



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 AM UTC

PDB ID : 4B2X / pdb_00004b2x
Title : Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
Authors : Alphey, M.S.; Pirrie, L.; Torrie, L.S.; Gardiner, M.; Sarkar, A.; Brenk, R.;
Westwood, N.J.; Gray, D.; Naismith, J.H.
Deposited on : 2012-07-18
Resolution : 1.70 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

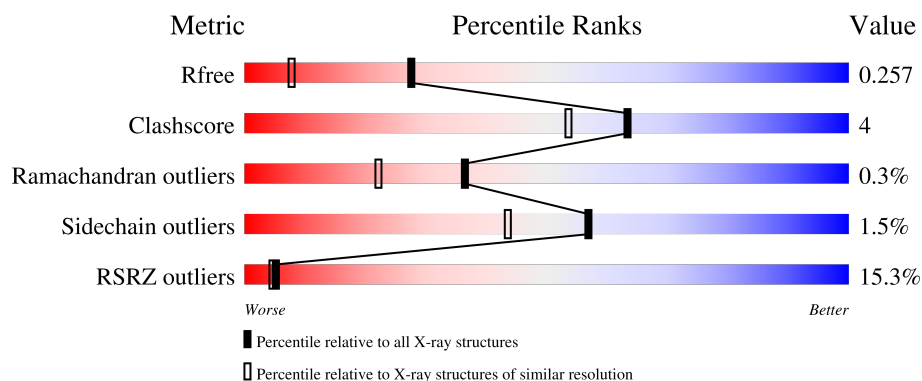
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	303	
1	B	303	
1	C	303	
1	D	303	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10293 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	2	0
			2365	1511	406	443	5			
1	B	302	Total	C	N	O	S	0	1	0
			2372	1514	406	446	6			
1	C	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	D	293	Total	C	N	O	S	0	2	0
			2305	1475	388	437	5			

There are 40 discrepancies between the modelled and reference sequences:

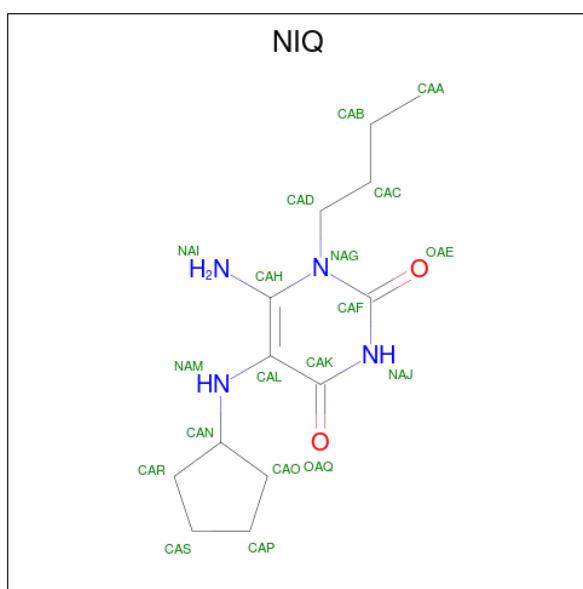
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q9HU22
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	GLY	-	expression tag	UNP Q9HU22
A	-3	SER	-	expression tag	UNP Q9HU22
A	-2	MET	-	expression tag	UNP Q9HU22
A	-1	ALA	-	expression tag	UNP Q9HU22
B	-9	HIS	-	expression tag	UNP Q9HU22
B	-8	HIS	-	expression tag	UNP Q9HU22
B	-7	HIS	-	expression tag	UNP Q9HU22
B	-6	HIS	-	expression tag	UNP Q9HU22
B	-5	HIS	-	expression tag	UNP Q9HU22
B	-4	HIS	-	expression tag	UNP Q9HU22
B	-3	GLY	-	expression tag	UNP Q9HU22
B	-2	SER	-	expression tag	UNP Q9HU22
B	-1	MET	-	expression tag	UNP Q9HU22
B	0	ALA	-	expression tag	UNP Q9HU22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP Q9HU22
C	-8	HIS	-	expression tag	UNP Q9HU22
C	-7	HIS	-	expression tag	UNP Q9HU22
C	-6	HIS	-	expression tag	UNP Q9HU22
C	-5	HIS	-	expression tag	UNP Q9HU22
C	-4	HIS	-	expression tag	UNP Q9HU22
C	-3	GLY	-	expression tag	UNP Q9HU22
C	-2	SER	-	expression tag	UNP Q9HU22
C	-1	MET	-	expression tag	UNP Q9HU22
C	0	ALA	-	expression tag	UNP Q9HU22
D	-9	HIS	-	expression tag	UNP Q9HU22
D	-8	HIS	-	expression tag	UNP Q9HU22
D	-7	HIS	-	expression tag	UNP Q9HU22
D	-6	HIS	-	expression tag	UNP Q9HU22
D	-5	HIS	-	expression tag	UNP Q9HU22
D	-4	HIS	-	expression tag	UNP Q9HU22
D	-3	GLY	-	expression tag	UNP Q9HU22
D	-2	SER	-	expression tag	UNP Q9HU22
D	-1	MET	-	expression tag	UNP Q9HU22
D	0	ALA	-	expression tag	UNP Q9HU22

- Molecule 2 is 6-amino-1-butyl-5-(cyclopentylamino)pyrimidine-2,4(1H,3H)-dione (CCD ID: NIQ) (formula: C₁₃H₂₂N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			24	18	4	2		

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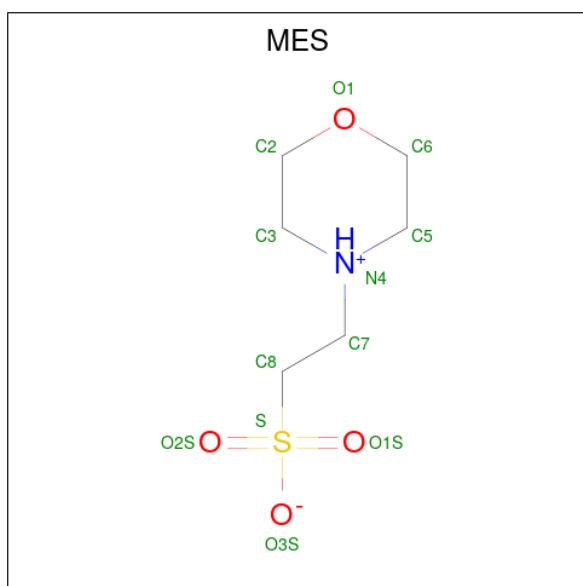
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			24	18	4	2		
2	C	1	Total	C	N	O	0	1
			24	18	4	2		
2	D	1	Total	C	N	O	0	1
			24	18	4	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

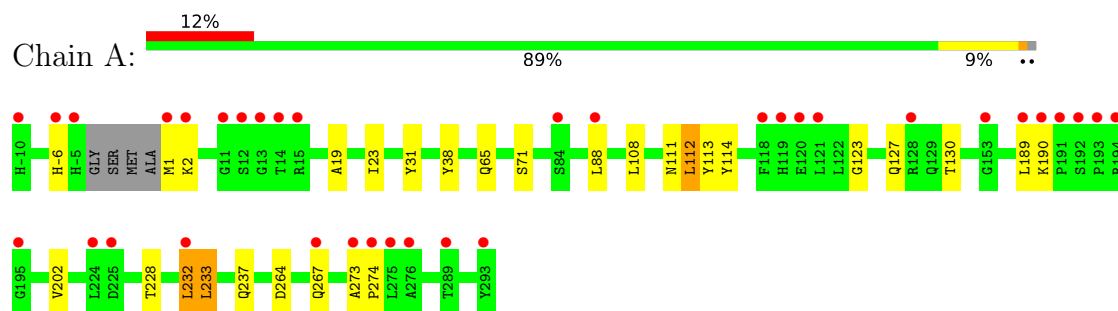
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total 265	O 265	0	0
5	B	199	Total 199	O 199	0	0
5	C	200	Total 200	O 200	0	0
5	D	176	Total 176	O 176	0	0

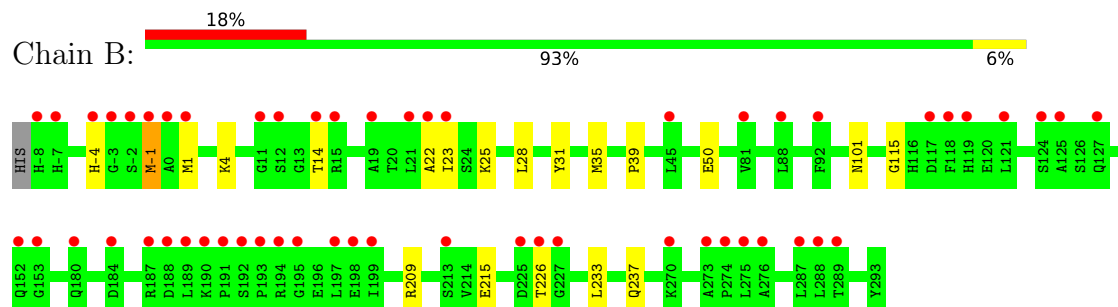
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

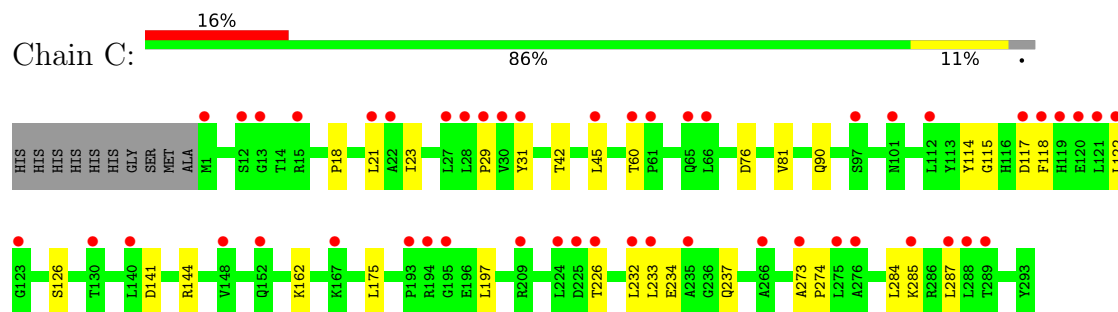
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



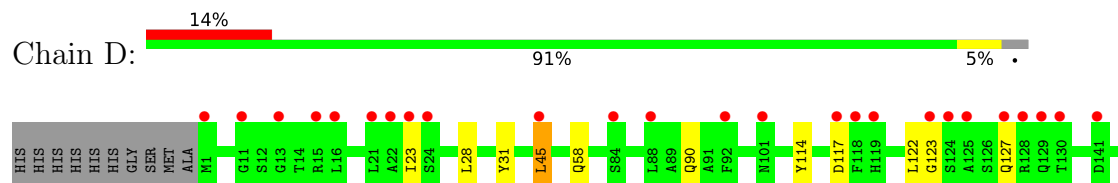
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

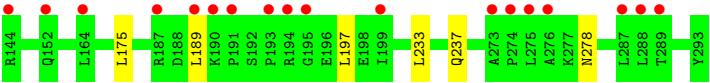


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.23Å 154.83Å 134.49Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	67.20 – 1.70 67.20 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (67.20-1.70) 96.3 (67.20-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.253 0.223 , 0.257	Depositor DCC
R_{free} test set	6998 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10293	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: NIQ, MES, CL

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	0.69	0/2426	0.72	0/3289
1	B	0.68	0/2430	0.72	0/3295
1	C	0.58	0/2352	0.70	0/3190
1	D	0.58	0/2361	0.68	0/3202
All	All	0.64	0/9569	0.71	0/12976

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	2365	0	2343	22	0
1	B	2372	0	2348	19	0
1	C	2299	0	2292	26	0
1	D	2305	0	2300	17	0
2	A	24	0	20	6	0
2	B	24	0	20	6	0
2	C	24	0	19	5	0
2	D	24	0	19	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	12	0	13	0	0
5	A	265	0	0	4	0
5	B	199	0	0	2	0
5	C	200	0	0	4	0
5	D	176	0	0	1	0
All	All	10293	0	9374	76	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 (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:23:ILE:CD1	1:D:23:ILE:HD12	2.09	0.82
1:C:141:ASP:OD2	1:C:144:ARG:HD3	1.83	0.79
1:A:232:LEU:HD23	5:A:2041:HOH:O	1.88	0.74
1:C:114:TYR:CD1	2:C:400[B]:NIQ:HAS1	2.24	0.73
1:C:45:LEU:HD11	2:C:400[A]:NIQ:HAN	1.70	0.71
1:D:23:ILE:HD13	1:D:28:LEU:HD23	1.74	0.69
1:B:23:ILE:HG12	1:D:23:ILE:HD12	1.75	0.69
1:C:45:LEU:CD1	2:C:400[A]:NIQ:HAN	2.24	0.68
1:B:23:ILE:HD13	1:D:23:ILE:HB	1.75	0.66
1:B:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.78	0.66
1:C:60:THR:HG23	5:C:2037:HOH:O	1.96	0.66
1:B:215:GLU:HG2	5:B:2104:HOH:O	1.96	0.64
1:B:23:ILE:CG1	1:D:23:ILE:HD12	2.28	0.63
1:B:115:GLY:H	2:B:400[B]:NIQ:HAS2	1.65	0.62
1:D:114:TYR:CD1	2:D:400[B]:NIQ:HAP2	2.36	0.60
1:C:60:THR:HG21	5:C:2024:HOH:O	2.00	0.60
1:A:38:TYR:HB2	1:A:112:LEU:HD22	1.84	0.60
1:B:-1:MET:HE2	1:B:-1:MET:HA	1.85	0.59
1:A:233:LEU:HD11	1:C:237[A]:GLN:HG3	1.84	0.59
1:C:115:GLY:H	2:C:400[B]:NIQ:HAS2	1.68	0.58
1:B:23:ILE:HD11	1:D:23:ILE:HD12	1.85	0.57
1:C:284:LEU:HA	1:C:287:LEU:HD12	1.86	0.57
1:B:233:LEU:HD21	1:D:237[B]:GLN:HA	1.88	0.56
1:A:114:TYR:CD1	2:A:400[B]:NIQ:HAS1	2.41	0.55
1:D:123:GLY:O	1:D:127:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237[B]:GLN:HA	1:C:233:LEU:HD21	1.90	0.54
1:A:237[A]:GLN:HA	1:C:233:LEU:HD21	1.91	0.53
1:B:1:MET:HE1	1:B:101:ASN:O	2.09	0.53
1:D:90:GLN:HG2	1:D:197:LEU:HD12	1.91	0.52
1:B:233:LEU:HD21	1:D:237[A]:GLN:HA	1.91	0.52
1:C:122:LEU:CD2	1:C:175:LEU:HD21	2.39	0.51
1:B:22:ALA:O	1:B:23:ILE:HG23	2.10	0.51
1:A:38:TYR:CB	1:A:112:LEU:HD22	2.41	0.50
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.94	0.49
1:B:25:LYS:NZ	1:B:226:THR:O	2.41	0.49
1:A:123:GLY:O	1:A:127:GLN:HG2	2.12	0.49
1:A:1:MET:HE1	5:A:2138:HOH:O	2.12	0.49
1:C:234:GLU:HA	1:C:237[A]:GLN:HE21	1.77	0.49
1:A:65:GLN:HB3	5:A:2074:HOH:O	2.13	0.49
1:A:228:THR:O	1:A:232:LEU:HD12	2.12	0.48
1:B:23:ILE:HD11	1:B:28:LEU:HD23	1.95	0.47
1:C:18:PRO:CB	1:C:21:LEU:HD12	2.45	0.47
1:C:141:ASP:OD2	1:C:144:ARG:NH1	2.44	0.46
1:C:114:TYR:HA	2:C:400[A]:NIQ:HAP2	1.97	0.46
1:A:190:LYS:HA	1:A:190:LYS:HE2	1.97	0.45
1:B:4:HIS:HE2	1:C:76:ASP:CG	2.25	0.45
1:A:233:LEU:HD13	1:C:233:LEU:CD1	2.47	0.45
1:C:42:THR:HG23	1:C:118:PHE:CE2	2.51	0.45
1:D:122:LEU:CD2	1:D:175:LEU:HD21	2.46	0.45
1:A:264:ASP:OD1	1:A:267[B]:GLN:HG2	2.16	0.45
2:B:400[B]:NIQ:HAS1	5:B:2199:HOH:O	2.17	0.44
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.99	0.44
1:C:122:LEU:HD21	1:C:175:LEU:HD21	1.99	0.44
1:A:88:LEU:HD13	1:A:108:LEU:HD21	2.00	0.44
1:A:19:ALA:HB1	1:C:29:PRO:HB3	2.00	0.43
1:A:23:ILE:CD1	1:C:23:ILE:HB	2.49	0.43
1:C:81:VAL:HG22	5:C:2055:HOH:O	2.18	0.42
1:D:189:LEU:HD23	5:D:2043:HOH:O	2.20	0.42
1:B:4:LYS:HD3	1:B:50:GLU:OE1	2.20	0.41
1:A:130:THR:HG22	5:A:2137:HOH:O	2.20	0.41
1:B:35:MET:O	1:B:39:PRO:HD2	2.21	0.41
1:A:189:LEU:HD11	1:A:202:VAL:HG23	2.03	0.41
1:B:14:THR:O	1:D:278:ASN:ND2	2.54	0.41
1:C:90:GLN:HG2	1:C:197:LEU:HD12	2.03	0.41
1:C:162:LYS:NZ	5:C:2108:HOH:O	2.54	0.41
1:A:113:TYR:O	2:A:400[A]:NIQ:HAP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:HB3	1:D:58[A]:GLN:HE21	1.87	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	297/303 (98%)	294 (99%)	2 (1%)	1 (0%)	36	22
1	B	301/303 (99%)	295 (98%)	5 (2%)	1 (0%)	36	22
1	C	292/303 (96%)	288 (99%)	3 (1%)	1 (0%)	36	22
1	D	293/303 (97%)	288 (98%)	4 (1%)	1 (0%)	36	22
All	All	1183/1212 (98%)	1165 (98%)	14 (1%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	TYR
1	D	31	TYR
1	A	31	TYR
1	C	31	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/248 (100%)	242 (98%)	6 (2%)	43	26
1	B	248/248 (100%)	246 (99%)	2 (1%)	73	65
1	C	241/248 (97%)	236 (98%)	5 (2%)	47	30
1	D	242/248 (98%)	240 (99%)	2 (1%)	73	65
All	All	979/992 (99%)	964 (98%)	15 (2%)	57	43

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	2	LYS
1	A	111	ASN
1	A	112	LEU
1	A	232	LEU
1	A	233	LEU
1	B	-1	MET
1	B	209	ARG
1	C	117	ASP
1	C	126	SER
1	C	226	THR
1	C	232	LEU
1	C	285	LYS
1	D	45	LEU
1	D	117	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	82	GLN
1	A	90	GLN
1	A	229	HIS
1	B	26	GLN
1	B	78	GLN
1	B	82	GLN
1	B	101	ASN
1	C	82	GLN
1	C	90	GLN
1	C	181	GLN
1	C	211	GLN

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Mol	Chain	Res	Type
1	D	119	HIS
1	D	129	GLN
1	D	181	GLN
1	D	211	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	NIQ	A	400[B]	-	20,20,20	1.04	1 (5%)	22,27,27	2.75	13 (59%)
2	NIQ	D	400[A]	-	20,20,20	1.14	3 (15%)	22,27,27	2.86	12 (54%)
2	NIQ	C	400[B]	-	20,20,20	1.14	3 (15%)	22,27,27	2.74	13 (59%)
2	NIQ	B	400[B]	-	20,20,20	1.00	1 (5%)	22,27,27	2.18	8 (36%)
4	MES	D	1295	-	12,12,12	1.92	1 (8%)	15,16,16	6.23	6 (40%)
2	NIQ	D	400[B]	-	20,20,20	1.23	4 (20%)	22,27,27	2.69	12 (54%)
2	NIQ	A	400[A]	-	20,20,20	1.01	2 (10%)	22,27,27	2.88	13 (59%)
2	NIQ	B	400[A]	-	20,20,20	0.93	1 (5%)	22,27,27	2.30	10 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NIQ	C	400[A]	-	20,20,20	0.87	1 (5%)	22,27,27	2.43	9 (40%)

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	NIQ	A	400[B]	-	-	3/8/15/15	0/2/2/2
2	NIQ	D	400[A]	-	-	3/8/15/15	0/2/2/2
2	NIQ	C	400[B]	-	-	3/8/15/15	0/2/2/2
2	NIQ	B	400[B]	-	-	0/8/15/15	0/2/2/2
4	MES	D	1295	-	-	2/6/14/14	0/1/1/1
2	NIQ	D	400[B]	-	-	3/8/15/15	0/2/2/2
2	NIQ	A	400[A]	-	-	2/8/15/15	0/2/2/2
2	NIQ	B	400[A]	-	-	3/8/15/15	0/2/2/2
2	NIQ	C	400[A]	-	-	2/8/15/15	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1295	MES	C8-S	-6.06	1.69	1.77
2	D	400[B]	NIQ	CAR-CAN	2.78	1.60	1.52
2	A	400[A]	NIQ	CAR-CAN	2.66	1.59	1.52
2	C	400[B]	NIQ	CAP-CAO	-2.57	1.41	1.51
2	B	400[A]	NIQ	CAF-NAG	-2.56	1.35	1.39
2	B	400[B]	NIQ	CAF-NAG	-2.56	1.35	1.39
2	D	400[A]	NIQ	CAF-NAJ	2.33	1.42	1.38
2	D	400[B]	NIQ	CAF-NAJ	2.33	1.42	1.38
2	D	400[A]	NIQ	CAF-NAG	-2.31	1.35	1.39
2	D	400[B]	NIQ	CAF-NAG	-2.31	1.35	1.39
2	C	400[A]	NIQ	CAH-NAG	-2.30	1.34	1.39
2	C	400[B]	NIQ	CAH-NAG	-2.30	1.34	1.39
2	C	400[B]	NIQ	CAR-CAN	-2.22	1.46	1.52
2	D	400[A]	NIQ	CAH-NAG	-2.09	1.35	1.39
2	D	400[B]	NIQ	CAH-NAG	-2.09	1.35	1.39
2	A	400[A]	NIQ	CAH-NAG	-2.08	1.35	1.39
2	A	400[B]	NIQ	CAH-NAG	-2.08	1.35	1.39

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1295	MES	O1S-S-C8	-15.52	83.28	106.73
4	D	1295	MES	O3S-S-O1S	-12.21	80.84	111.40
4	D	1295	MES	O2S-S-O1S	-8.67	85.63	113.82
4	D	1295	MES	O3S-S-C8	8.04	121.73	106.00
4	D	1295	MES	O2S-S-C8	6.75	116.94	106.73
2	C	400[A]	NIQ	CAK-NAJ-CAF	-5.94	119.56	127.34
2	C	400[B]	NIQ	CAK-NAJ-CAF	-5.94	119.56	127.34
2	A	400[A]	NIQ	CAK-NAJ-CAF	-5.77	119.77	127.34
2	A	400[B]	NIQ	CAK-NAJ-CAF	-5.77	119.77	127.34
2	D	400[A]	NIQ	CAK-NAJ-CAF	-5.71	119.86	127.34
2	D	400[B]	NIQ	CAK-NAJ-CAF	-5.71	119.86	127.34
2	D	400[A]	NIQ	CAP-CAO-CAN	-5.57	87.15	104.38
2	B	400[A]	NIQ	CAK-NAJ-CAF	-5.51	120.12	127.34
2	B	400[B]	NIQ	CAK-NAJ-CAF	-5.51	120.12	127.34
2	C	400[B]	NIQ	CAP-CAO-CAN	-5.04	88.80	104.38
2	A	400[A]	NIQ	CAP-CAO-CAN	-4.83	89.43	104.38
2	A	400[B]	NIQ	CAS-CAR-CAN	-4.52	90.41	104.38
2	D	400[A]	NIQ	CAP-CAS-CAR	-4.33	91.55	105.97
2	A	400[A]	NIQ	CAD-NAG-CAF	4.04	121.93	117.31
2	A	400[B]	NIQ	CAD-NAG-CAF	4.04	121.93	117.31
2	B	400[A]	NIQ	CAP-CAS-CAR	-3.86	93.11	105.97
2	B	400[B]	NIQ	CAR-CAN-CAO	-3.79	96.29	103.38
2	D	400[B]	NIQ	CAP-CAS-CAR	-3.72	93.61	105.97
2	C	400[A]	NIQ	NAI-CAH-NAG	3.69	123.50	116.29
2	C	400[B]	NIQ	NAI-CAH-NAG	3.69	123.50	116.29
2	A	400[A]	NIQ	CAL-CAH-NAI	-3.67	116.17	123.34
2	A	400[B]	NIQ	CAL-CAH-NAI	-3.67	116.17	123.34
2	C	400[A]	NIQ	CAP-CAS-CAR	-3.53	94.22	105.97
2	D	400[A]	NIQ	CAL-CAH-NAI	-3.53	116.45	123.34
2	D	400[B]	NIQ	CAL-CAH-NAI	-3.53	116.45	123.34
2	B	400[A]	NIQ	CAC-CAD-NAG	-3.46	104.18	112.36
2	B	400[B]	NIQ	CAC-CAD-NAG	-3.46	104.18	112.36
2	D	400[A]	NIQ	CAD-NAG-CAF	3.45	121.26	117.31
2	D	400[B]	NIQ	CAD-NAG-CAF	3.45	121.26	117.31
2	A	400[A]	NIQ	NAJ-CAF-NAG	3.40	121.56	115.45
2	A	400[B]	NIQ	NAJ-CAF-NAG	3.40	121.56	115.45
2	D	400[A]	NIQ	CAC-CAD-NAG	-3.40	104.31	112.36
2	D	400[B]	NIQ	CAC-CAD-NAG	-3.40	104.31	112.36
2	A	400[A]	NIQ	CAC-CAD-NAG	-3.39	104.34	112.36
2	A	400[B]	NIQ	CAC-CAD-NAG	-3.39	104.34	112.36
2	C	400[A]	NIQ	NAJ-CAF-NAG	3.35	121.48	115.45
2	C	400[B]	NIQ	NAJ-CAF-NAG	3.35	121.48	115.45
2	D	400[A]	NIQ	NAJ-CAF-NAG	3.28	121.34	115.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400[B]	NIQ	NAJ-CAF-NAG	3.28	121.34	115.45
2	D	400[A]	NIQ	NAI-CAH-NAG	3.24	122.63	116.29
2	D	400[B]	NIQ	NAI-CAH-NAG	3.24	122.63	116.29
2	C	400[A]	NIQ	CAL-CAH-NAI	-3.22	117.05	123.34
2	C	400[B]	NIQ	CAL-CAH-NAI	-3.22	117.05	123.34
2	C	400[A]	NIQ	CAC-CAD-NAG	-3.21	104.77	112.36
2	C	400[B]	NIQ	CAC-CAD-NAG	-3.21	104.77	112.36
2	C	400[A]	NIQ	CAD-NAG-CAF	3.20	120.98	117.31
2	C	400[B]	NIQ	CAD-NAG-CAF	3.20	120.98	117.31
2	A	400[A]	NIQ	CAR-CAN-CAO	-3.14	97.50	103.38
2	A	400[A]	NIQ	CAL-CAH-NAG	3.12	121.95	119.02
2	A	400[B]	NIQ	CAL-CAH-NAG	3.12	121.95	119.02
2	A	400[A]	NIQ	CAP-CAS-CAR	-3.11	95.61	105.97
2	D	400[B]	NIQ	CAN-NAM-CAL	3.09	142.22	126.61
2	D	400[B]	NIQ	CAS-CAP-CAO	-3.04	95.84	105.97
2	B	400[A]	NIQ	NAJ-CAF-NAG	2.99	120.83	115.45
2	B	400[B]	NIQ	NAJ-CAF-NAG	2.99	120.83	115.45
2	B	400[A]	NIQ	OAQ-CAK-CAL	-2.96	120.12	127.26
2	B	400[B]	NIQ	OAQ-CAK-CAL	-2.96	120.12	127.26
2	A	400[A]	NIQ	NAI-CAH-NAG	2.86	121.88	116.29
2	A	400[B]	NIQ	NAI-CAH-NAG	2.86	121.88	116.29
2	D	400[A]	NIQ	OAQ-CAK-CAL	-2.80	120.51	127.26
2	D	400[B]	NIQ	OAQ-CAK-CAL	-2.80	120.51	127.26
2	A	400[B]	NIQ	CAR-CAN-NAM	2.74	117.58	111.98
2	A	400[B]	NIQ	CAN-NAM-CAL	-2.70	112.97	126.61
2	A	400[A]	NIQ	CAS-CAP-CAO	-2.69	97.01	105.97
2	C	400[B]	NIQ	CAR-CAN-NAM	2.69	117.48	111.98
2	A	400[A]	NIQ	OAE-CAF-NAJ	-2.64	116.62	121.49
2	A	400[B]	NIQ	OAE-CAF-NAJ	-2.64	116.62	121.49
2	C	400[B]	NIQ	CAN-NAM-CAL	2.61	139.78	126.61
2	D	400[B]	NIQ	CAP-CAO-CAN	-2.55	96.49	104.38
2	A	400[A]	NIQ	CAO-CAN-NAM	2.52	117.13	111.98
2	C	400[B]	NIQ	CAR-CAN-CAO	-2.47	98.76	103.38
2	B	400[A]	NIQ	CAD-NAG-CAF	2.41	120.08	117.31
2	B	400[B]	NIQ	CAD-NAG-CAF	2.41	120.08	117.31
2	C	400[B]	NIQ	CAS-CAR-CAN	-2.40	96.95	104.38
2	A	400[B]	NIQ	CAO-CAN-NAM	2.40	116.88	111.98
2	B	400[A]	NIQ	CAS-CAP-CAO	-2.36	98.13	105.97
2	D	400[A]	NIQ	CAR-CAN-CAO	-2.34	98.99	103.38
2	C	400[A]	NIQ	OAE-CAF-NAJ	-2.33	117.19	121.49
2	C	400[B]	NIQ	OAE-CAF-NAJ	-2.33	117.19	121.49
4	D	1295	MES	O3S-S-O2S	2.32	117.19	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400[A]	NIQ	CAS-CAP-CAO	-2.26	98.46	105.97
2	B	400[A]	NIQ	CAL-CAK-NAJ	2.25	118.31	112.13
2	B	400[B]	NIQ	CAL-CAK-NAJ	2.25	118.31	112.13
2	C	400[A]	NIQ	OAQ-CAK-CAL	-2.20	121.96	127.26
2	C	400[B]	NIQ	OAQ-CAK-CAL	-2.20	121.96	127.26
2	B	400[A]	NIQ	CAP-CAO-CAN	-2.10	97.87	104.38
2	B	400[A]	NIQ	OAE-CAF-NAJ	-2.08	117.65	121.49
2	B	400[B]	NIQ	OAE-CAF-NAJ	-2.08	117.65	121.49
2	D	400[A]	NIQ	CAL-CAH-NAG	2.02	120.92	119.02
2	D	400[B]	NIQ	CAL-CAH-NAG	2.02	120.92	119.02
2	A	400[B]	NIQ	CAP-CAS-CAR	-2.00	99.31	105.97

There are no chirality outliers.

All (21) torsion outliers are listed below:

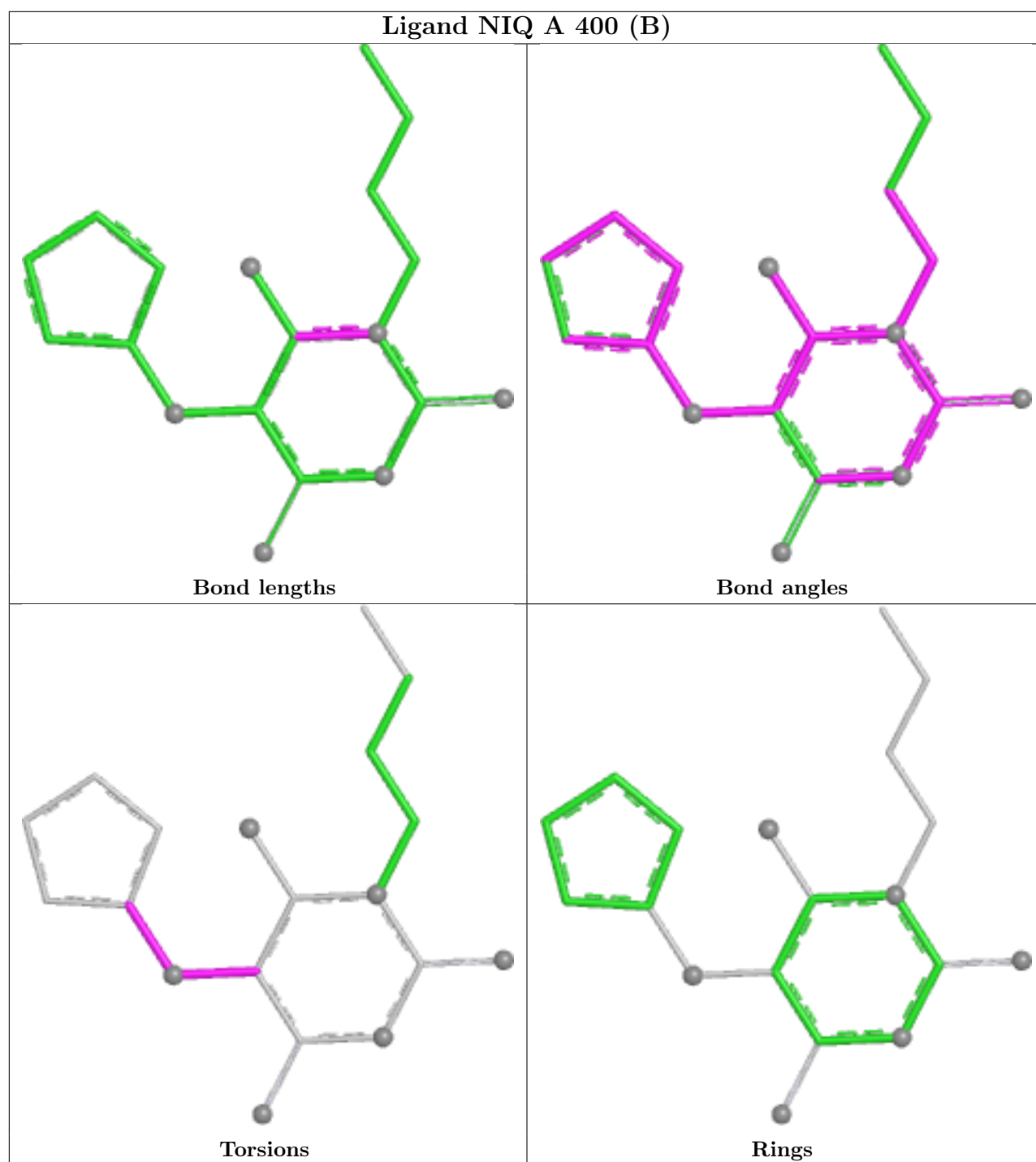
Mol	Chain	Res	Type	Atoms
2	A	400[B]	NIQ	CAH-CAL-NAM-CAN
2	A	400[B]	NIQ	CAK-CAL-NAM-CAN
2	A	400[B]	NIQ	CAO-CAN-NAM-CAL
2	B	400[A]	NIQ	CAH-CAL-NAM-CAN
2	B	400[A]	NIQ	CAK-CAL-NAM-CAN
2	B	400[A]	NIQ	CAR-CAN-NAM-CAL
2	C	400[A]	NIQ	CAH-CAL-NAM-CAN
2	C	400[A]	NIQ	CAK-CAL-NAM-CAN
2	C	400[B]	NIQ	CAH-CAL-NAM-CAN
2	C	400[B]	NIQ	CAK-CAL-NAM-CAN
2	D	400[A]	NIQ	CAH-CAL-NAM-CAN
2	D	400[A]	NIQ	CAK-CAL-NAM-CAN
2	D	400[A]	NIQ	CAR-CAN-NAM-CAL
2	D	400[B]	NIQ	CAK-CAL-NAM-CAN
2	D	400[B]	NIQ	CAR-CAN-NAM-CAL
4	D	1295	MES	C7-C8-S-O2S
2	A	400[A]	NIQ	CAK-CAL-NAM-CAN
2	D	400[B]	NIQ	CAH-CAL-NAM-CAN
4	D	1295	MES	C7-C8-S-O3S
2	A	400[A]	NIQ	CAR-CAN-NAM-CAL
2	C	400[B]	NIQ	CAO-CAN-NAM-CAL

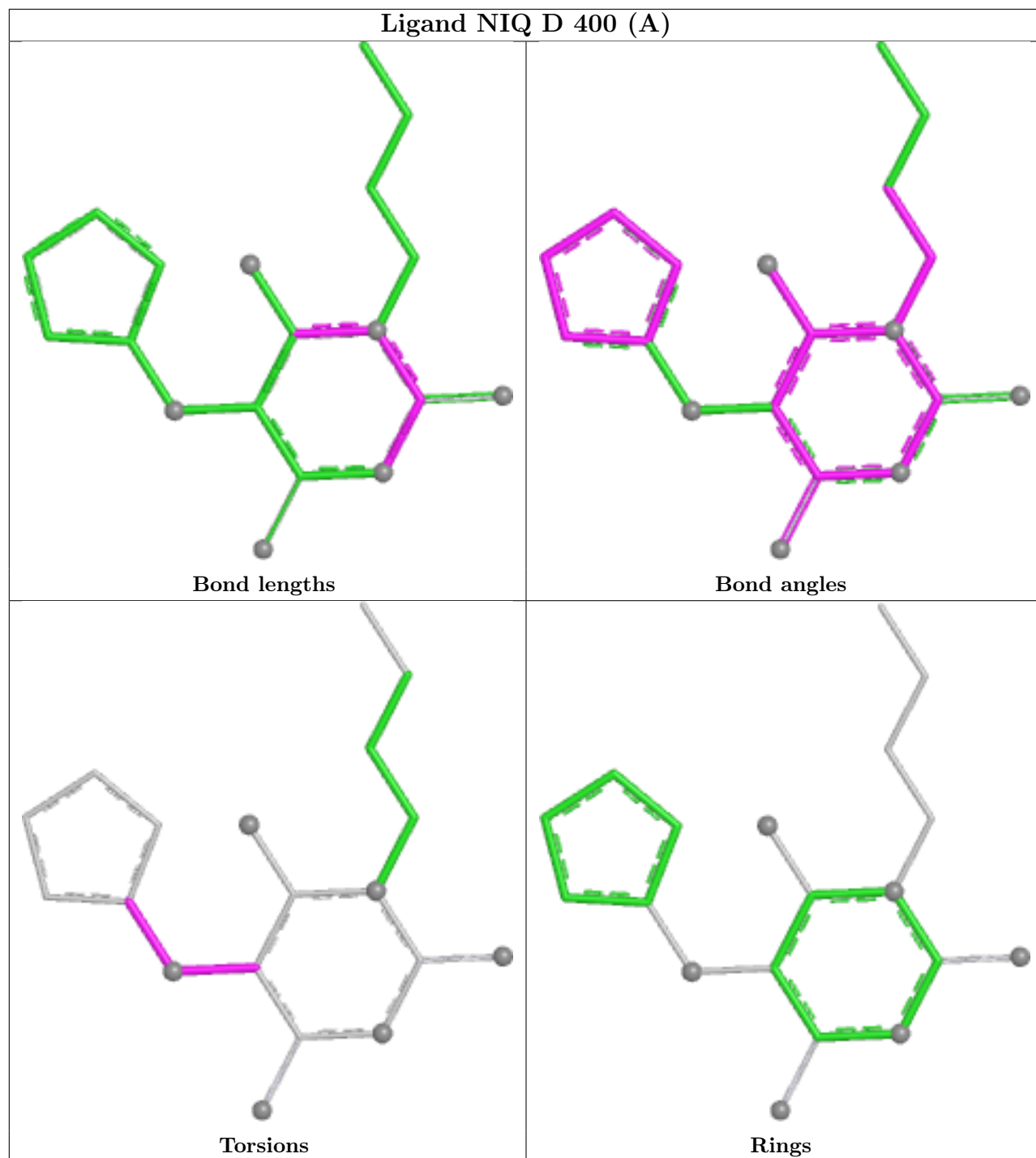
There are no ring outliers.

6 monomers are involved in 18 short contacts:

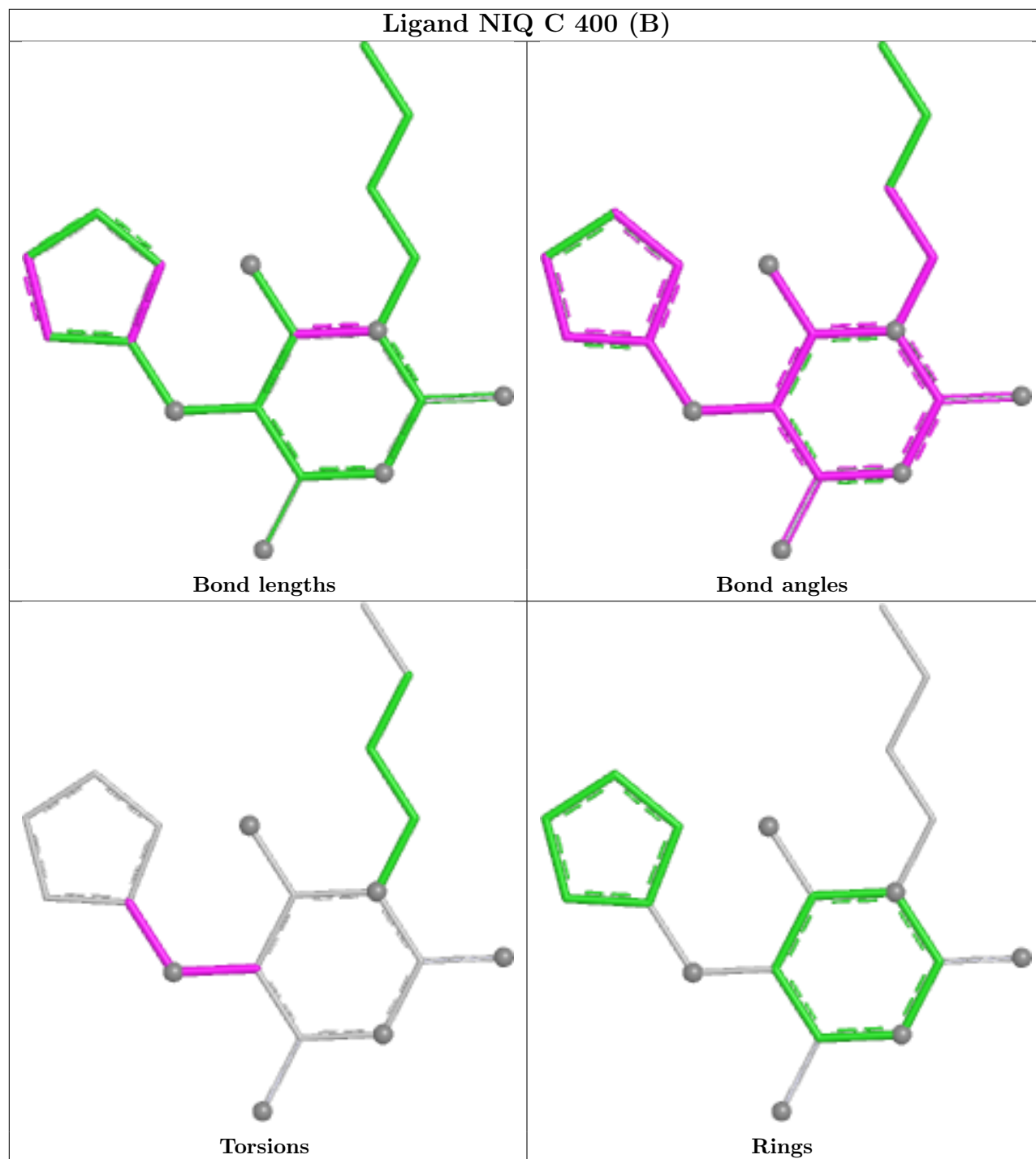
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400[B]	NIQ	4	0
2	C	400[B]	NIQ	2	0
2	B	400[B]	NIQ	6	0
2	D	400[B]	NIQ	1	0
2	A	400[A]	NIQ	2	0
2	C	400[A]	NIQ	3	0

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.

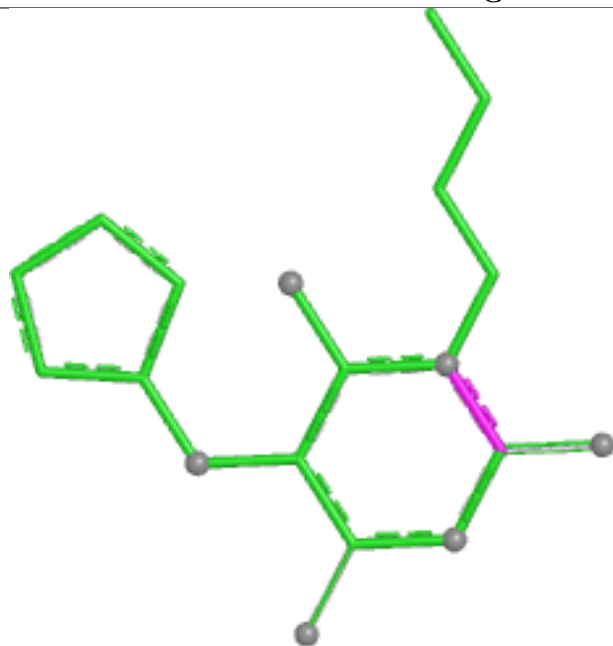




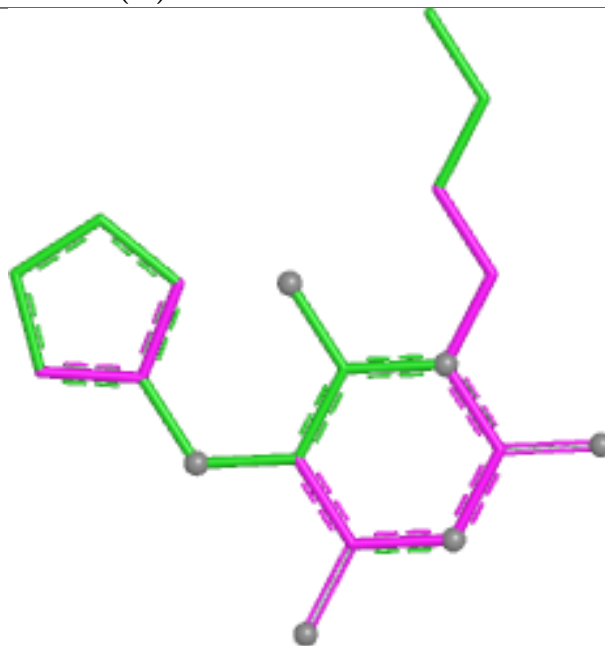
Ligand NIQ C 400 (B)



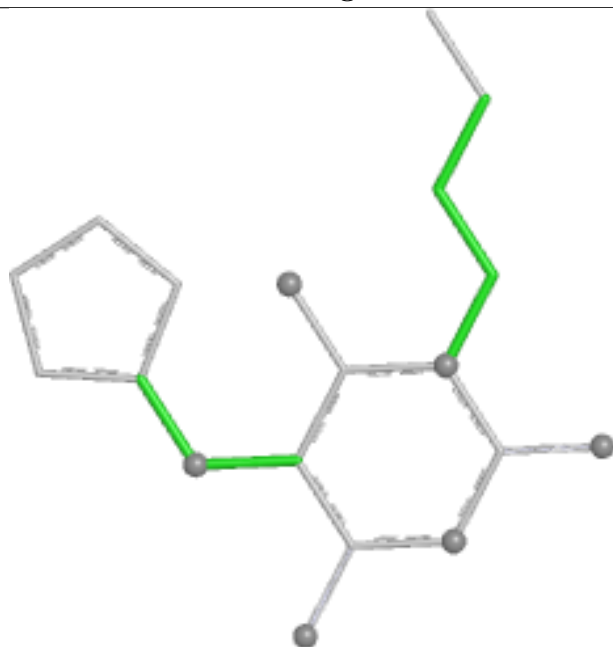
Ligand NIQ B 400 (B)



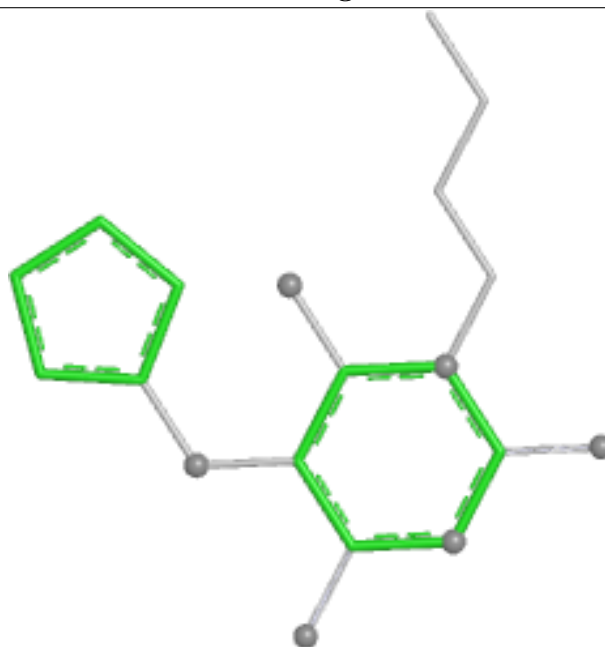
Bond lengths



Bond angles

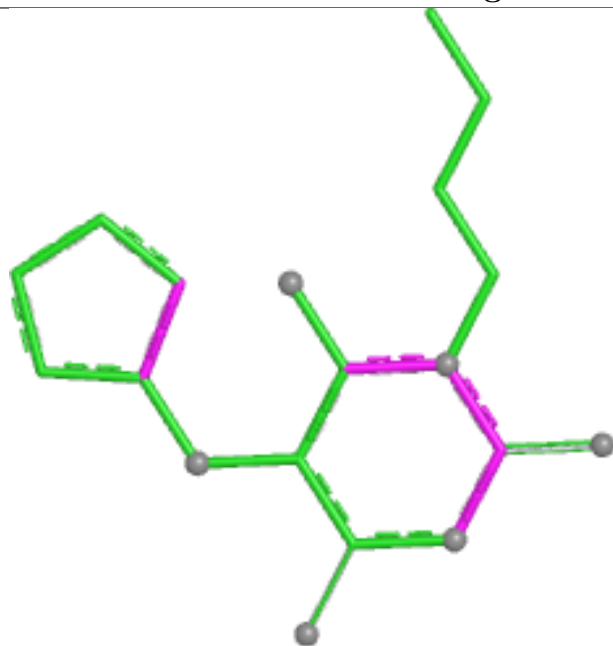


Torsions

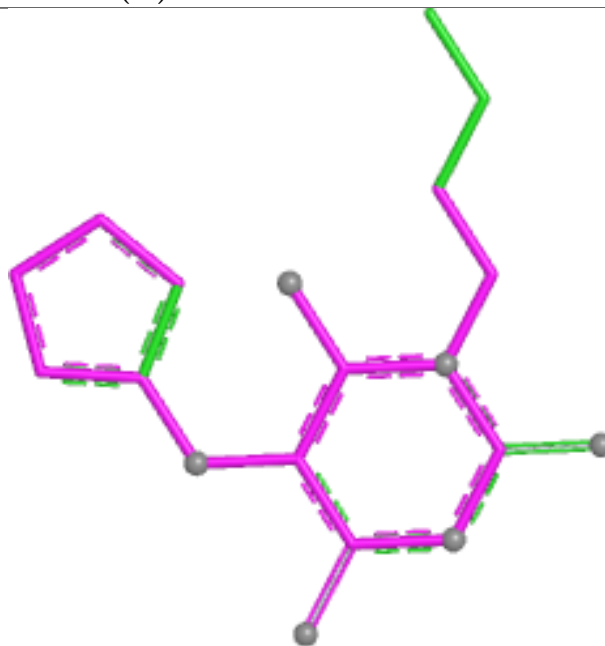


Rings

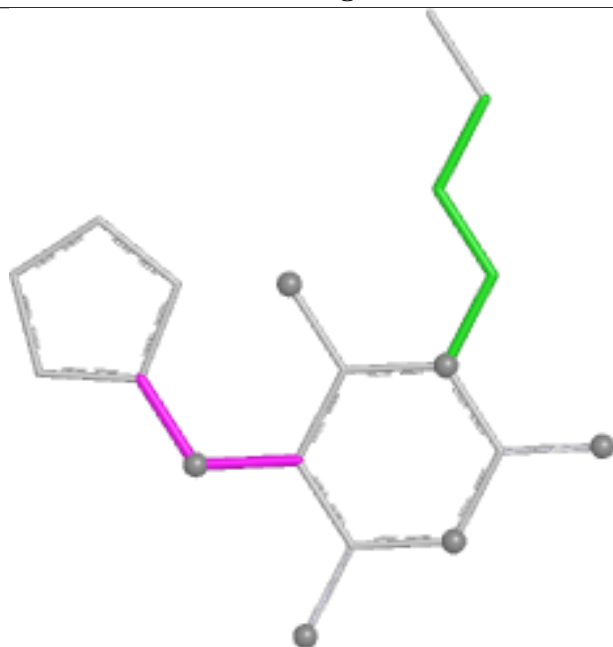
Ligand NIQ D 400 (B)



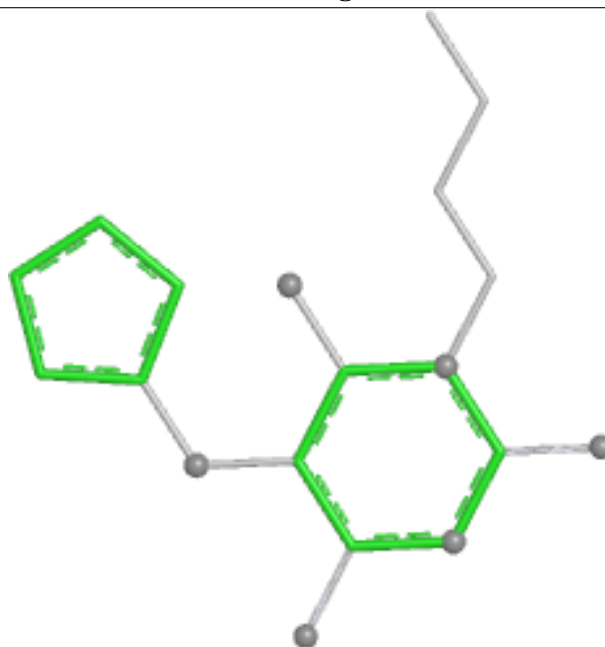
Bond lengths



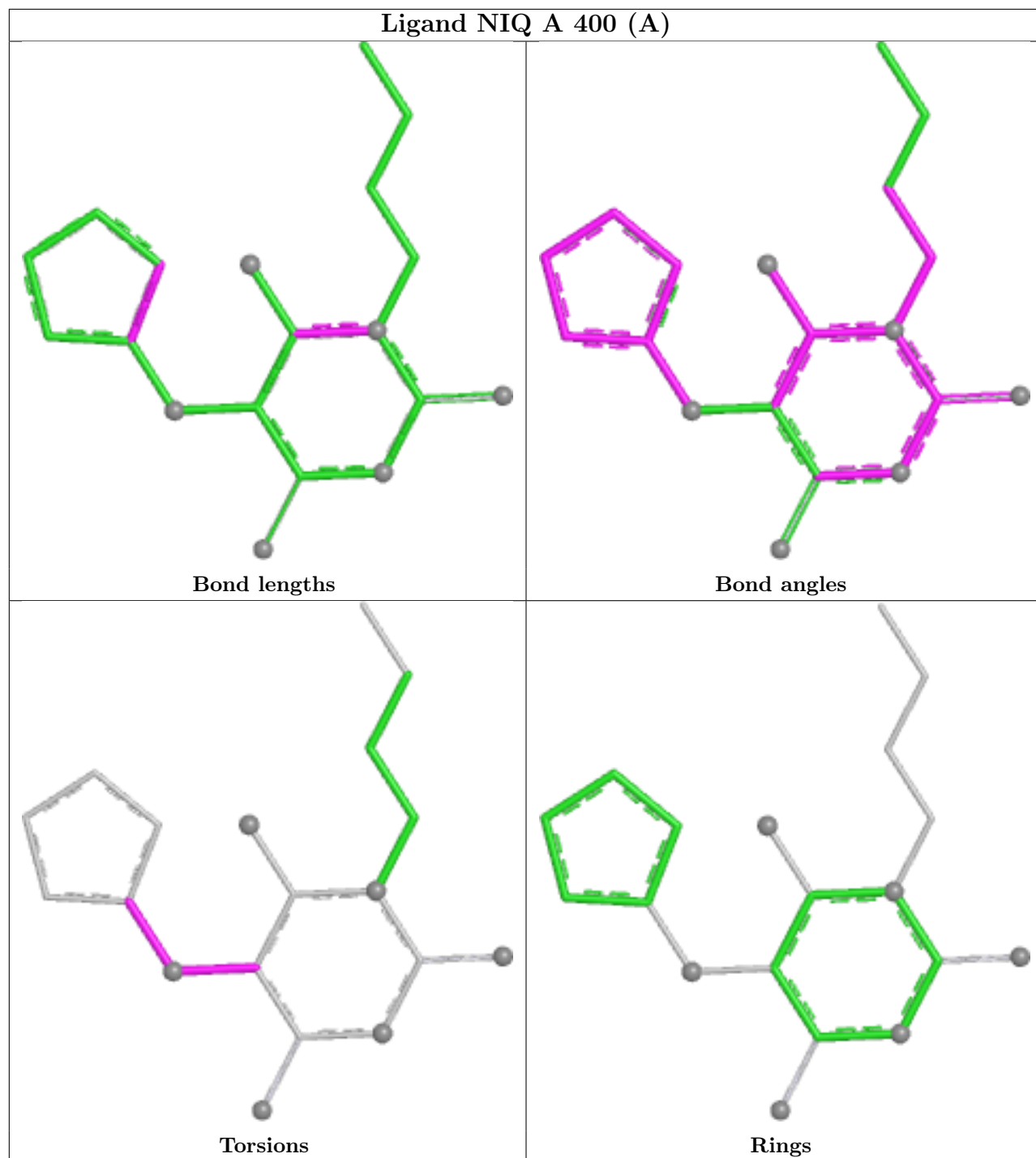
Bond angles

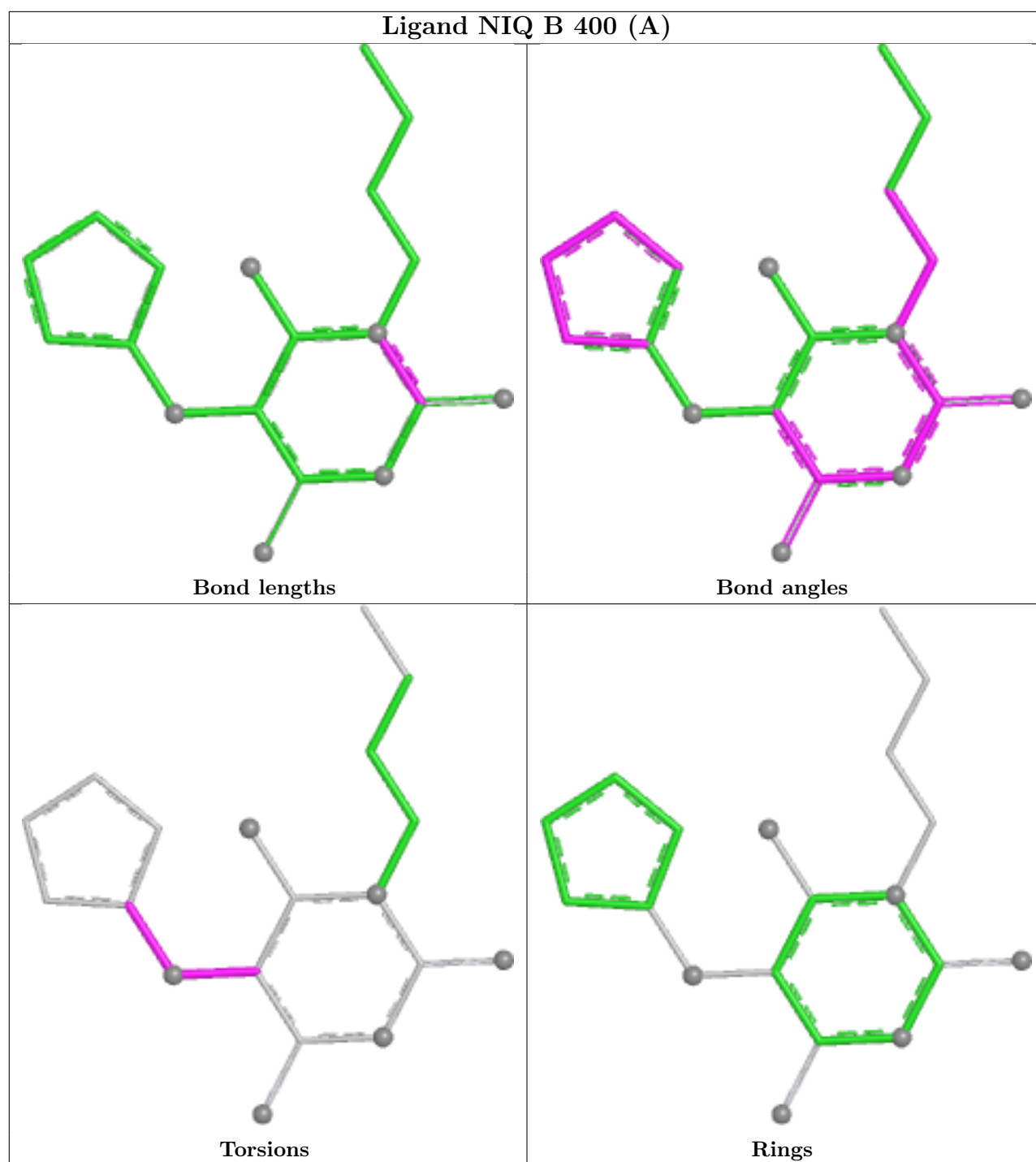


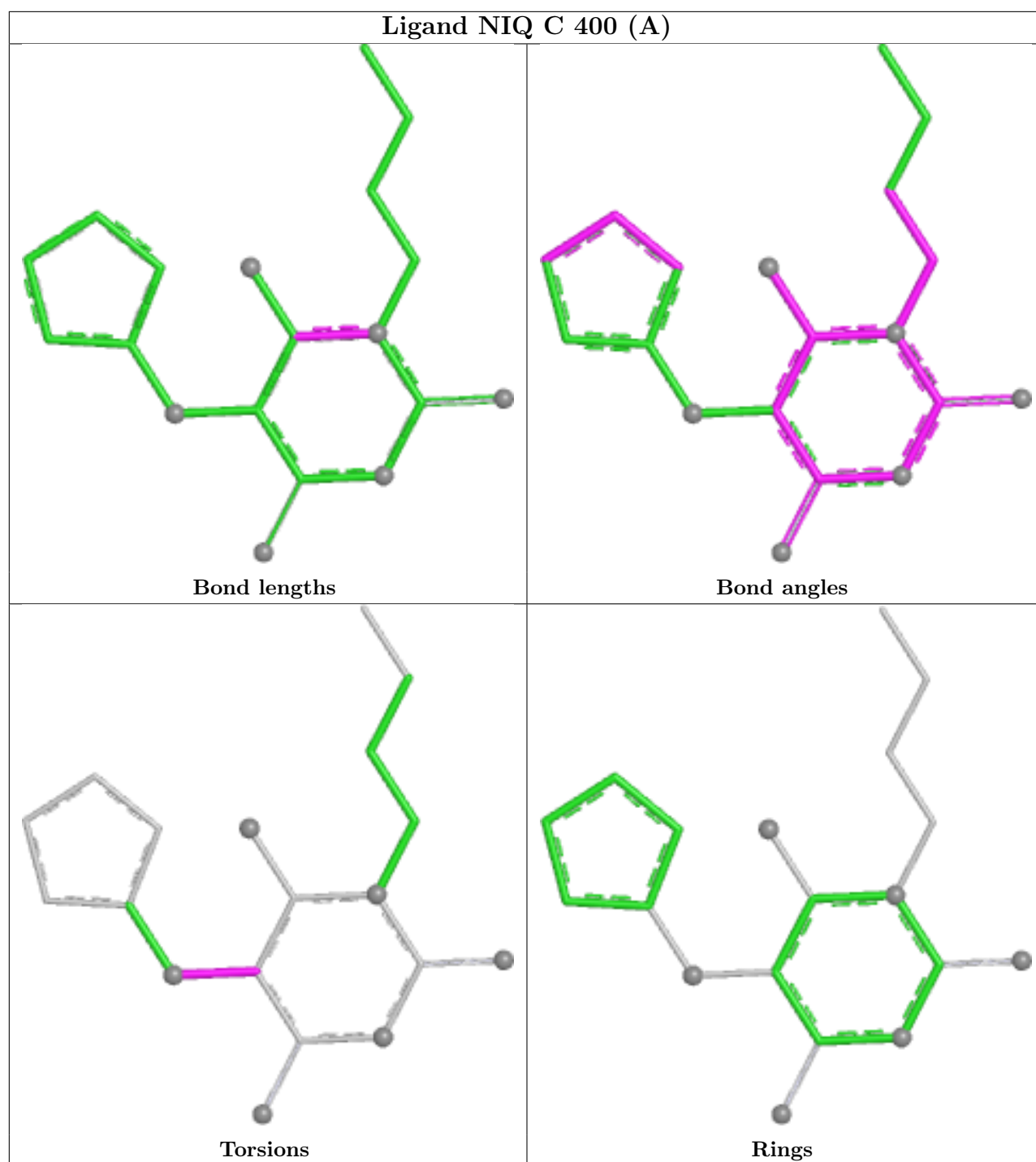
Torsions



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	299/303 (98%)	0.87	35 (11%) 9 9	10, 28, 47, 68	2 (0%)
1	B	302/303 (99%)	1.03	55 (18%) 3 3	12, 30, 55, 82	1 (0%)
1	C	293/303 (96%)	1.16	49 (16%) 4 4	15, 32, 47, 66	1 (0%)
1	D	293/303 (96%)	1.05	43 (14%) 6 5	13, 32, 49, 75	2 (0%)
All	All	1187/1212 (97%)	1.02	182 (15%) 5 4	10, 30, 51, 82	6 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	7.4
1	B	189	LEU	6.1
1	C	118	PHE	5.8
1	D	118	PHE	5.6
1	B	-8	HIS	5.2
1	A	118	PHE	5.0
1	B	23	ILE	4.8
1	C	121	LEU	4.5
1	B	11	GLY	4.4
1	B	195	GLY	4.4
1	B	191	PRO	4.4
1	B	193	PRO	4.4
1	C	123	GLY	4.4
1	A	-6	HIS	4.3
1	B	88	LEU	4.3
1	D	23	ILE	4.3
1	A	-10	HIS	4.1
1	D	189	LEU	4.1
1	B	117	ASP	4.0
1	A	189	LEU	4.0
1	B	118	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	3.9
1	A	1	MET	3.8
1	A	13	GLY	3.7
1	A	121	LEU	3.7
1	C	225	ASP	3.5
1	B	190	LYS	3.5
1	A	191	PRO	3.5
1	A	11	GLY	3.5
1	A	193	PRO	3.5
1	D	13	GLY	3.5
1	B	0	ALA	3.5
1	B	197	LEU	3.5
1	A	120	GLU	3.4
1	A	275	LEU	3.4
1	B	22	ALA	3.4
1	C	232	LEU	3.4
1	D	289	THR	3.3
1	D	1	MET	3.3
1	D	130	THR	3.2
1	C	287	LEU	3.2
1	B	-3	GLY	3.2
1	B	275	LEU	3.2
1	C	224	LEU	3.2
1	A	2	LYS	3.2
1	A	119	HIS	3.2
1	A	190	LYS	3.2
1	B	21	LEU	3.2
1	A	289	THR	3.2
1	C	193	PRO	3.1
1	A	88	LEU	3.1
1	C	122	LEU	3.1
1	D	11	GLY	3.1
1	A	-5	HIS	3.1
1	A	12	SER	3.1
1	B	12	SER	3.1
1	C	66	LEU	3.0
1	D	21	LEU	3.0
1	C	15	ARG	3.0
1	C	117	ASP	3.0
1	C	112	LEU	3.0
1	C	119	HIS	2.9
1	C	22	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	21	LEU	2.9
1	D	45	LEU	2.9
1	A	225	ASP	2.9
1	D	128	ARG	2.9
1	D	119	HIS	2.9
1	D	195	GLY	2.8
1	B	45	LEU	2.8
1	C	288	LEU	2.8
1	D	24	SER	2.8
1	B	194	ARG	2.8
1	C	130	THR	2.8
1	C	289	THR	2.8
1	B	92	PHE	2.8
1	A	232	LEU	2.8
1	C	275	LEU	2.8
1	B	225	ASP	2.8
1	B	226	THR	2.8
1	B	192	SER	2.8
1	B	-4	HIS	2.7
1	B	198	GLU	2.7
1	C	29	PRO	2.7
1	D	141	ASP	2.7
1	D	199	ILE	2.7
1	C	167	LYS	2.7
1	A	293	TYR	2.7
1	C	1	MET	2.7
1	B	-2	SER	2.6
1	A	224	LEU	2.6
1	B	287	LEU	2.6
1	A	128	ARG	2.6
1	D	117	ASP	2.6
1	B	213	SER	2.6
1	C	27	LEU	2.6
1	C	28	LEU	2.6
1	D	16	LEU	2.6
1	D	164	LEU	2.6
1	D	194	ARG	2.6
1	D	287	LEU	2.6
1	C	152	GLN	2.6
1	A	276	ALA	2.6
1	B	19	ALA	2.6
1	D	190	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	193	PRO	2.6
1	D	274	PRO	2.6
1	B	-1	MET	2.6
1	B	121	LEU	2.6
1	D	84	SER	2.6
1	D	15	ARG	2.6
1	C	195	GLY	2.5
1	C	60	THR	2.5
1	C	120	GLU	2.5
1	C	235	ALA	2.5
1	D	273	ALA	2.5
1	B	127	GLN	2.5
1	B	199	ILE	2.5
1	C	13	GLY	2.5
1	D	127	GLN	2.5
1	C	65	GLN	2.4
1	B	1	MET	2.4
1	A	267[A]	GLN	2.4
1	C	194	ARG	2.4
1	B	288	LEU	2.4
1	D	129	GLN	2.4
1	D	288	LEU	2.4
1	C	266	ALA	2.4
1	C	30	VAL	2.4
1	D	124	SER	2.3
1	A	84	SER	2.3
1	A	195	GLY	2.3
1	B	227	GLY	2.3
1	B	270	LYS	2.3
1	A	153	GLY	2.3
1	B	274	PRO	2.3
1	C	61	PRO	2.3
1	B	125	ALA	2.3
1	C	233	LEU	2.3
1	B	15	ARG	2.3
1	D	187	ARG	2.3
1	B	184	ASP	2.3
1	A	274	PRO	2.2
1	C	273	ALA	2.2
1	D	88	LEU	2.2
1	B	188	ASP	2.2
1	A	15	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	101	ASN	2.2
1	A	273	ALA	2.2
1	C	45	LEU	2.2
1	D	275	LEU	2.2
1	D	92	PHE	2.2
1	B	187	ARG	2.2
1	C	31	TYR	2.2
1	B	289	THR	2.2
1	B	81	VAL	2.2
1	B	276	ALA	2.2
1	D	152	GLN	2.2
1	D	123	GLY	2.2
1	B	-7	HIS	2.2
1	C	226	THR	2.2
1	C	101	ASN	2.1
1	C	285	LYS	2.1
1	A	192	SER	2.1
1	B	14	THR	2.1
1	B	273	ALA	2.1
1	C	276	ALA	2.1
1	D	276	ALA	2.1
1	B	153	GLY	2.1
1	C	12	SER	2.1
1	A	14	THR	2.1
1	D	191	PRO	2.1
1	B	119	HIS	2.1
1	B	152	GLN	2.1
1	B	124	SER	2.1
1	D	125	ALA	2.0
1	C	97	SER	2.0
1	D	144	ARG	2.0
1	C	140	LEU	2.0
1	B	180	GLN	2.0
1	C	209	ARG	2.0
1	C	148	VAL	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 oligosaccharides in this entry.

6.4 Ligands

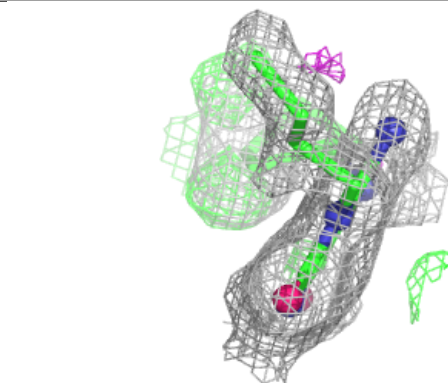
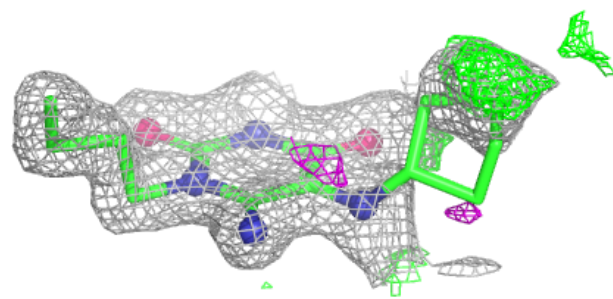
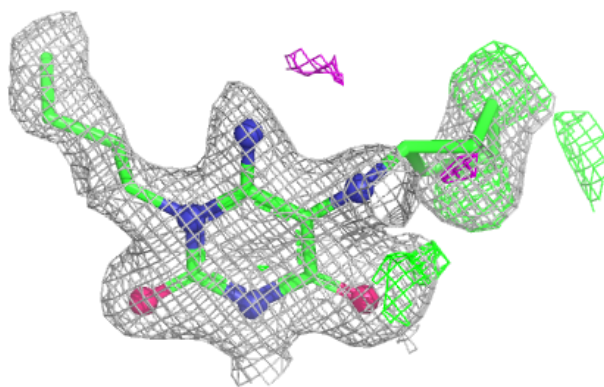
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NIQ	D	400[A]	19/19	0.80	0.19	35,36,40,41	5
2	NIQ	D	400[B]	19/19	0.80	0.19	33,36,40,41	5
2	NIQ	C	400[A]	19/19	0.81	0.19	37,38,39,41	5
2	NIQ	C	400[B]	19/19	0.81	0.19	36,38,39,41	5
4	MES	D	1295	12/12	0.83	0.16	55,57,61,61	0
2	NIQ	B	400[B]	19/19	0.86	0.15	29,31,32,32	5
2	NIQ	B	400[A]	19/19	0.86	0.15	29,31,33,33	5
2	NIQ	A	400[B]	19/19	0.89	0.14	29,30,31,32	5
2	NIQ	A	400[A]	19/19	0.89	0.14	29,31,33,33	5
3	CL	A	1294	1/1	0.96	0.09	37,37,37,37	0
3	CL	D	1294	1/1	0.97	0.07	40,40,40,40	0
3	CL	B	1294	1/1	0.97	0.07	32,32,32,32	0
3	CL	C	1294	1/1	0.98	0.05	34,34,34,34	0

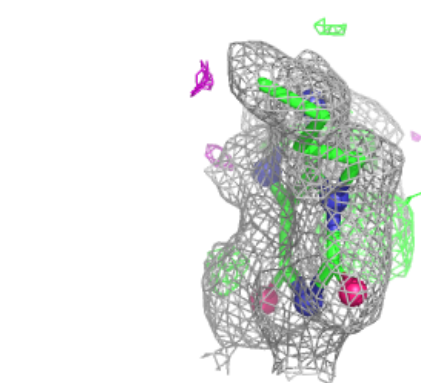
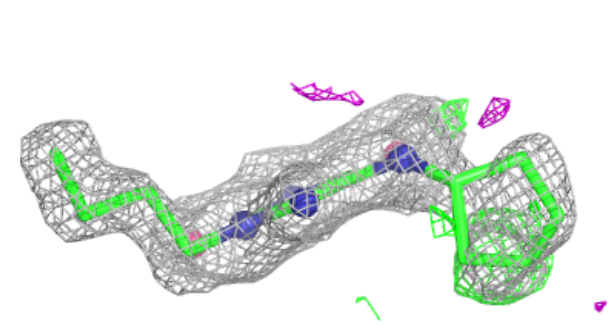
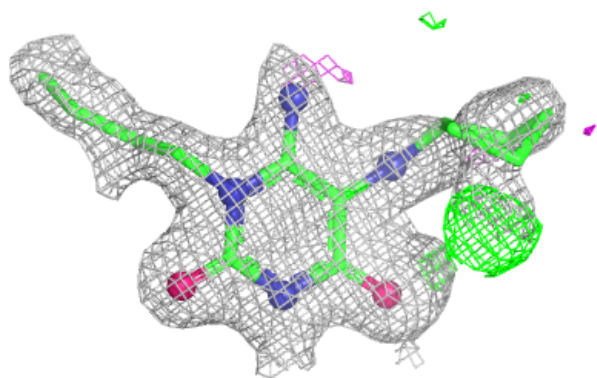
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NIQ D 400 (A):

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

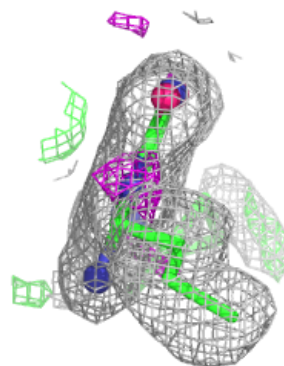
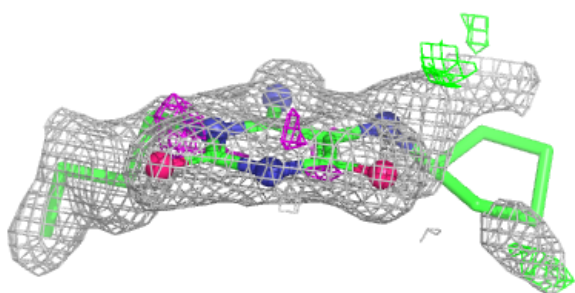
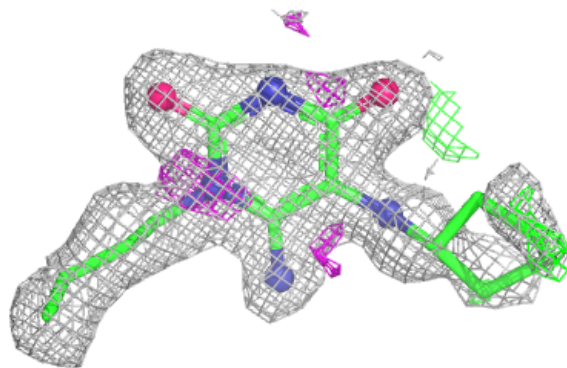
**Electron density around NIQ D 400 (B):**

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

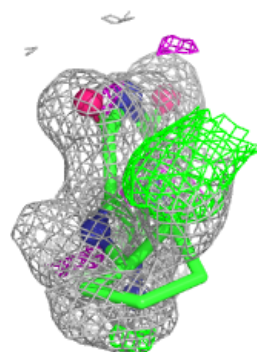
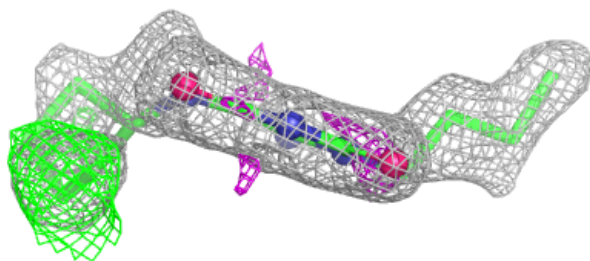
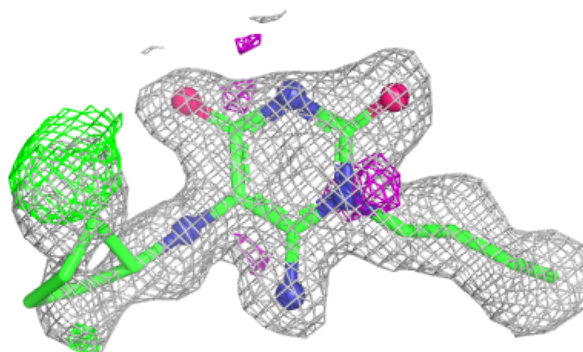


Electron density around NIQ C 400 (A):

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

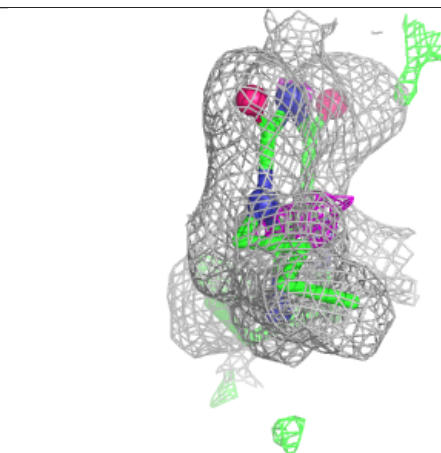
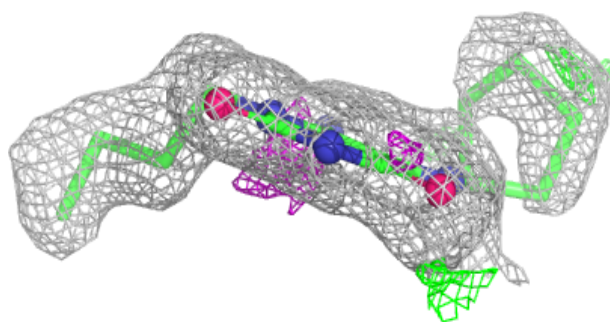
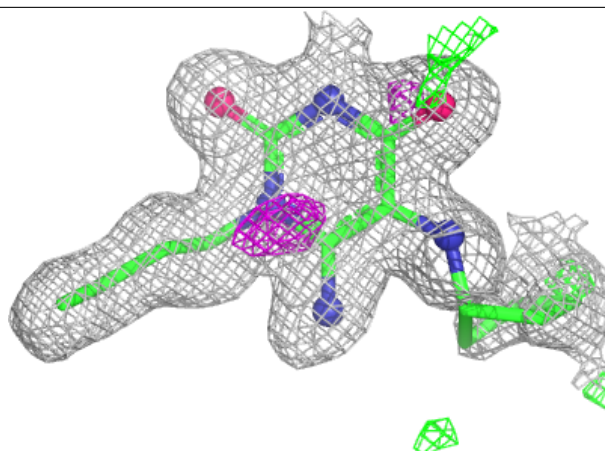
**Electron density around NIQ C 400 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

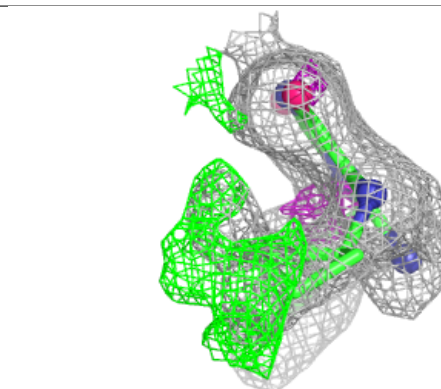
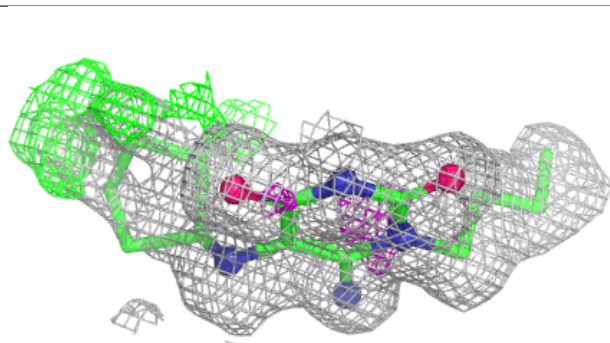
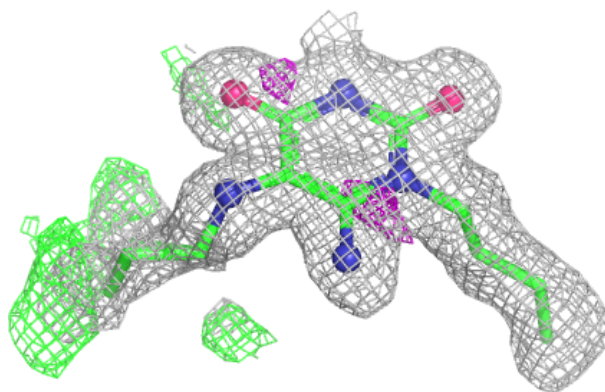


Electron density around NIQ B 400 (B):

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

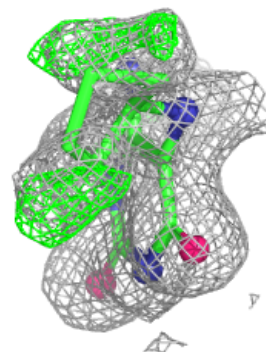
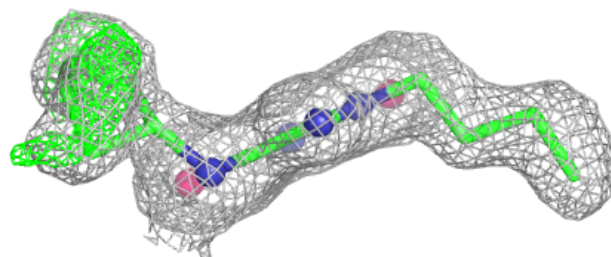
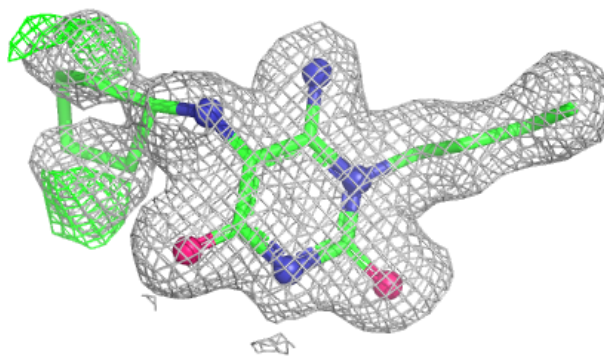
**Electron density around NIQ B 400 (A):**

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

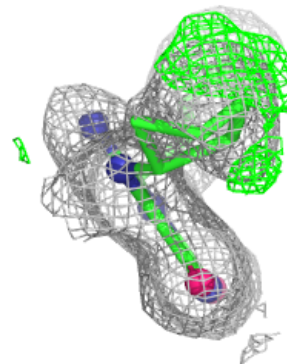
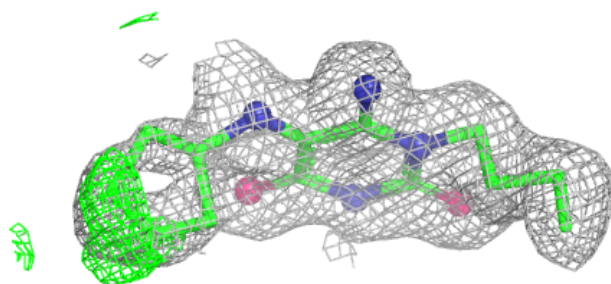
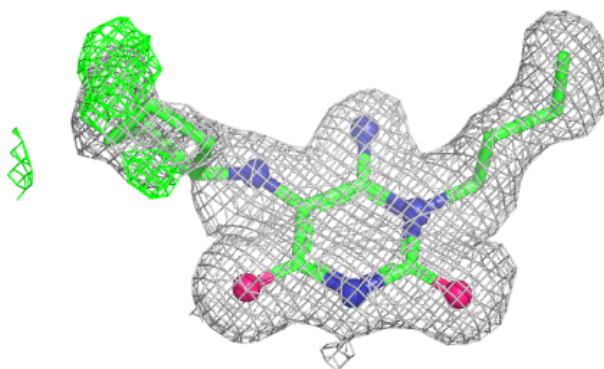


Electron density around NIQ A 400 (B):

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

**Electron density around NIQ A 400 (A):**

$2mF_o - DF_c$ (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.