



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:19 AM UTC

PDB ID : 7SQL / pdb_00007sql
Title : Crystal structure of human uridine-cytidine kinase 2 complexed with a weak small molecule inhibitor
Authors : Mashayekh, S.; Stunkard, L.M.; Kienle, M.; Mathews, I.I.; Khosla, C.
Deposited on : 2021-11-05
Resolution : 2.40 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

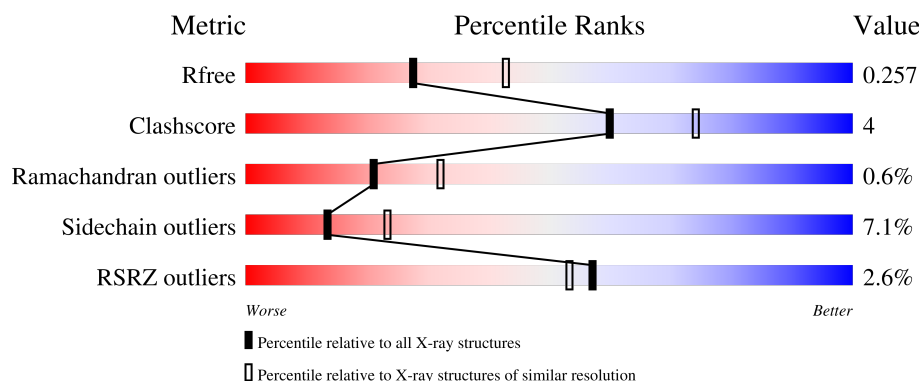
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	250	<div> <div>2%</div> <div>71% 12% • 15%</div> </div>
1	B	250	<div> <div>3%</div> <div>67% 17% • 15%</div> </div>
1	C	250	<div> <div>3%</div> <div>72% 12% • 15%</div> </div>
1	D	250	<div> <div>•</div> <div>73% 10% • 15%</div> </div>

2 Entry composition [i](#)

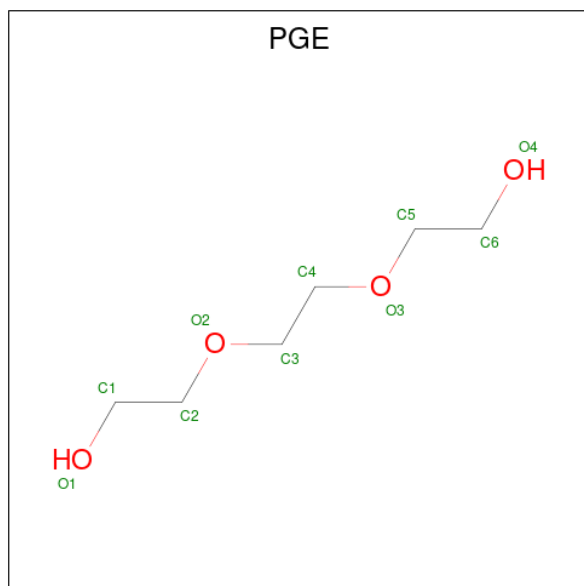
There are 7 unique types of molecules in this entry. The entry contains 7321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine-cytidine kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	5	0
			1732	1109	290	330	3			
1	B	212	Total	C	N	O	S	0	4	0
			1725	1104	289	329	3			
1	C	212	Total	C	N	O	S	0	1	0
			1695	1084	288	320	3			
1	D	212	Total	C	N	O	S	0	0	0
			1699	1088	285	323	3			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



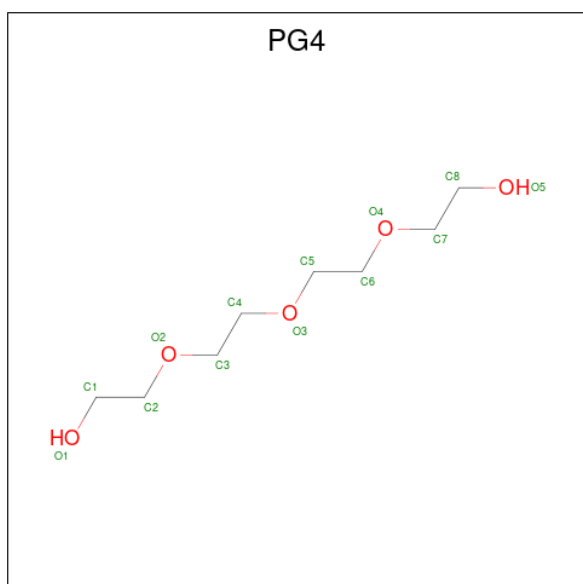
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		

- 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		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



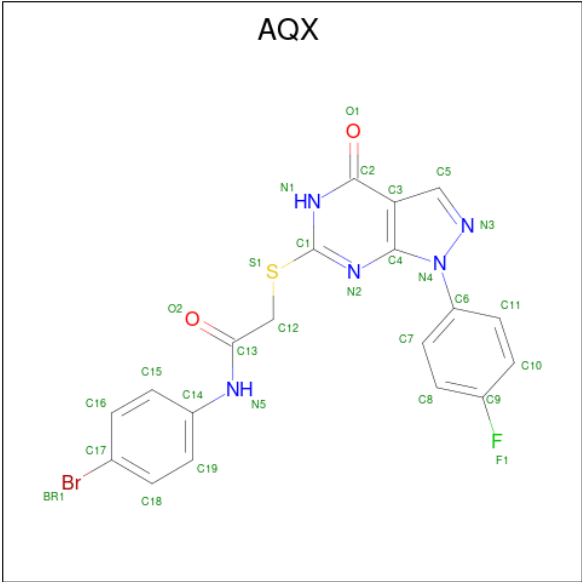
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is N-(4-bromophenyl)-2-{{[1-(4-fluorophenyl)-4-oxo-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-6-yl]sulfanyl}acetamide (CCD ID: AQX) (formula: C₁₉H₁₃BrFN₅O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	F	N	O	S		
6	C	1	58	2	38	2	10	4	2	0	1
6	D	1	87	3	57	3	15	6	3	0	1

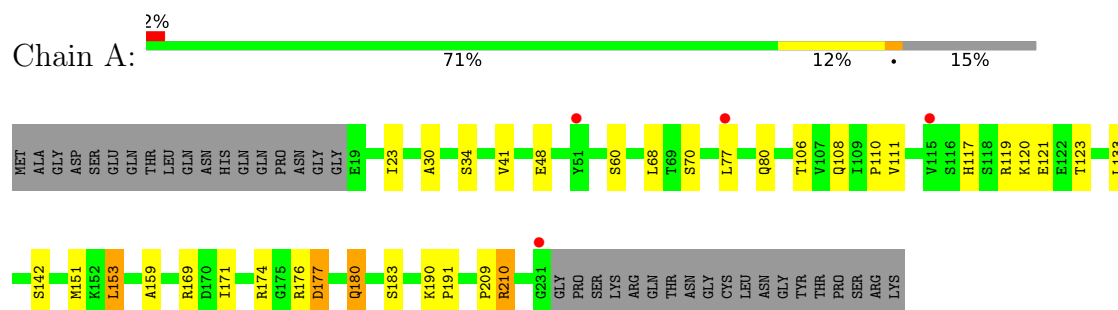
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total	O	0	0
			51	51		
7	B	66	Total	O	0	1
			67	67		
7	C	61	Total	O	0	0
			61	61		
7	D	55	Total	O	0	0
			55	55		

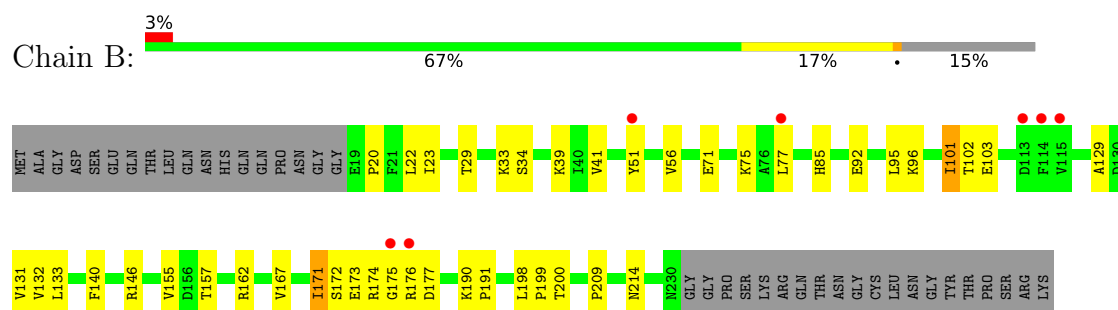
3 Residue-property plots [i](#)

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.

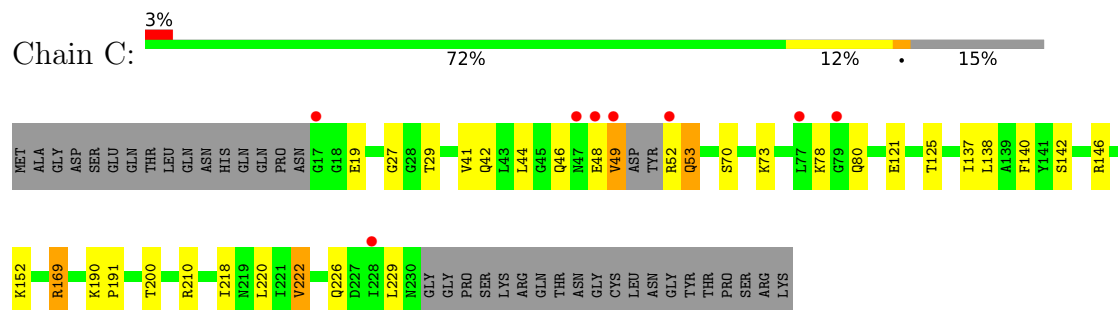
• Molecule 1: Uridine-cytidine kinase 2



• Molecule 1: Uridine-cytidine kinase 2

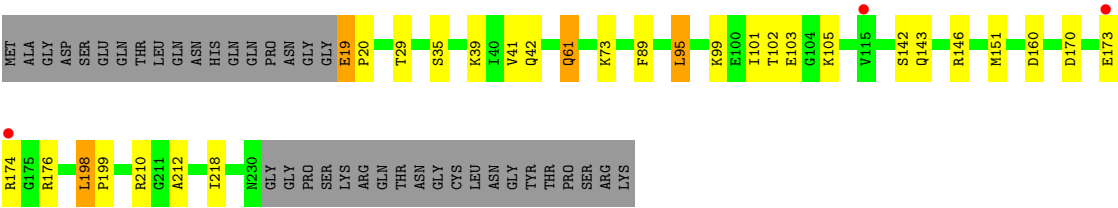


• Molecule 1: Uridine-cytidine kinase 2



• Molecule 1: Uridine-cytidine kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	84.09Å 93.89Å 157.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.40 39.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.70-2.40) 99.0 (39.70-2.40)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.257 0.204 , 0.257	Depositor DCC
R_{free} test set	2414 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: PEG, AQX, PGE, PG4, 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	1.01	0/1776	1.42	3/2401 (0.1%)
1	B	1.02	0/1763	1.44	3/2384 (0.1%)
1	C	1.04	0/1725	1.41	2/2329 (0.1%)
1	D	1.04	0/1728	1.45	3/2337 (0.1%)
All	All	1.03	0/6992	1.43	11/9451 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	177	ASP	CB-CA-C	5.83	119.49	109.51
1	C	121	GLU	N-CA-C	-5.60	104.57	111.40
1	B	101	ILE	CA-C-N	5.48	128.17	120.28
1	B	101	ILE	C-N-CA	5.48	128.17	120.28
1	D	61	GLN	CA-C-N	5.46	127.53	120.44
1	D	61	GLN	C-N-CA	5.46	127.53	120.44
1	D	160	ASP	CA-CB-CG	5.36	117.95	112.60
1	A	180	GLN	CB-CA-C	5.24	119.48	110.79
1	B	85	HIS	CB-CA-C	5.15	116.83	109.26
1	C	27	GLY	CA-C-O	-5.12	116.76	122.14

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	1732	0	1758	18	0
1	B	1725	0	1746	17	1
1	C	1695	0	1722	14	0
1	D	1699	0	1717	10	0
2	A	20	0	28	0	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	B	13	0	18	0	0
4	D	13	0	18	0	0
5	B	7	0	10	1	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
6	C	58	0	0	1	0
6	D	87	0	0	3	0
7	A	51	0	0	4	0
7	B	67	0	0	3	0
7	C	61	0	0	1	0
7	D	55	0	0	2	0
All	All	7321	0	7069	61	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (61) 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:210[B]:ARG:HB2	1:A:210[B]:ARG:HH11	1.46	0.80
1:B:162:ARG:NH2	7:B:402:HOH:O	2.17	0.77
1:B:92:GLU:OE2	7:B:401:HOH:O	2.09	0.71
6:D:301[A]:AQX:S1	7:D:407:HOH:O	2.50	0.70
6:D:301[A]:AQX:N1	6:D:301[A]:AQX:O2	2.27	0.68
1:A:210[A]:ARG:NH2	7:A:401:HOH:O	2.22	0.64
1:C:169[B]:ARG:HG3	7:C:427:HOH:O	2.00	0.61
1:A:108:GLN:NE2	1:A:123:THR:OG1	2.34	0.61
1:C:137:ILE:HG13	1:C:138:LEU:HG	1.84	0.60
1:B:157:THR:O	1:B:162:ARG:HD3	2.04	0.58
1:B:23:ILE:HB	1:B:133:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:SER:HB3	5:B:302:PEG:H22	1.85	0.57
1:A:30:ALA:H	3:A:303:GOL:H2	1.70	0.55
1:A:209:PRO:HB2	1:A:210[B]:ARG:HD3	1.88	0.55
1:A:210[A]:ARG:NE	7:A:401:HOH:O	2.36	0.54
1:D:212:ALA:HA	1:D:218:ILE:HD11	1.90	0.54
1:B:172:SER:O	1:B:174:ARG:N	2.41	0.54
1:C:53:GLN:HE21	1:C:53:GLN:HA	1.72	0.54
1:A:169:ARG:HD3	7:A:443:HOH:O	2.09	0.53
1:C:220:LEU:HD13	1:D:151:MET:HE1	1.91	0.53
1:A:68:LEU:HD12	1:A:117:HIS:HB3	1.92	0.53
1:B:172:SER:O	1:B:175:GLY:N	2.42	0.52
1:D:29:THR:HG23	7:D:422:HOH:O	2.10	0.52
1:B:29[A]:THR:HG23	7:B:445:HOH:O	2.10	0.52
1:C:49:VAL:HG21	1:C:52:ARG:CA	2.42	0.50
1:A:210[B]:ARG:HH11	1:A:210[B]:ARG:CB	2.23	0.49
1:C:49:VAL:HG21	1:C:52:ARG:N	2.27	0.49
1:B:33:LYS:HA	1:B:155:VAL:HG21	1.94	0.49
1:A:174:ARG:CG	1:A:176:ARG:HG3	2.43	0.48
1:B:140:PHE:HB2	1:B:200:THR:HB	1.95	0.48
1:B:167:VAL:O	1:B:171:ILE:HB	2.13	0.48
1:D:20:PRO:HG2	1:D:101:ILE:O	2.14	0.48
1:C:70:SER:HA	1:C:73:LYS:HE2	1.97	0.47
1:A:190:LYS:HB3	1:A:191:PRO:HD3	1.95	0.47
1:D:95:LEU:HD22	1:D:99:LYS:HE2	1.96	0.47
6:D:301[B]:AQX:S1	6:D:301[B]:AQX:C14	3.03	0.47
1:B:101:ILE:HG21	1:B:132:VAL:HG21	1.96	0.47
1:C:44:LEU:C	1:C:46:GLN:H	2.24	0.46
1:C:190:LYS:HB3	1:C:191:PRO:HD3	1.97	0.46
1:A:23:ILE:HB	1:A:133:LEU:HD23	1.98	0.46
1:C:140:PHE:HB2	1:C:200:THR:HB	1.98	0.46
1:C:78:LYS:HE2	1:C:80:GLN:NE2	2.32	0.45
1:D:198:LEU:N	1:D:199:PRO:CD	2.79	0.45
1:D:103:GLU:OE1	1:D:105:LYS:NZ	2.50	0.45
1:B:209:PRO:HD2	1:B:214:ASN:ND2	2.32	0.45
1:D:61:GLN:HG2	1:D:89:PHE:CD1	2.52	0.45
1:A:111:VAL:HG12	1:A:120:LYS:HD2	1.99	0.45
1:C:218:ILE:O	1:C:222:VAL:HG13	2.17	0.44
1:D:19:GLU:HG3	1:D:102:THR:O	2.18	0.44
1:A:210[A]:ARG:CZ	7:A:401:HOH:O	2.63	0.44
1:A:159:ALA:HB3	6:C:301[B]:AQX:C5	2.49	0.43
1:B:20:PRO:HB3	1:B:129:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:N	3:A:303:GOL:H2	2.33	0.42
1:D:170:ASP:HA	1:D:174:ARG:HD3	2.01	0.42
1:C:53:GLN:HE21	1:C:53:GLN:CA	2.32	0.42
1:C:146:ARG:O	1:C:152:LYS:HE3	2.19	0.41
1:B:190:LYS:HB3	1:B:191:PRO:HD3	2.00	0.41
1:B:56:VAL:HA	1:B:131:VAL:O	2.21	0.41
1:A:151:MET:HG2	1:A:153:LEU:HD13	2.03	0.41
1:A:110:PRO:HB3	1:A:119:ARG:HD3	2.03	0.40
1:B:198:LEU:N	1:B:199:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:OE2	1:B:103:GLU:OE2[2_565]	1.93	0.27

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	216/250 (86%)	213 (99%)	1 (0%)	2 (1%)	14	22
1	B	214/250 (86%)	206 (96%)	6 (3%)	2 (1%)	14	22
1	C	209/250 (84%)	202 (97%)	6 (3%)	1 (0%)	24	37
1	D	210/250 (84%)	201 (96%)	7 (3%)	2 (1%)	12	20
All	All	849/1000 (85%)	822 (97%)	20 (2%)	7 (1%)	21	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173[A]	GLU

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Mol	Chain	Res	Type
1	B	173[B]	GLU
1	C	210	ARG
1	A	210[A]	ARG
1	A	210[B]	ARG
1	D	173	GLU
1	D	210	ARG

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	195/220 (89%)	180 (92%)	15 (8%)	12	20
1	B	194/220 (88%)	180 (93%)	14 (7%)	13	23
1	C	189/220 (86%)	175 (93%)	14 (7%)	13	22
1	D	190/220 (86%)	178 (94%)	12 (6%)	16	29
All	All	768/880 (87%)	713 (93%)	55 (7%)	13	23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	41	VAL
1	A	48	GLU
1	A	60	SER
1	A	70	SER
1	A	77	LEU
1	A	80	GLN
1	A	106	THR
1	A	121	GLU
1	A	142	SER
1	A	153	LEU
1	A	171	ILE
1	A	177	ASP
1	A	180	GLN
1	A	183	SER

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Mol	Chain	Res	Type
1	B	22	LEU
1	B	39	LYS
1	B	41	VAL
1	B	51	TYR
1	B	71	GLU
1	B	75	LYS
1	B	77	LEU
1	B	95	LEU
1	B	96	LYS
1	B	102	THR
1	B	146	ARG
1	B	171	ILE
1	B	176	ARG
1	B	177	ASP
1	C	19	GLU
1	C	29	THR
1	C	41	VAL
1	C	42	GLN
1	C	48	GLU
1	C	49	VAL
1	C	53	GLN
1	C	125	THR
1	C	142	SER
1	C	169[A]	ARG
1	C	169[B]	ARG
1	C	222	VAL
1	C	226	GLN
1	C	229	LEU
1	D	19	GLU
1	D	35	SER
1	D	39	LYS
1	D	41	VAL
1	D	42	GLN
1	D	73	LYS
1	D	95	LEU
1	D	142	SER
1	D	143	GLN
1	D	146	ARG
1	D	176	ARG
1	D	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	117	HIS
1	B	184	GLN
1	C	53	GLN
1	C	80	GLN
1	C	91	ASN
1	C	223	GLN
1	C	226	GLN
1	D	42	GLN
1	D	80	GLN
1	D	108	GLN
1	D	117	HIS

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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	303	-	5,5,5	0.23	0	5,5,5	0.53	0
4	PG4	D	302	-	12,12,12	0.37	0	11,11,11	0.17	0
2	PGE	A	302	-	9,9,9	0.24	0	8,8,8	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	303	-	5,5,5	0.15	0	5,5,5	0.34	0
6	AQX	D	301[C]	-	32,32,32	0.98	4 (12%)	44,45,45	1.97	11 (25%)
2	PGE	A	301	-	9,9,9	0.33	0	8,8,8	0.28	0
6	AQX	C	301[B]	-	32,32,32	1.03	4 (12%)	44,45,45	1.94	11 (25%)
5	PEG	C	302	-	6,6,6	0.22	0	5,5,5	0.19	0
3	GOL	C	303	-	5,5,5	0.21	0	5,5,5	0.47	0
3	GOL	A	303	-	5,5,5	0.25	0	5,5,5	0.43	0
6	AQX	C	301[C]	-	32,32,32	1.02	4 (12%)	44,45,45	2.03	12 (27%)
5	PEG	B	302	-	6,6,6	0.28	0	5,5,5	0.19	0
6	AQX	D	301[A]	-	32,32,32	1.03	4 (12%)	44,45,45	1.98	12 (27%)
4	PG4	B	301	-	12,12,12	0.23	0	11,11,11	0.10	0
5	PEG	D	304	-	6,6,6	0.26	0	5,5,5	0.18	0
6	AQX	D	301[B]	-	32,32,32	1.04	4 (12%)	44,45,45	1.93	12 (27%)

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
3	GOL	D	303	-	-	4/4/4/4	-
4	PG4	D	302	-	-	3/10/10/10	-
2	PGE	A	302	-	-	2/7/7/7	-
3	GOL	B	303	-	-	2/4/4/4	-
6	AQX	D	301[C]	-	-	7/13/13/13	0/4/4/4
2	PGE	A	301	-	-	6/7/7/7	-
6	AQX	C	301[B]	-	-	6/13/13/13	0/4/4/4
5	PEG	C	302	-	-	3/4/4/4	-
3	GOL	C	303	-	-	2/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
6	AQX	C	301[C]	-	-	6/13/13/13	0/4/4/4
5	PEG	B	302	-	-	2/4/4/4	-
6	AQX	D	301[A]	-	-	5/13/13/13	0/4/4/4
4	PG4	B	301	-	-	5/10/10/10	-
5	PEG	D	304	-	-	3/4/4/4	-
6	AQX	D	301[B]	-	-	8/13/13/13	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301[A]	AQX	C2-N1	-3.05	1.33	1.38
6	C	301[C]	AQX	C2-N1	-3.01	1.33	1.38
6	D	301[B]	AQX	C2-N1	-2.99	1.33	1.38
6	C	301[B]	AQX	C2-N1	-2.97	1.33	1.38
6	C	301[B]	AQX	C3-C2	-2.84	1.39	1.45
6	D	301[A]	AQX	C3-C2	-2.79	1.39	1.45
6	C	301[C]	AQX	C5-N3	2.76	1.37	1.32
6	D	301[C]	AQX	C5-N3	2.70	1.36	1.32
6	D	301[C]	AQX	C2-N1	-2.65	1.33	1.38
6	D	301[C]	AQX	C3-C2	-2.55	1.40	1.45
6	D	301[B]	AQX	C3-C2	-2.47	1.40	1.45
6	C	301[B]	AQX	C3-C4	-2.38	1.39	1.45
6	D	301[B]	AQX	C5-N3	2.36	1.36	1.32
6	D	301[A]	AQX	C5-N3	2.32	1.36	1.32
6	C	301[C]	AQX	C3-C2	-2.32	1.40	1.45
6	C	301[B]	AQX	C5-N3	2.27	1.36	1.32
6	C	301[C]	AQX	C3-C4	-2.27	1.39	1.45
6	D	301[B]	AQX	C3-C4	-2.22	1.39	1.45
6	D	301[A]	AQX	C3-C4	-2.21	1.39	1.45
6	D	301[C]	AQX	C3-C4	-2.15	1.39	1.45

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301[B]	AQX	C5-N3-N4	6.39	109.69	104.59
6	D	301[A]	AQX	C5-N3-N4	6.20	109.54	104.59
6	C	301[C]	AQX	S1-C1-N2	-5.94	116.72	121.98
6	C	301[B]	AQX	C5-N3-N4	5.80	109.22	104.59
6	D	301[C]	AQX	C5-N3-N4	5.73	109.16	104.59
6	C	301[C]	AQX	C5-N3-N4	5.42	108.91	104.59
6	D	301[B]	AQX	C3-C4-N2	-4.93	123.71	127.44
6	C	301[B]	AQX	C3-C4-N2	-4.88	123.74	127.44
6	C	301[B]	AQX	S1-C1-N2	-4.46	118.03	121.98
6	D	301[C]	AQX	S1-C1-N2	-4.46	118.03	121.98
6	D	301[A]	AQX	C3-C4-N2	-4.44	124.08	127.44
6	C	301[C]	AQX	C3-C4-N2	-4.34	124.16	127.44
6	D	301[C]	AQX	C6-N4-N3	4.15	123.90	118.85
6	D	301[A]	AQX	S1-C1-N2	-4.15	118.30	121.98
6	D	301[B]	AQX	C3-C5-N3	-3.86	107.66	112.45
6	C	301[C]	AQX	C6-N4-N3	3.84	123.52	118.85
6	D	301[C]	AQX	C3-C5-N3	-3.82	107.71	112.45
6	D	301[C]	AQX	C3-C4-N2	-3.80	124.56	127.44
6	D	301[A]	AQX	C3-C5-N3	-3.75	107.79	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301[B]	AQX	C3-C5-N3	-3.71	107.84	112.45
6	D	301[B]	AQX	C5-C3-C4	3.70	107.33	104.57
6	D	301[A]	AQX	C6-N4-N3	3.62	123.25	118.85
6	D	301[C]	AQX	C2-C3-C4	-3.61	116.12	118.35
6	C	301[C]	AQX	C2-C3-C4	-3.56	116.14	118.35
6	D	301[A]	AQX	C5-C3-C4	3.48	107.17	104.57
6	C	301[C]	AQX	C3-C5-N3	-3.47	108.14	112.45
6	C	301[B]	AQX	C5-C3-C4	3.46	107.15	104.57
6	D	301[A]	AQX	C2-C3-C4	-3.40	116.25	118.35
6	D	301[C]	AQX	C5-C3-C4	3.39	107.10	104.57
6	D	301[A]	AQX	C3-C2-N1	3.35	120.31	114.45
6	D	301[B]	AQX	C4-N4-N3	-3.30	107.06	111.12
6	C	301[C]	AQX	C3-C2-N1	3.29	120.20	114.45
6	D	301[B]	AQX	C3-C2-N1	3.24	120.11	114.45
6	D	301[C]	AQX	C3-C2-N1	3.22	120.09	114.45
6	C	301[B]	AQX	C3-C2-N1	3.18	120.01	114.45
6	D	301[A]	AQX	C4-N4-N3	-3.13	107.27	111.12
6	C	301[B]	AQX	C6-N4-N3	2.97	122.46	118.85
6	C	301[B]	AQX	C4-N4-N3	-2.94	107.50	111.12
6	C	301[C]	AQX	C5-C3-C4	2.86	106.70	104.57
6	C	301[B]	AQX	C1-N1-C2	-2.84	117.74	123.46
6	D	301[B]	AQX	C6-N4-N3	2.83	122.29	118.85
6	D	301[B]	AQX	C2-C3-C4	-2.78	116.63	118.35
6	D	301[B]	AQX	C1-N1-C2	-2.77	117.89	123.46
6	C	301[C]	AQX	C1-N1-C2	-2.73	117.96	123.46
6	D	301[C]	AQX	C4-N4-N3	-2.73	107.75	111.12
6	D	301[A]	AQX	C1-N1-C2	-2.72	117.98	123.46
6	C	301[C]	AQX	C4-N4-N3	-2.70	107.80	111.12
6	D	301[C]	AQX	C1-N1-C2	-2.69	118.05	123.46
6	D	301[B]	AQX	S1-C1-N2	-2.50	119.77	121.98
6	D	301[B]	AQX	N1-C1-N2	2.31	127.82	123.84
6	C	301[B]	AQX	N1-C1-N2	2.29	127.78	123.84
6	D	301[A]	AQX	N1-C1-N2	2.25	127.71	123.84
6	C	301[C]	AQX	N1-C1-N2	2.25	127.71	123.84
6	C	301[B]	AQX	C2-C3-C4	-2.24	116.96	118.35
6	D	301[C]	AQX	N1-C1-N2	2.22	127.67	123.84
6	C	301[C]	AQX	O1-C2-N1	-2.18	116.01	120.11
6	D	301[A]	AQX	O1-C2-N1	-2.14	116.09	120.11
6	D	301[B]	AQX	O1-C2-N1	-2.06	116.24	120.11

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	GOL	O1-C1-C2-C3
3	C	303	GOL	O1-C1-C2-C3
3	D	303	GOL	O1-C1-C2-C3
3	D	303	GOL	C1-C2-C3-O3
6	C	301[B]	AQX	N1-C1-S1-C12
6	C	301[B]	AQX	N2-C1-S1-C12
6	C	301[B]	AQX	C12-C13-N5-C14
6	C	301[B]	AQX	O2-C13-N5-C14
6	C	301[C]	AQX	N1-C1-S1-C12
6	C	301[C]	AQX	N2-C1-S1-C12
6	C	301[C]	AQX	C12-C13-N5-C14
6	D	301[A]	AQX	N1-C1-S1-C12
6	D	301[A]	AQX	N2-C1-S1-C12
6	D	301[A]	AQX	C12-C13-N5-C14
6	D	301[B]	AQX	N1-C1-S1-C12
6	D	301[B]	AQX	N2-C1-S1-C12
6	D	301[B]	AQX	C12-C13-N5-C14
6	D	301[C]	AQX	N1-C1-S1-C12
6	D	301[C]	AQX	N2-C1-S1-C12
6	D	301[C]	AQX	C12-C13-N5-C14
6	D	301[C]	AQX	O2-C13-N5-C14
6	D	301[A]	AQX	O2-C13-N5-C14
6	D	301[B]	AQX	O2-C13-N5-C14
6	C	301[C]	AQX	O2-C13-N5-C14
2	A	301	PGE	O2-C3-C4-O3
6	C	301[B]	AQX	C19-C14-N5-C13
6	C	301[B]	AQX	C15-C14-N5-C13
4	B	301	PG4	O2-C3-C4-O3
4	B	301	PG4	O1-C1-C2-O2
4	B	301	PG4	O3-C5-C6-O4
2	A	301	PGE	O1-C1-C2-O2
2	A	301	PGE	O3-C5-C6-O4
2	A	302	PGE	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-O2
3	C	303	GOL	O1-C1-C2-O2
3	D	303	GOL	O1-C1-C2-O2
5	B	302	PEG	O2-C3-C4-O4
6	D	301[B]	AQX	S1-C12-C13-N5
5	C	302	PEG	O2-C3-C4-O4
3	D	303	GOL	O2-C2-C3-O3
4	B	301	PG4	C3-C4-O3-C5
2	A	301	PGE	C4-C3-O2-C2
2	A	301	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
6	D	301[B]	AQX	S1-C12-C13-O2
2	A	302	PGE	C6-C5-O3-C4
6	D	301[A]	AQX	C13-C12-S1-C1
6	C	301[C]	AQX	C7-C6-N4-N3
6	D	301[C]	AQX	C7-C6-N4-C4
4	D	302	PG4	O1-C1-C2-O2
6	D	301[C]	AQX	C11-C6-N4-C4
4	B	301	PG4	C5-C6-O4-C7
6	C	301[C]	AQX	C11-C6-N4-N3
5	B	302	PEG	C4-C3-O2-C2
5	C	302	PEG	O1-C1-C2-O2
4	D	302	PG4	O4-C7-C8-O5
6	D	301[B]	AQX	C7-C6-N4-C4
6	D	301[C]	AQX	C15-C14-N5-C13
6	D	301[B]	AQX	C11-C6-N4-C4
5	D	304	PEG	C1-C2-O2-C3
4	D	302	PG4	C1-C2-O2-C3
5	C	302	PEG	C4-C3-O2-C2
3	B	303	GOL	C1-C2-C3-O3
5	D	304	PEG	O1-C1-C2-O2
5	D	304	PEG	O2-C3-C4-O4
2	A	301	PGE	C6-C5-O3-C4
3	B	303	GOL	O2-C2-C3-O3

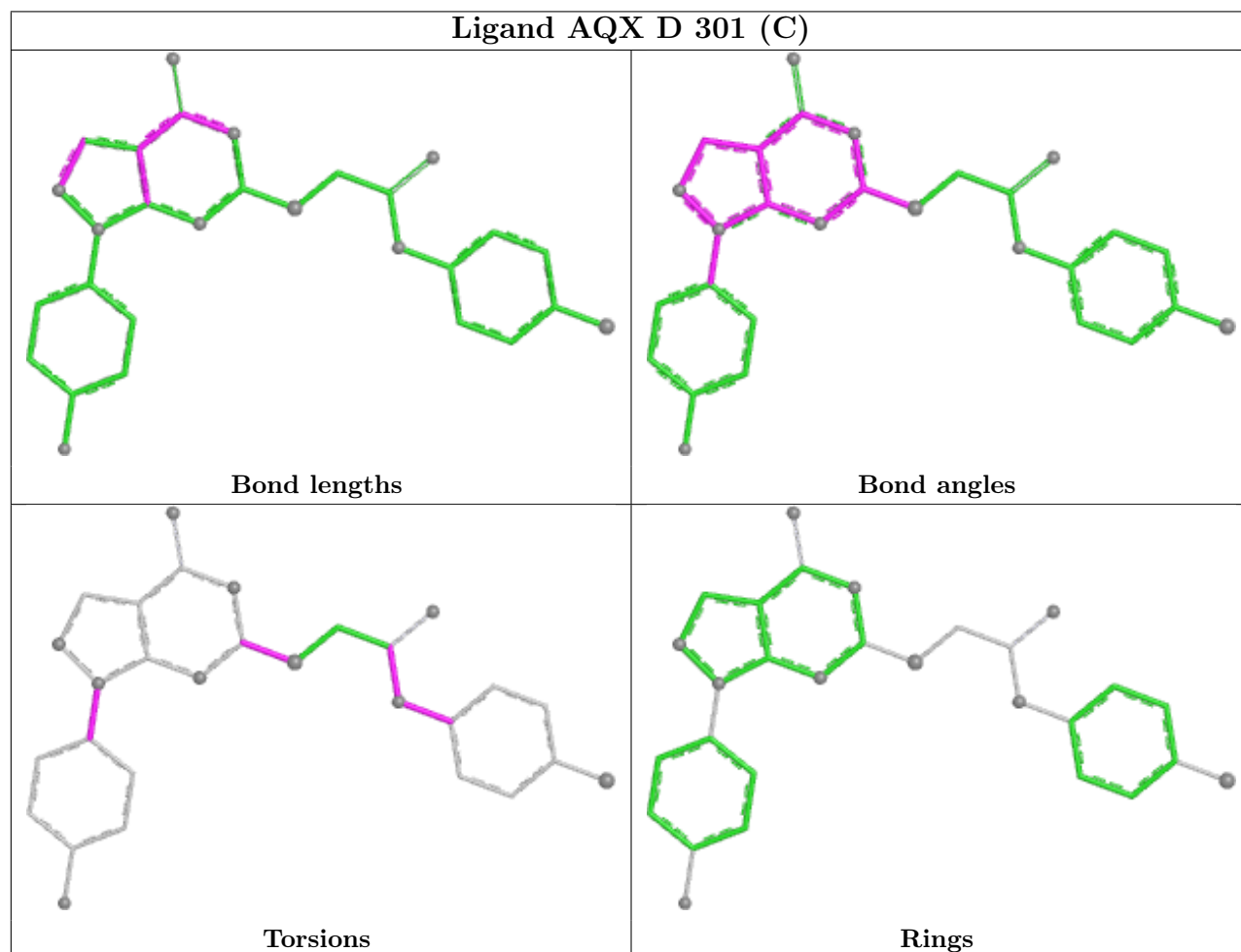
There are no ring outliers.

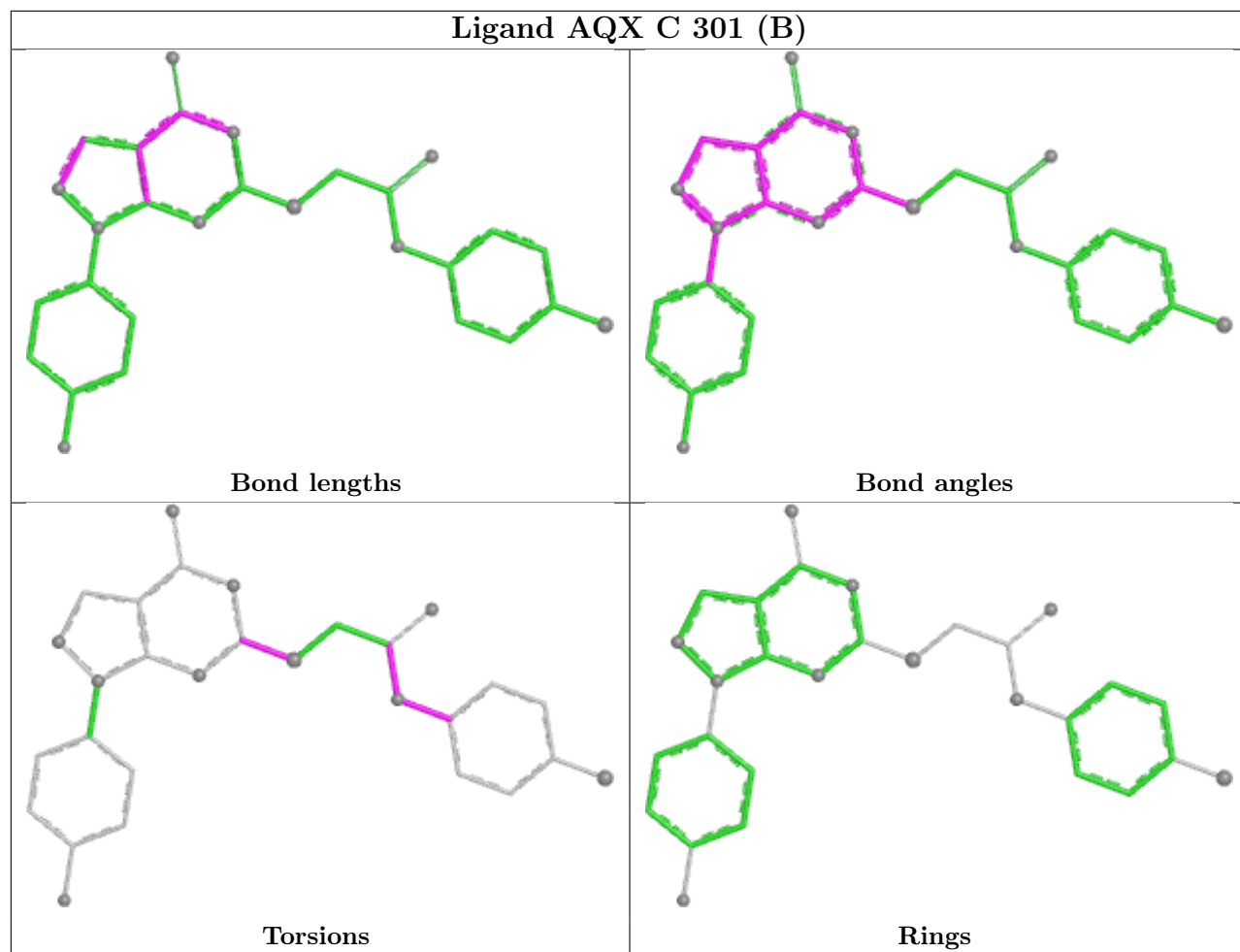
5 monomers are involved in 7 short contacts:

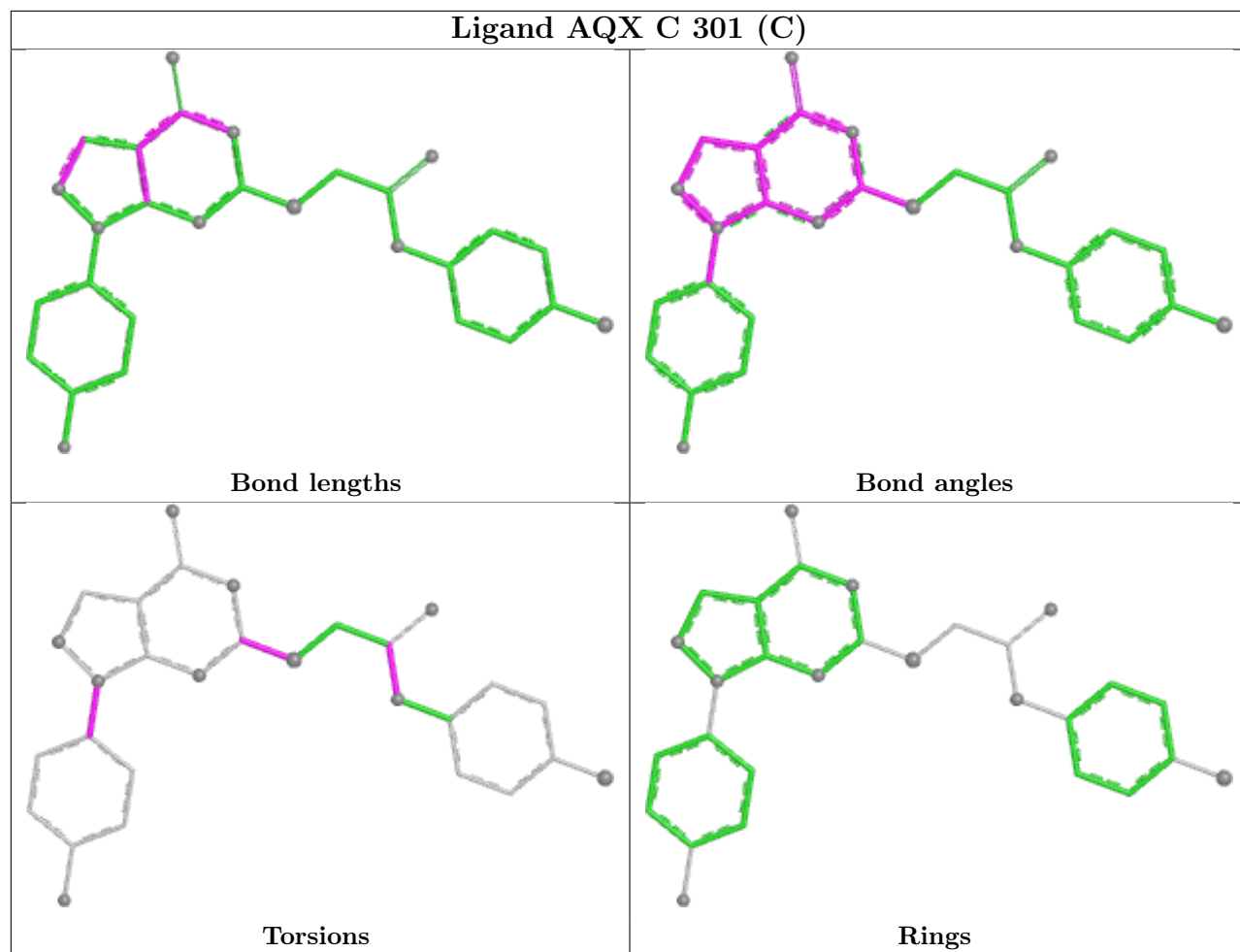
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301[B]	AQX	1	0
3	A	303	GOL	2	0
5	B	302	PEG	1	0
6	D	301[A]	AQX	2	0
6	D	301[B]	AQX	1	0

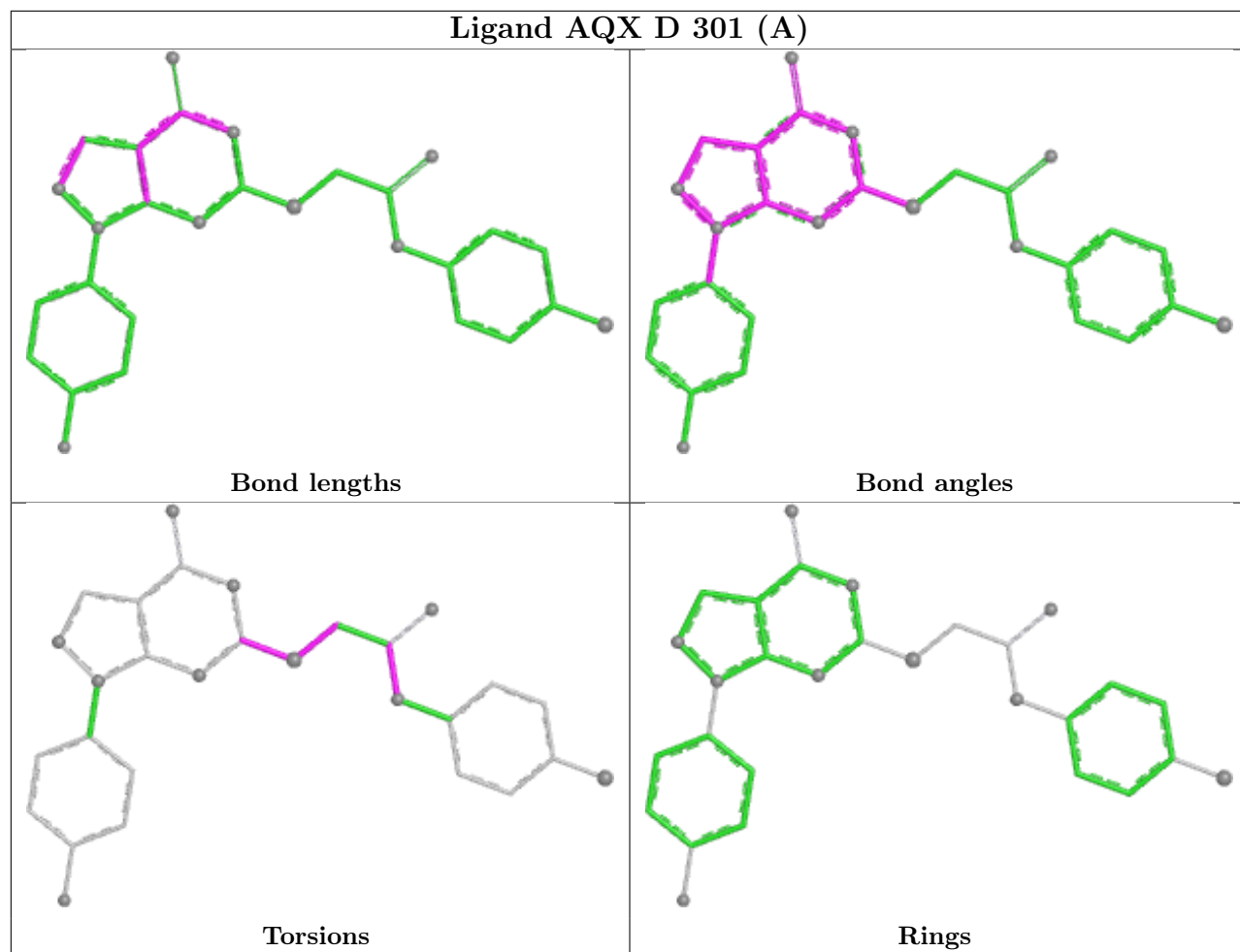
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

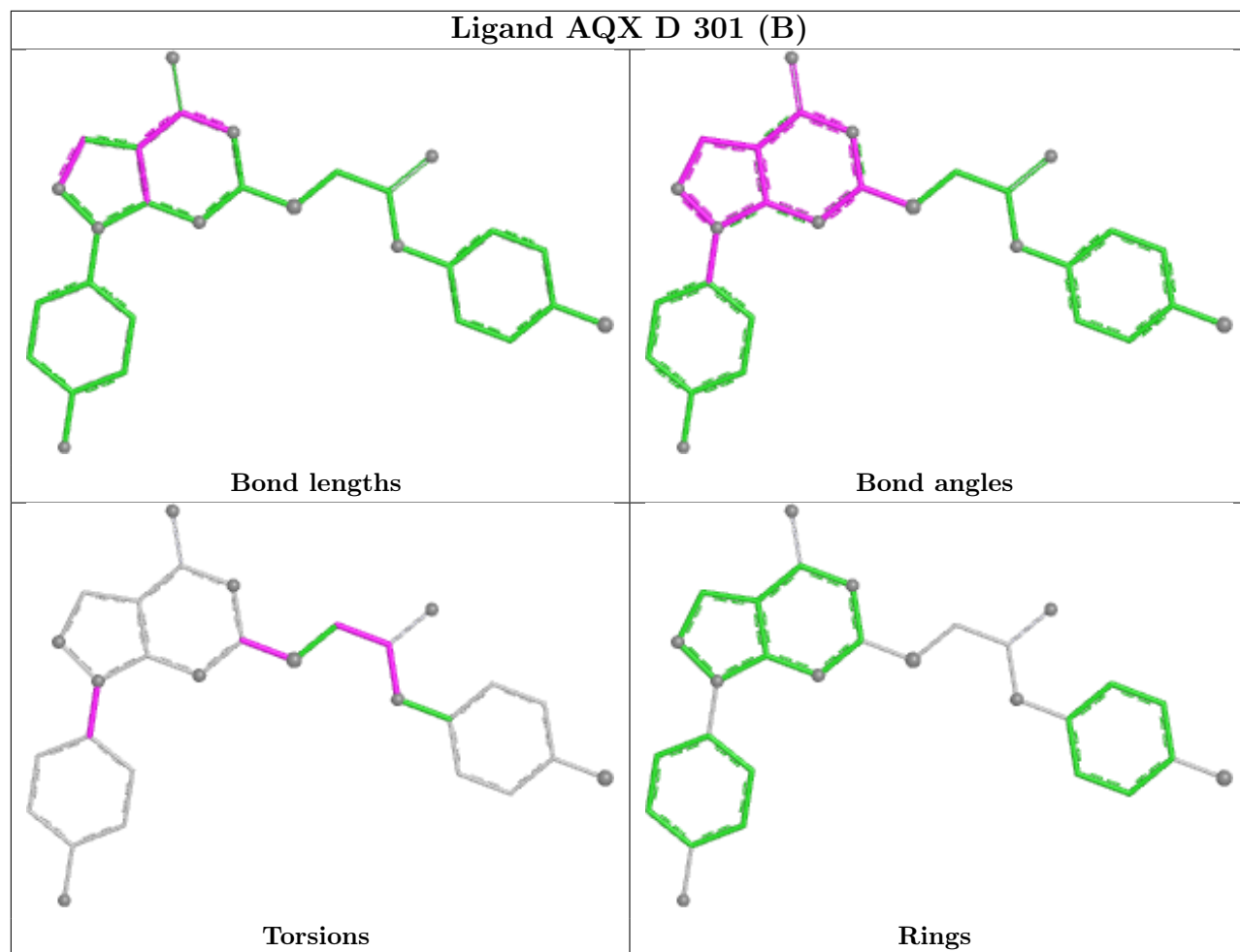
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents 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	213/250 (85%)	-0.03	4 (1%) 66 62	22, 46, 81, 110	5 (2%)
1	B	212/250 (84%)	0.01	7 (3%) 49 45	21, 43, 83, 116	4 (1%)
1	C	212/250 (84%)	-0.00	8 (3%) 44 40	28, 46, 81, 124	1 (0%)
1	D	212/250 (84%)	0.00	3 (1%) 73 69	32, 50, 75, 96	0
All	All	849/1000 (84%)	-0.00	22 (2%) 57 53	21, 46, 81, 124	10 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TYR	4.2
1	C	49	VAL	4.2
1	C	52	ARG	3.7
1	C	79	GLY	3.5
1	B	51	TYR	3.1
1	B	114	PHE	3.1
1	C	47	ASN	3.1
1	A	77	LEU	3.0
1	B	115	VAL	2.9
1	A	231	GLY	2.9
1	B	77	LEU	2.8
1	C	17	GLY	2.8
1	C	48	GLU	2.7
1	C	228	ILE	2.6
1	D	115	VAL	2.5
1	B	175	GLY	2.3
1	D	174	ARG	2.3
1	A	115	VAL	2.3
1	C	77	LEU	2.1
1	B	176	ARG	2.1
1	D	173	GLU	2.0
1	B	113	ASP	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 ⓘ

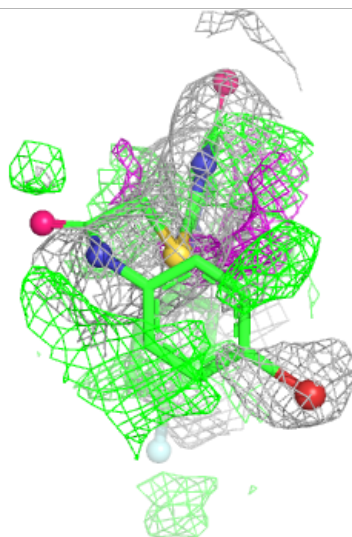
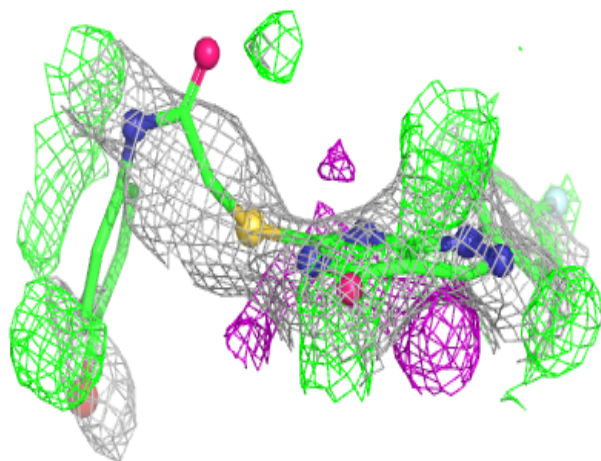
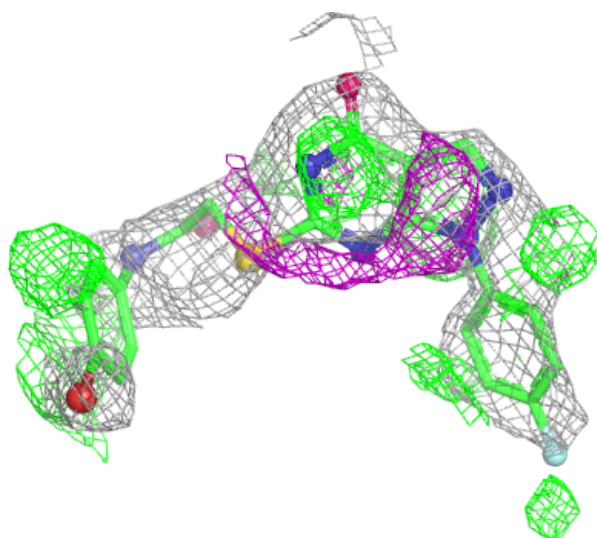
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AQX	C	301[B]	29/29	0.73	0.37	73,93,124,126	29
6	AQX	C	301[C]	29/29	0.73	0.37	71,91,102,111	29
6	AQX	D	301[A]	29/29	0.78	0.33	50,64,81,82	29
6	AQX	D	301[B]	29/29	0.78	0.33	52,61,71,73	29
6	AQX	D	301[C]	29/29	0.78	0.33	77,92,109,114	29
5	PEG	B	302	7/7	0.85	0.21	43,53,63,69	0
5	PEG	D	304	7/7	0.86	0.18	60,65,78,79	0
3	GOL	D	303	6/6	0.87	0.19	56,58,62,67	0
5	PEG	C	302	7/7	0.87	0.17	67,68,71,71	0
2	PGE	A	302	10/10	0.88	0.20	51,64,71,71	10
4	PG4	D	302	13/13	0.89	0.15	51,61,89,96	0
3	GOL	B	303	6/6	0.90	0.15	56,66,70,74	0
3	GOL	C	303	6/6	0.90	0.15	44,48,54,55	0
2	PGE	A	301	10/10	0.90	0.12	57,63,69,70	0
3	GOL	A	303	6/6	0.91	0.18	51,54,64,68	0
4	PG4	B	301	13/13	0.92	0.11	62,65,71,76	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.

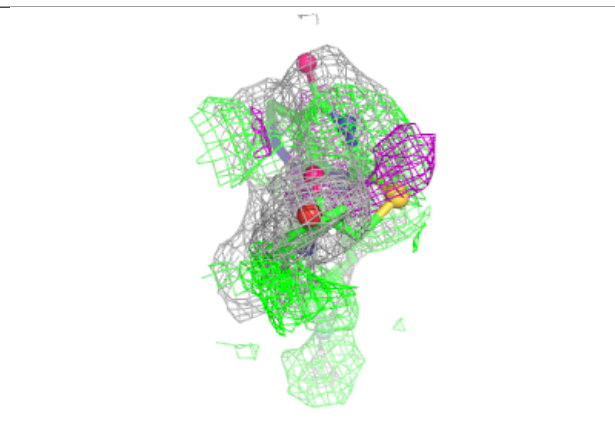
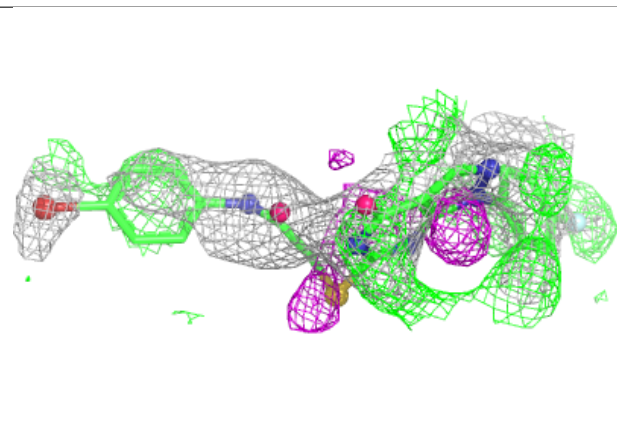
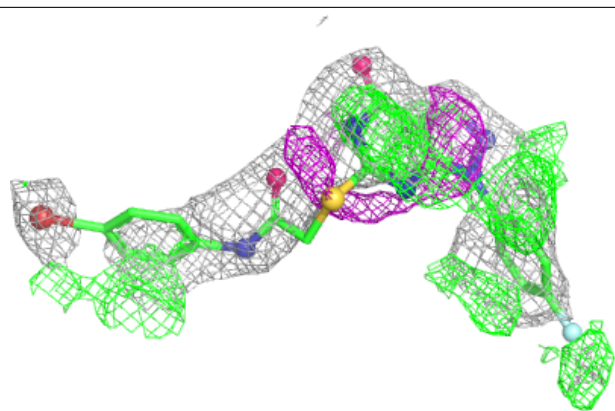
Electron density around AQX C 301 (B):

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

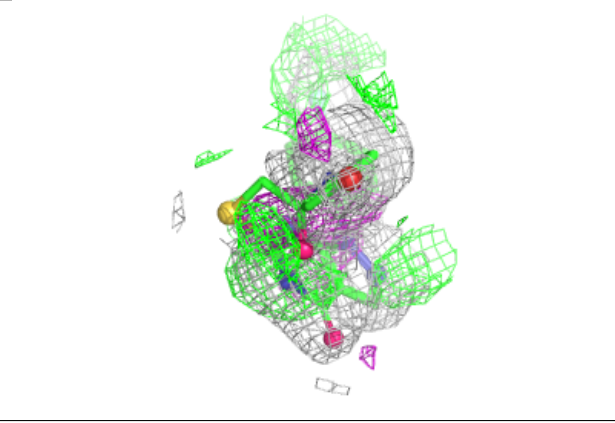
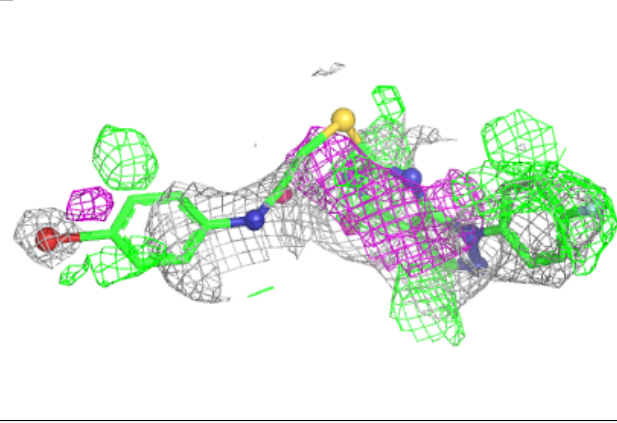
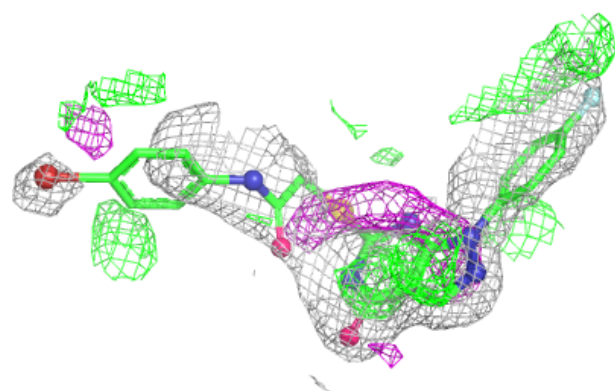


Electron density around AQX C 301 (C):

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

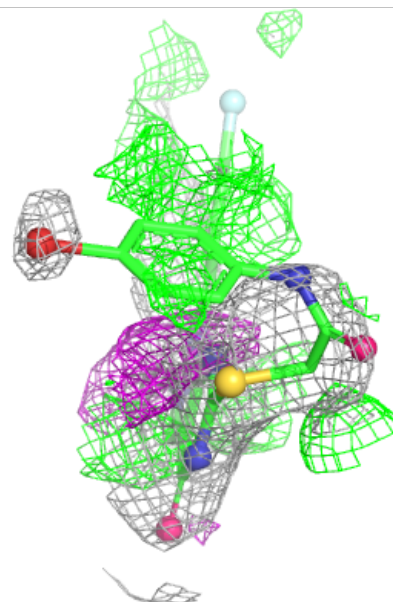
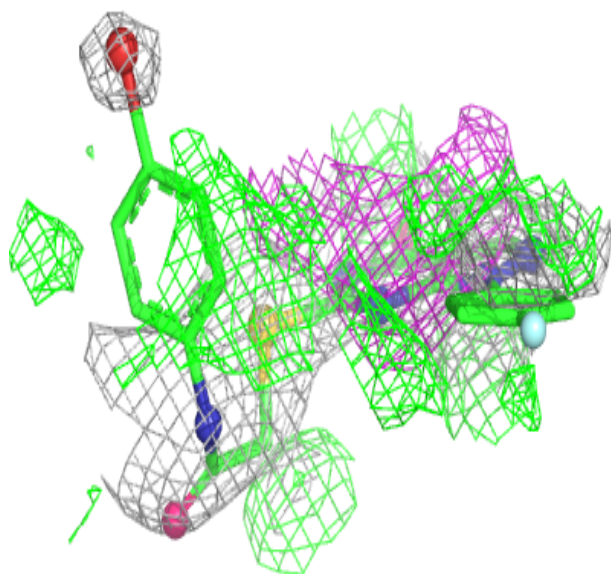
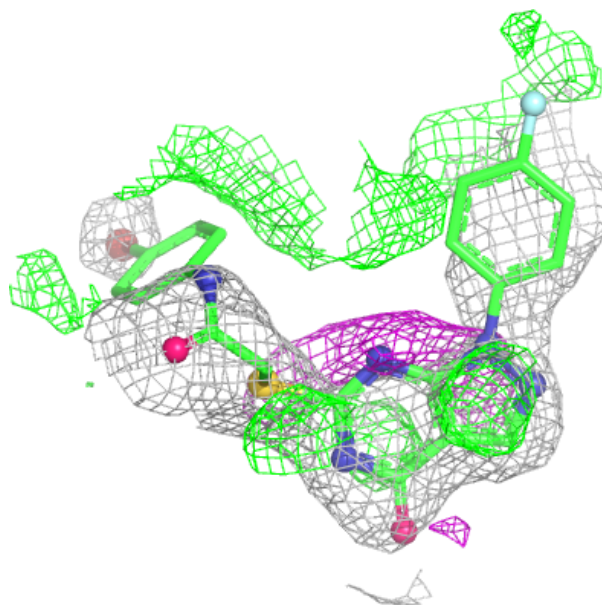
**Electron density around AQX D 301 (A):**

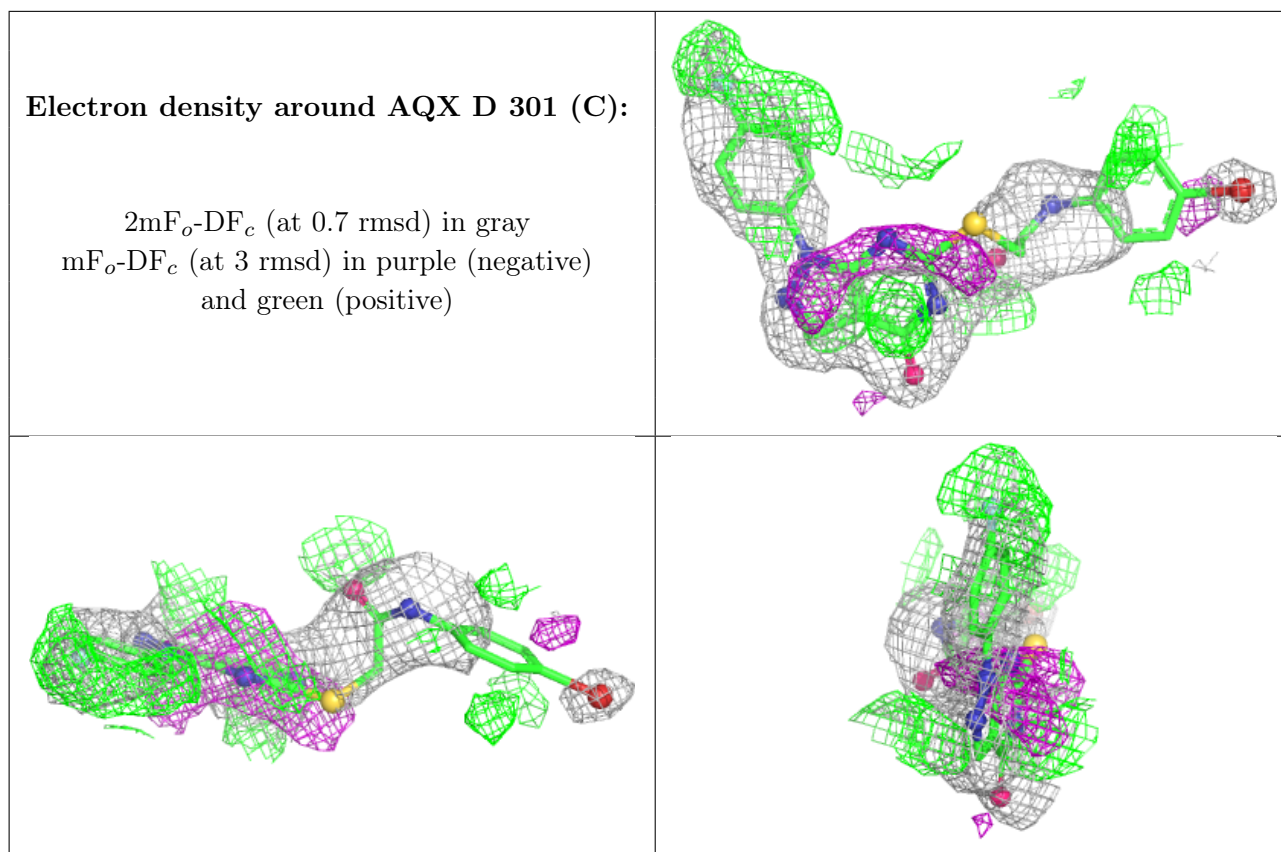
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AQX D 301 (B):

$2mF_o-DF_c$ (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.