



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:47 PM EDT

PDB ID : 7A3L / pdb_00007a3l
Title : Crystal structure of DPP8 in complex with a 4-oxo-b-lactam based inhibitor, A241
Authors : Ross, B.H.; Huber, R.
Deposited on : 2020-08-18
Resolution : 2.80 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

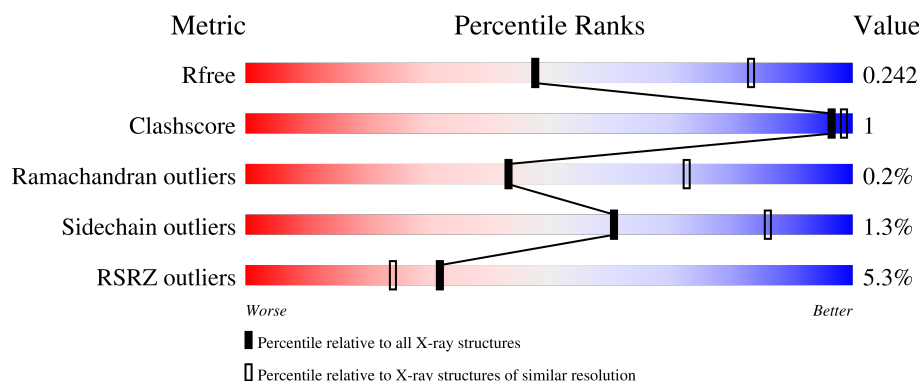
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	898	5% 91% 5%
1	B	898	4% 88% 8%
1	C	898	6% 91% 5%

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	TMO	A	903	-	-	-	X
4	TMO	B	904	-	-	-	X

2 Entry composition [i](#)

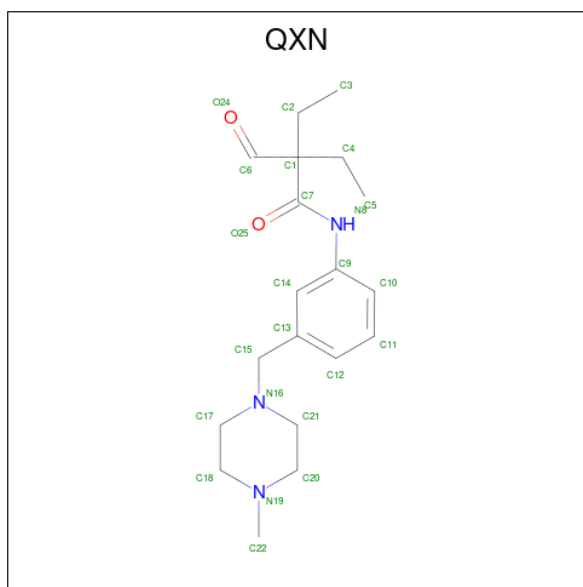
There are 6 unique types of molecules in this entry. The entry contains 20714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 8.

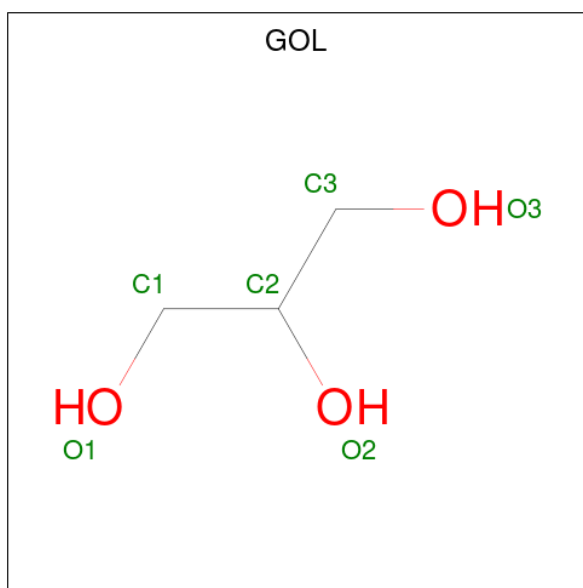
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6910	4436	1160	1285	29			
1	B	826	Total	C	N	O	S	0	1	0
			6717	4318	1125	1246	28			
1	C	850	Total	C	N	O	S	0	0	0
			6910	4436	1160	1285	29			

- Molecule 2 is 2-ethyl-2-methanoyl- {N}-[3-[(4-methylpiperazin-1-yl)methyl]phenyl]butanam ide (CCD ID: QXN) (formula: C₁₉H₂₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



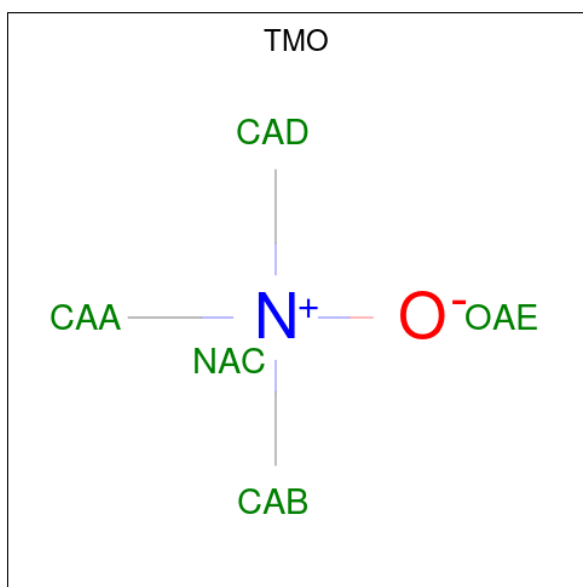
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	3	2		
2	B	1	Total	C	N	O	0	0
			24	19	3	2		
2	C	1	Total	C	N	O	0	0
			24	19	3	2		

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

- Molecule 4 is trimethylamine oxide (CCD ID: TMO) (formula: C_3H_9NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	3	1	1		
4	B	1	Total	C	N	O	0	0
			5	3	1	1		
4	B	1	Total	C	N	O	0	0
			5	3	1	1		
4	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	16	Total	O	0	0
			16	16		

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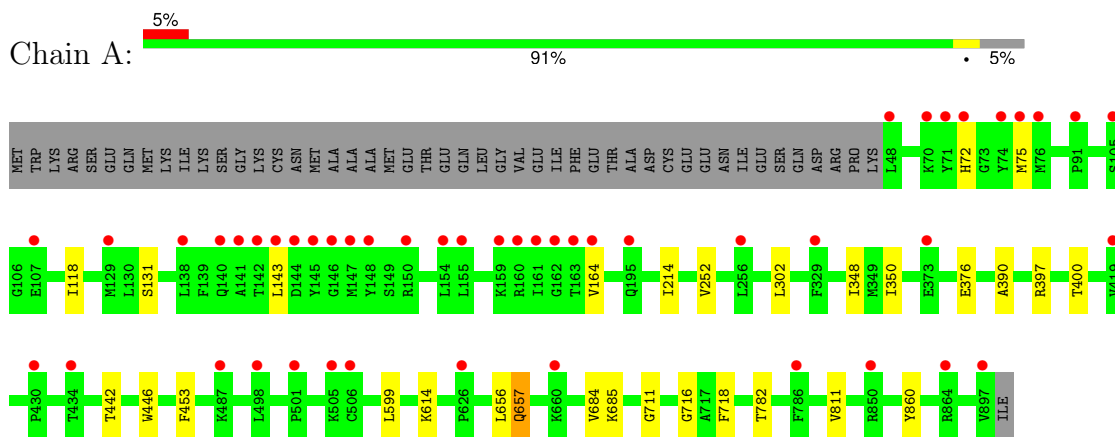
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	13	Total	O	0	0
			13	13		

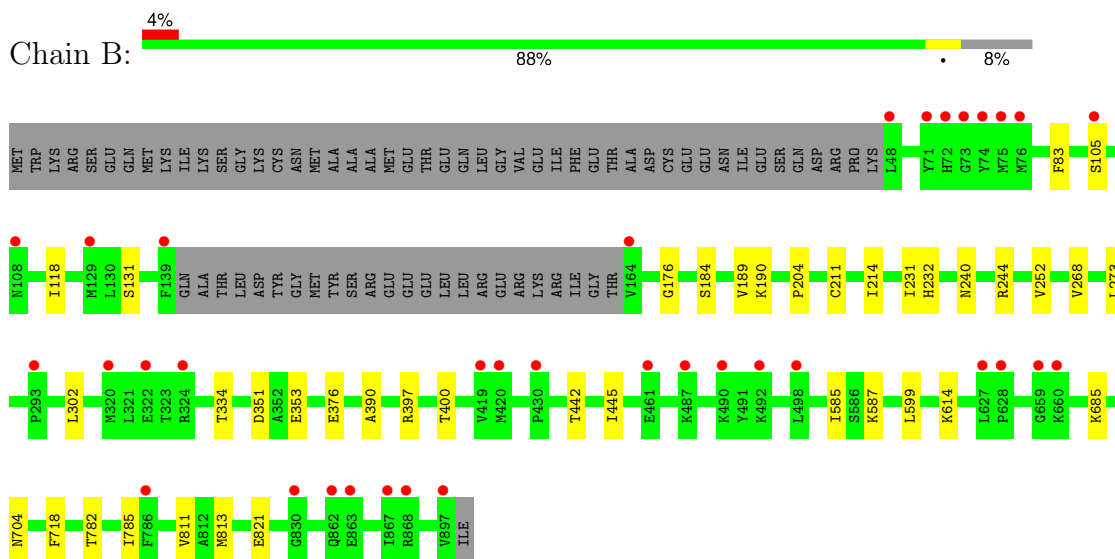
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 8

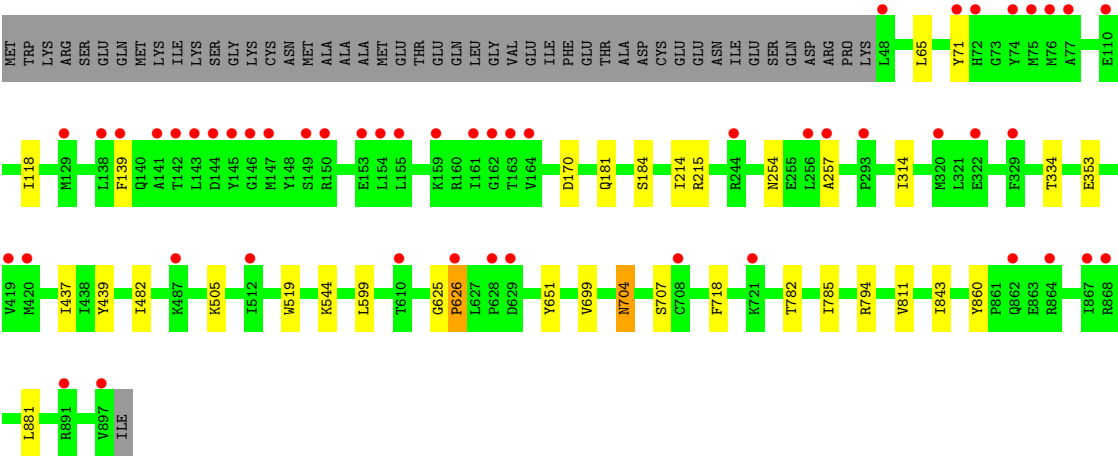


• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	164.03Å 252.78Å 261.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 2.80 44.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.07-2.80) 100.0 (44.07-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.213 , 0.245 0.213 , 0.242	Depositor DCC
R_{free} test set	6645 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20714	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: QXN, GOL, CL, TMO

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	0.98	0/7102	1.30	4/9634 (0.0%)
1	B	0.98	0/6907	1.30	0/9373
1	C	0.98	0/7102	1.31	1/9634 (0.0%)
All	All	0.98	0/21111	1.30	5/28641 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	VAL	CA-C-N	5.63	125.48	121.65
1	A	164	VAL	C-N-CA	5.63	125.48	121.65
1	C	860	TYR	CB-CA-C	5.36	116.22	110.65
1	A	711	GLY	CA-C-O	-5.14	118.68	122.23
1	A	860	TYR	CB-CA-C	5.03	115.88	110.65

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	6910	0	6724	10	0
1	B	6717	0	6527	17	0
1	C	6910	0	6724	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	24	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	16	2	0
3	C	12	0	16	0	0
4	A	5	0	9	0	0
4	B	10	0	18	0	0
4	C	5	0	9	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	17	0	0	0	0
6	B	16	0	0	0	0
6	C	13	0	0	0	0
All	All	20714	0	20059	41	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 1.

All (41) 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:376:GLU:HG3	1:A:397:ARG:HB2	1.78	0.65
1:B:587:LYS:HZ1	3:B:902:GOL:C1	2.16	0.58
1:C:651:TYR:HB2	1:C:699:VAL:HB	1.87	0.55
1:C:334:THR:CG2	1:C:785:ILE:HA	2.36	0.54
1:A:657:GLN:HE21	1:A:657:GLN:HA	1.72	0.54
1:C:782:THR:HA	1:C:811:VAL:HG22	1.92	0.51
1:B:587:LYS:HZ1	3:B:902:GOL:H12	1.74	0.51
1:C:118:ILE:HD12	1:C:599:LEU:HD22	1.92	0.51
1:A:782:THR:HA	1:A:811:VAL:HG22	1.92	0.50
1:B:176:GLY:O	1:B:190:LYS:HA	2.12	0.50
1:B:376:GLU:HG3	1:B:397:ARG:HB2	1.93	0.49
1:A:72:HIS:HB3	1:A:75:MET:HE2	1.95	0.49
1:B:118:ILE:HD12	1:B:599:LEU:CD2	2.43	0.48
1:B:240:ASN:O	1:B:244:ARG:HA	2.14	0.48
1:C:704:ASN:O	1:C:707:SER:OG	2.26	0.47
1:B:189:VAL:CG1	1:B:204:PRO:HA	2.45	0.47
1:B:351:ASP:OD1	1:B:351:ASP:C	2.59	0.46
1:B:400:THR:O	1:B:442:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HG22	1:A:350:ILE:CD1	2.46	0.46
1:C:625:GLY:O	1:C:626:PRO:C	2.59	0.46
1:C:254:ASN:HD22	1:C:257:ALA:HB2	1.81	0.45
1:C:118:ILE:HD12	1:C:599:LEU:CD2	2.46	0.45
1:A:302:LEU:HD22	1:A:390:ALA:HB1	2.00	0.44
1:B:782:THR:HA	1:B:811:VAL:HG22	2.00	0.43
1:B:231:ILE:HG21	1:B:268:VAL:CG2	2.49	0.43
1:C:519:TRP:CG	1:C:544:LYS:HA	2.53	0.43
1:C:65:LEU:HD21	1:C:881:LEU:HD22	2.00	0.42
1:A:400:THR:O	1:A:442:THR:HA	2.19	0.42
1:B:83:PHE:CD1	1:B:585:ILE:HD13	2.53	0.42
1:A:446:TRP:CH2	1:A:716:GLY:HA2	2.55	0.42
1:B:211:CYS:HB3	1:B:232:HIS:CD2	2.55	0.42
1:B:813:MET:HA	1:B:813:MET:HE2	2.02	0.42
1:C:181:GLN:NE2	1:C:215:ARG:O	2.52	0.42
1:B:302:LEU:HD22	1:B:390:ALA:HB1	2.01	0.41
1:B:184:SER:HA	1:B:214:ILE:CD1	2.50	0.41
1:C:184:SER:HA	1:C:214:ILE:CD1	2.50	0.41
1:A:376:GLU:HG3	1:A:397:ARG:CB	2.50	0.41
1:C:439:TYR:CE1	1:C:482:ILE:HD13	2.56	0.41
1:C:437:ILE:HB	1:C:505:LYS:HA	2.03	0.40
1:A:118:ILE:HD12	1:A:599:LEU:HD22	2.02	0.40
1:B:334:THR:CG2	1:B:785:ILE:HA	2.51	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	848/898 (94%)	805 (95%)	42 (5%)	1 (0%)	48 77
1	B	823/898 (92%)	787 (96%)	35 (4%)	1 (0%)	48 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	848/898 (94%)	803 (95%)	43 (5%)	2 (0%)	43	72
All	All	2519/2694 (94%)	2395 (95%)	120 (5%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	139	PHE
1	A	453	PHE
1	B	445	ILE
1	C	626	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	753/795 (95%)	743 (99%)	10 (1%)	61	86
1	B	733/795 (92%)	723 (99%)	10 (1%)	59	85
1	C	753/795 (95%)	745 (99%)	8 (1%)	65	87
All	All	2239/2385 (94%)	2211 (99%)	28 (1%)	61	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	SER
1	A	143	LEU
1	A	214	ILE
1	A	252	VAL
1	A	614	LYS
1	A	656	LEU
1	A	657	GLN
1	A	684	VAL
1	A	685	LYS
1	A	718	PHE
1	B	105	SER

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Mol	Chain	Res	Type
1	B	131	SER
1	B	252	VAL
1	B	273	LEU
1	B	353	GLU
1	B	614	LYS
1	B	685	LYS
1	B	704	ASN
1	B	718	PHE
1	B	821	GLU
1	C	71	TYR
1	C	170	ASP
1	C	314	ILE
1	C	353	GLU
1	C	704	ASN
1	C	718	PHE
1	C	794	ARG
1	C	843	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	195	GLN
1	A	199	GLN
1	A	200	GLN
1	A	258	ASN
1	A	423	GLN
1	A	559	ASN
1	A	595	HIS
1	A	654	HIS
1	A	657	GLN
1	A	673	GLN
1	A	801	GLN
1	A	837	HIS
1	A	840	HIS
1	A	858	GLN
1	A	875	HIS
1	A	882	HIS
1	B	111	ASN
1	B	199	GLN
1	B	258	ASN
1	B	423	GLN

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Mol	Chain	Res	Type
1	B	559	ASN
1	B	595	HIS
1	B	654	HIS
1	B	801	GLN
1	B	858	GLN
1	C	123	ASN
1	C	140	GLN
1	C	195	GLN
1	C	199	GLN
1	C	200	GLN
1	C	254	ASN
1	C	403	GLN
1	C	423	GLN
1	C	550	HIS
1	C	837	HIS
1	C	858	GLN
1	C	882	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](#)

Of 16 ligands modelled in this entry, 3 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
4	TMO	B	903	-	4,4,4	6.35	1 (25%)	6,6,6	0.20	0
4	TMO	B	904	-	4,4,4	6.34	1 (25%)	6,6,6	0.22	0
2	QXN	A	901	1	23,25,25	0.66	0	28,34,34	0.93	1 (3%)
3	GOL	B	905	-	5,5,5	0.12	0	5,5,5	0.43	0
3	GOL	C	902	-	5,5,5	0.11	0	5,5,5	0.29	0
3	GOL	C	904	-	5,5,5	0.10	0	5,5,5	0.28	0
3	GOL	A	902	-	5,5,5	0.14	0	5,5,5	0.36	0
2	QXN	B	901	1	23,25,25	0.64	0	28,34,34	0.90	1 (3%)
3	GOL	B	902	-	5,5,5	0.13	0	5,5,5	0.41	0
2	QXN	C	901	1	23,25,25	0.67	0	28,34,34	0.97	1 (3%)
4	TMO	A	903	-	4,4,4	6.16	1 (25%)	6,6,6	0.28	0
4	TMO	C	903	-	4,4,4	6.30	1 (25%)	6,6,6	0.24	0
3	GOL	A	904	-	5,5,5	0.12	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QXN	A	901	1	-	2/20/33/33	0/2/2/2
3	GOL	B	905	-	-	4/4/4/4	-
3	GOL	C	902	-	-	0/4/4/4	-
3	GOL	C	904	-	-	2/4/4/4	-
3	GOL	A	902	-	-	4/4/4/4	-
2	QXN	B	901	1	-	3/20/33/33	0/2/2/2
3	GOL	B	902	-	-	2/4/4/4	-
2	QXN	C	901	1	-	2/20/33/33	0/2/2/2
3	GOL	A	904	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	TMO	OAE-NAC	-12.66	1.25	1.42
4	B	904	TMO	OAE-NAC	-12.65	1.25	1.42
4	C	903	TMO	OAE-NAC	-12.56	1.25	1.42
4	A	903	TMO	OAE-NAC	-12.30	1.25	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	QXN	C1-C7-N8	2.70	119.24	115.68
2	B	901	QXN	C1-C7-N8	2.50	118.98	115.68
2	A	901	QXN	C1-C7-N8	2.37	118.81	115.68

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	QXN	C2-C1-C6-O24
2	A	901	QXN	C4-C1-C6-O24
2	B	901	QXN	C2-C1-C6-O24
2	C	901	QXN	C2-C1-C6-O24
3	A	902	GOL	O1-C1-C2-C3
3	A	902	GOL	C1-C2-C3-O3
3	A	902	GOL	O2-C2-C3-O3
3	B	902	GOL	C1-C2-C3-O3
3	B	905	GOL	O1-C1-C2-C3
3	B	905	GOL	C1-C2-C3-O3
3	B	902	GOL	O2-C2-C3-O3
3	A	904	GOL	O1-C1-C2-C3
3	C	904	GOL	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-O2
3	A	904	GOL	O1-C1-C2-O2
3	B	905	GOL	O1-C1-C2-O2
3	B	905	GOL	O2-C2-C3-O3
3	C	904	GOL	O2-C2-C3-O3
2	B	901	QXN	C4-C1-C6-O24
2	C	901	QXN	C4-C1-C2-C3
2	B	901	QXN	C4-C1-C2-C3

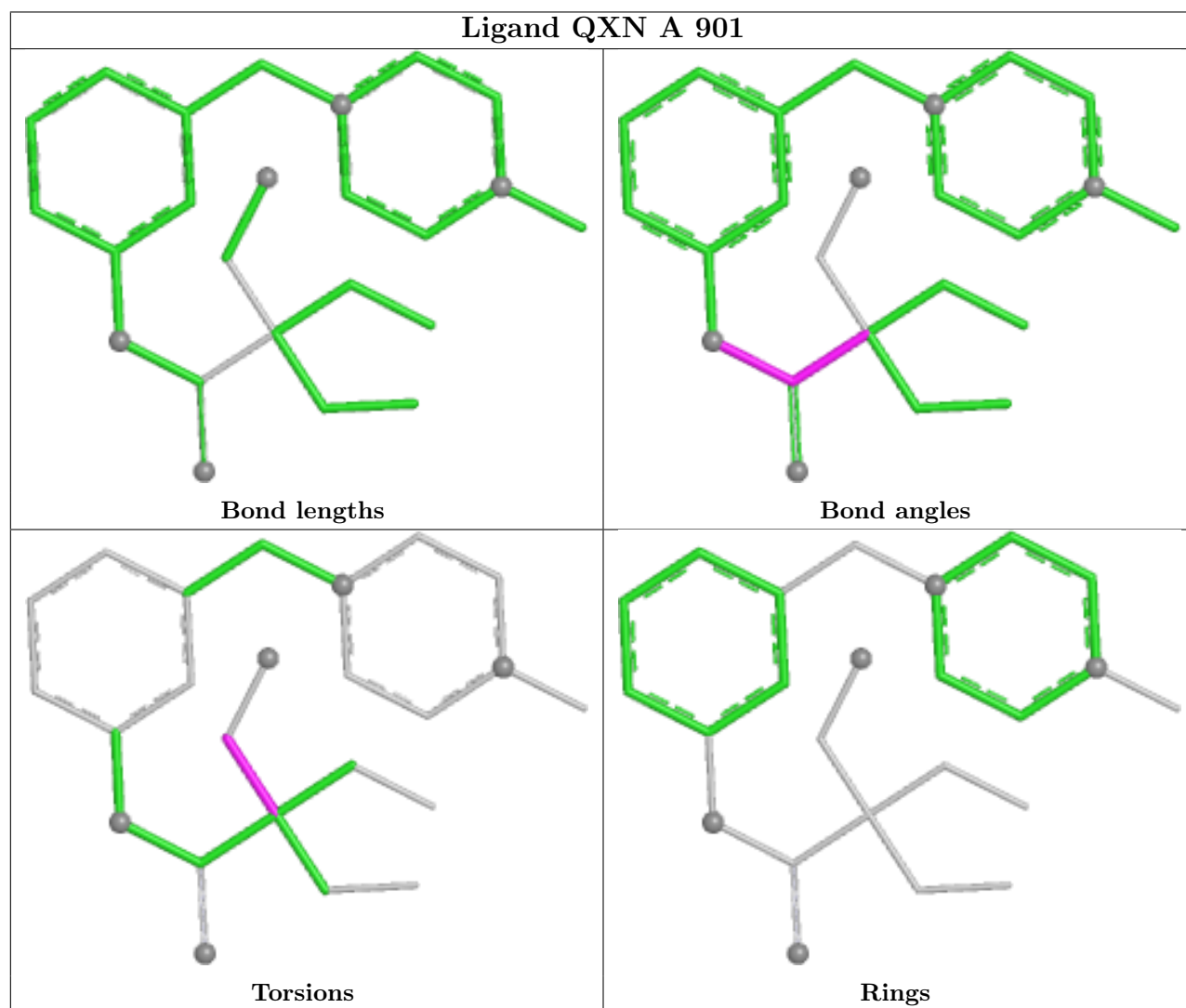
There are no ring outliers.

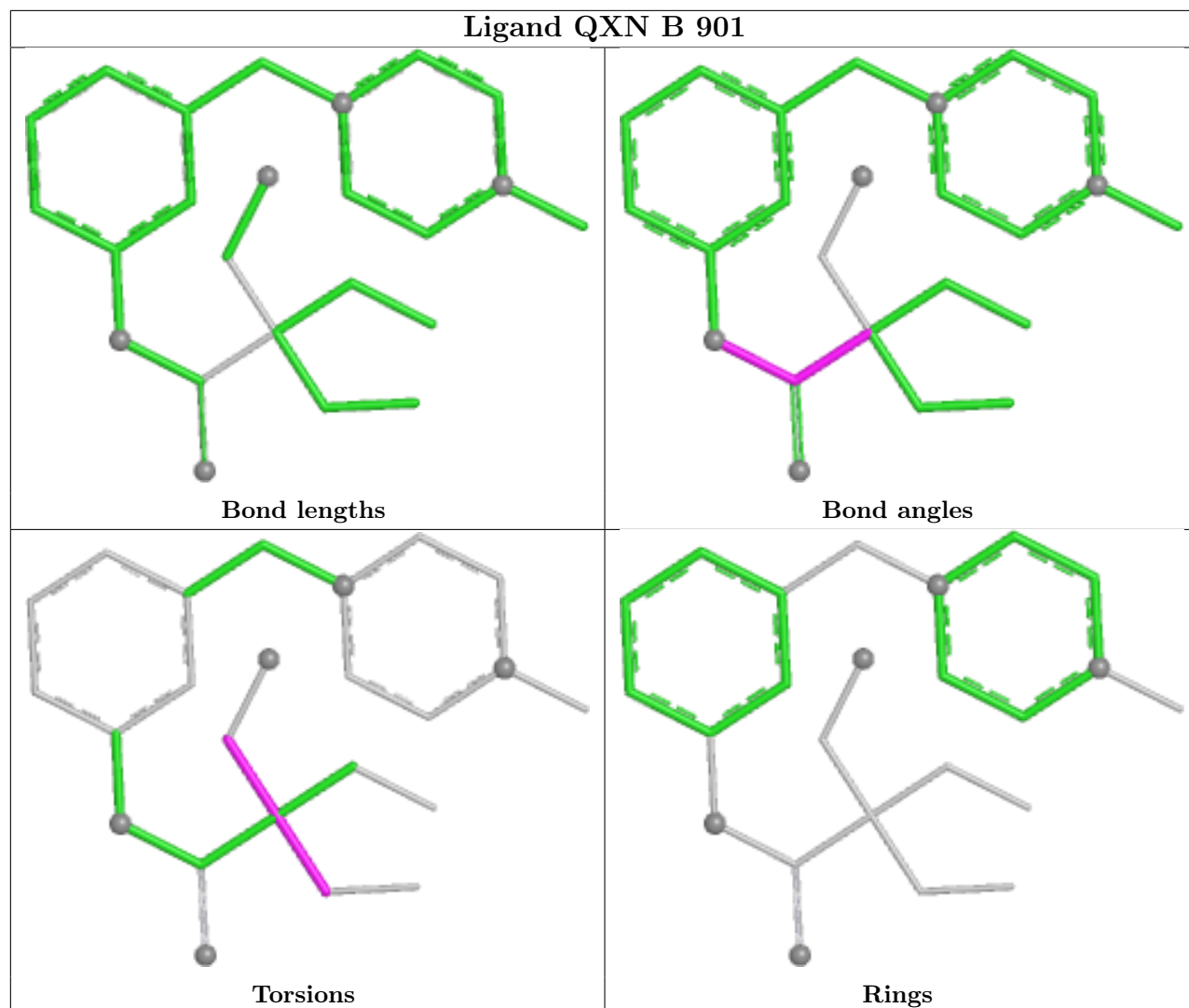
1 monomer is involved in 2 short contacts:

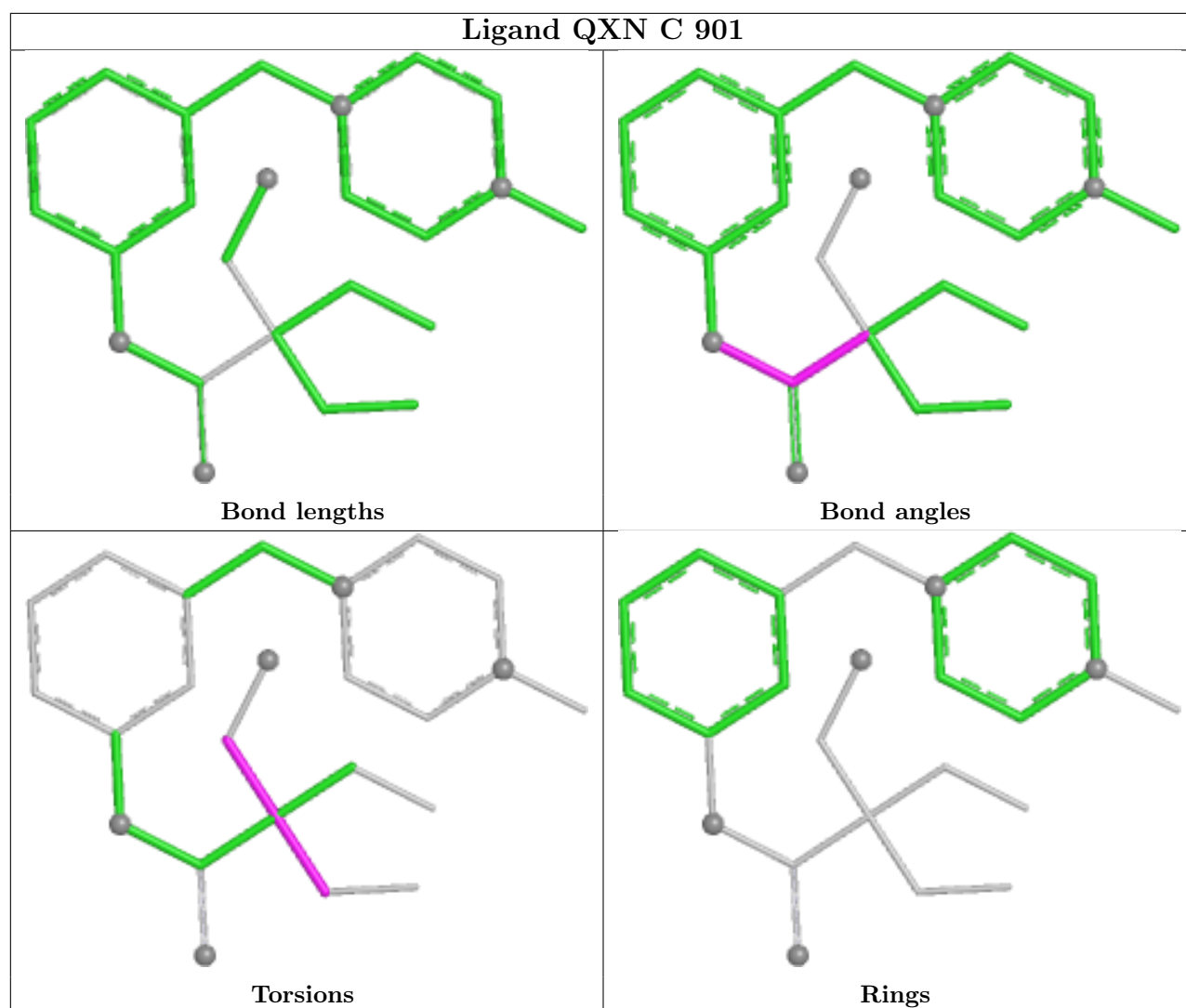
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	GOL	2	0

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	850/898 (94%)	0.35	48 (5%)	30	23	51, 73, 128, 195	0
1	B	826/898 (91%)	0.27	35 (4%)	40	32	30, 70, 118, 156	1 (0%)
1	C	850/898 (94%)	0.46	51 (6%)	27	21	51, 75, 136, 191	0
All	All	2526/2694 (93%)	0.36	134 (5%)	32	24	30, 73, 126, 195	1 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	LEU	6.8
1	C	141	ALA	6.0
1	C	143	LEU	5.4
1	A	145	TYR	5.2
1	B	139	PHE	5.1
1	A	155	LEU	5.1
1	A	141	ALA	4.8
1	A	76	MET	4.7
1	A	142	THR	4.5
1	C	155	LEU	4.4
1	C	897	VAL	4.3
1	A	897	VAL	4.2
1	C	74	TYR	4.2
1	B	862	GLN	4.2
1	C	419	VAL	4.0
1	A	146	GLY	4.0
1	C	142	THR	4.0
1	C	75	MET	3.9
1	A	164	VAL	3.9
1	B	48	LEU	3.8
1	B	76	MET	3.7
1	A	71	TYR	3.7
1	B	419	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	154	LEU	3.6
1	C	163	THR	3.6
1	B	897	VAL	3.6
1	C	145	TYR	3.5
1	C	48	LEU	3.4
1	A	75	MET	3.4
1	C	138	LEU	3.3
1	B	628	PRO	3.2
1	A	147	MET	3.2
1	C	144	ASP	3.2
1	A	154	LEU	3.1
1	C	161	ILE	3.1
1	C	626	PRO	3.1
1	B	108	ASN	3.1
1	B	164	VAL	3.1
1	C	129	MET	3.0
1	A	159	LYS	3.0
1	A	329	PHE	3.0
1	C	71	TYR	3.0
1	A	419	VAL	3.0
1	A	505	LYS	2.9
1	A	74	TYR	2.9
1	B	105	SER	2.9
1	C	420	MET	2.9
1	A	626	PRO	2.9
1	A	150	ARG	2.9
1	A	161	ILE	2.9
1	C	629	ASP	2.9
1	C	72	HIS	2.9
1	A	148	TYR	2.8
1	C	329	PHE	2.8
1	B	75	MET	2.8
1	C	76	MET	2.8
1	B	660	LYS	2.8
1	C	244	ARG	2.7
1	A	144	ASP	2.7
1	A	48	LEU	2.7
1	C	322	GLU	2.7
1	A	786	PHE	2.6
1	C	159	LYS	2.6
1	B	498	LEU	2.6
1	C	149	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	867	ILE	2.6
1	C	164	VAL	2.6
1	C	162	GLY	2.6
1	C	628	PRO	2.5
1	B	129	MET	2.5
1	A	487	LYS	2.5
1	B	72	HIS	2.5
1	B	74	TYR	2.5
1	B	868	ARG	2.5
1	B	487	LYS	2.5
1	B	324	ARG	2.5
1	C	862	GLN	2.5
1	A	256	LEU	2.4
1	A	498	LEU	2.4
1	C	708	CYS	2.4
1	A	162	GLY	2.4
1	C	146	GLY	2.4
1	C	147	MET	2.4
1	A	430	PRO	2.4
1	C	150	ARG	2.4
1	C	487	LYS	2.4
1	B	73	GLY	2.4
1	C	77	ALA	2.4
1	B	71	TYR	2.4
1	B	320	MET	2.4
1	B	420	MET	2.4
1	A	72	HIS	2.4
1	C	256	LEU	2.4
1	B	627	LEU	2.3
1	A	70	LYS	2.3
1	B	293	PRO	2.3
1	A	138	LEU	2.3
1	B	659	GLY	2.3
1	C	610	THR	2.3
1	A	160	ARG	2.3
1	A	91	PRO	2.3
1	A	195	GLN	2.3
1	B	492	LYS	2.3
1	A	163	THR	2.3
1	A	660	LYS	2.2
1	A	107	GLU	2.2
1	A	373	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLU	2.2
1	A	105	SER	2.2
1	A	850	ARG	2.2
1	C	868	ARG	2.2
1	C	864	ARG	2.1
1	C	320	MET	2.1
1	A	434	THR	2.1
1	A	506	CYS	2.1
1	B	461	GLU	2.1
1	C	891	ARG	2.1
1	A	140	GLN	2.1
1	C	293	PRO	2.1
1	B	786	PHE	2.1
1	B	863	GLU	2.1
1	C	110	GLU	2.1
1	A	864	ARG	2.1
1	C	257	ALA	2.1
1	C	867	ILE	2.1
1	A	129	MET	2.1
1	B	490	LYS	2.1
1	A	501	PRO	2.1
1	B	430	PRO	2.1
1	C	139	PHE	2.1
1	C	512	ILE	2.0
1	C	153	GLU	2.0
1	C	721	LYS	2.0
1	B	830	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,

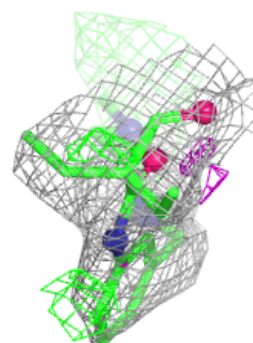
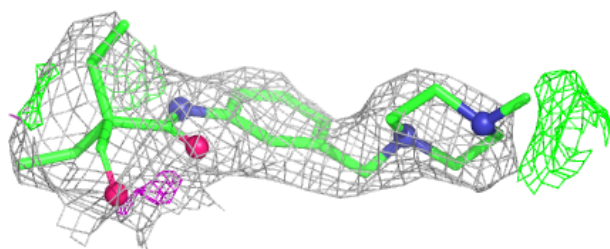
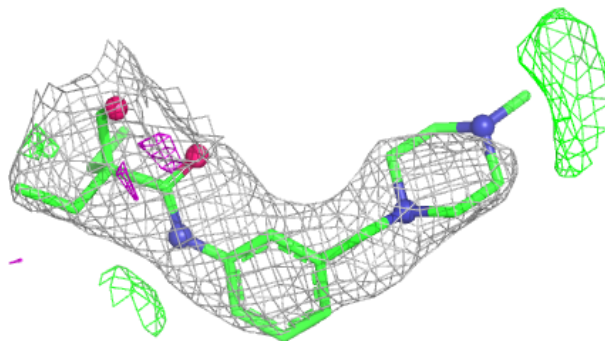
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	902	6/6	0.59	0.27	87,91,93,96	0
4	TMO	B	904	5/5	0.71	0.54	104,104,105,106	0
3	GOL	C	902	6/6	0.73	0.27	90,95,97,97	0
3	GOL	B	905	6/6	0.75	0.21	96,99,99,100	0
4	TMO	A	903	5/5	0.77	0.44	87,88,89,90	0
3	GOL	C	904	6/6	0.78	0.18	96,99,100,101	0
3	GOL	A	902	6/6	0.81	0.25	90,91,93,94	0
4	TMO	C	903	5/5	0.81	0.46	98,99,101,101	0
3	GOL	A	904	6/6	0.85	0.18	97,102,103,104	0
2	QXN	C	901	24/24	0.88	0.25	66,102,131,134	0
4	TMO	B	903	5/5	0.88	0.34	98,99,101,102	0
2	QXN	A	901	24/24	0.89	0.25	65,95,124,125	0
2	QXN	B	901	24/24	0.92	0.18	59,85,112,114	0
5	CL	C	905	1/1	0.92	0.10	92,92,92,92	0
5	CL	A	905	1/1	0.93	0.20	87,87,87,87	0
5	CL	B	906	1/1	0.94	0.10	84,84,84,84	0

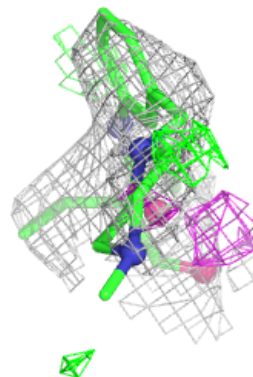
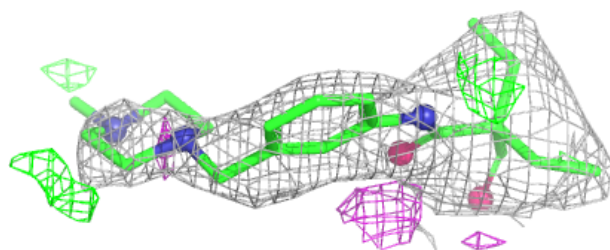
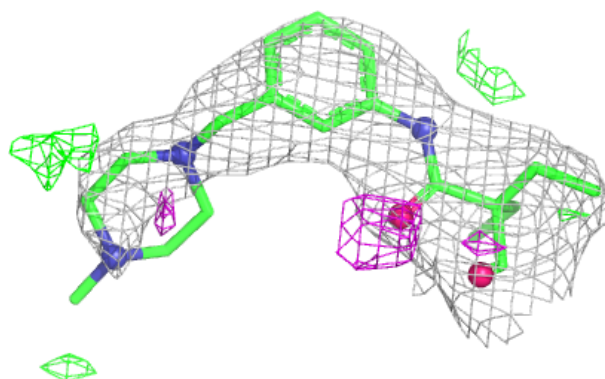
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QXN C 901:

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

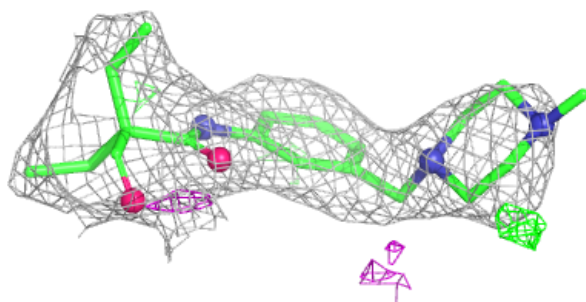
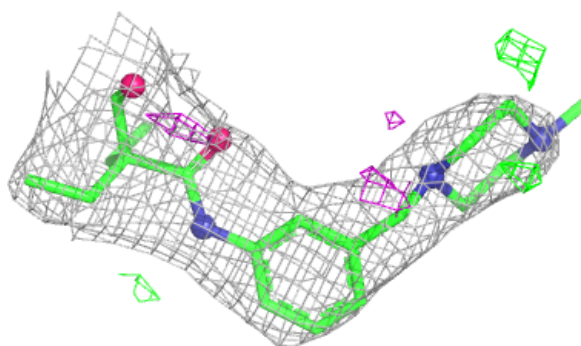
**Electron density around QXN A 901:**

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



Electron density around QXN B 901:

$2mF_o-DF_c$ (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.