Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2022 – 04:47 pm BST

PDB ID	:	7A3G
Title	:	Crystal structure of DPP8 in complex with a 4-oxo-b-lactam based inhibitor, 91
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 (i) 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 (i)) were used in the production of this report:

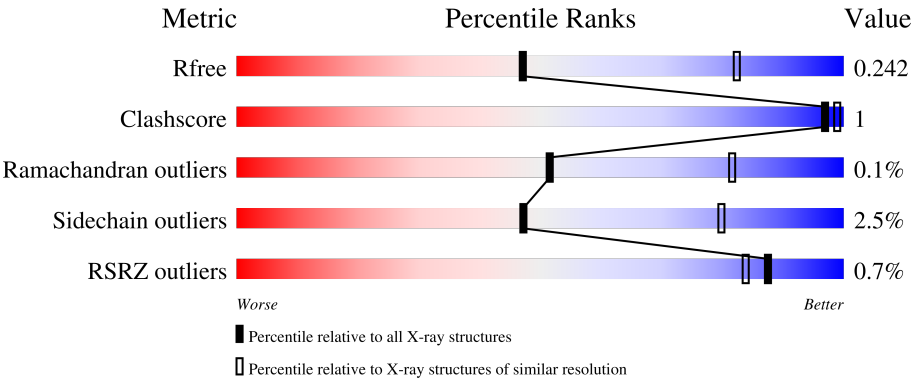
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

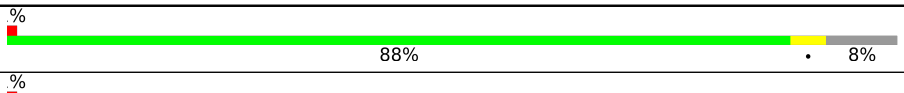
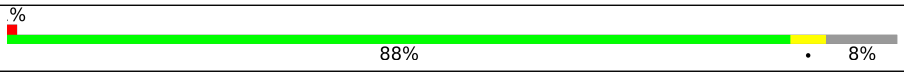
The reported resolution of this entry is 2.80 Å.

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	
1	B	898	

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	PO4	A	1009	-	-	-	X

2 Entry composition

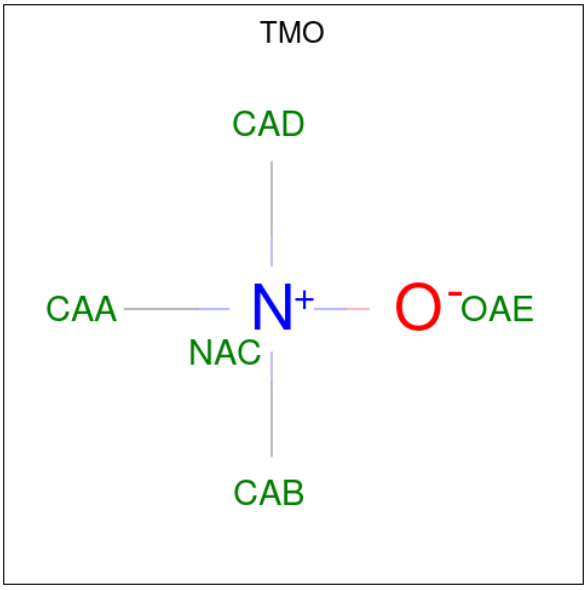
There are 8 unique types of molecules in this entry. The entry contains 13651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

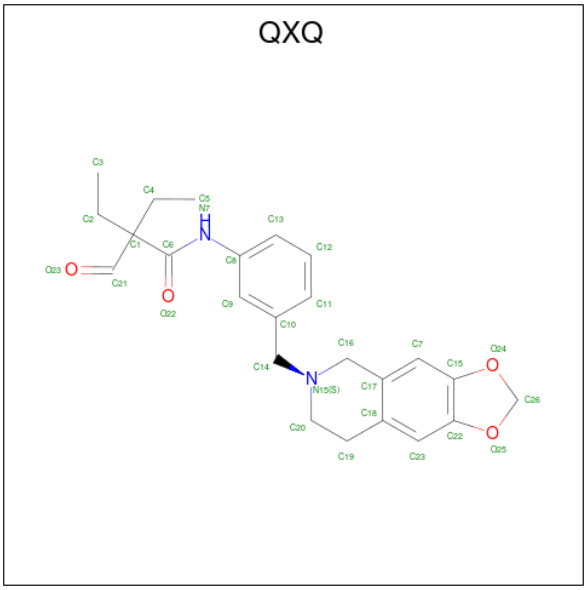
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	828	Total	C	N	O	S	0	0	0
			6723	4323	1125	1247	28			
1	A	827	Total	C	N	O	S	0	0	0
			6712	4314	1124	1246	28			

- Molecule 2 is trimethylamine oxide (three-letter code: TMO) (formula: C_3H_9NO).



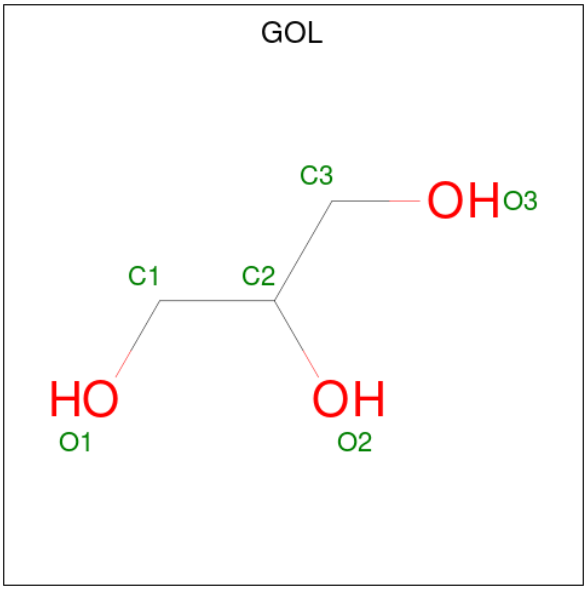
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 3 is {N}-[3-(7,8-dihydro-5 {H}-[1,3]dioxolo[4,5-g]isoquinolin-6-ylmethyl)phenyl]-2-ethyl-2-methanoyl-butanamide (three-letter code: QXQ) (formula: $C_{24}H_{28}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



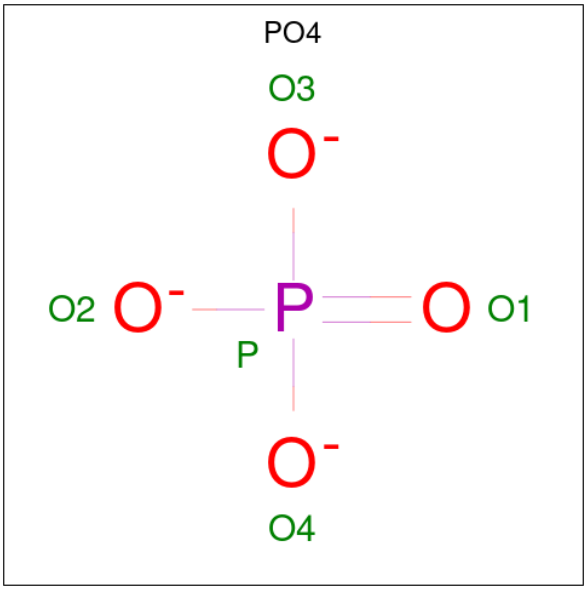
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	24	2	4		
3	A	1	Total	C	N	O	0	0
			30	24	2	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



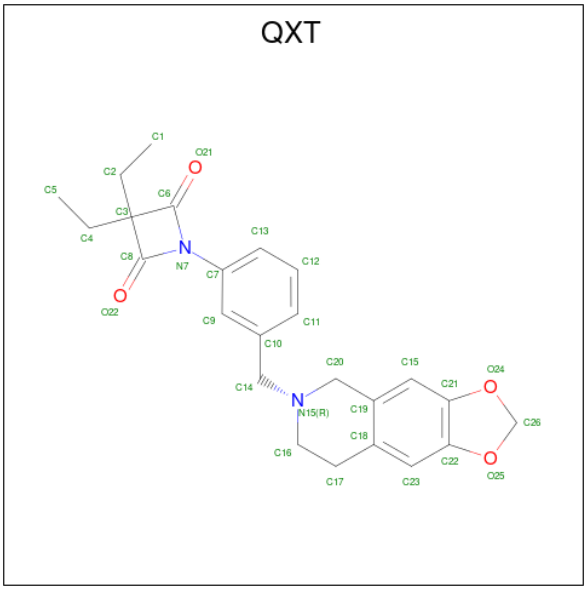
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is 1-[3-(7,8-dihydro-5 {H}-[1,3]dioxolo[4,5-g]isoquinolin-6-ylmethyl)phenyl]-3, 3-diethyl-azetidine-2,4-dione (three-letter code: QXT) (formula: $C_{24}H_{26}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 30 24 2 4	0	0
6	A	1	Total C N O 30 24 2 4	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

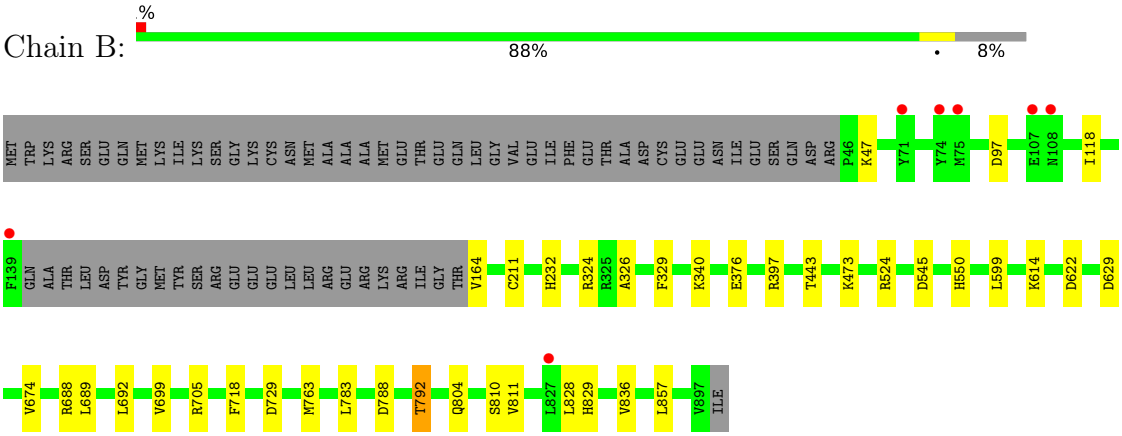
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	5	Total O 5 5	0	0
8	A	5	Total O 5 5	0	0

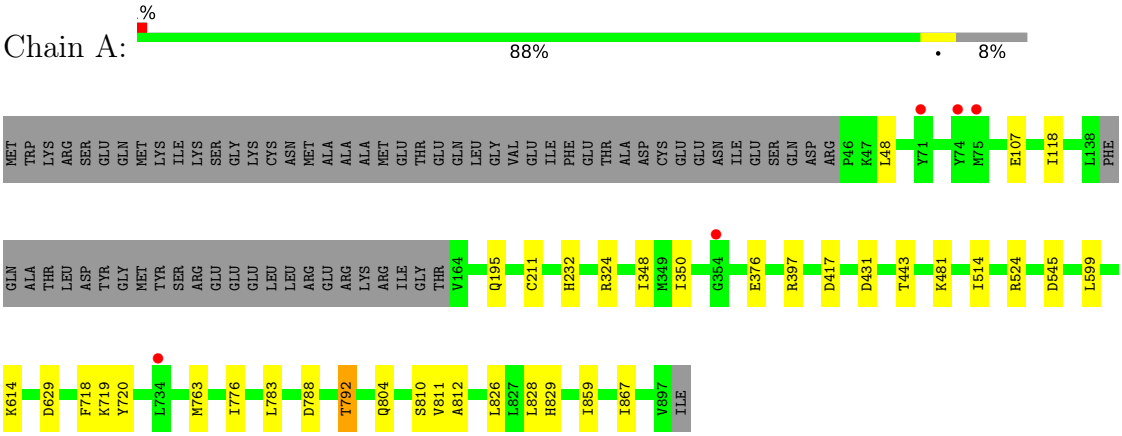
3 Residue-property plots (i)

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	153.60Å 153.60Å 270.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 2.80 49.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.43-2.80) 100.0 (49.43-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.209 , 0.242 0.212 , 0.242	Depositor DCC
R_{free} test set	4421 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13651	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, CL, QXT, GOL, TMO, QXQ

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	0.37	0/6901	0.60	0/9364
1	B	0.37	0/6913	0.60	0/9380
All	All	0.37	0/13814	0.60	0/18744

There are no bond length outliers.

There are no bond angle outliers.

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	6712	0	6533	13	0
1	B	6723	0	6542	11	0
2	A	10	0	18	1	0
2	B	10	0	18	1	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
5	A	20	0	0	0	0
5	B	20	0	0	0	0
6	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
All	All	13651	0	13143	23	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 (23) 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:B:376:GLU:HG3	1:B:397:ARG:HB2	1.89	0.55
1:A:783:LEU:HD13	1:A:812:ALA:HB3	1.93	0.49
1:A:867:ILE:HD12	2:A:1003:TMO:HABB	1.93	0.48
1:B:689:LEU:HG	1:B:699:VAL:HG11	1.95	0.48
1:A:788:ASP:O	1:A:792:THR:HG22	2.14	0.47
1:B:857:LEU:HD21	1:A:859:ILE:HD12	1.97	0.46
1:A:481:LYS:HB2	1:A:514:ILE:HD11	1.97	0.46
1:B:783:LEU:HD12	1:B:810:SER:HB3	1.99	0.45
1:A:719:LYS:HG2	1:A:720:TYR:CD2	2.53	0.44
1:B:705:ARG:HD3	1:B:729:ASP:OD2	2.19	0.43
1:B:326:ALA:HB2	2:B:901:TMO:HAAB	2.01	0.43
1:B:788:ASP:O	1:B:792:THR:HG22	2.19	0.43
1:A:376:GLU:HG3	1:A:397:ARG:HB2	2.00	0.43
1:B:763:MET:SD	1:B:811:VAL:HG12	2.59	0.42
1:B:118:ILE:HD12	1:B:599:LEU:HD22	2.00	0.42
1:A:348:ILE:HG22	1:A:350:ILE:CD1	2.49	0.42
1:A:776:ILE:HG23	1:A:826:LEU:HD23	2.02	0.42
1:A:783:LEU:HD12	1:A:810:SER:HB3	2.02	0.42
1:A:211:CYS:HB3	1:A:232:HIS:CD2	2.55	0.41
1:A:118:ILE:HD12	1:A:599:LEU:HD22	2.03	0.41
1:A:763:MET:SD	1:A:811:VAL:HG12	2.61	0.41
1:B:211:CYS:HB3	1:B:232:HIS:CD2	2.56	0.40
1:B:118:ILE:HD12	1:B:599:LEU:CD2	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	823/898 (92%)	779 (95%)	42 (5%)	2 (0%)	47 78
1	B	824/898 (92%)	779 (94%)	45 (6%)	0	100 100
All	All	1647/1796 (92%)	1558 (95%)	87 (5%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	107	GLU

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	733/795 (92%)	719 (98%)	14 (2%)	57 85
1	B	734/795 (92%)	711 (97%)	23 (3%)	40 74
All	All	1467/1590 (92%)	1430 (98%)	37 (2%)	47 80

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	LYS
1	B	97	ASP
1	B	164	VAL
1	B	324	ARG

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Mol	Chain	Res	Type
1	B	329	PHE
1	B	340	LYS
1	B	443	THR
1	B	473	LYS
1	B	524	ARG
1	B	545	ASP
1	B	550	HIS
1	B	614	LYS
1	B	622	ASP
1	B	629	ASP
1	B	674	VAL
1	B	688	ARG
1	B	692	LEU
1	B	718	PHE
1	B	792	THR
1	B	804	GLN
1	B	828	LEU
1	B	829	HIS
1	B	836	VAL
1	A	195	GLN
1	A	324	ARG
1	A	417	ASP
1	A	431	ASP
1	A	443	THR
1	A	524	ARG
1	A	545	ASP
1	A	614	LYS
1	A	629	ASP
1	A	718	PHE
1	A	792	THR
1	A	804	GLN
1	A	828	LEU
1	A	829	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	B	199	GLN
1	B	200	GLN
1	B	403	GLN
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	199	GLN
1	A	200	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	TMO	B	901	-	4,4,4	6.31	1 (25%)	6,6,6	0.29	0
5	PO4	B	906	-	4,4,4	0.89	0	6,6,6	0.35	0
4	GOL	B	905	-	5,5,5	0.29	0	5,5,5	0.33	0
5	PO4	B	909	-	4,4,4	0.76	0	6,6,6	0.46	0
5	PO4	A	1009	-	4,4,4	0.79	0	6,6,6	0.45	0
3	QXQ	A	1002	1	31,33,33	1.27	2 (6%)	43,47,47	1.46	7 (16%)
2	TMO	B	903	-	4,4,4	6.37	1 (25%)	6,6,6	0.24	0
3	QXQ	B	902	1	31,33,33	1.27	2 (6%)	43,47,47	1.49	8 (18%)
2	TMO	A	1001	-	4,4,4	6.38	1 (25%)	6,6,6	0.29	0
5	PO4	A	1008	-	4,4,4	0.87	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	QXT	B	910	-	30,34,34	1.33	2 (6%)	41,51,51	1.68	10 (24%)
5	PO4	A	1006	-	4,4,4	0.82	0	6,6,6	0.43	0
4	GOL	A	1005	-	5,5,5	0.43	0	5,5,5	0.23	0
5	PO4	A	1007	-	4,4,4	0.89	0	6,6,6	0.42	0
5	PO4	B	908	-	4,4,4	0.89	0	6,6,6	0.45	0
5	PO4	B	907	-	4,4,4	0.84	0	6,6,6	0.47	0
6	QXT	A	1010	-	30,34,34	1.32	2 (6%)	41,51,51	1.62	8 (19%)
2	TMO	A	1003	-	4,4,4	6.31	1 (25%)	6,6,6	0.24	0
4	GOL	B	904	-	5,5,5	0.38	0	5,5,5	0.26	0
4	GOL	A	1004	-	5,5,5	0.23	0	5,5,5	0.23	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	GOL	B	904	-	-	0/4/4/4	-
4	GOL	B	905	-	-	0/4/4/4	-
4	GOL	A	1005	-	-	4/4/4/4	-
3	QXQ	A	1002	1	-	5/20/38/38	0/4/4/4
3	QXQ	B	902	1	-	5/20/38/38	0/4/4/4
4	GOL	A	1004	-	-	0/4/4/4	-
6	QXT	A	1010	-	-	2/14/49/49	0/5/5/5
6	QXT	B	910	-	-	5/14/49/49	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903	TMO	OAE-NAC	-12.68	1.25	1.42
2	A	1001	TMO	OAE-NAC	-12.66	1.25	1.42
2	A	1003	TMO	OAE-NAC	-12.57	1.25	1.42
2	B	901	TMO	OAE-NAC	-12.51	1.25	1.42
6	B	910	QXT	C19-C18	5.70	1.51	1.40
6	A	1010	QXT	C19-C18	5.65	1.51	1.40
3	A	1002	QXQ	C18-C17	5.36	1.50	1.40
3	B	902	QXQ	C18-C17	5.34	1.50	1.40
6	A	1010	QXT	C22-C21	2.95	1.46	1.39
3	A	1002	QXQ	C22-C15	2.85	1.46	1.39
3	B	902	QXQ	C22-C15	2.84	1.46	1.39
6	B	910	QXT	C22-C21	2.84	1.46	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	910	QXT	C17-C16-N15	-4.84	105.80	111.07
6	A	1010	QXT	C17-C16-N15	-4.08	106.63	111.07
3	B	902	QXQ	C14-N15-C16	-3.62	105.18	111.62
6	B	910	QXT	O22-C8-N7	3.52	135.95	132.19
6	A	1010	QXT	O21-C6-N7	3.40	135.82	132.19
3	A	1002	QXQ	C14-N15-C16	-3.26	105.82	111.62
6	B	910	QXT	C26-O24-C21	3.18	109.47	105.34
6	B	910	QXT	C26-O25-C22	3.12	109.39	105.34
6	A	1010	QXT	C10-C14-N15	-3.03	107.24	113.12
3	A	1002	QXQ	C26-O24-C15	2.92	109.13	105.34
3	B	902	QXQ	C26-O24-C15	2.90	109.11	105.34
3	B	902	QXQ	C26-O25-C22	2.88	109.09	105.34
6	A	1010	QXT	C26-O24-C21	2.87	109.07	105.34
3	A	1002	QXQ	C26-O25-C22	2.81	108.99	105.34
6	A	1010	QXT	C26-O25-C22	2.70	108.85	105.34
6	A	1010	QXT	C9-C7-N7	2.52	122.24	119.12
6	B	910	QXT	O21-C6-N7	2.50	134.87	132.19
6	A	1010	QXT	O22-C8-N7	2.41	134.77	132.19
6	B	910	QXT	C10-C14-N15	-2.29	108.68	113.12
3	A	1002	QXQ	C19-C20-N15	2.27	113.54	111.07
6	A	1010	QXT	C22-C23-C18	-2.25	117.49	121.09
3	B	902	QXQ	C13-C8-C9	-2.24	116.99	119.65
6	B	910	QXT	O24-C21-C15	2.19	130.78	127.85
3	A	1002	QXQ	C13-C8-C9	-2.15	117.10	119.65
6	B	910	QXT	C22-C23-C18	-2.14	117.67	121.09
3	B	902	QXQ	O24-C15-C7	2.14	130.71	127.85
3	B	902	QXQ	C1-C6-N7	2.11	118.57	115.43
3	A	1002	QXQ	O22-C6-C1	-2.09	117.84	121.21
3	A	1002	QXQ	O24-C15-C7	2.09	130.65	127.85
6	B	910	QXT	C9-C7-N7	2.05	121.65	119.12
3	B	902	QXQ	O22-C6-C1	-2.03	117.94	121.21
3	B	902	QXQ	C19-C20-N15	2.03	113.28	111.07
6	B	910	QXT	C19-C20-N15	-2.01	109.77	112.14

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	QXQ	C4-C1-C2-C3
3	B	902	QXQ	C21-C1-C2-C3
3	B	902	QXQ	C2-C1-C21-O23

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Mol	Chain	Res	Type	Atoms
3	B	902	QXQ	C4-C1-C21-O23
3	A	1002	QXQ	C2-C1-C4-C5
3	A	1002	QXQ	C21-C1-C4-C5
3	A	1002	QXQ	C2-C1-C21-O23
3	A	1002	QXQ	C4-C1-C21-O23
4	A	1005	GOL	O1-C1-C2-C3
4	A	1005	GOL	C1-C2-C3-O3
6	B	910	QXT	C1-C2-C3-C6
6	B	910	QXT	C8-C3-C4-C5
3	B	902	QXQ	C6-C1-C2-C3
6	A	1010	QXT	C10-C14-N15-C20
4	A	1005	GOL	O1-C1-C2-O2
3	A	1002	QXQ	C6-C1-C4-C5
6	B	910	QXT	C10-C14-N15-C20
4	A	1005	GOL	O2-C2-C3-O3
6	B	910	QXT	C2-C3-C4-C5
6	A	1010	QXT	C10-C14-N15-C16
6	B	910	QXT	C10-C14-N15-C16

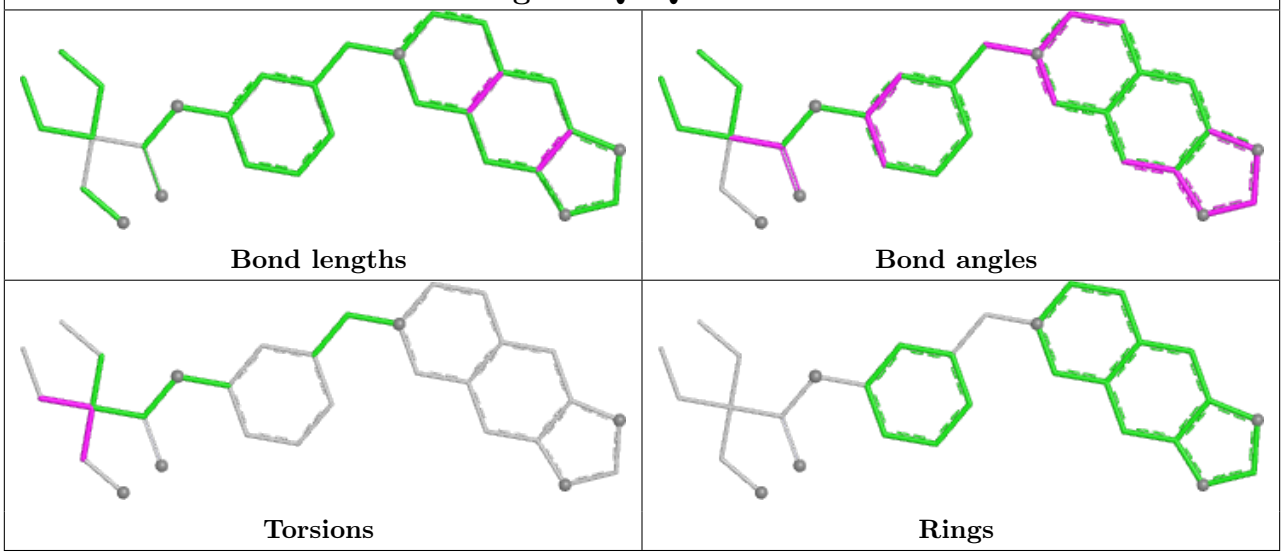
There are no ring outliers.

2 monomers are involved in 2 short contacts:

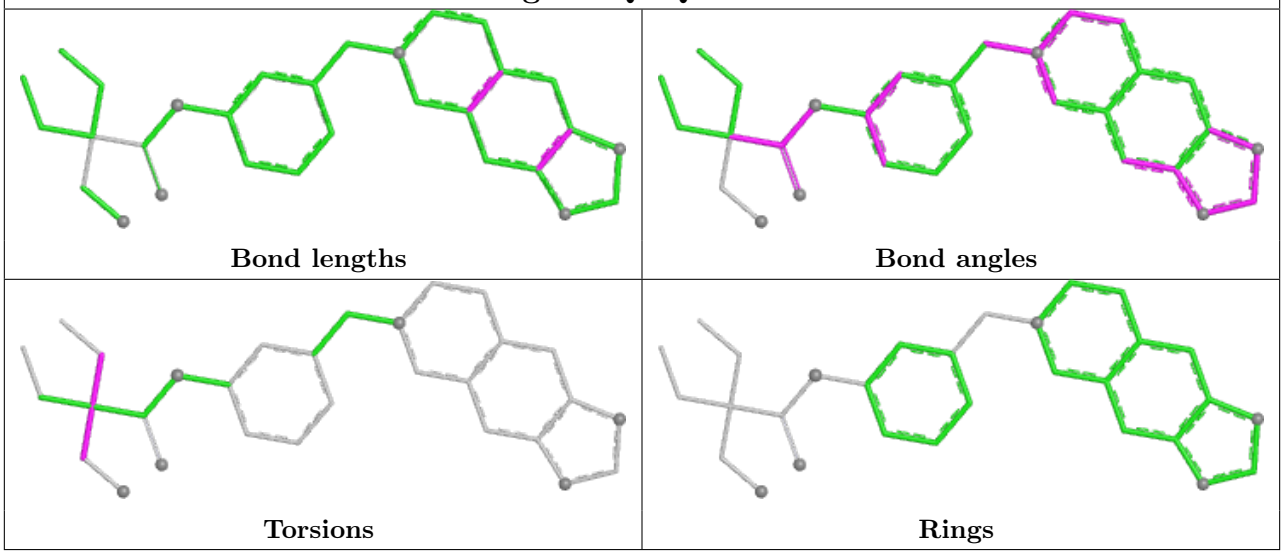
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	TMO	1	0
2	A	1003	TMO	1	0

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 then 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.

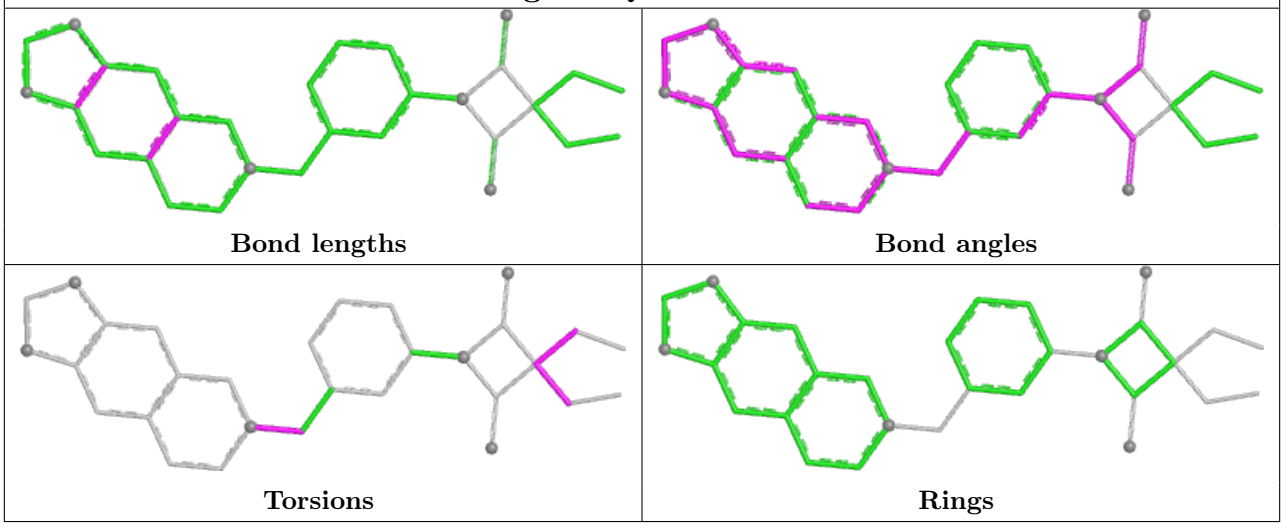
Ligand QXQ A 1002

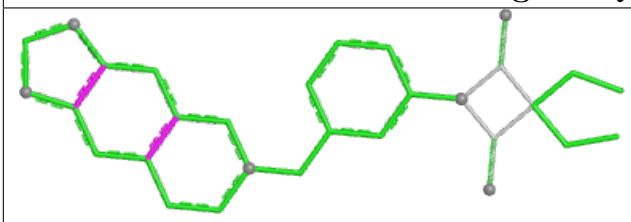
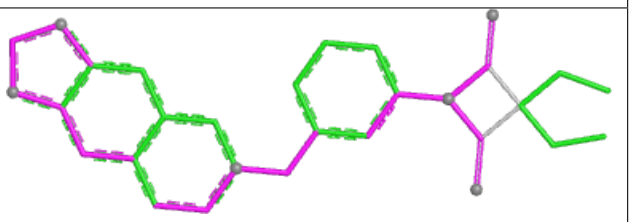
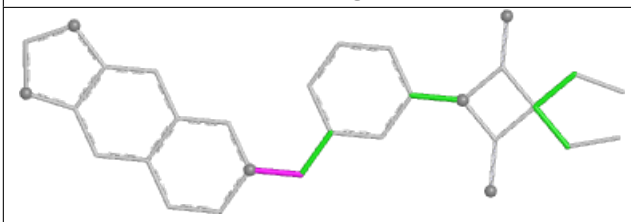
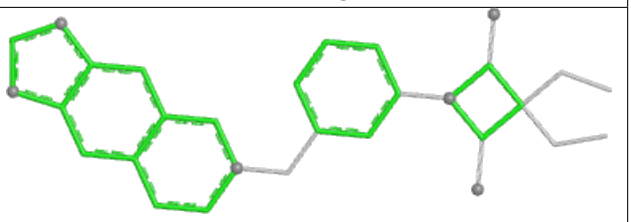


Ligand QXQ B 902



Ligand QXT B 910



Ligand QXT A 1010	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} 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	827/898 (92%)	0.07	5 (0%)	89	86	60, 85, 125, 189	0
1	B	828/898 (92%)	0.05	7 (0%)	86	81	60, 86, 126, 190	0
All	All	1655/1796 (92%)	0.06	12 (0%)	87	84	60, 85, 125, 190	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	TYR	6.2
1	A	71	TYR	4.3
1	B	71	TYR	4.0
1	B	74	TYR	3.8
1	A	75	MET	3.3
1	B	107	GLU	3.0
1	A	734	LEU	2.8
1	B	108	ASN	2.7
1	A	354	GLY	2.5
1	B	139	PHE	2.4
1	B	827	LEU	2.3
1	B	75	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

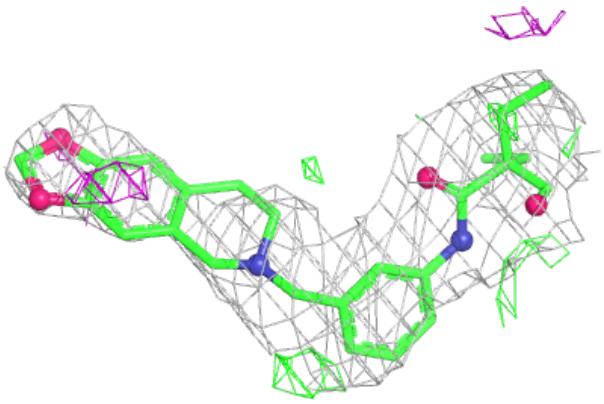
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

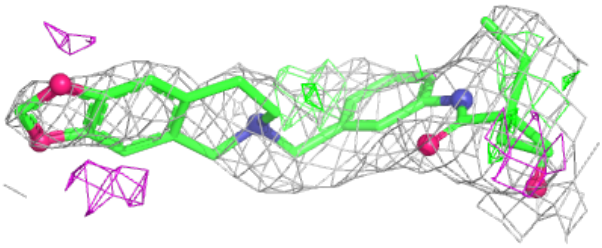
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	B	911	1/1	0.74	0.28	106,106,106,106	0
5	PO4	A	1009	5/5	0.76	0.45	131,134,138,143	0
4	GOL	B	905	6/6	0.77	0.18	106,107,107,107	0
5	PO4	B	909	5/5	0.78	0.35	140,140,144,152	0
4	GOL	A	1005	6/6	0.80	0.16	111,115,116,117	0
5	PO4	A	1008	5/5	0.80	0.32	159,159,160,164	0
5	PO4	B	906	5/5	0.84	0.42	128,130,133,133	0
2	TMO	A	1003	5/5	0.84	0.34	114,116,117,118	0
5	PO4	A	1006	5/5	0.84	0.39	128,130,132,137	0
5	PO4	B	908	5/5	0.85	0.41	153,156,158,162	0
3	QXQ	A	1002	30/30	0.86	0.33	83,127,155,156	0
3	QXQ	B	902	30/30	0.86	0.28	83,120,154,155	0
7	CL	A	1011	1/1	0.86	0.13	101,101,101,101	0
4	GOL	B	904	6/6	0.88	0.11	108,109,110,110	0
5	PO4	B	907	5/5	0.89	0.25	138,138,144,144	0
2	TMO	B	901	5/5	0.89	0.37	82,83,85,93	0
6	QXT	B	910	30/30	0.90	0.26	81,89,112,118	0
2	TMO	B	903	5/5	0.90	0.24	112,112,115,116	0
4	GOL	A	1004	6/6	0.90	0.14	116,118,119,119	0
5	PO4	A	1007	5/5	0.92	0.22	143,144,147,147	0
6	QXT	A	1010	30/30	0.92	0.21	80,91,116,119	0
2	TMO	A	1001	5/5	0.93	0.33	84,85,89,91	0

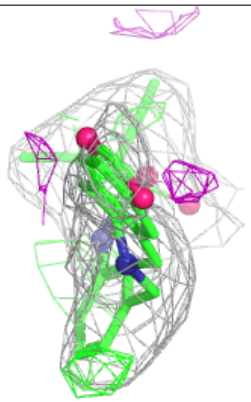
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QXQ A 1002:

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

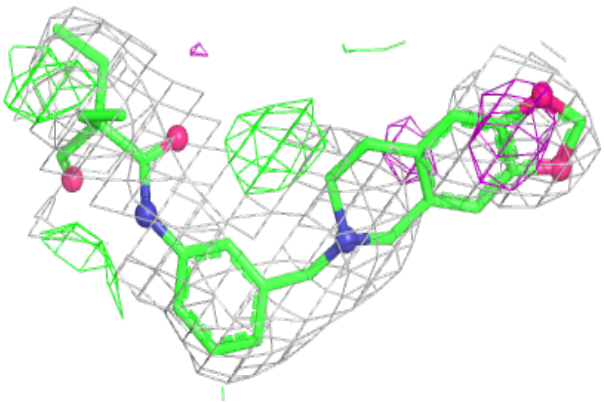


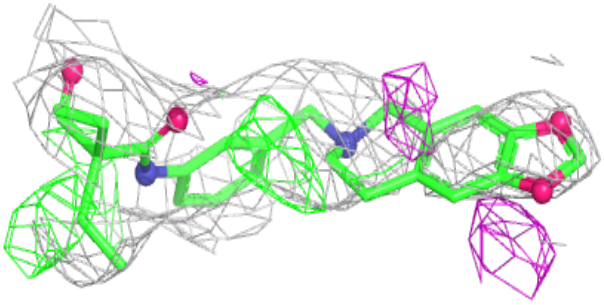




Electron density around QXQ B 902:

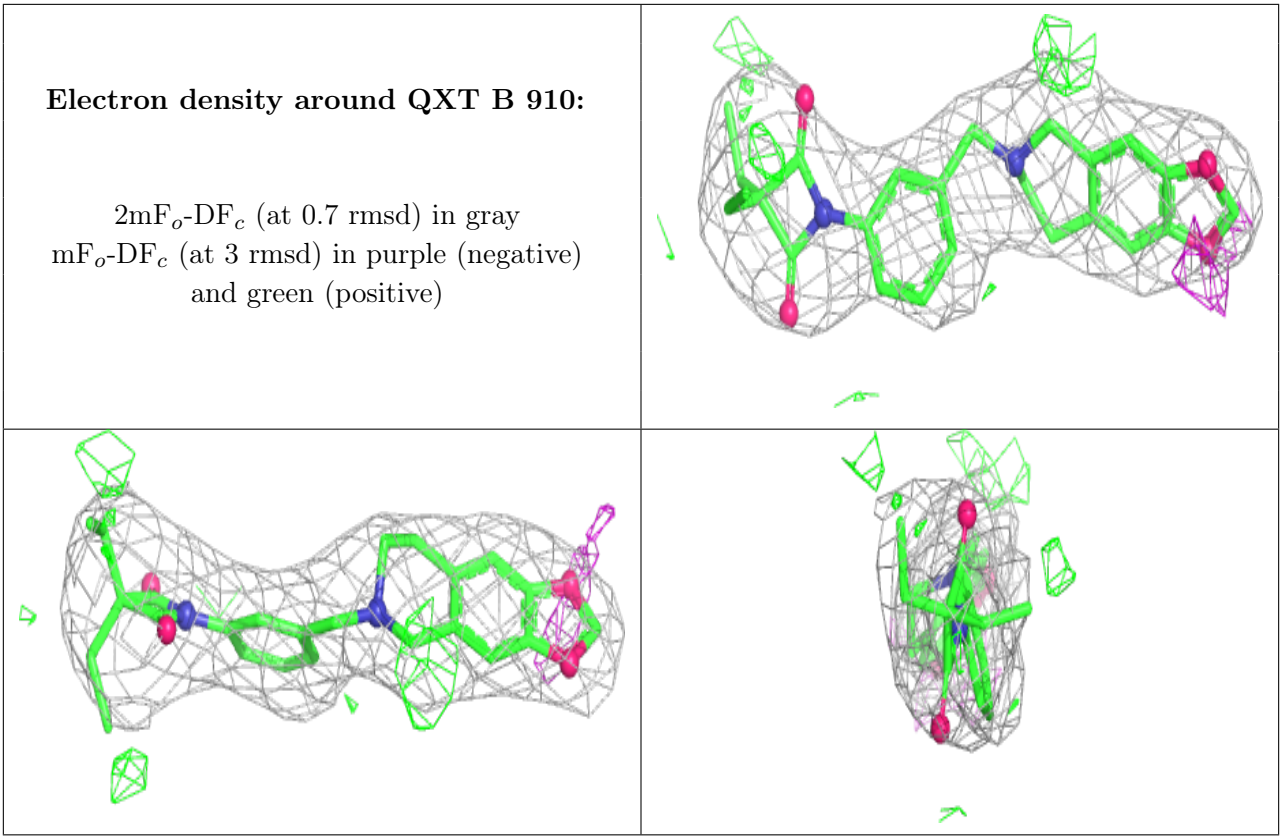
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





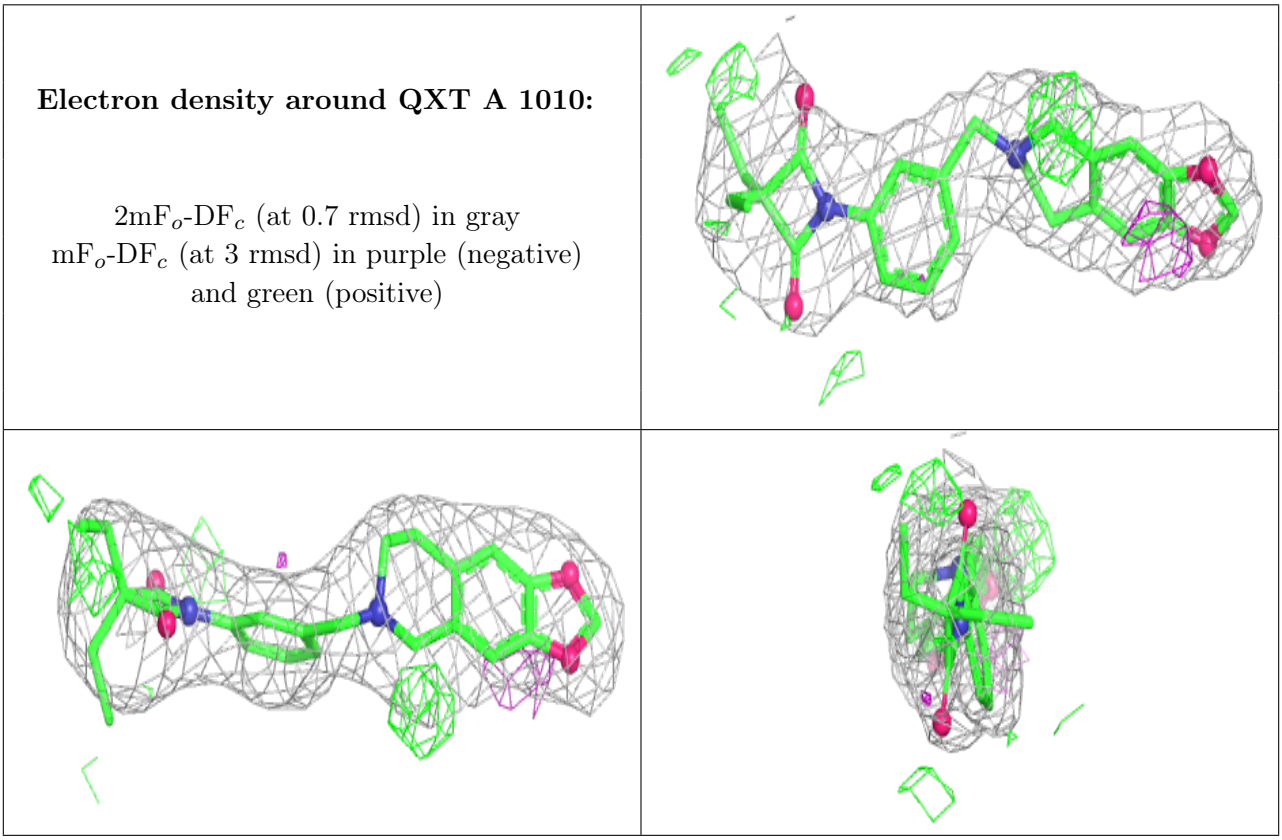
Electron density around QXT B 910:

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



Electron density around QXT A 1010:

$2mF_o$-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.