



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 7B48 / pdb_00007b48
Title : Structural basis of reactivation of oncogenic p53 mutants by a small molecule: methylene quinuclidinone (MQ). Human p53DBD-R273H mutant bound to MQ: R273H-MQ (II)
Authors : Degtjarik, O.; Rozenberg, H.; Shakked, Z.
Deposited on : 2020-12-02
Resolution : 2.05 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

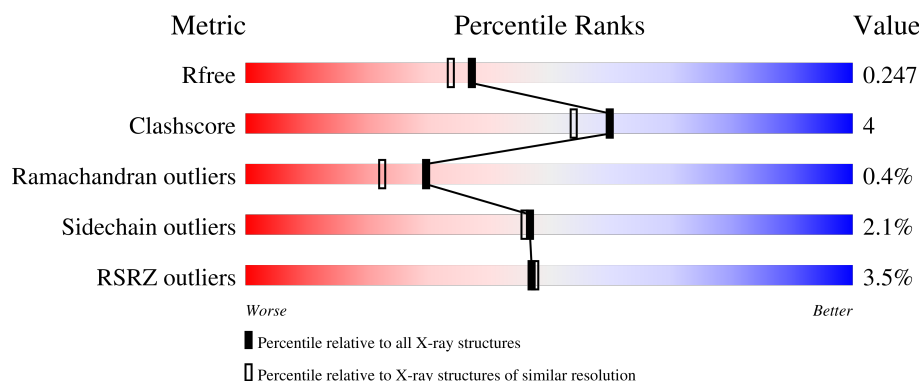
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	200	3% 78% 18% .
1	B	200	3% 82% 14% .
1	C	200	4% 79% 15% ..
1	D	200	4% 84% 10% 6%

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
4	EDO	B	303	-	-	X	-
6	PEG	C	305	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6615 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	4	0
			1526	941	277	289	19			
1	B	193	Total	C	N	O	S	0	3	0
			1519	937	277	286	19			
1	C	192	Total	C	N	O	S	0	3	0
			1517	936	277	285	19			
1	D	189	Total	C	N	O	S	0	5	0
			1499	924	276	281	18			

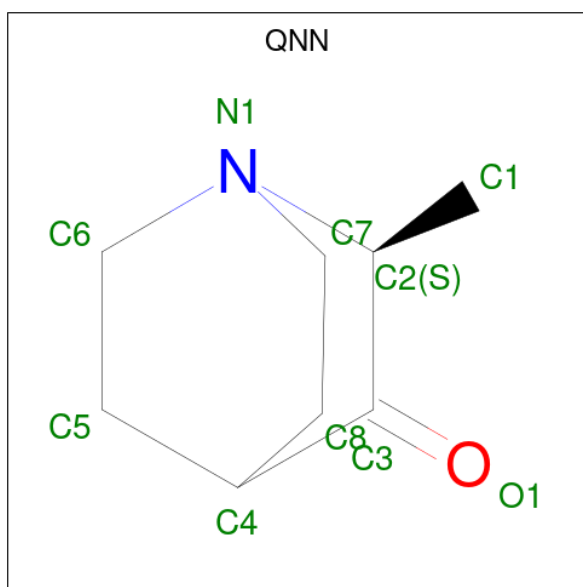
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	HIS	ARG	engineered mutation	UNP P04637
B	273	HIS	ARG	engineered mutation	UNP P04637
C	273	HIS	ARG	engineered mutation	UNP P04637
D	273	HIS	ARG	engineered mutation	UNP P04637

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is (2 {S})-2-methyl-1-azabicyclo[2.2.2]octan-3-one (CCD ID: QNN) (formula: C₈H₁₃NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	1
			10	8	1	1		
3	C	1	Total	C	N	O	0	1
			10	8	1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



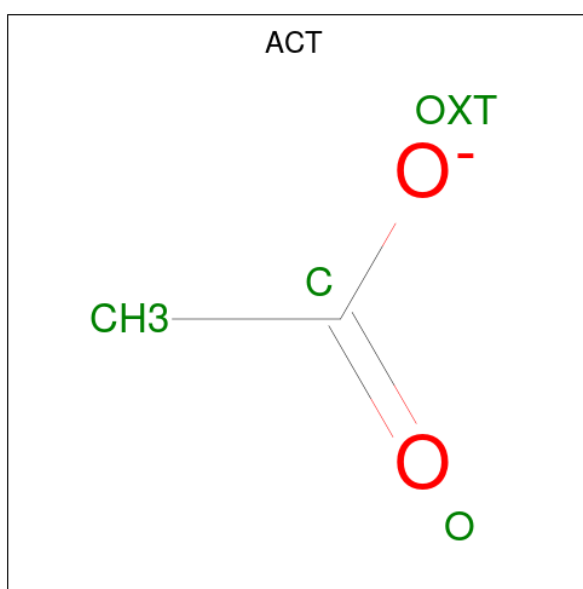
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

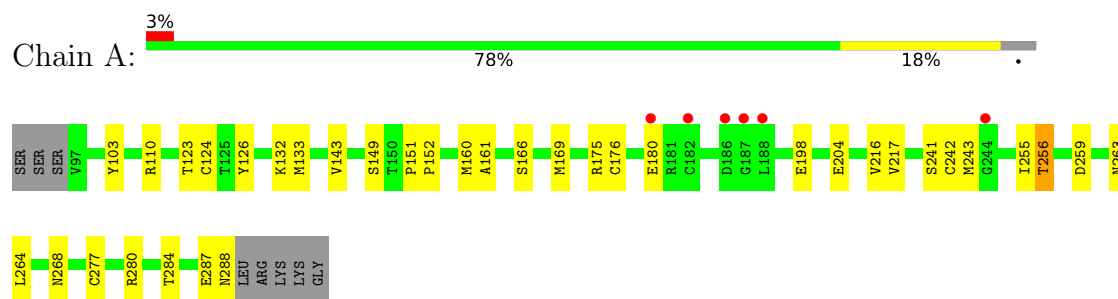
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total	O	0	2
			144	144		
7	B	83	Total	O	0	0
			83	83		
7	C	110	Total	O	0	2
			112	112		
7	D	134	Total	O	0	4
			138	138		

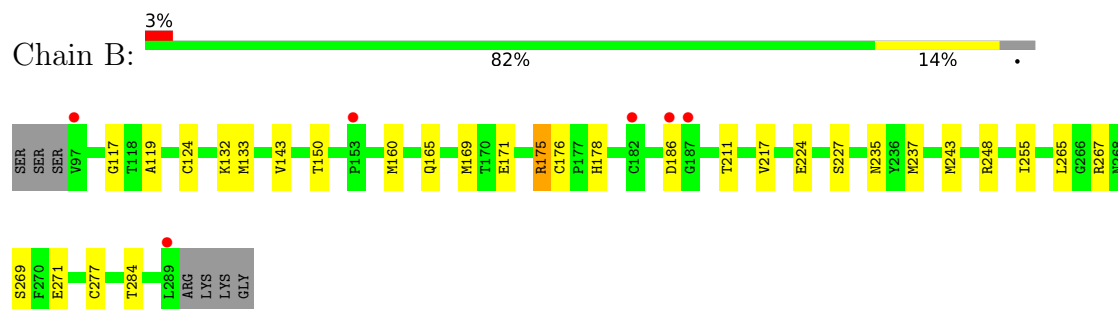
3 Residue-property plots [i](#)

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.

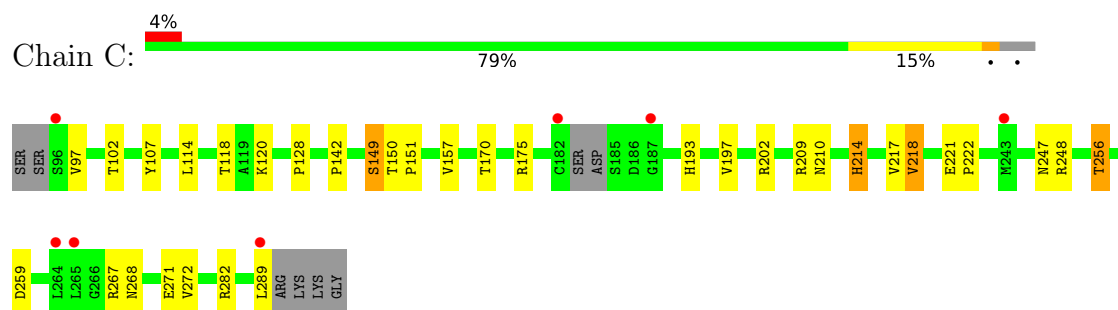
• Molecule 1: Cellular tumor antigen p53



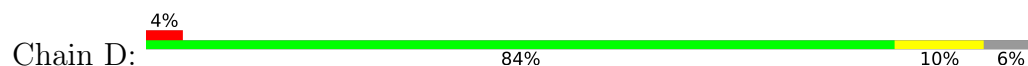
• Molecule 1: Cellular tumor antigen p53

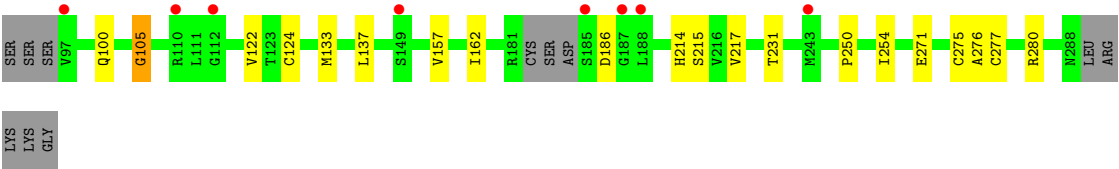


• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.25Å 72.00Å 85.23Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	36.67 – 2.05 36.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.9 (36.67-2.05) 98.2 (36.67-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.176 , 0.228 0.193 , 0.247	Depositor DCC
R_{free} test set	2503 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.049 for h,-k,-l	Xtriage
Reported twinning fraction	0.756 for H, K, L 0.244 for -h,-k,l	Depositor
Outliers	0 of 51884 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6615	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PEG, ZN, QNN, EDO

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	1.31	8/1562 (0.5%)	1.39	5/2122 (0.2%)
1	B	1.28	5/1555 (0.3%)	1.48	9/2115 (0.4%)
1	C	1.24	3/1552 (0.2%)	1.41	7/2107 (0.3%)
1	D	1.27	4/1533 (0.3%)	1.43	7/2081 (0.3%)
All	All	1.28	20/6202 (0.3%)	1.43	28/8425 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ALA	C-O	9.50	1.35	1.23
1	B	171	GLU	C-O	8.79	1.35	1.23
1	C	120	LYS	C-O	-8.33	1.14	1.24
1	B	255	ILE	C-O	8.31	1.33	1.24
1	B	143	VAL	C-O	7.23	1.31	1.24
1	A	216	VAL	C-O	6.91	1.31	1.24
1	D	217	VAL	C-O	6.46	1.30	1.24
1	A	160	MET	C-O	6.34	1.31	1.23
1	D	157	VAL	C-O	6.05	1.30	1.24
1	A	268	ASN	C-O	5.67	1.30	1.23
1	A	143	VAL	C-O	5.62	1.30	1.24
1	B	267	ARG	C-O	5.35	1.30	1.23
1	C	170	THR	C-O	-5.30	1.17	1.24
1	A	126	TYR	C-O	5.28	1.30	1.23
1	A	132	LYS	C-O	5.25	1.29	1.23
1	C	214	HIS	C-O	5.23	1.30	1.23
1	D	214	HIS	CE1-NE2	5.20	1.37	1.32
1	B	265	LEU	C-O	5.19	1.30	1.23
1	A	255	ILE	C-O	5.14	1.29	1.24
1	D	215	SER	C-O	5.09	1.30	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	VAL	CA-C-N	8.11	131.14	120.28
1	D	122	VAL	C-N-CA	8.11	131.14	120.28
1	C	118	THR	CA-C-O	-6.36	112.83	120.65
1	C	259	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	105	GLY	CA-C-N	6.14	128.80	120.38
1	D	105	GLY	C-N-CA	6.14	128.80	120.38
1	D	275	CYS	CA-C-N	5.97	128.43	120.55
1	D	275	CYS	C-N-CA	5.97	128.43	120.55
1	B	150	THR	CA-CB-OG1	-5.94	100.69	109.60
1	B	217	VAL	CB-CA-C	5.91	119.60	110.50
1	A	256	THR	CA-CB-OG1	-5.90	100.75	109.60
1	D	231	THR	CB-CA-C	5.78	119.78	109.38
1	B	175	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	C	175	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	152	PRO	N-CA-C	5.49	117.39	110.70
1	C	218	VAL	N-CA-C	-5.46	102.84	109.01
1	B	117	GLY	CA-C-O	-5.43	116.26	122.78
1	C	271	GLU	CB-CA-C	5.36	119.33	109.46
1	B	235	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	123	THR	CB-CA-C	-5.33	100.94	110.70
1	B	165	GLN	CA-C-N	5.28	127.61	120.38
1	B	165	GLN	C-N-CA	5.28	127.61	120.38
1	A	175	ARG	NE-CZ-NH1	-5.12	116.39	121.50
1	A	198	GLU	CB-CA-C	5.10	118.05	109.48
1	C	256	THR	CA-CB-OG1	-5.10	101.95	109.60
1	B	119	ALA	CA-C-N	5.07	128.43	120.82
1	B	119	ALA	C-N-CA	5.07	128.43	120.82
1	C	222	PRO	N-CA-C	-5.04	104.55	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1526	0	1455	15	0
1	B	1519	0	1451	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1517	0	1449	17	0
1	D	1499	0	1422	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	B	8	0	12	5	0
4	C	8	0	12	0	0
4	D	8	0	12	2	0
5	B	4	0	3	0	0
5	D	4	0	3	0	0
6	B	7	0	10	0	0
6	C	7	0	10	5	0
6	D	7	0	10	1	0
7	A	144	0	0	1	0
7	B	83	0	0	1	0
7	C	112	0	0	1	0
7	D	138	0	0	0	0
All	All	6615	0	5849	52	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 (52) 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:D:280:ARG:HG2	1:D:280:ARG:HH11	1.45	0.81
1:D:124:CYS:SG	1:D:133[A]:MET:SD	2.93	0.67
1:D:271:GLU:OE2	6:D:305:PEG:O4	2.14	0.65
1:B:211:THR:OG1	4:B:303:EDO:H22	1.98	0.64
1:C:202:ARG:NH2	1:C:221:GLU:OE2	2.30	0.62
1:A:264:LEU:HD23	1:B:243:MET:CE	2.30	0.62
1:A:277[B]:CYS:SG	1:A:280:ARG:NH2	2.70	0.59
1:D:250:PRO:HA	4:D:302:EDO:C2	2.33	0.59
1:A:264:LEU:HD23	1:B:243:MET:HE1	1.86	0.58
1:C:157:VAL:O	1:C:217:VAL:HA	2.06	0.54
1:B:211:THR:HG1	4:B:303:EDO:H22	1.72	0.53
1:D:162[B]:ILE:HD12	1:D:254:ILE:HD11	1.89	0.53
1:B:124:CYS:SG	1:B:133:MET:SD	3.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HD3	1:B:237:MET:HB2	1.92	0.52
1:A:124:CYS:SG	1:A:133[A]:MET:SD	3.07	0.51
1:B:248:ARG:HB3	1:B:248:ARG:CZ	2.40	0.51
1:B:160:MET:HE1	4:B:303:EDO:C1	2.41	0.50
1:C:247:ASN:OD1	1:C:248:ARG:NH1	2.46	0.49
1:A:264:LEU:CD2	1:B:243:MET:HE1	2.43	0.49
1:D:137:LEU:HD22	4:D:303:EDO:H11	1.95	0.48
1:A:241:SER:O	1:A:242:CYS:C	2.57	0.47
1:C:256:THR:HG22	1:C:267:ARG:HG3	1.97	0.47
1:B:160:MET:HE1	4:B:303:EDO:H11	1.96	0.47
1:C:268:ASN:HB3	7:C:460:HOH:O	2.14	0.47
1:C:102:THR:HG23	1:C:268:ASN:OD1	2.15	0.46
1:A:103:TYR:CG	1:B:243:MET:HE3	2.51	0.46
1:B:176:CYS:SG	1:B:178:HIS:HB3	2.56	0.46
1:C:114:LEU:HD12	1:C:142:PRO:HG2	1.96	0.46
1:D:100:GLN:NE2	1:D:162[A]:ILE:HD12	2.30	0.46
1:D:280:ARG:HG2	1:D:280:ARG:NH1	2.22	0.46
1:C:282:ARG:NH2	6:C:305:PEG:C2	2.79	0.45
1:B:277[B]:CYS:SG	7:B:483:HOH:O	2.62	0.45
1:C:128:PRO:CD	6:C:305:PEG:H22	2.47	0.45
1:C:193:HIS:CE1	1:C:214:HIS:HB3	2.53	0.44
1:A:204:GLU:HB3	1:A:217:VAL:HG13	1.99	0.44
1:C:282:ARG:HH22	6:C:305:PEG:C2	2.30	0.44
1:B:132:LYS:HG3	1:B:271:GLU:HG2	2.00	0.44
1:A:259:ASP:OD2	1:A:263:ASN:HB2	2.18	0.43
1:C:128:PRO:HD3	6:C:305:PEG:H41	2.00	0.43
1:A:284:THR:O	1:A:287:GLU:HG2	2.17	0.43
1:C:282:ARG:NH2	6:C:305:PEG:H21	2.34	0.42
1:A:176:CYS:O	1:A:180:GLU:HG3	2.19	0.42
1:B:277[B]:CYS:SG	1:B:277[B]:CYS:O	2.77	0.42
1:C:209:ARG:HG3	1:C:210:ASN:OD1	2.20	0.42
1:A:256:THR:HG23	7:A:506:HOH:O	2.19	0.42
1:A:149:SER:O	1:A:151:PRO:HD3	2.19	0.42
1:B:160:MET:HE1	4:B:303:EDO:H12	2.02	0.41
1:C:149:SER:HB3	1:D:276:ALA:HB1	2.02	0.41
1:A:166:SER:HA	1:A:169:MET:HE3	2.03	0.41
1:A:103:TYR:CD2	1:B:243:MET:HE3	2.56	0.41
1:C:197:VAL:HG11	1:C:218:VAL:HG11	2.02	0.40
1:C:107:TYR:CE2	1:C:151:PRO:HA	2.56	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	194/200 (97%)	190 (98%)	4 (2%)	0	100	100
1	B	194/200 (97%)	188 (97%)	5 (3%)	1 (0%)	24	16
1	C	191/200 (96%)	184 (96%)	6 (3%)	1 (0%)	24	16
1	D	190/200 (95%)	183 (96%)	6 (3%)	1 (0%)	24	16
All	All	769/800 (96%)	745 (97%)	21 (3%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	VAL
1	B	186	ASP
1	D	105	GLY

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	173/179 (97%)	170 (98%)	3 (2%)	53	53
1	B	172/179 (96%)	167 (97%)	5 (3%)	37	33
1	C	172/179 (96%)	168 (98%)	4 (2%)	44	42
1	D	167/179 (93%)	164 (98%)	3 (2%)	51	51
All	All	684/716 (96%)	669 (98%)	15 (2%)	47	44

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

Mol	Chain	Res	Type
1	A	110	ARG
1	A	243	MET
1	A	288	ASN
1	B	169	MET
1	B	224	GLU
1	B	227	SER
1	B	269	SER
1	B	284	THR
1	C	149	SER
1	C	150	THR
1	C	272	VAL
1	C	289	LEU
1	D	186	ASP
1	D	277[A]	CYS
1	D	277[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	GLN
1	B	131	ASN
1	B	268	ASN
1	B	288	ASN
1	D	168	HIS
1	D	178	HIS

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, 4 are monoatomic - leaving 13 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	$\# Z > 2$
5	ACT	B	305	-	3,3,3	1.23	0	3,3,3	0.74	0
4	EDO	C	303	-	3,3,3	0.24	0	2,2,2	0.30	0
3	QNN	B	302[A]	1	10,11,11	1.52	3 (30%)	14,16,16	1.29	3 (21%)
4	EDO	D	302	-	3,3,3	0.35	0	2,2,2	0.29	0
6	PEG	D	305	-	6,6,6	0.19	0	5,5,5	0.32	0
6	PEG	C	305	-	6,6,6	0.63	0	5,5,5	0.73	0
3	QNN	C	302[A]	1	10,11,11	1.25	1 (10%)	14,16,16	1.39	1 (7%)
4	EDO	B	303	-	3,3,3	0.15	0	2,2,2	0.52	0
6	PEG	B	306	-	6,6,6	0.20	0	5,5,5	0.19	0
4	EDO	C	304	-	3,3,3	0.42	0	2,2,2	0.19	0
5	ACT	D	304	-	3,3,3	1.05	0	3,3,3	0.76	0
4	EDO	D	303	-	3,3,3	0.15	0	2,2,2	0.19	0
4	EDO	B	304	-	3,3,3	0.25	0	2,2,2	0.37	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
4	EDO	C	303	-	-	1/1/1/1	-
3	QNN	B	302[A]	1	-	-	0/3/2/2
4	EDO	D	302	-	-	1/1/1/1	-
6	PEG	D	305	-	-	3/4/4/4	-
6	PEG	C	305	-	-	3/4/4/4	-
3	QNN	C	302[A]	1	-	-	0/3/2/2
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
6	PEG	B	306	-	-	1/4/4/4	-
4	EDO	D	303	-	-	1/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[A]	QNN	C7-N1	3.17	1.53	1.47
3	C	302[A]	QNN	C7-N1	2.67	1.52	1.47
3	B	302[A]	QNN	C6-N1	2.23	1.51	1.47
3	B	302[A]	QNN	C1-C2	-2.20	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302[A]	QNN	O1-C3-C2	3.33	127.09	121.72
3	B	302[A]	QNN	C6-N1-C2	-2.59	106.10	111.22
3	B	302[A]	QNN	O1-C3-C2	2.56	125.85	121.72
3	B	302[A]	QNN	C7-N1-C6	-2.17	105.00	109.13

There are no chirality outliers.

All (13) torsion outliers are listed below:

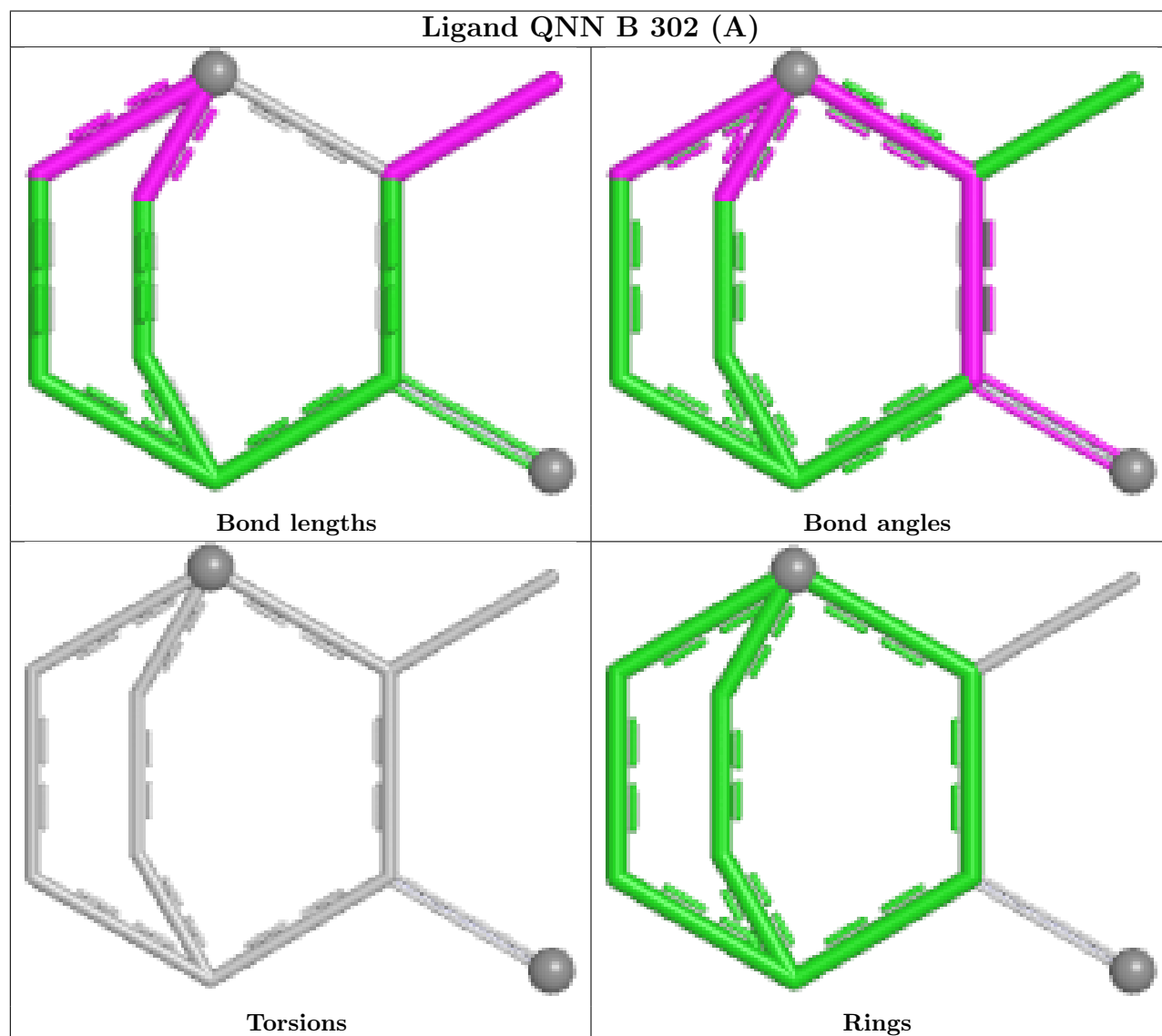
Mol	Chain	Res	Type	Atoms
6	C	305	PEG	O2-C3-C4-O4
6	D	305	PEG	O1-C1-C2-O2
6	B	306	PEG	O2-C3-C4-O4
4	C	303	EDO	O1-C1-C2-O2
6	D	305	PEG	O2-C3-C4-O4
4	B	304	EDO	O1-C1-C2-O2
4	D	303	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
6	C	305	PEG	C4-C3-O2-C2
6	D	305	PEG	C4-C3-O2-C2
4	B	303	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
6	C	305	PEG	O1-C1-C2-O2

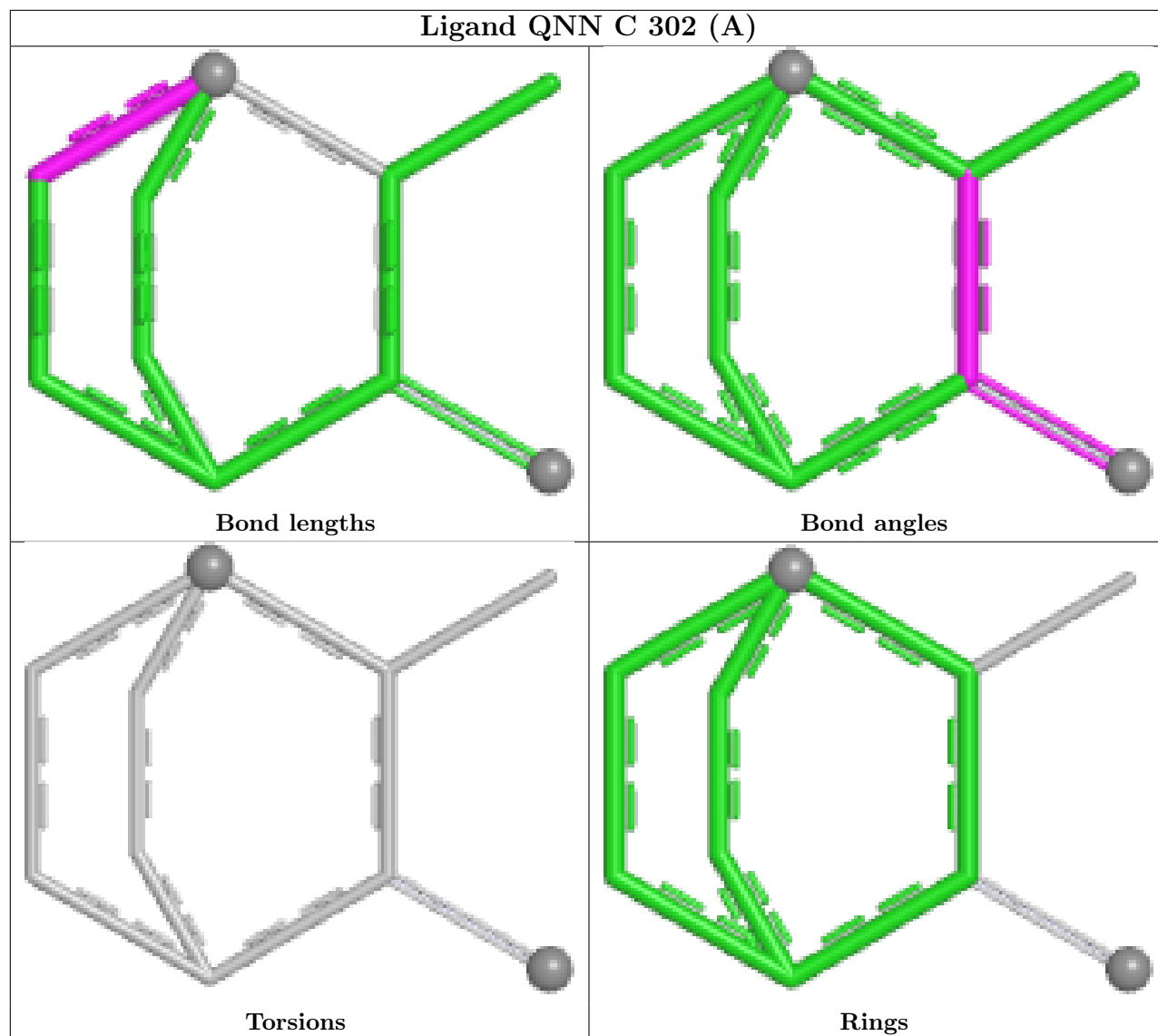
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	EDO	1	0
6	D	305	PEG	1	0
6	C	305	PEG	5	0
4	B	303	EDO	5	0
4	D	303	EDO	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	192/200 (96%)	0.13	6 (3%) 51 52	12, 28, 54, 69	4 (2%)
1	B	193/200 (96%)	0.34	6 (3%) 51 52	12, 34, 53, 64	3 (1%)
1	C	192/200 (96%)	0.31	7 (3%) 46 46	12, 33, 54, 62	3 (1%)
1	D	189/200 (94%)	0.32	8 (4%) 40 40	13, 32, 51, 65	5 (2%)
All	All	766/800 (95%)	0.28	27 (3%) 47 48	12, 32, 54, 69	15 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110[A]	ARG	6.1
1	D	188	LEU	3.9
1	A	187	GLY	3.1
1	C	264	LEU	2.9
1	C	182	CYS	2.7
1	C	96	SER	2.6
1	D	97	VAL	2.5
1	D	112	GLY	2.5
1	D	185	SER	2.5
1	C	265	LEU	2.4
1	B	182[A]	CYS	2.3
1	C	289	LEU	2.3
1	A	186	ASP	2.3
1	B	97	VAL	2.3
1	C	187	GLY	2.3
1	D	187	GLY	2.3
1	A	188	LEU	2.3
1	D	149	SER	2.2
1	B	153	PRO	2.2
1	C	243	MET	2.2
1	B	186	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	182	CYS	2.1
1	D	243	MET	2.1
1	A	180	GLU	2.1
1	B	187	GLY	2.1
1	B	289	LEU	2.1
1	A	244	GLY	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](#)

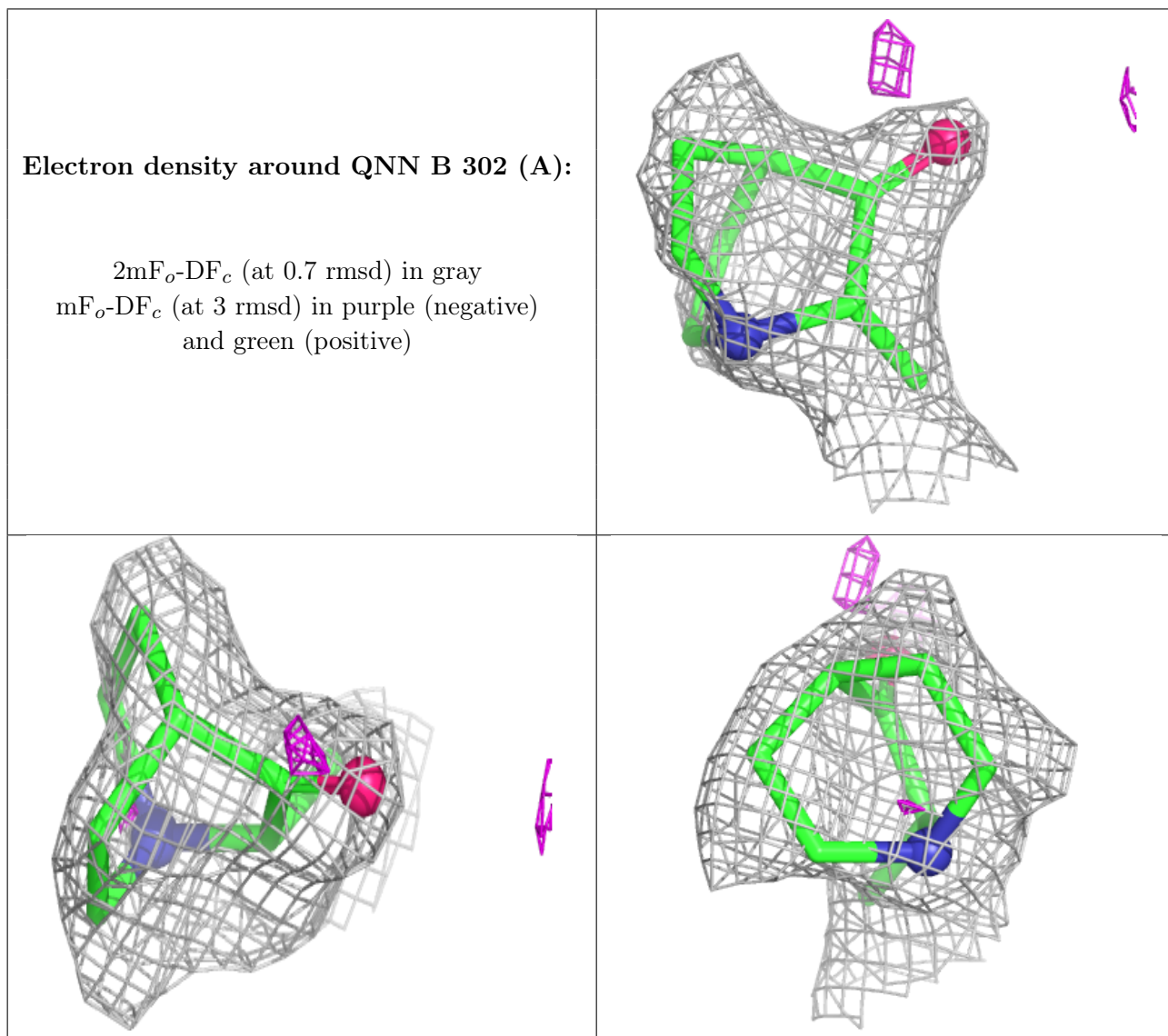
There are no oligosaccharides in this entry.

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.

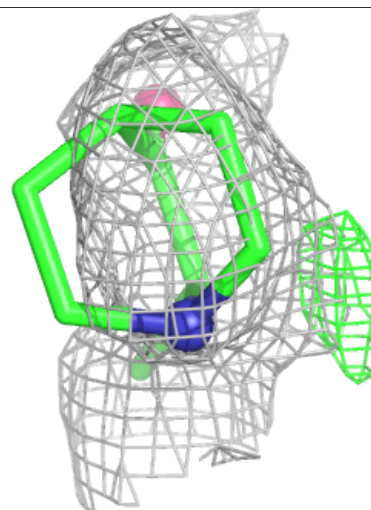
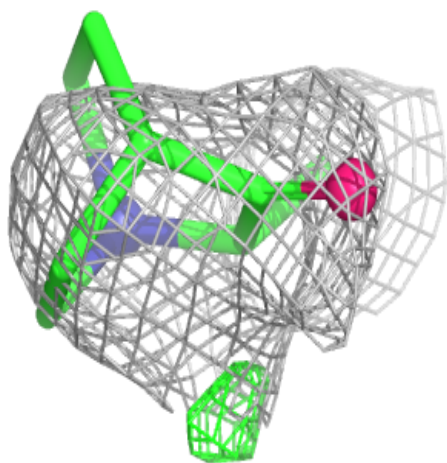
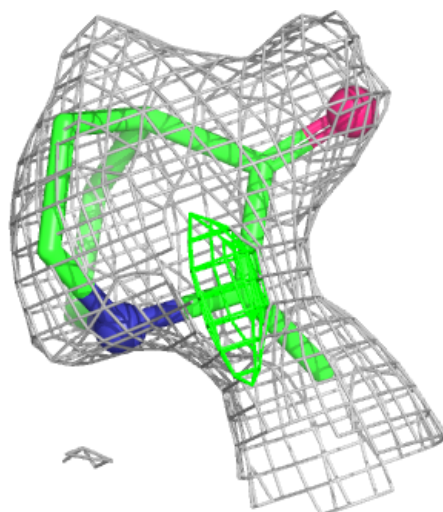
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	D	304	4/4	0.71	0.20	43,46,46,47	4
4	EDO	D	303	4/4	0.72	0.28	45,46,47,47	4
3	QNN	B	302[A]	10/10	0.73	0.17	31,37,38,39	10
4	EDO	D	302	4/4	0.74	0.17	36,36,37,39	4
3	QNN	C	302[A]	10/10	0.77	0.18	37,53,55,57	10
5	ACT	B	305	4/4	0.83	0.14	36,36,40,41	0
4	EDO	B	304	4/4	0.83	0.16	42,43,43,45	4
6	PEG	B	306	7/7	0.87	0.17	30,33,35,36	7
6	PEG	C	305	7/7	0.87	0.13	17,19,22,22	7
6	PEG	D	305	7/7	0.87	0.13	35,37,39,39	7
4	EDO	C	304	4/4	0.89	0.21	21,22,22,22	4
4	EDO	B	303	4/4	0.91	0.10	31,35,35,37	4
4	EDO	C	303	4/4	0.93	0.12	23,25,26,28	4
2	ZN	B	301	1/1	0.97	0.04	28,28,28,28	0
2	ZN	D	301	1/1	0.98	0.03	34,34,34,34	0
2	ZN	C	301	1/1	0.98	0.04	27,27,27,27	0
2	ZN	A	301	1/1	0.99	0.03	30,30,30,30	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 QNN C 302 (A):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.