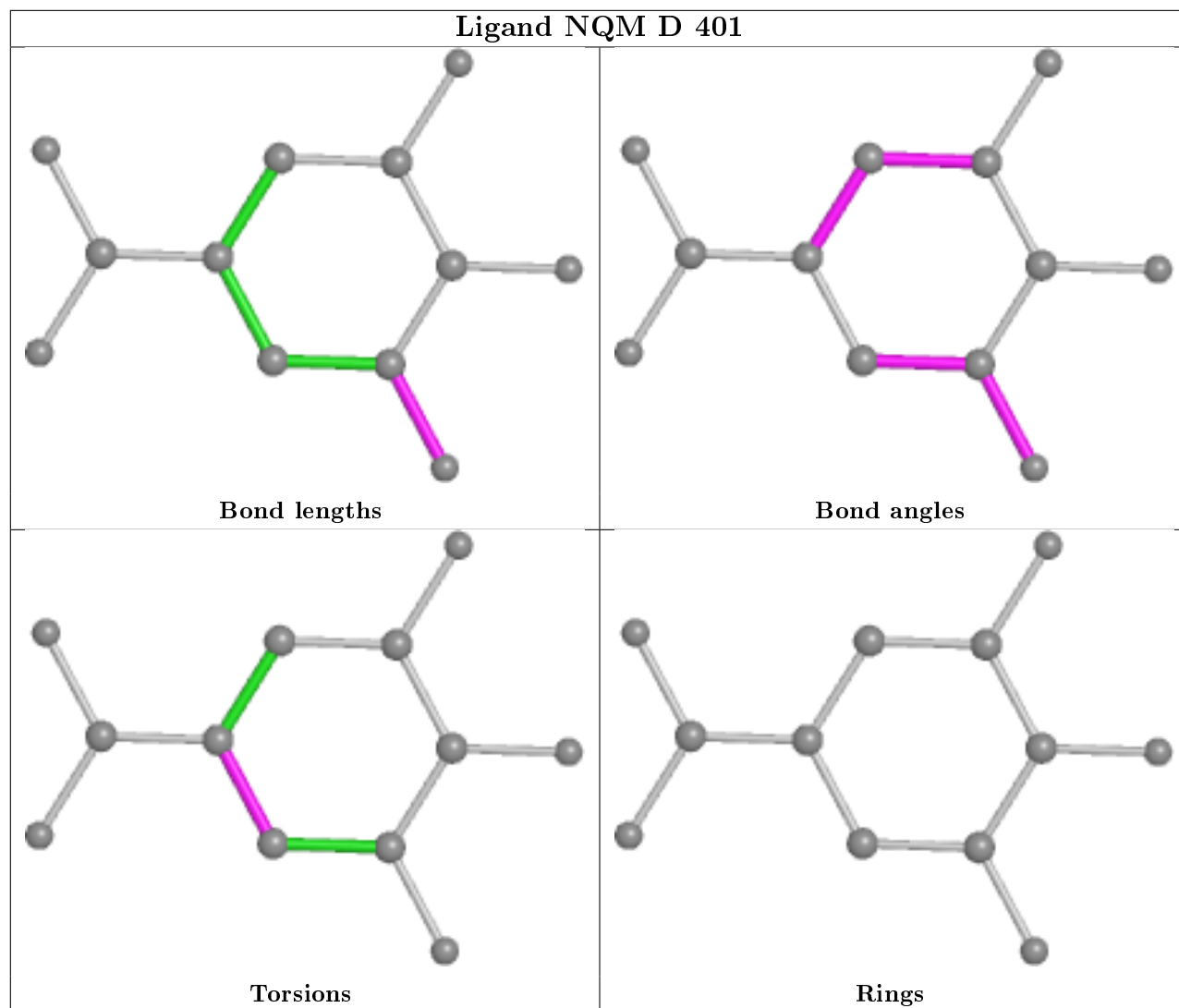
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	351/365 (96%)	-0.12	16 (4%) 32 29	16, 30, 52, 88	0
1	B	351/365 (96%)	-0.54	3 (0%) 84 84	14, 20, 31, 57	0
1	C	352/365 (96%)	-0.44	3 (0%) 84 84	15, 21, 37, 60	0
1	D	351/365 (96%)	0.12	37 (10%) 6 5	15, 32, 65, 88	0
All	All	1405/1460 (96%)	-0.24	59 (4%) 36 32	14, 24, 55, 88	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	7.1
1	D	193	GLY	6.5
1	D	188	VAL	5.9
1	A	335	ALA	5.7
1	A	194	LEU	5.3
1	D	244	LEU	5.0
1	D	190	VAL	4.9
1	D	187	ALA	4.8
1	D	334	ASP	4.6
1	A	191	VAL	4.2
1	D	335	ALA	4.1
1	D	299	PRO	4.0
1	D	184	SER	3.9
1	A	300	GLY	3.9
1	D	236	ALA	3.8
1	A	188	VAL	3.8
1	D	186	ASN	3.7
1	D	191	VAL	3.7
1	D	234	ILE	3.6
1	A	334	ASP	3.6
1	D	232	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	3.4
1	D	196	VAL	3.3
1	D	189	ASP	3.2
1	D	300	GLY	3.1
1	A	299	PRO	3.1
1	A	244	LEU	3.1
1	C	7	ASN	3.1
1	B	335	ALA	3.0
1	D	230	LEU	3.0
1	A	187	ALA	2.9
1	D	250	VAL	2.8
1	A	76	PRO	2.7
1	C	335	ALA	2.6
1	D	183	PRO	2.6
1	D	185	GLY	2.6
1	D	240	ALA	2.5
1	D	237	ILE	2.5
1	D	298	ILE	2.5
1	C	334	ASP	2.5
1	A	336	GLY	2.5
1	D	239	LEU	2.5
1	A	186	ASN	2.4
1	D	241	VAL	2.4
1	D	242	GLY	2.4
1	B	334	ASP	2.4
1	D	195	PRO	2.4
1	A	184	SER	2.3
1	D	245	MET	2.2
1	D	235	GLU	2.2
1	D	8	MET	2.1
1	D	248	GLY	2.1
1	B	8	MET	2.1
1	D	243	GLU	2.1
1	A	185	GLY	2.1
1	A	189	ASP	2.1
1	D	182	LEU	2.0
1	D	198	LEU	2.0
1	D	301	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

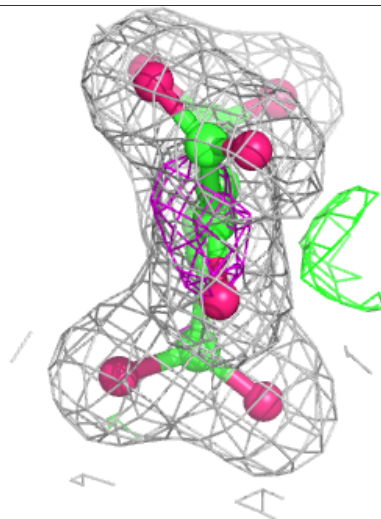
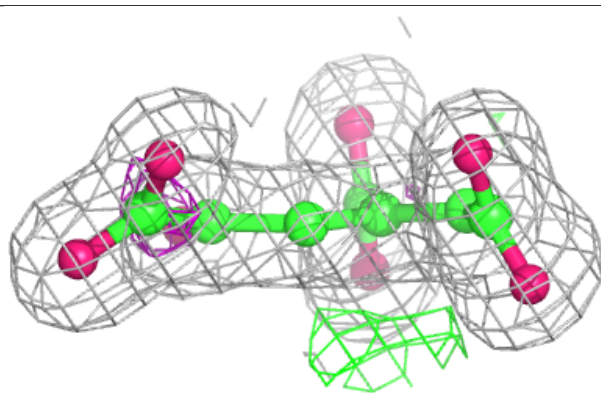
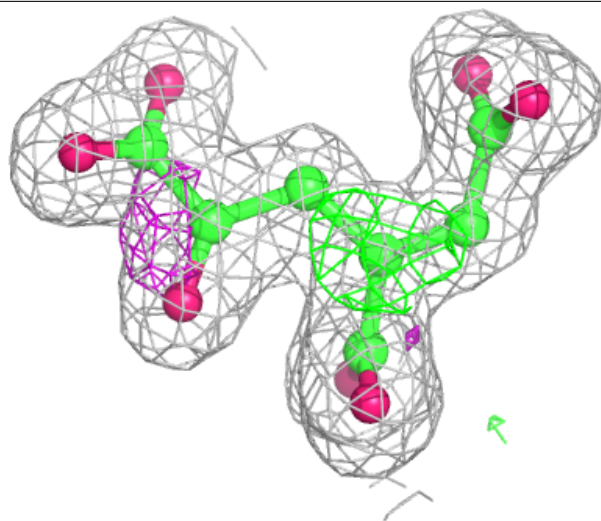
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	B	402	1/1	0.94	0.06	39,39,39,39	0
3	CL	A	403	1/1	0.96	0.10	49,49,49,49	0
2	NQM	D	401	14/14	0.97	0.06	22,25,35,35	0
2	NQM	B	401	14/14	0.98	0.08	14,17,26,29	0
2	NQM	C	401	14/14	0.98	0.09	16,18,28,28	0
2	NQM	A	401	14/14	0.98	0.07	22,25,33,34	0
3	CL	D	402	1/1	0.99	0.09	33,33,33,33	0
3	CL	C	402	1/1	0.99	0.04	30,30,30,30	0
3	CL	A	402	1/1	0.99	0.09	33,33,33,33	0
3	CL	B	403	1/1	1.00	0.04	28,28,28,28	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 NQM D 401:**

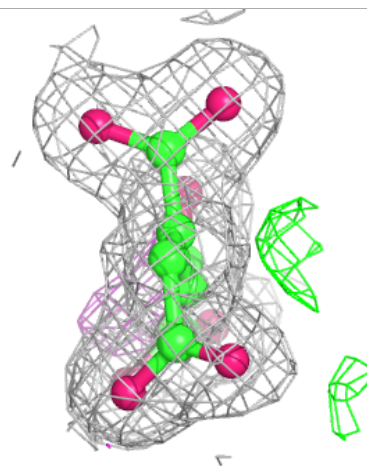
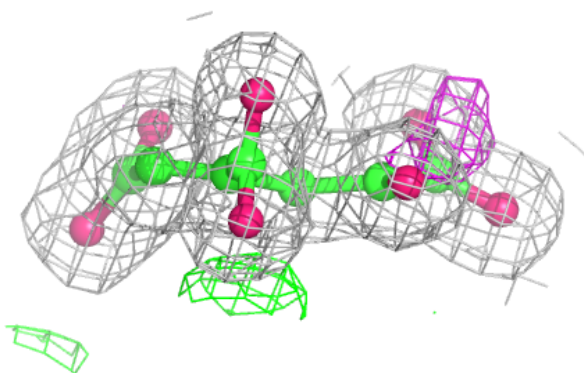
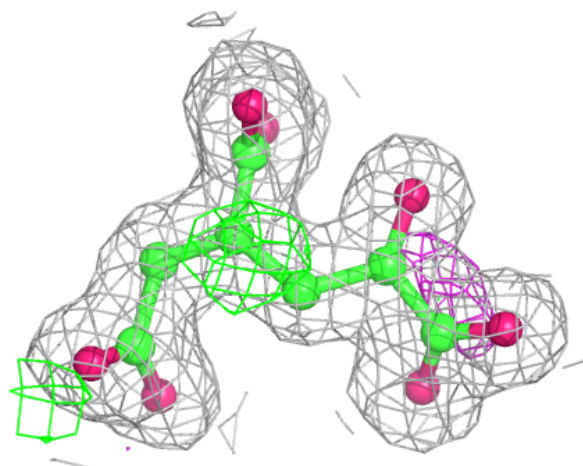
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





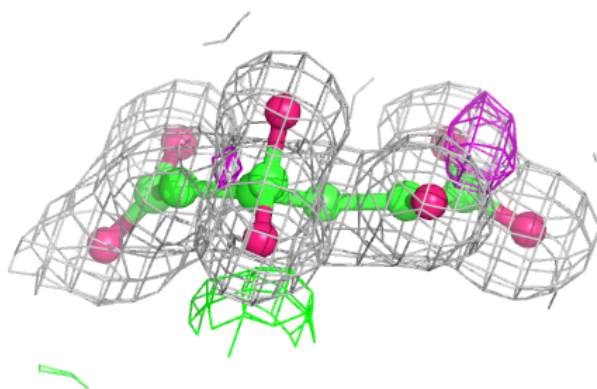
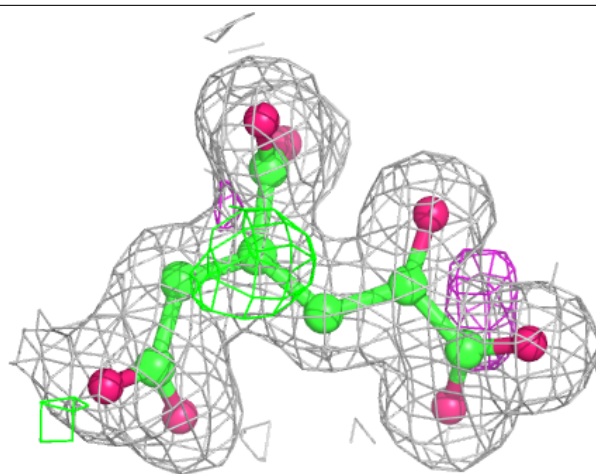
**Electron density around NQM B 401:**

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



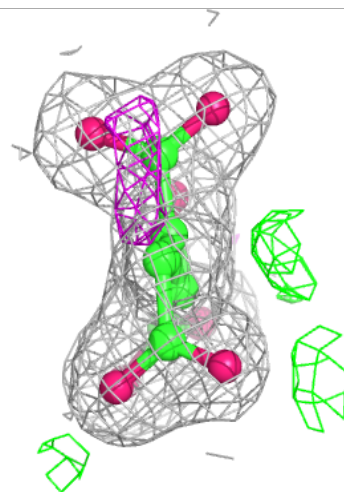
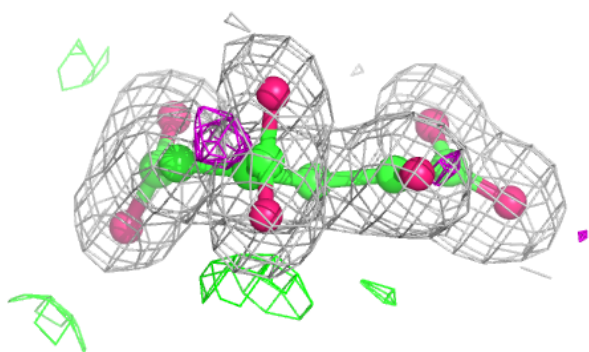
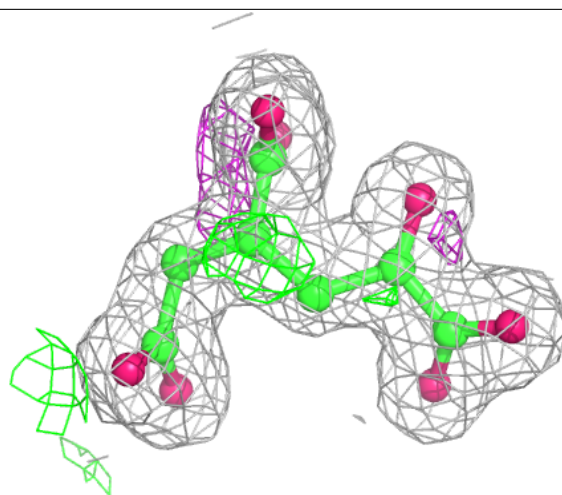
**Electron density around NQM C 401:**

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



**Electron density around NQM 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.