



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:15 AM UTC

PDB ID : 8ADJ / pdb_00008adj
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

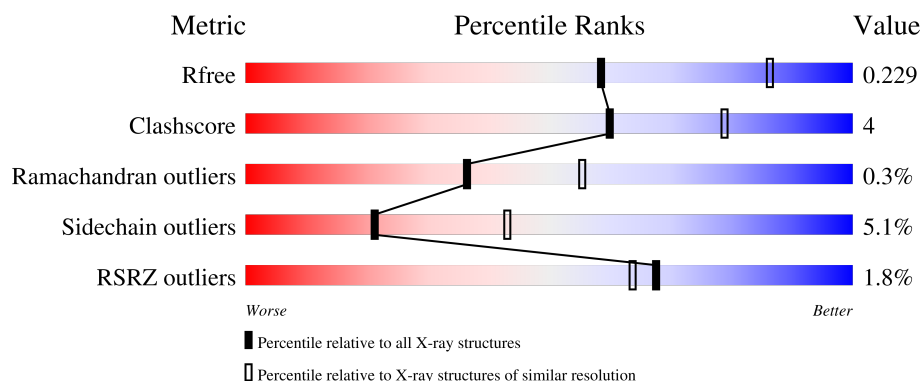
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	0% 74% 13% • 11%
1	B	578	2% 74% 13% • 11%
1	C	578	2% 75% 12% • 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

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
1	A	515	Total	C	N	O	S	0	1	0
			4170	2656	732	761	21			
1	B	515	Total	C	N	O	S	0	0	0
			4167	2654	732	761	20			
1	C	515	Total	C	N	O	S	0	3	0
			4184	2668	732	762	22			

There are 60 discrepancies between the modelled and reference sequences:

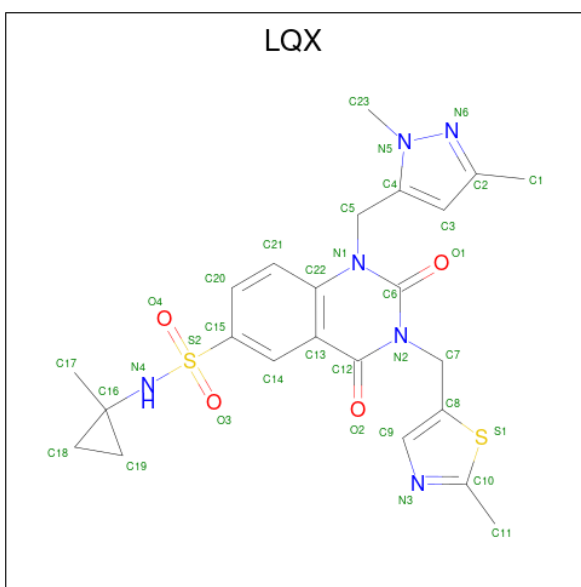
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O46043
A	-18	GLY	-	expression tag	UNP O46043
A	-17	SER	-	expression tag	UNP O46043
A	-16	SER	-	expression tag	UNP O46043
A	-15	HIS	-	expression tag	UNP O46043
A	-14	HIS	-	expression tag	UNP O46043
A	-13	HIS	-	expression 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

Continued on next page...

Continued from previous page...

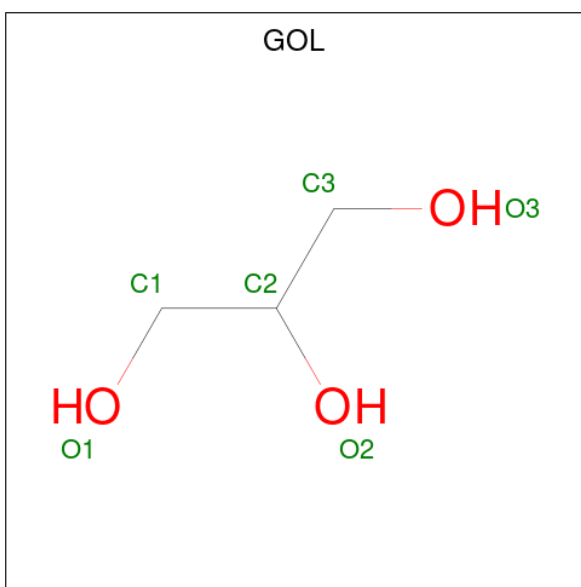
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O46043
B	-15	HIS	-	expression tag	UNP O46043
B	-14	HIS	-	expression tag	UNP O46043
B	-13	HIS	-	expression tag	UNP O46043
B	-12	HIS	-	expression tag	UNP O46043
B	-11	HIS	-	expression tag	UNP O46043
B	-10	HIS	-	expression tag	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 (CCD ID: LQX) (formula: C₂₃H₂₆N₆O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



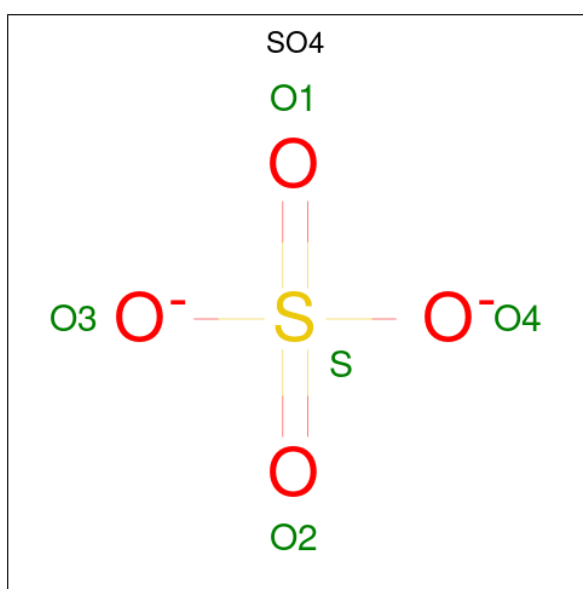
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: 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

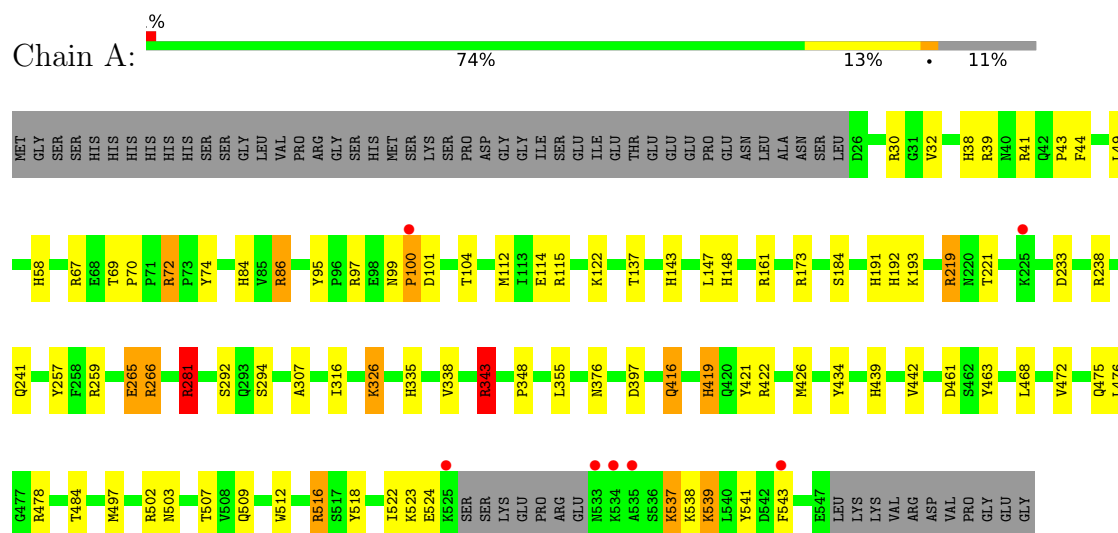
- Molecule 6 is water.

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

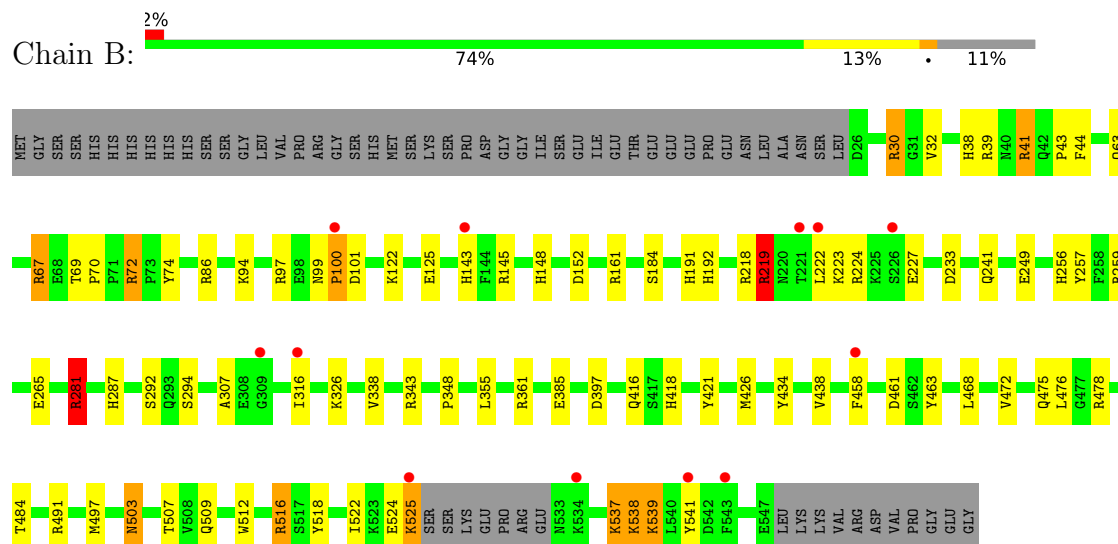
3 Residue-property plots [i](#)

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.

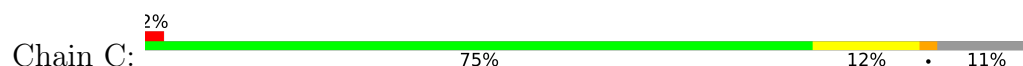
• Molecule 1: Poly(ADP-ribose) glycohydrolase

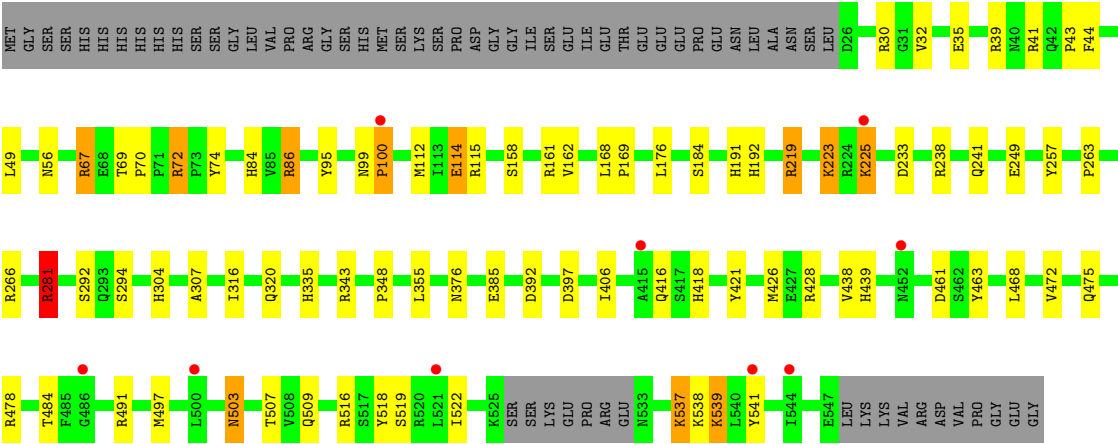


• Molecule 1: Poly(ADP-ribose) glycohydrolase



• 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 59.02 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.02-2.51) 99.8 (59.02-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.51Å)	Xtriage
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	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
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

Xtriage'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: SO4, LQX, GOL, 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	0.74	10/4283 (0.2%)	1.16	6/5809 (0.1%)
1	B	0.75	8/4277 (0.2%)	1.18	6/5801 (0.1%)
1	C	0.74	7/4304 (0.2%)	1.15	3/5838 (0.1%)
All	All	0.74	25/12864 (0.2%)	1.16	15/17448 (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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	HIS	CE1-NE2	7.08	1.39	1.32
1	B	418	HIS	CE1-NE2	6.86	1.39	1.32
1	B	256	HIS	CE1-NE2	6.57	1.39	1.32
1	B	191	HIS	CE1-NE2	6.42	1.39	1.32
1	C	192	HIS	CE1-NE2	6.38	1.39	1.32
1	A	191	HIS	CE1-NE2	6.28	1.38	1.32
1	A	192	HIS	CE1-NE2	6.20	1.38	1.32
1	A	143	HIS	CE1-NE2	5.99	1.38	1.32
1	B	148	HIS	CE1-NE2	5.94	1.38	1.32
1	C	335	HIS	CE1-NE2	5.91	1.38	1.32
1	B	287	HIS	CE1-NE2	5.79	1.38	1.32
1	C	418	HIS	CE1-NE2	5.57	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	HIS	CE1-NE2	5.50	1.38	1.32
1	B	192	HIS	CE1-NE2	5.49	1.38	1.32
1	C	191	HIS	CE1-NE2	5.41	1.38	1.32
1	A	419	HIS	CE1-NE2	5.34	1.37	1.32
1	A	58	HIS	CE1-NE2	5.34	1.37	1.32
1	A	335	HIS	CE1-NE2	5.29	1.37	1.32
1	C	439	HIS	CE1-NE2	5.29	1.37	1.32
1	C	304	HIS	CE1-NE2	5.28	1.37	1.32
1	A	439	HIS	CE1-NE2	5.22	1.37	1.32
1	A	84	HIS	CE1-NE2	5.21	1.37	1.32
1	B	143	HIS	CE1-NE2	5.18	1.37	1.32
1	C	84	HIS	CE1-NE2	5.07	1.37	1.32
1	A	148	HIS	CE1-NE2	5.05	1.37	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	CA-CB-CG	7.49	120.08	112.60
1	C	233	ASP	CA-CB-CG	6.81	119.41	112.60
1	B	219	ARG	NE-CZ-NH2	-6.36	113.47	119.20
1	C	397	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	397	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	233	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	104	THR	CA-CB-OG1	-5.55	101.27	109.60
1	A	137	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	397	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	458	PHE	CB-CA-C	5.20	119.70	109.72
1	B	152	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	543	PHE	CB-CA-C	5.06	120.88	110.31
1	A	221	THR	CA-CB-OG1	-5.05	102.02	109.60
1	C	392	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	418	HIS	CA-CB-CG	5.04	118.83	113.80

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

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	34	0
1	B	4167	0	4084	35	0
1	C	4184	0	4107	37	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
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	107	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 (107) 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:497:MET:HE3	1:A:537:LYS:HG3	1.51	0.91
1:C:497:MET:HE3	1:C:537:LYS:HG3	1.56	0.85
1:B:497:MET:HE3	1:B:537:LYS:HG3	1.64	0.79
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:A:497:MET:HE3	1:A:537:LYS:CG	2.26	0.66
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:421:TYR:HA	1:B:426:MET:HE3	1.83	0.59
1:B:227:GLU:HG2	6:B:718:HOH:O	2.02	0.59
1:C:421:TYR:HA	1:C:426:MET:HE3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:TRP:CE2	1:B:516:ARG:HD2	2.40	0.57
1:A:421:TYR:HA	1:A:426:MET:HE3	1.85	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:497:MET:HE3	1:C:537:LYS:CG	2.33	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
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: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:C:69:THR:HA	1:C:70:PRO:C	2.37	0.48
1:A:463:TYR:HD2	1:A:537:LYS:HD2	1.79	0.48
1:B:69:THR:HA	1:B:70:PRO:C	2.38	0.48
1:B:125:GLU:HG2	6:B:762:HOH:O	2.12	0.48
1:C:99:ASN:O	1:C:100:PRO:C	2.56	0.48
1:C:257:TYR:HB2	1:C:348:PRO:HG2	1.96	0.47
1:A:99:ASN:O	1:A:100:PRO:C	2.57	0.47
1:B:257:TYR:HB2	1:B:348:PRO:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HA	1:A:70:PRO:C	2.38	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:99:ASN:O	1:B:100:PRO:C	2.58	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:95:TYR:HD2	1:A:112:MET:HE1	1.81	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:C:112[B]:MET:HE2	1:C:115:ARG:HH22	1.81	0.45
1:B:538:LYS:HA	1:B:538:LYS:HD3	1.65	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: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
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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112[B]:MET:HE2	1:C:115:ARG:NH2	2.36	0.41
1:C:168:LEU:HB3	1:C:169:PRO:HD3	2.03	0.41
1:C:428:ARG:C	1:C:428:ARG:HD3	2.46	0.41
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%)	30	49
1	B	511/578 (88%)	492 (96%)	17 (3%)	2 (0%)	30	49
1	C	514/578 (89%)	491 (96%)	22 (4%)	1 (0%)	43	63
All	All	1537/1734 (89%)	1471 (96%)	61 (4%)	5 (0%)	36	55

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 ⓘ

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%)	427 (94%)	26 (6%)	18	39
1	B	452/507 (89%)	431 (95%)	21 (5%)	24	48
1	C	455/507 (90%)	432 (95%)	23 (5%)	21	43
All	All	1360/1521 (89%)	1290 (95%)	70 (5%)	21	43

All (70) 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	49	LEU
1	A	72	ARG
1	A	101	ASP
1	A	114	GLU
1	A	122	LYS
1	A	193	LYS
1	A	241	GLN
1	A	265	GLU
1	A	266	ARG
1	A	281	ARG
1	A	316	ILE
1	A	326	LYS
1	A	343	ARG
1	A	376	ASN
1	A	416	GLN
1	A	442	VAL
1	A	503	ASN
1	A	507	THR
1	A	522	ILE
1	A	523	LYS
1	A	524	GLU
1	A	537	LYS
1	A	539	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	ARG
1	B	32	VAL
1	B	67	ARG
1	B	94	LYS
1	B	101	ASP
1	B	122	LYS
1	B	222	LEU
1	B	223	LYS
1	B	241	GLN
1	B	281	ARG
1	B	316	ILE
1	B	326	LYS
1	B	416	GLN
1	B	503	ASN
1	B	507	THR
1	B	522	ILE
1	B	524	GLU
1	B	525	LYS
1	B	537	LYS
1	B	538	LYS
1	B	539	LYS
1	C	30	ARG
1	C	32	VAL
1	C	35	GLU
1	C	49	LEU
1	C	56	ASN
1	C	67	ARG
1	C	72	ARG
1	C	95[A]	TYR
1	C	95[B]	TYR
1	C	114	GLU
1	C	223	LYS
1	C	225	LYS
1	C	241	GLN
1	C	266	ARG
1	C	281	ARG
1	C	316	ILE
1	C	376	ASN
1	C	416	GLN
1	C	503	ASN
1	C	507	THR
1	C	522	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	537	LYS
1	C	539	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	210	ASN
1	A	237	ASN
1	A	241	GLN
1	A	325	ASN
1	A	416	GLN
1	A	475	GLN
1	A	503	ASN
1	B	38	HIS
1	B	63	GLN
1	B	143	HIS
1	B	149	GLN
1	B	419	HIS
1	B	452	ASN
1	B	475	GLN
1	B	503	ASN
1	C	38	HIS
1	C	99	ASN
1	C	237	ASN
1	C	241	GLN
1	C	475	GLN
1	C	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	601	-	39,39,39	1.22	4 (10%)	51,61,61	2.77	20 (39%)
4	SO4	A	604	-	4,4,4	0.75	0	6,6,6	0.60	0
2	LQX	C	601	-	39,39,39	1.06	3 (7%)	51,61,61	2.07	11 (21%)
4	SO4	A	606	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	B	604	-	4,4,4	0.62	0	6,6,6	0.51	0
4	SO4	C	603	-	4,4,4	0.33	0	6,6,6	0.63	0
3	GOL	B	602	-	5,5,5	0.24	0	5,5,5	0.65	0
3	GOL	B	603	-	5,5,5	0.26	0	5,5,5	0.69	0
3	GOL	A	602	-	5,5,5	0.20	0	5,5,5	0.43	0
3	GOL	A	603	-	5,5,5	0.29	0	5,5,5	0.62	0
4	SO4	A	605	-	4,4,4	0.66	0	6,6,6	0.60	0
4	SO4	C	604	-	4,4,4	0.34	0	6,6,6	0.42	0
3	GOL	C	602	-	5,5,5	0.13	0	5,5,5	0.28	0
2	LQX	A	601	-	39,39,39	1.20	4 (10%)	51,61,61	2.18	11 (21%)

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	B	601	-	-	4/17/24/24	0/5/5/5
2	LQX	C	601	-	-	4/17/24/24	0/5/5/5
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	A	602	-	-	1/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
2	LQX	A	601	-	-	3/17/24/24	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	LQX	C4-N5	3.23	1.40	1.36
2	A	601	LQX	C16-N4	-3.08	1.44	1.49
2	A	601	LQX	C10-S1	-2.98	1.66	1.73
2	C	601	LQX	C16-N4	-2.93	1.44	1.49
2	A	601	LQX	C7-N2	2.75	1.50	1.46
2	B	601	LQX	C16-N4	-2.70	1.44	1.49
2	C	601	LQX	C10-S1	-2.18	1.68	1.73
2	B	601	LQX	C10-S1	-2.13	1.68	1.73
2	A	601	LQX	C20-C15	2.08	1.42	1.38
2	C	601	LQX	C20-C15	2.07	1.42	1.38
2	B	601	LQX	C7-N2	2.05	1.49	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LQX	S1-C10-N3	-12.69	106.01	114.63
2	C	601	LQX	S1-C10-N3	-10.82	107.28	114.63
2	A	601	LQX	S1-C10-N3	-10.54	107.46	114.63
2	B	601	LQX	C5-N1-C6	6.16	120.85	116.65
2	A	601	LQX	C12-N2-C6	-4.84	121.80	125.33
2	B	601	LQX	C16-N4-S2	-4.62	119.29	128.36
2	B	601	LQX	C23-N5-C4	4.33	131.32	128.18
2	A	601	LQX	N2-C6-N1	4.13	119.95	117.04
2	B	601	LQX	C11-C10-S1	3.79	130.64	122.51
2	B	601	LQX	C8-S1-C10	3.79	97.71	90.71
2	B	601	LQX	C9-C8-S1	-3.66	105.25	108.93
2	B	601	LQX	C18-C16-N4	3.45	120.28	115.60
2	B	601	LQX	C12-N2-C6	-3.44	122.82	125.33
2	C	601	LQX	O4-S2-O3	-3.22	115.61	119.52
2	C	601	LQX	C23-N5-C4	3.19	130.50	128.18
2	B	601	LQX	N2-C6-N1	3.10	119.22	117.04
2	C	601	LQX	C5-N1-C6	3.10	118.76	116.65
2	A	601	LQX	C5-N1-C6	3.09	118.75	116.65
2	C	601	LQX	O3-S2-N4	2.94	114.08	107.36
2	A	601	LQX	C8-S1-C10	2.78	95.85	90.71
2	A	601	LQX	C23-N5-C4	2.73	130.16	128.18
2	C	601	LQX	C8-S1-C10	2.69	95.68	90.71
2	A	601	LQX	C16-N4-S2	-2.67	123.13	128.36
2	B	601	LQX	C7-C8-S1	2.64	126.40	121.50
2	B	601	LQX	C1-C2-N6	-2.61	116.96	120.24
2	A	601	LQX	C18-C16-N4	2.52	119.02	115.60
2	B	601	LQX	C23-N5-N6	-2.50	115.55	119.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LQX	O3-S2-N4	2.43	112.92	107.36
2	B	601	LQX	O3-S2-N4	2.34	112.70	107.36
2	B	601	LQX	C5-N1-C22	-2.25	117.69	120.20
2	C	601	LQX	C7-C8-C9	2.25	130.89	128.14
2	C	601	LQX	C16-N4-S2	-2.24	123.97	128.36
2	C	601	LQX	O4-S2-C15	2.21	110.77	107.98
2	B	601	LQX	C15-S2-N4	-2.20	104.19	108.11
2	C	601	LQX	C8-C9-N3	-2.19	112.89	117.00
2	A	601	LQX	C8-C9-N3	-2.13	113.00	117.00
2	B	601	LQX	C8-C7-N2	-2.12	110.45	112.69
2	A	601	LQX	O1-C6-N1	-2.11	119.41	122.15
2	C	601	LQX	O4-S2-N4	-2.11	102.55	107.36
2	B	601	LQX	O1-C6-N1	-2.10	119.44	122.15
2	B	601	LQX	C7-N2-C6	2.07	119.20	116.71
2	B	601	LQX	C20-C15-S2	-2.01	117.55	119.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

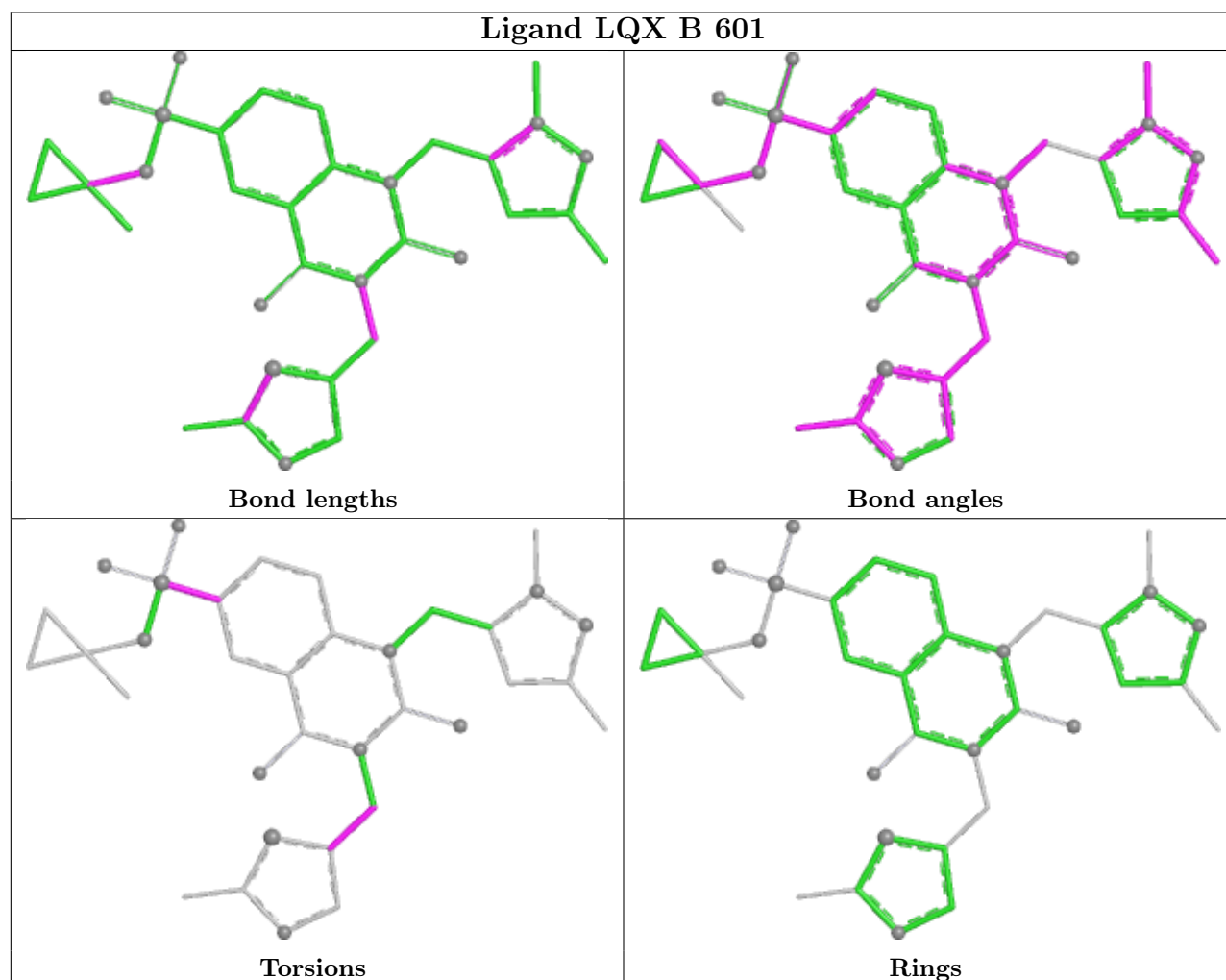
Mol	Chain	Res	Type	Atoms
2	A	601	LQX	C8-C7-N2-C6
2	C	601	LQX	N2-C7-C8-C9
3	C	602	GOL	C1-C2-C3-O3
2	C	601	LQX	N2-C7-C8-S1
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
2	A	601	LQX	N2-C7-C8-C9
3	C	602	GOL	O2-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
2	B	601	LQX	N2-C7-C8-C9
3	A	602	GOL	O1-C1-C2-C3
2	B	601	LQX	C14-C15-S2-O4
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
2	B	601	LQX	N2-C7-C8-S1

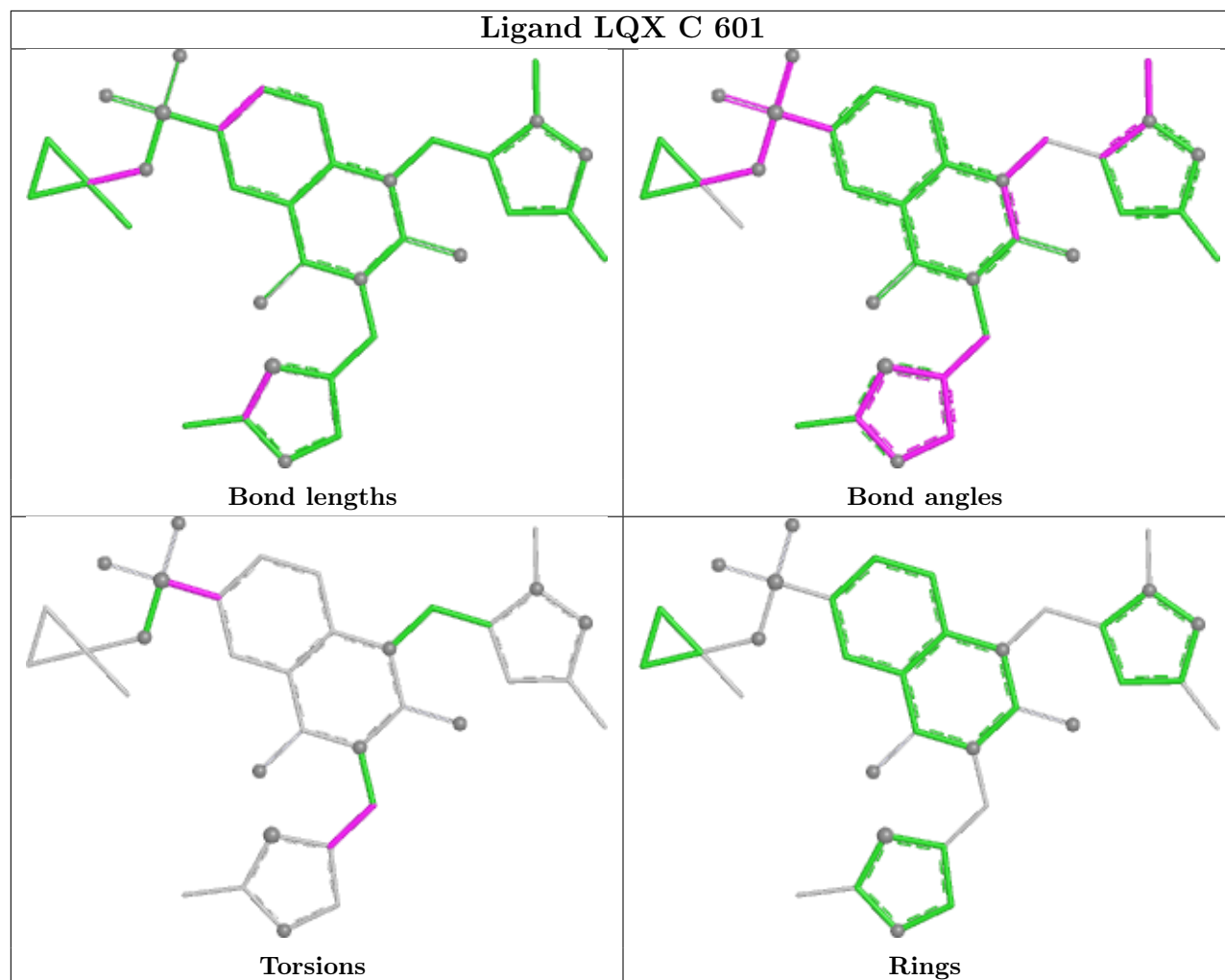
There are no ring outliers.

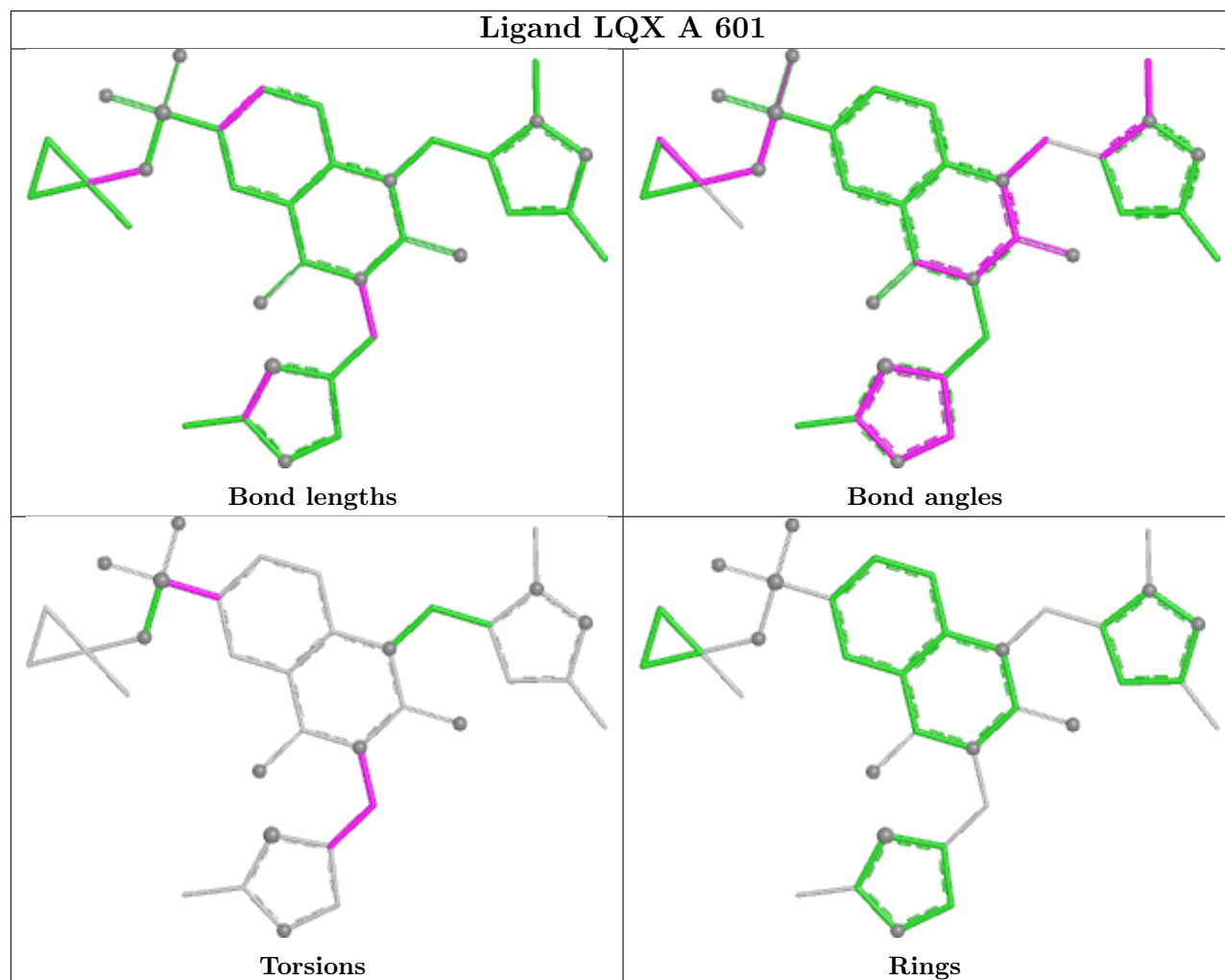
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	1	0
3	A	602	GOL	1	0
3	C	602	GOL	1	0
2	A	601	LQX	2	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%)	-0.07	7 (1%) 73 70	34, 65, 112, 146	1 (0%)
1	B	515/578 (89%)	-0.01	12 (2%) 61 57	41, 67, 112, 163	0
1	C	515/578 (89%)	0.02	9 (1%) 69 65	37, 67, 120, 153	3 (0%)
All	All	1545/1734 (89%)	-0.02	28 (1%) 67 64	34, 66, 115, 163	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	LEU	3.7
1	A	543	PHE	3.4
1	B	458	PHE	3.4
1	C	100	PRO	3.3
1	B	316	ILE	3.2
1	B	525	LYS	3.1
1	A	100	PRO	2.9
1	C	486	GLY	2.6
1	B	543	PHE	2.6
1	A	535	ALA	2.4
1	C	415	ALA	2.4
1	B	226	SER	2.4
1	B	534	LYS	2.4
1	C	452	ASN	2.3
1	B	309	GLY	2.3
1	A	225	LYS	2.2
1	B	143	HIS	2.2
1	B	100	PRO	2.2
1	A	525	LYS	2.2
1	B	541	TYR	2.2
1	C	225	LYS	2.2
1	C	500	LEU	2.2
1	C	541	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	521	LEU	2.1
1	C	544	ILE	2.1
1	A	533	ASN	2.1
1	B	221	THR	2.1
1	A	534	LYS	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](#)

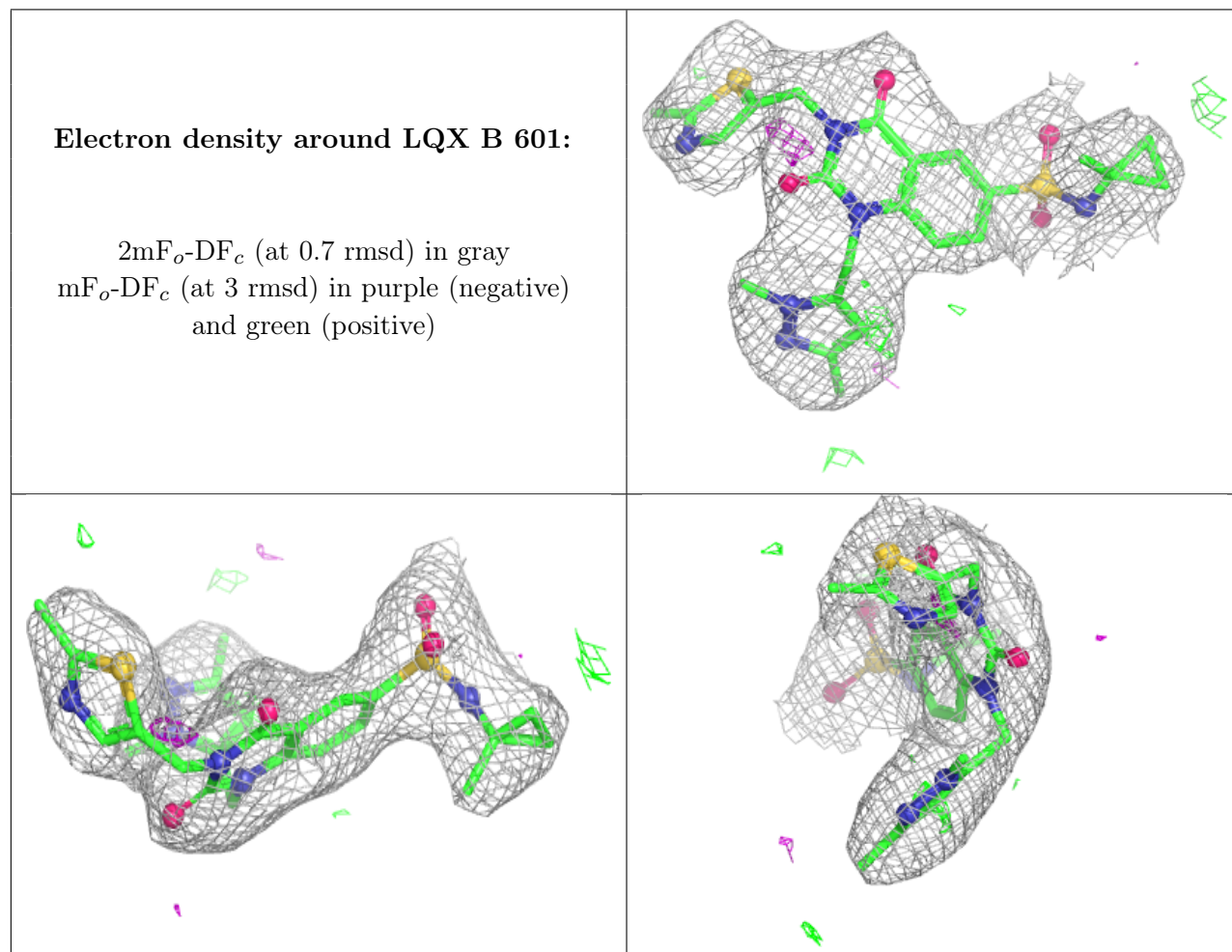
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

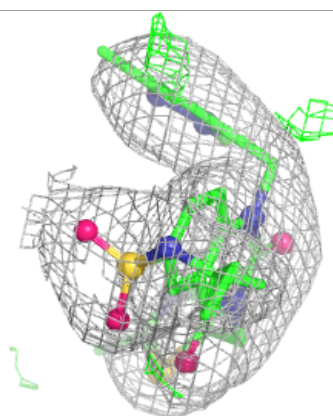
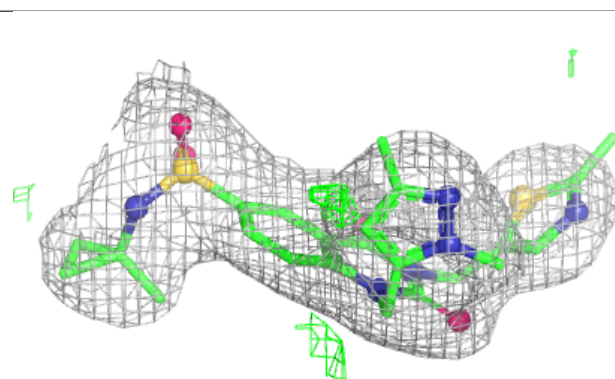
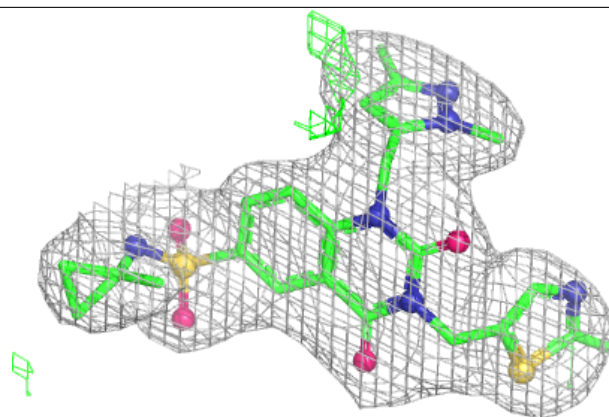
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	606	5/5	0.70	0.11	140,146,162,192	0
3	GOL	A	603	6/6	0.81	0.16	94,102,120,126	0
3	GOL	B	602	6/6	0.84	0.10	77,84,94,95	0
4	SO4	A	605	5/5	0.85	0.13	72,77,79,154	0
3	GOL	B	603	6/6	0.88	0.15	88,93,102,103	0
4	SO4	C	604	5/5	0.88	0.13	74,95,102,149	0
3	GOL	C	602	6/6	0.89	0.12	67,87,93,93	0
3	GOL	A	602	6/6	0.89	0.12	74,80,84,90	0
4	SO4	B	604	5/5	0.91	0.12	60,67,99,130	0
5	CL	C	605	1/1	0.91	0.11	88,88,88,88	0
4	SO4	C	603	5/5	0.93	0.08	64,68,76,79	0
4	SO4	A	604	5/5	0.95	0.07	44,57,62,65	0
5	CL	B	605	1/1	0.96	0.08	88,88,88,88	0
2	LQX	B	601	35/35	0.96	0.09	54,71,90,94	0
2	LQX	C	601	35/35	0.97	0.07	56,68,102,104	0
2	LQX	A	601	35/35	0.97	0.07	52,63,79,85	0
5	CL	A	607	1/1	0.98	0.06	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.



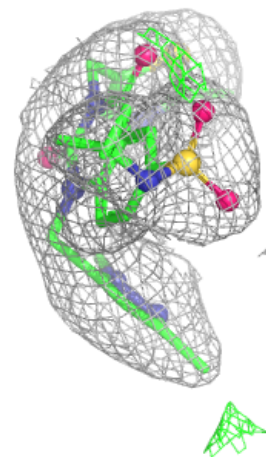
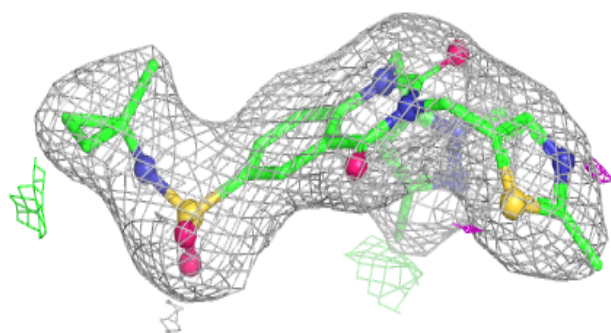
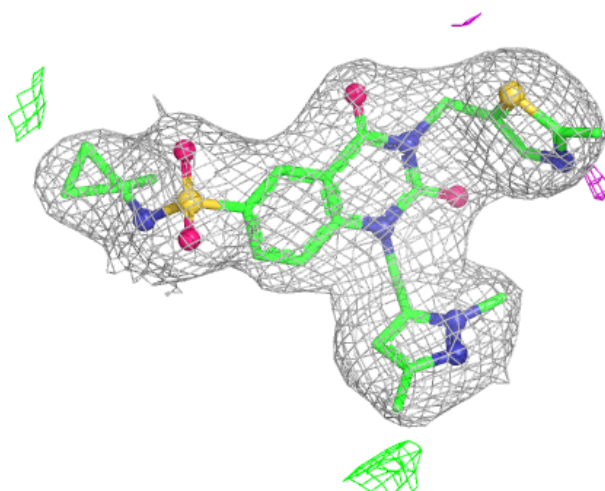
Electron density around LQX C 601:

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



Electron density around LQX A 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.