



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2023 – 04:38 pm BST

PDB ID : 8ADJ
Title : Poly(ADP-ribose) glycohydrolase (PARG) from *Drosophila melanogaster* in complex with PARG inhibitor PDD00017272
Authors : Ariza, A.; Fontana, P.
Deposited on : 2022-07-08
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

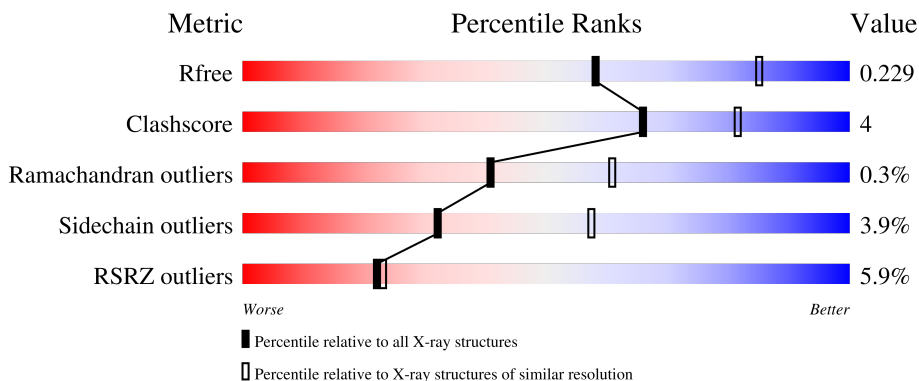
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	578	 2% 76% 11% .. 11%
1	B	578	 5% 77% 10% .. 11%
1	C	578	 8% 77% 10% .. 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	607	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12890 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 Poly(ADP-ribose) glycohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	4170	2656	732	761	21	0	1	0
1	B	515	4167	2654	732	761	20	0	0	0
1	C	515	4184	2668	732	762	22	0	3	0

There are 60 discrepancies between the modelled and reference sequences:

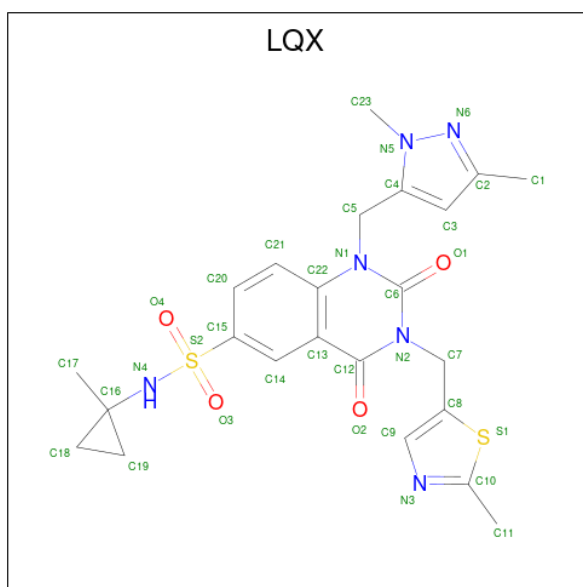
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O46043
A	-18	GLY	-	expression tag	UNP O46043
A	-17	SER	-	expression tag	UNP O46043
A	-16	SER	-	expression tag	UNP O46043
A	-15	HIS	-	expression tag	UNP O46043
A	-14	HIS	-	expression tag	UNP O46043
A	-13	HIS	-	expression tag	UNP O46043
A	-12	HIS	-	expression tag	UNP O46043
A	-11	HIS	-	expression tag	UNP O46043
A	-10	HIS	-	expression tag	UNP O46043
A	-9	SER	-	expression tag	UNP O46043
A	-8	SER	-	expression tag	UNP O46043
A	-7	GLY	-	expression tag	UNP O46043
A	-6	LEU	-	expression tag	UNP O46043
A	-5	VAL	-	expression tag	UNP O46043
A	-4	PRO	-	expression tag	UNP O46043
A	-3	ARG	-	expression tag	UNP O46043
A	-2	GLY	-	expression tag	UNP O46043
A	-1	SER	-	expression tag	UNP O46043
A	0	HIS	-	expression tag	UNP O46043
B	-19	MET	-	initiating methionine	UNP O46043
B	-18	GLY	-	expression tag	UNP O46043
B	-17	SER	-	expression tag	UNP O46043

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O46043
B	-15	HIS	-	expression tag	UNP O46043
B	-14	HIS	-	expression tag	UNP O46043
B	-13	HIS	-	expression tag	UNP O46043
B	-12	HIS	-	expression tag	UNP O46043
B	-11	HIS	-	expression tag	UNP O46043
B	-10	HIS	-	expression tag	UNP O46043
B	-9	SER	-	expression tag	UNP O46043
B	-8	SER	-	expression tag	UNP O46043
B	-7	GLY	-	expression tag	UNP O46043
B	-6	LEU	-	expression tag	UNP O46043
B	-5	VAL	-	expression tag	UNP O46043
B	-4	PRO	-	expression tag	UNP O46043
B	-3	ARG	-	expression tag	UNP O46043
B	-2	GLY	-	expression tag	UNP O46043
B	-1	SER	-	expression tag	UNP O46043
B	0	HIS	-	expression tag	UNP O46043
C	-19	MET	-	initiating methionine	UNP O46043
C	-18	GLY	-	expression tag	UNP O46043
C	-17	SER	-	expression tag	UNP O46043
C	-16	SER	-	expression tag	UNP O46043
C	-15	HIS	-	expression tag	UNP O46043
C	-14	HIS	-	expression tag	UNP O46043
C	-13	HIS	-	expression tag	UNP O46043
C	-12	HIS	-	expression tag	UNP O46043
C	-11	HIS	-	expression tag	UNP O46043
C	-10	HIS	-	expression tag	UNP O46043
C	-9	SER	-	expression tag	UNP O46043
C	-8	SER	-	expression tag	UNP O46043
C	-7	GLY	-	expression tag	UNP O46043
C	-6	LEU	-	expression tag	UNP O46043
C	-5	VAL	-	expression tag	UNP O46043
C	-4	PRO	-	expression tag	UNP O46043
C	-3	ARG	-	expression tag	UNP O46043
C	-2	GLY	-	expression tag	UNP O46043
C	-1	SER	-	expression tag	UNP O46043
C	0	HIS	-	expression tag	UNP O46043

- Molecule 2 is 1-[(2,5-dimethylpyrazol-3-yl)methyl]-N-(1-methylcyclopropyl)-3-[(2-methyl-1,3-thiazol-5-yl)methyl]-2,4-bis(oxidanylidene)quinazoline-6-sulfonamide (three-letter code: LQX) (formula: C₂₃H₂₆N₆O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			35	23	6	4	2		
2	B	1	Total	C	N	O	S	0	0
			35	23	6	4	2		
2	C	1	Total	C	N	O	S	0	0
			35	23	6	4	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



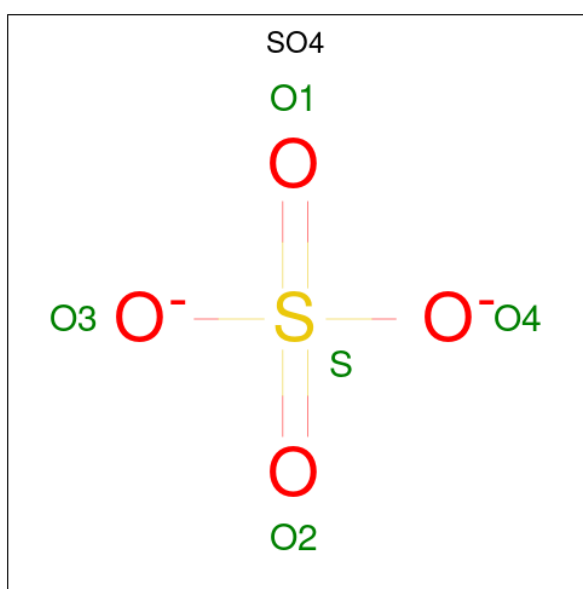
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

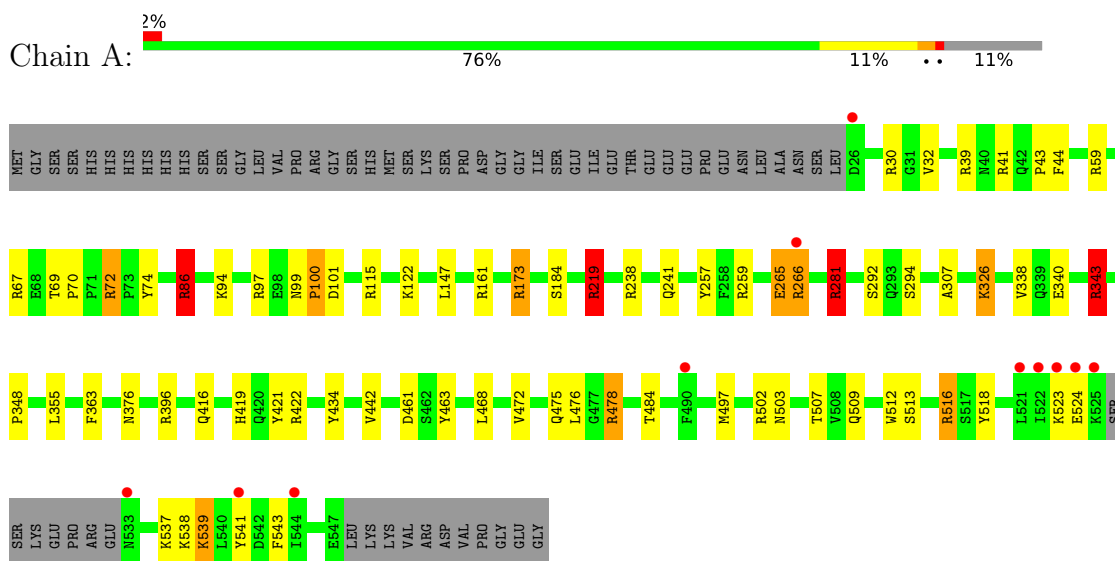
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	71	Total O 71 71	0	0
6	B	88	Total O 88 88	0	0
6	C	41	Total O 42 42	0	1

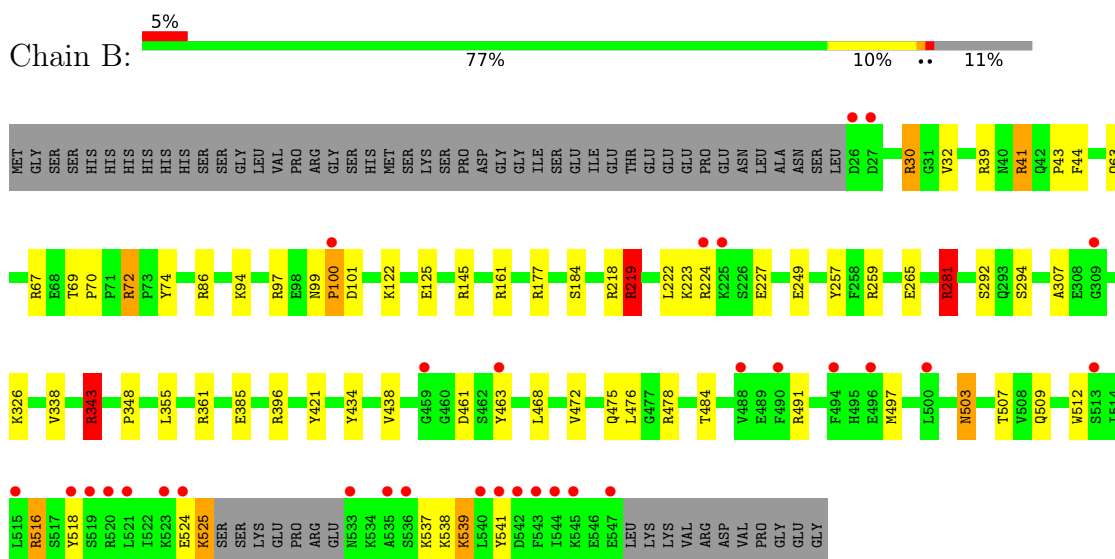
3 Residue-property plots [i](#)

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.

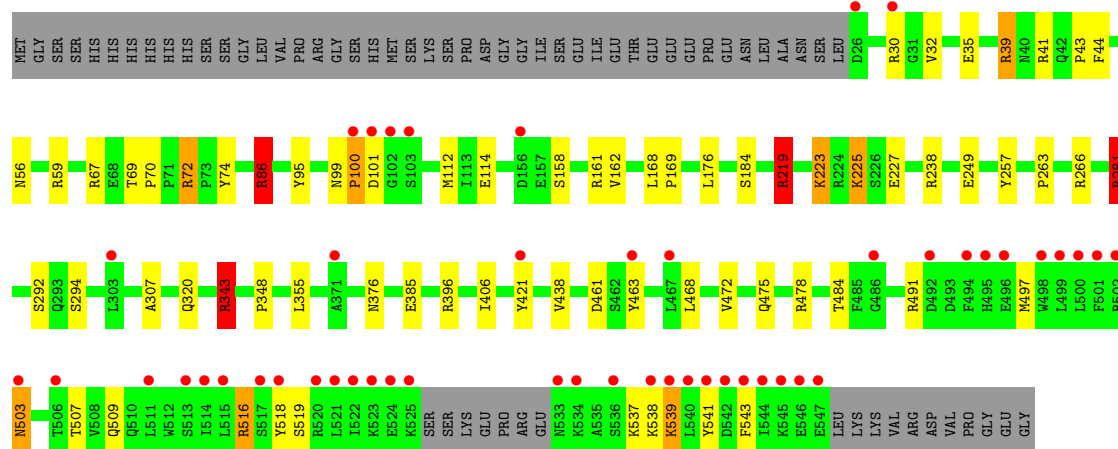
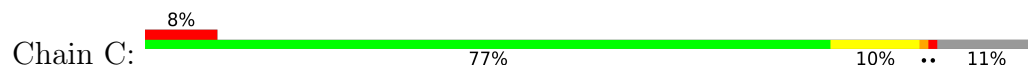
- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.39Å 115.92Å 123.27Å 90.00° 112.20° 90.00°	Depositor
Resolution (Å)	59.02 – 2.51 59.01 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.02-2.51) 99.8 (59.01-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.183 , 0.223 0.189 , 0.229	Depositor DCC
R_{free} test set	4262 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12890	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, LQX, GOL

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	0.51	1/4283 (0.0%)	0.91	10/5809 (0.2%)
1	B	0.52	0/4277	0.92	6/5801 (0.1%)
1	C	0.53	2/4304 (0.0%)	0.91	9/5838 (0.2%)
All	All	0.52	3/12864 (0.0%)	0.91	25/17448 (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	A	0	14
1	B	0	16
1	C	0	11
All	All	0	41

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	GLU	CD-OE1	7.19	1.33	1.25
1	C	227	GLU	CD-OE2	6.96	1.33	1.25
1	A	340	GLU	CD-OE2	5.35	1.31	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ARG	NE-CZ-NH2	-13.65	113.47	120.30
1	A	219	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	C	86	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	C	39	ARG	NE-CZ-NH2	-7.79	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	219	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	478	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	396	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	177	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	219	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	478	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	396	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	C	343	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	219	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	343	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	C	59	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	281	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	173	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	516	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	281	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	543	PHE	CB-CA-C	5.24	120.88	110.40
1	A	343	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	59	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	543	PHE	CB-CA-C	5.07	120.54	110.40
1	B	396	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	259	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	422	ARG	Sidechain
1	A	478	ARG	Sidechain
1	A	516	ARG	Sidechain
1	A	67	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	86	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	161	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	219	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	259	ARG	Sidechain
1	B	281	ARG	Sidechain
1	B	30	ARG	Sidechain
1	B	343	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	478	ARG	Sidechain
1	B	491	ARG	Sidechain
1	B	516	ARG	Sidechain
1	B	67	ARG	Sidechain
1	B	72	ARG	Sidechain
1	B	86	ARG	Sidechain
1	C	161	ARG	Sidechain
1	C	219	ARG	Sidechain
1	C	238	ARG	Sidechain
1	C	281	ARG	Sidechain
1	C	343	ARG	Sidechain
1	C	39	ARG	Sidechain
1	C	41	ARG	Sidechain
1	C	478	ARG	Sidechain
1	C	491	ARG	Sidechain
1	C	67	ARG	Sidechain
1	C	86	ARG	Sidechain

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	4170	0	4089	31	0
1	B	4167	0	4084	35	0
1	C	4184	0	4107	34	0
2	A	35	0	0	2	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
3	A	12	0	16	1	0
3	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	1	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
5	A	1	0	0	2	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	71	0	0	2	0
6	B	88	0	0	3	0
6	C	42	0	0	1	0
All	All	12890	0	12320	101	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 (101) 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:A:265:GLU:HG2	1:A:266:ARG:N	2.05	0.71
1:A:115:ARG:NH2	5:A:607:CL:CL	2.64	0.67
1:C:225:LYS:O	1:C:225:LYS:HG2	1.97	0.64
1:B:421:TYR:OH	1:B:461:ASP:OD2	2.17	0.62
1:C:421:TYR:OH	1:C:461:ASP:OD2	2.16	0.61
1:A:502:ARG:NH1	6:A:701:HOH:O	2.34	0.60
1:B:63:GLN:HE22	1:B:72:ARG:HH11	1.50	0.59
1:B:227:GLU:HG2	6:B:718:HOH:O	2.02	0.59
1:B:512:TRP:CE2	1:B:516:ARG:HD2	2.40	0.57
1:A:512:TRP:CE2	1:A:516:ARG:HD2	2.39	0.57
1:B:219:ARG:NH2	1:B:355:LEU:O	2.38	0.57
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.72	0.54
1:A:421:TYR:OH	1:A:461:ASP:OD2	2.23	0.54
1:A:97:ARG:NE	5:A:607:CL:CL	2.77	0.54
1:A:538:LYS:O	1:A:541:TYR:HB2	2.08	0.54
1:C:281:ARG:HH11	1:C:281:ARG:HG3	1.73	0.53
1:B:518:TYR:CD1	1:B:539:LYS:HG2	2.43	0.53
2:A:601:LQX:C9	2:A:601:LQX:O1	2.56	0.53
1:B:538:LYS:O	1:B:541:TYR:HB2	2.09	0.53
1:C:538:LYS:O	1:C:541:TYR:HB2	2.08	0.53
1:B:265:GLU:HB2	6:B:777:HOH:O	2.09	0.52
1:C:223:LYS:HB3	1:C:223:LYS:NZ	2.25	0.52
1:A:518:TYR:CD1	1:A:539:LYS:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ARG:HH11	1:C:281:ARG:CG	2.23	0.51
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.75	0.51
1:B:281:ARG:HD3	1:B:438:VAL:CG2	2.41	0.51
1:C:518:TYR:CD1	1:C:539:LYS:HG2	2.46	0.51
1:A:343:ARG:HG2	2:A:601:LQX:C19	2.41	0.50
1:C:86:ARG:HH12	3:C:602:GOL:H12	1.76	0.50
1:A:219:ARG:NH2	1:A:355:LEU:O	2.43	0.50
1:A:326:LYS:HE2	6:A:718:HOH:O	2.10	0.50
1:C:219:ARG:NH2	1:C:355:LEU:O	2.44	0.49
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.26	0.49
1:C:43:PRO:O	1:C:44:PHE:HB2	2.13	0.49
1:B:43:PRO:O	1:B:44:PHE:HB2	2.12	0.49
1:C:497:MET:HE3	1:C:537:LYS:HG3	1.94	0.49
1:B:307:ALA:HA	1:B:484:THR:OG1	2.12	0.49
1:A:86:ARG:HH12	3:A:602:GOL:H31	1.78	0.48
1:C:307:ALA:HA	1:C:484:THR:OG1	2.13	0.48
1:B:281:ARG:HH11	1:B:281:ARG:CG	2.26	0.48
1:A:463:TYR:HD2	1:A:537:LYS:HD2	1.79	0.48
1:B:125:GLU:HG2	6:B:762:HOH:O	2.12	0.48
1:C:257:TYR:HB2	1:C:348:PRO:HG2	1.96	0.47
1:B:257:TYR:HB2	1:B:348:PRO:HG2	1.96	0.47
1:A:74:TYR:O	1:A:184:SER:HB2	2.14	0.46
1:A:416:GLN:HB2	1:A:419:HIS:ND1	2.31	0.46
1:C:468:LEU:O	1:C:472:VAL:HG23	2.16	0.46
1:B:463:TYR:HD2	1:B:537:LYS:HD2	1.81	0.46
1:C:294:SER:OG	1:C:475:GLN:NE2	2.49	0.46
1:A:307:ALA:HA	1:A:484:THR:OG1	2.15	0.45
1:A:538:LYS:HD2	1:A:538:LYS:HA	1.74	0.45
1:C:463:TYR:HD2	1:C:537:LYS:HD2	1.81	0.45
1:A:497:MET:CE	1:A:537:LYS:HG3	2.47	0.45
1:B:538:LYS:HA	1:B:538:LYS:HD3	1.65	0.45
1:C:69:THR:HA	1:C:70:PRO:C	2.37	0.45
1:C:263:PRO:HG2	6:C:731:HOH:O	2.16	0.45
1:C:503:ASN:HD22	1:C:503:ASN:H	1.65	0.45
1:A:43:PRO:O	1:A:44:PHE:HB2	2.16	0.45
1:A:294:SER:OG	1:A:475:GLN:NE2	2.50	0.45
1:B:74:TYR:O	1:B:184:SER:HB2	2.17	0.44
1:A:292:SER:O	1:A:509:GLN:HB2	2.17	0.44
1:B:497:MET:CE	1:B:537:LYS:HG3	2.47	0.44
1:A:257:TYR:HB2	1:A:348:PRO:HG2	2.00	0.44
1:A:468:LEU:O	1:A:472:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112[A]:MET:HE3	1:C:112[A]:MET:HB3	1.89	0.43
1:C:497:MET:CE	1:C:537:LYS:HG3	2.48	0.43
1:B:69:THR:HA	1:B:70:PRO:C	2.38	0.43
1:B:503:ASN:HD22	1:B:503:ASN:H	1.66	0.43
1:C:158:SER:O	1:C:162:VAL:HG23	2.19	0.43
1:B:43:PRO:O	1:B:44:PHE:CB	2.66	0.43
1:C:99:ASN:O	1:C:100:PRO:C	2.56	0.43
1:A:434:TYR:CE1	1:A:476:LEU:HD21	2.53	0.43
1:C:249:GLU:HG3	1:C:385:GLU:HA	2.00	0.43
1:C:292:SER:O	1:C:509:GLN:HB2	2.18	0.43
1:B:218:ARG:HH22	3:B:602:GOL:C3	2.32	0.43
1:A:99:ASN:O	1:A:100:PRO:C	2.57	0.42
1:A:518:TYR:HD1	1:A:539:LYS:HG2	1.84	0.42
1:C:225:LYS:O	1:C:225:LYS:CG	2.65	0.42
1:A:69:THR:HA	1:A:70:PRO:C	2.38	0.42
1:B:292:SER:O	1:B:509:GLN:HB2	2.19	0.42
1:B:468:LEU:O	1:B:472:VAL:HG23	2.19	0.42
1:C:114:GLU:HG3	1:C:176:LEU:HD22	2.02	0.42
1:B:97:ARG:HH21	1:B:97:ARG:CB	2.32	0.42
1:C:74:TYR:O	1:C:184:SER:HB2	2.18	0.42
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.87	0.42
1:B:434:TYR:CE1	1:B:476:LEU:HD21	2.55	0.41
1:B:99:ASN:O	1:B:100:PRO:C	2.58	0.41
1:B:294:SER:OG	1:B:475:GLN:NE2	2.54	0.41
1:B:525:LYS:HB3	1:B:525:LYS:NZ	2.35	0.41
1:B:249:GLU:HG3	1:B:385:GLU:HA	2.02	0.41
1:C:43:PRO:O	1:C:44:PHE:CB	2.68	0.41
1:C:72:ARG:HG2	1:C:72:ARG:HH21	1.86	0.41
1:B:97:ARG:NH2	1:B:97:ARG:HB3	2.36	0.41
1:C:168:LEU:HB3	1:C:169:PRO:HD3	2.03	0.41
1:B:497:MET:HE3	1:B:537:LYS:HG3	2.02	0.40
1:B:39:ARG:HB2	1:B:41:ARG:HH11	1.86	0.40
1:C:320:GLN:O	1:C:406:ILE:HA	2.21	0.40
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.37	0.40
1:B:518:TYR:HD1	1:B:539:LYS:HG2	1.84	0.40
1:C:281:ARG:HD3	1:C:438:VAL:CG2	2.51	0.40
1:C:516:ARG:O	1:C:519:SER:HB3	2.21	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	512/578 (89%)	488 (95%)	22 (4%)	2 (0%)	34	54
1	B	511/578 (88%)	492 (96%)	17 (3%)	2 (0%)	34	54
1	C	514/578 (89%)	491 (96%)	22 (4%)	1 (0%)	47	68
All	All	1537/1734 (89%)	1471 (96%)	61 (4%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	PRO
1	A	100	PRO
1	B	338	VAL
1	A	338	VAL
1	B	100	PRO

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	453/507 (89%)	431 (95%)	22 (5%)	25	47
1	B	452/507 (89%)	437 (97%)	15 (3%)	38	64
1	C	455/507 (90%)	438 (96%)	17 (4%)	34	60
All	All	1360/1521 (89%)	1306 (96%)	54 (4%)	32	56

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

Mol	Chain	Res	Type
1	A	30	ARG
1	A	32	VAL
1	A	39	ARG
1	A	72	ARG
1	A	94	LYS
1	A	101	ASP
1	A	122	LYS
1	A	241	GLN
1	A	265	GLU
1	A	266	ARG
1	A	281	ARG
1	A	326	LYS
1	A	343	ARG
1	A	363	PHE
1	A	376	ASN
1	A	442	VAL
1	A	503	ASN
1	A	507	THR
1	A	513	SER
1	A	523	LYS
1	A	524	GLU
1	A	539	LYS
1	B	30	ARG
1	B	32	VAL
1	B	94	LYS
1	B	101	ASP
1	B	122	LYS
1	B	222	LEU
1	B	223	LYS
1	B	281	ARG
1	B	326	LYS
1	B	343	ARG
1	B	503	ASN
1	B	507	THR
1	B	524	GLU
1	B	525	LYS
1	B	539	LYS
1	C	30	ARG
1	C	32	VAL
1	C	35	GLU
1	C	56	ASN
1	C	72	ARG
1	C	95[A]	TYR

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Mol	Chain	Res	Type
1	C	95[B]	TYR
1	C	101	ASP
1	C	223	LYS
1	C	225	LYS
1	C	266	ARG
1	C	281	ARG
1	C	343	ARG
1	C	376	ASN
1	C	503	ASN
1	C	507	THR
1	C	539	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	416	GLN
1	A	452	ASN
1	A	475	GLN
1	A	503	ASN
1	B	63	GLN
1	B	210	ASN
1	B	241	GLN
1	B	419	HIS
1	B	452	ASN
1	B	475	GLN
1	B	503	ASN
1	C	38	HIS
1	C	241	GLN
1	C	452	ASN
1	C	475	GLN
1	C	503	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	LQX	C	601	-	37,39,39	1.14	4 (10%)	47,61,61	1.72	9 (19%)
3	GOL	B	602	-	5,5,5	0.24	0	5,5,5	0.63	0
3	GOL	C	602	-	5,5,5	0.13	0	5,5,5	0.29	0
4	SO4	A	606	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	C	603	-	4,4,4	0.34	0	6,6,6	0.63	0
3	GOL	B	603	-	5,5,5	0.25	0	5,5,5	0.67	0
4	SO4	C	604	-	4,4,4	0.27	0	6,6,6	0.42	0
4	SO4	B	604	-	4,4,4	0.61	0	6,6,6	0.52	0
2	LQX	B	601	-	37,39,39	1.15	2 (5%)	47,61,61	2.33	11 (23%)
2	LQX	A	601	-	37,39,39	1.18	4 (10%)	47,61,61	1.57	9 (19%)
4	SO4	A	604	-	4,4,4	0.72	0	6,6,6	0.59	0
3	GOL	A	602	-	5,5,5	0.20	0	5,5,5	0.43	0
4	SO4	A	605	-	4,4,4	0.59	0	6,6,6	0.64	0
3	GOL	A	603	-	5,5,5	0.29	0	5,5,5	0.60	0

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	LQX	C	601	-	-	2/16/24/24	0/5/5/5
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LQX	B	601	-	-	2/16/24/24	0/5/5/5
2	LQX	A	601	-	-	2/16/24/24	0/5/5/5
3	GOL	A	602	-	-	1/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	LQX	C16-N4	-2.97	1.44	1.49
2	C	601	LQX	C8-S1	-2.90	1.67	1.73
2	B	601	LQX	C8-S1	-2.88	1.67	1.73
2	C	601	LQX	C16-N4	-2.83	1.44	1.49
2	B	601	LQX	C16-N4	-2.61	1.44	1.49
2	A	601	LQX	C8-S1	-2.46	1.68	1.73
2	A	601	LQX	C10-S1	-2.44	1.66	1.73
2	A	601	LQX	C20-C15	2.10	1.42	1.38
2	C	601	LQX	C20-C15	2.09	1.42	1.38
2	C	601	LQX	C9-N3	2.01	1.39	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LQX	C11-C10-S1	7.83	130.64	120.12
2	B	601	LQX	C9-C8-S1	-6.79	105.25	112.00
2	B	601	LQX	C5-N1-C6	6.53	120.85	116.77
2	C	601	LQX	C4-C5-N1	-6.44	104.81	113.00
2	B	601	LQX	C16-N4-S2	-4.47	119.29	128.61
2	A	601	LQX	C11-C10-S1	4.38	126.00	120.12
2	A	601	LQX	C9-C8-S1	-4.17	107.85	112.00
2	C	601	LQX	C11-C10-S1	4.09	125.61	120.12
2	B	601	LQX	C5-C4-C3	3.54	133.77	129.34
2	B	601	LQX	C18-C16-N4	3.41	120.28	115.64
2	C	601	LQX	O4-S2-O3	-3.20	115.61	119.55
2	C	601	LQX	C5-N1-C6	3.19	118.76	116.77
2	A	601	LQX	C5-N1-C6	3.18	118.75	116.77
2	C	601	LQX	C9-C8-S1	-3.14	108.88	112.00
2	C	601	LQX	O3-S2-N4	2.97	114.08	107.32
2	A	601	LQX	C4-C5-N1	-2.78	109.47	113.00
2	A	601	LQX	C5-C4-C3	2.76	132.80	129.34
2	A	601	LQX	C16-N4-S2	-2.63	123.13	128.61
2	A	601	LQX	C18-C16-N4	2.49	119.02	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LQX	O3-S2-N4	2.46	112.92	107.32
2	B	601	LQX	C15-S2-N4	-2.40	104.19	108.17
2	B	601	LQX	O3-S2-N4	2.36	112.70	107.32
2	C	601	LQX	O4-S2-C15	2.28	110.77	107.97
2	C	601	LQX	C16-N4-S2	-2.23	123.97	128.61
2	C	601	LQX	O4-S2-N4	-2.09	102.55	107.32
2	A	601	LQX	O1-C6-N1	-2.08	119.41	122.22
2	B	601	LQX	O1-C6-N1	-2.06	119.44	122.22
2	B	601	LQX	C20-C15-S2	-2.05	117.55	119.77
2	B	601	LQX	C23-N5-C4	2.02	131.32	128.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-C3
2	B	601	LQX	C14-C15-S2-O4
2	A	601	LQX	C8-C7-N2-C6
2	B	601	LQX	C20-C15-S2-O4
2	A	601	LQX	C14-C15-S2-O4
2	C	601	LQX	C14-C15-S2-O4
2	C	601	LQX	C20-C15-S2-O4

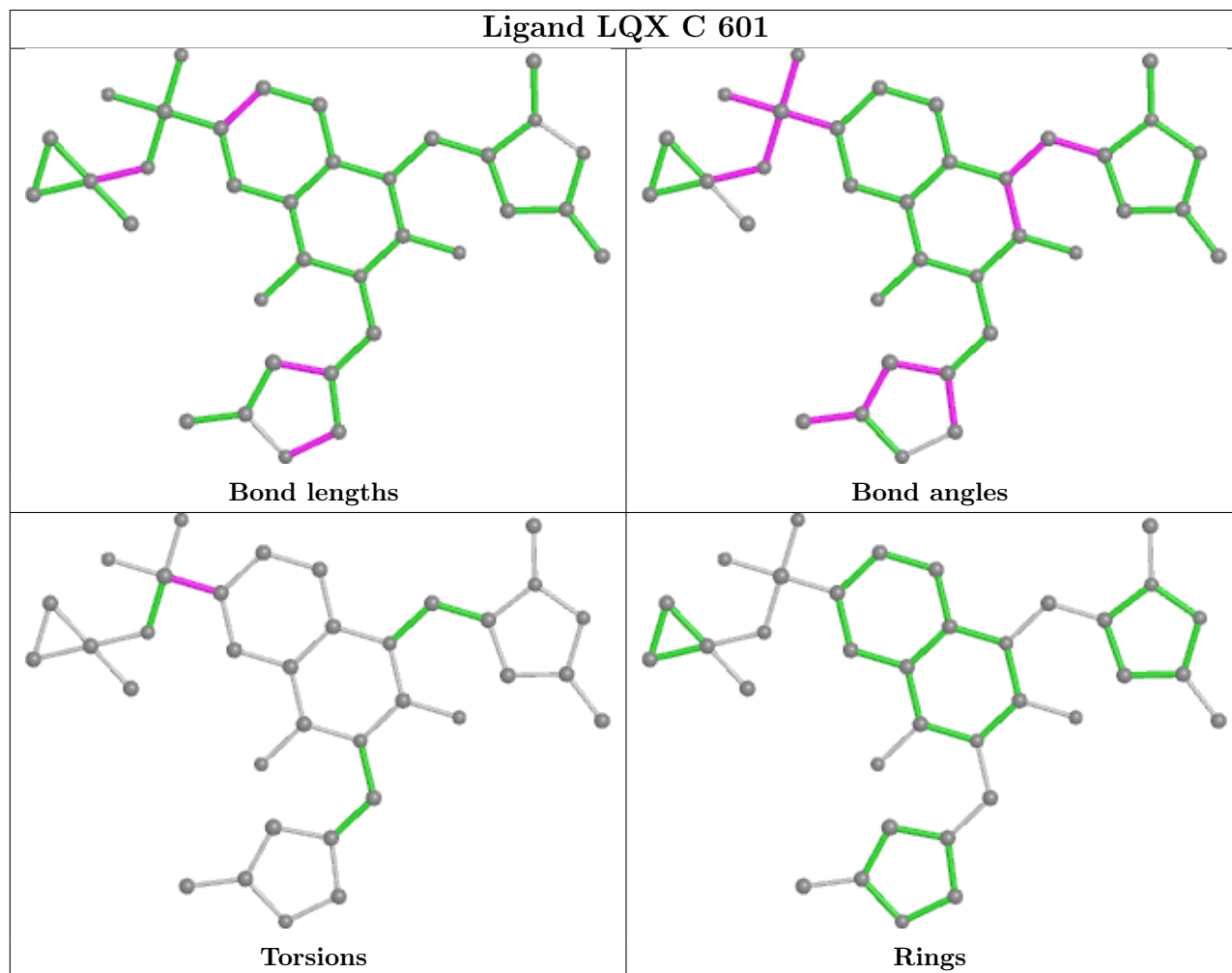
There are no ring outliers.

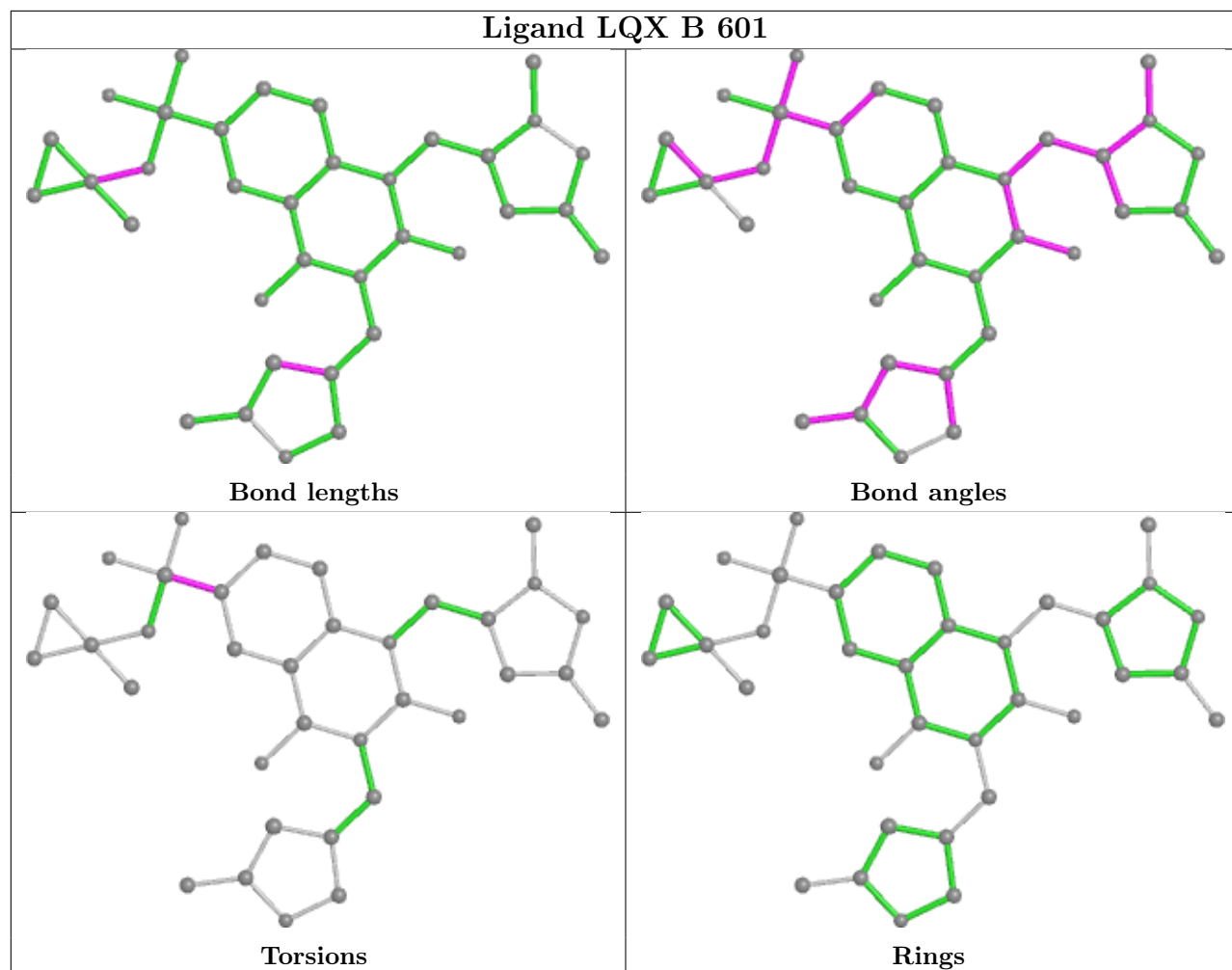
4 monomers are involved in 5 short contacts:

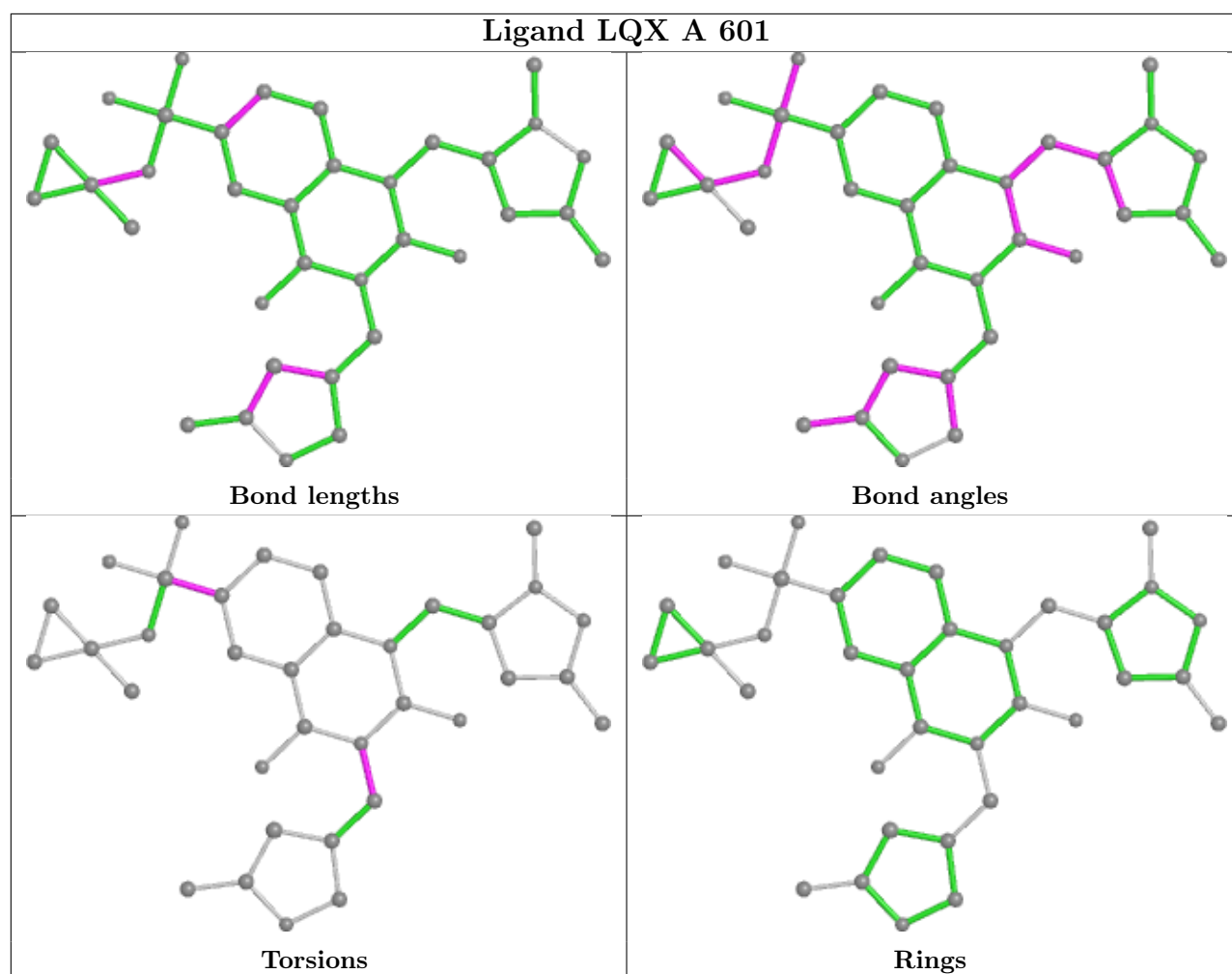
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	1	0
3	C	602	GOL	1	0
2	A	601	LQX	2	0
3	A	602	GOL	1	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	515/578 (89%)	0.13	11 (2%) 63 66	43, 65, 112, 146	0
1	B	515/578 (89%)	0.34	31 (6%) 21 22	41, 67, 112, 163	0
1	C	515/578 (89%)	0.62	49 (9%) 8 8	43, 67, 120, 153	0
All	All	1545/1734 (89%)	0.37	91 (5%) 22 23	41, 66, 115, 163	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	ASN	8.1
1	C	541	TYR	8.0
1	C	544	ILE	6.5
1	C	515	LEU	5.8
1	B	225	LYS	5.5
1	C	518	TYR	5.2
1	B	541	TYR	5.0
1	C	500	LEU	4.7
1	C	522	ILE	4.7
1	C	545	LYS	4.6
1	C	514	ILE	4.5
1	C	540	LEU	4.4
1	C	543	PHE	4.3
1	C	533	ASN	4.3
1	C	542	ASP	4.2
1	B	524	GLU	4.2
1	C	499	LEU	4.1
1	B	540	LEU	3.7
1	C	101	ASP	3.7
1	B	545	LYS	3.6
1	B	544	ILE	3.6
1	C	495	HIS	3.5
1	C	501	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	503	ASN	3.5
1	C	463	TYR	3.3
1	C	538	LYS	3.3
1	B	490	PHE	3.3
1	C	496	GLU	3.2
1	C	486	GLY	3.2
1	C	534	LYS	3.2
1	C	100	PRO	3.1
1	C	103	SER	3.1
1	B	542	ASP	3.1
1	B	459	GLY	3.1
1	C	536	SER	3.1
1	C	521	LEU	3.0
1	B	496	GLU	2.9
1	A	533	ASN	2.9
1	B	500	LEU	2.9
1	B	518	TYR	2.9
1	C	494	PHE	2.9
1	C	467	LEU	2.9
1	C	520	ARG	2.9
1	C	546	GLU	2.8
1	B	494	PHE	2.8
1	C	547	GLU	2.8
1	B	26	ASP	2.8
1	B	519	SER	2.8
1	C	102	GLY	2.7
1	A	544	ILE	2.7
1	B	543	PHE	2.7
1	B	520	ARG	2.7
1	B	513	SER	2.7
1	A	525	LYS	2.6
1	C	523	LYS	2.6
1	B	515	LEU	2.6
1	B	523	LYS	2.5
1	C	502	ARG	2.5
1	C	524	GLU	2.5
1	A	490	PHE	2.5
1	C	421	TYR	2.4
1	A	541	TYR	2.4
1	B	535	ALA	2.4
1	A	266	ARG	2.4
1	C	506	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	524	GLU	2.4
1	B	547	GLU	2.4
1	C	513	SER	2.4
1	B	488	VAL	2.3
1	B	463	TYR	2.3
1	C	26	ASP	2.3
1	C	30	ARG	2.3
1	C	511	LEU	2.3
1	C	492	ASP	2.2
1	C	498	TRP	2.2
1	C	517	SER	2.2
1	B	27	ASP	2.1
1	B	224	ARG	2.1
1	C	156	ASP	2.1
1	C	525	LYS	2.1
1	C	371	ALA	2.1
1	A	522	ILE	2.1
1	A	26	ASP	2.1
1	C	303	LEU	2.1
1	A	521	LEU	2.1
1	B	100	PRO	2.1
1	B	521	LEU	2.1
1	A	523	LYS	2.1
1	C	539	LYS	2.0
1	B	309	GLY	2.0
1	B	536	SER	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

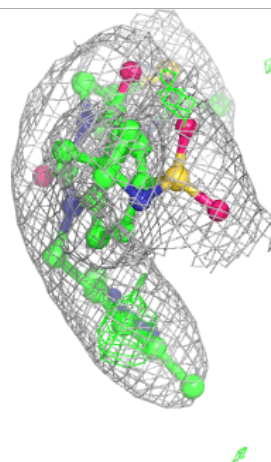
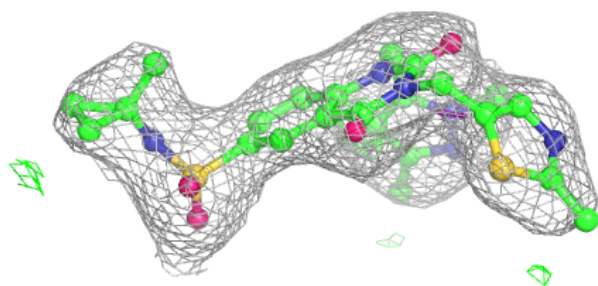
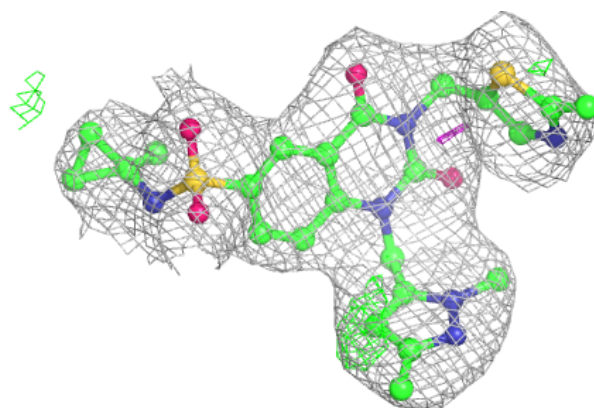
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	606	5/5	0.70	0.28	140,146,162,192	0
3	GOL	A	603	6/6	0.71	0.28	94,102,120,126	0
4	SO4	A	605	5/5	0.80	0.18	72,77,79,154	0
3	GOL	B	602	6/6	0.84	0.12	77,84,94,95	0
3	GOL	B	603	6/6	0.85	0.24	88,93,102,103	0
3	GOL	C	602	6/6	0.87	0.17	67,87,93,93	0
4	SO4	C	604	5/5	0.88	0.20	74,95,102,149	0
5	CL	C	605	1/1	0.89	0.13	88,88,88,88	0
3	GOL	A	602	6/6	0.91	0.14	74,80,84,90	0
4	SO4	B	604	5/5	0.92	0.18	60,67,99,130	0
5	CL	B	605	1/1	0.94	0.14	88,88,88,88	0
2	LQX	B	601	35/35	0.97	0.13	54,71,90,94	0
4	SO4	C	603	5/5	0.98	0.12	64,68,76,79	0
2	LQX	C	601	35/35	0.98	0.15	56,68,102,104	0
2	LQX	A	601	35/35	0.98	0.16	52,63,79,85	0
4	SO4	A	604	5/5	0.98	0.14	44,57,62,65	0
5	CL	A	607	1/1	0.99	0.09	68,68,68,68	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.

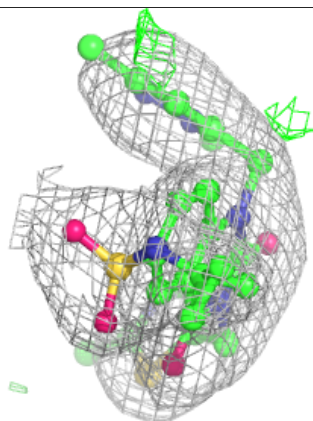
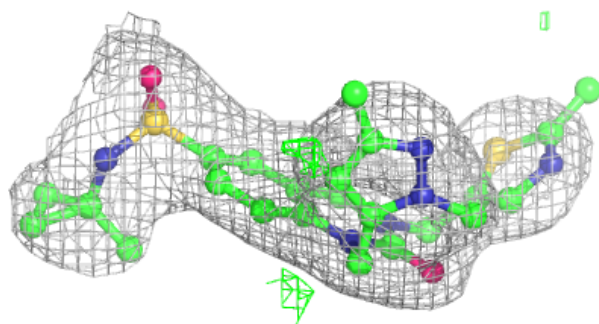
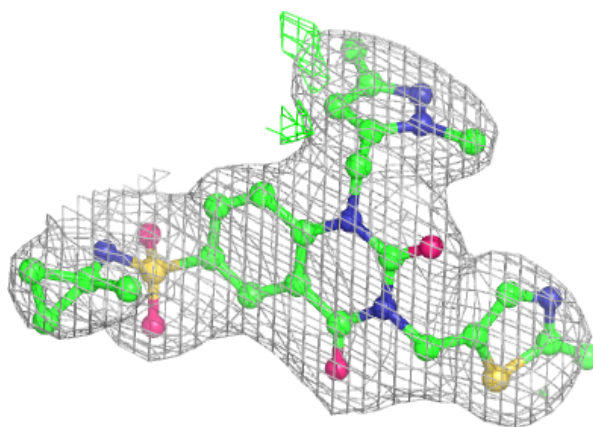
Electron density around LQX B 601:

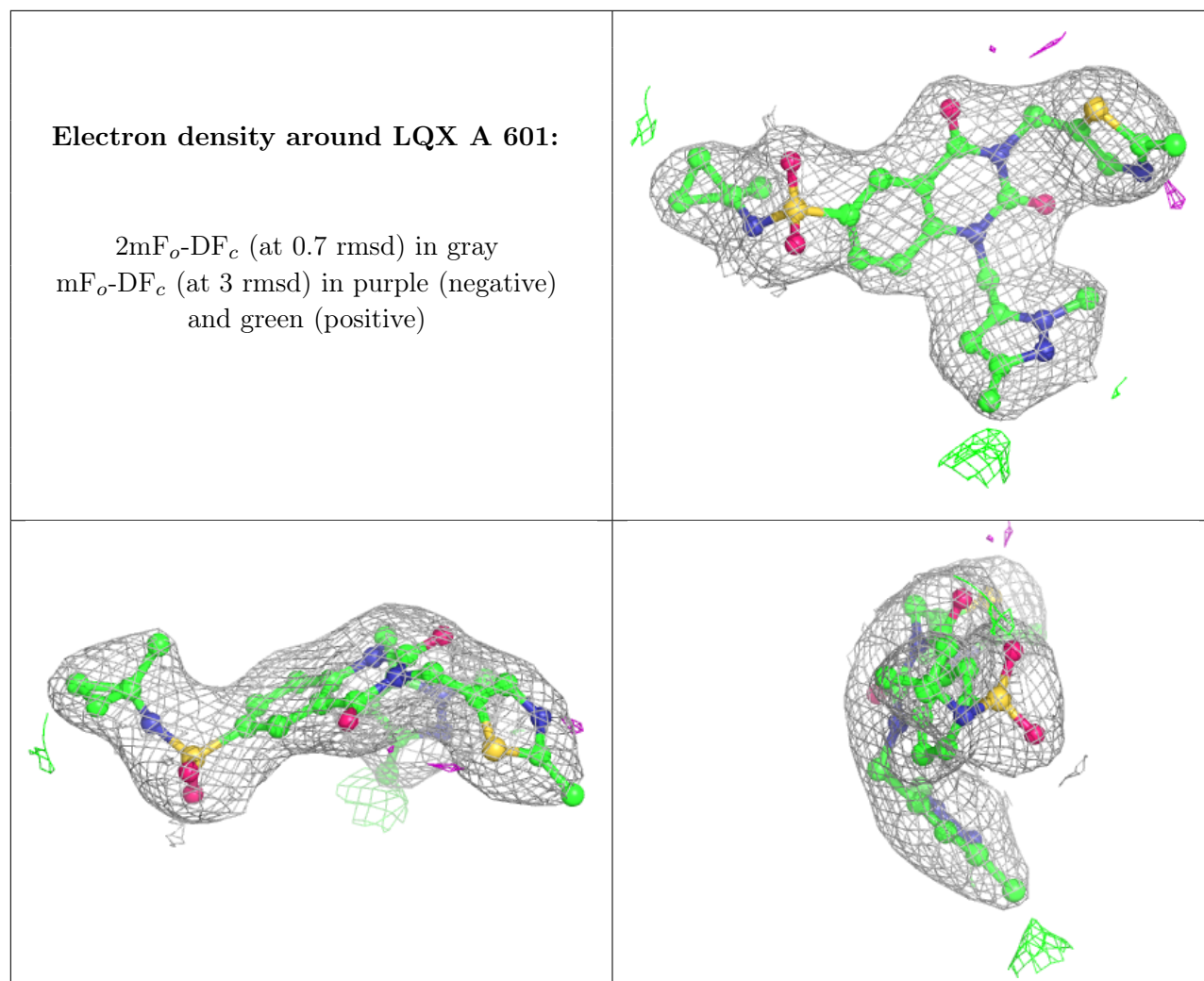
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LQX C 601:

$2mF_o-DF_c$ (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.