Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 02:17 pm GMT

PDB ID	:	7APG
Title	:	Crystal structure of JAK3 in complex with FM587 (compound 9a)
Authors	:	Chaikuad, A.; Forster, M.; Gehringer, M.; Laufer, S.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2020-10-16
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 following versions of software and data (see references ⓘ) were used in the production of this report:

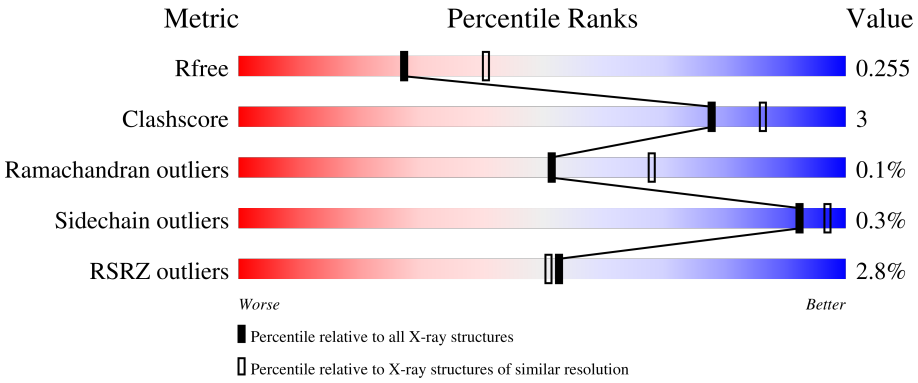
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	294	4% 88% 6% • 5%
1	B	294	4% 89% 5% • 5%
1	C	294	2% 90% 8% ••
1	D	294	% 88% 6% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9501 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.

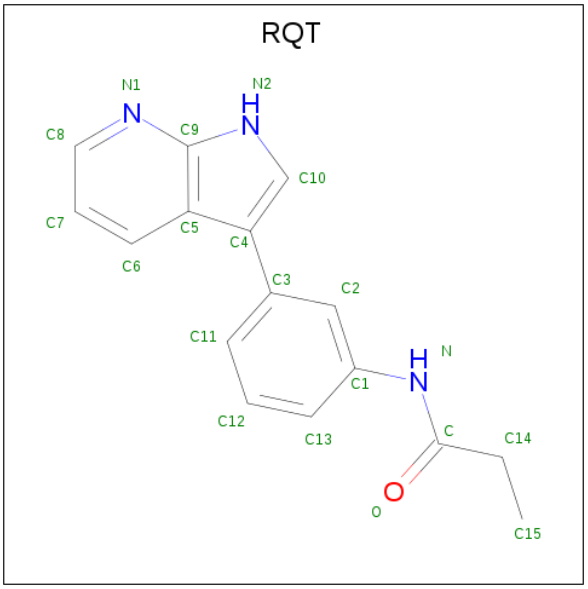
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	2	0
			2223	1420	386	402	15			
1	B	278	Total	C	N	O	S	0	1	0
			2220	1417	390	400	13			
1	C	289	Total	C	N	O	S	0	1	0
			2304	1466	405	418	15			
1	D	277	Total	C	N	O	S	0	1	0
			2205	1408	386	398	13			

There are 20 discrepancies between the modelled and reference sequences:

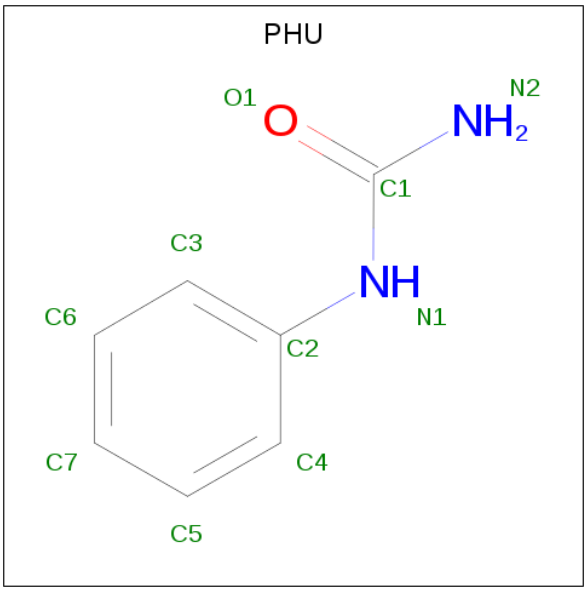
Chain	Residue	Modelled	Actual	Comment	Reference
A	810	SER	-	expression tag	UNP P52333
A	811	MET	-	expression tag	UNP P52333
A	949	ALA	ASP	conflict	UNP P52333
A	1040	SER	CYS	conflict	UNP P52333
A	1048	SER	CYS	conflict	UNP P52333
B	810	SER	-	expression tag	UNP P52333
B	811	MET	-	expression tag	UNP P52333
B	949	ALA	ASP	conflict	UNP P52333
B	1040	SER	CYS	conflict	UNP P52333
B	1048	SER	CYS	conflict	UNP P52333
C	810	SER	-	expression tag	UNP P52333
C	811	MET	-	expression tag	UNP P52333
C	949	ALA	ASP	conflict	UNP P52333
C	1040	SER	CYS	conflict	UNP P52333
C	1048	SER	CYS	conflict	UNP P52333
D	810	SER	-	expression tag	UNP P52333
D	811	MET	-	expression tag	UNP P52333
D	949	ALA	ASP	conflict	UNP P52333
D	1040	SER	CYS	conflict	UNP P52333
D	1048	SER	CYS	conflict	UNP P52333

- Molecule 2 is {N}-[3-(1 {H}-pyrrolo[2,3-b]pyridin-3-yl)phenyl]propanamide (three-letter code: RQT) (formula: $C_{16}H_{15}N_3O$) (labeled as "Ligand of Interest" by author).



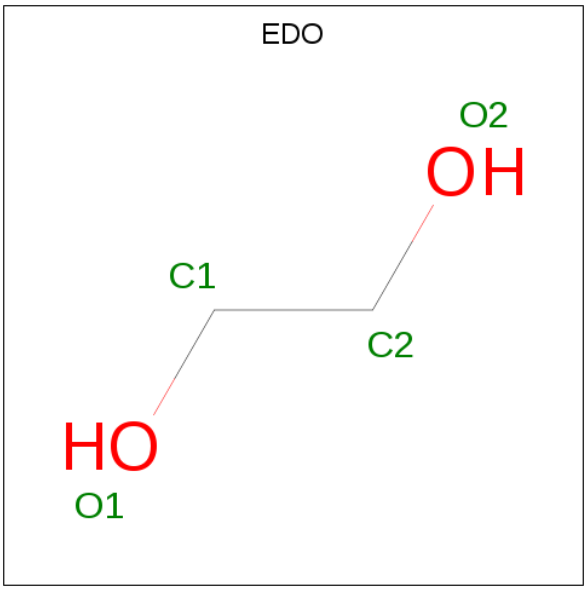
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			40	32	6	2		
2	B	1	Total	C	N	O	0	0
			20	16	3	1		
2	C	1	Total	C	N	O	0	0
			20	16	3	1		
2	D	1	Total	C	N	O	0	0
			20	16	3	1		

- Molecule 3 is 1-phenylurea (three-letter code: PHU) (formula: $C_7H_8N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 7 2 1	0	0
3	B	1	Total C N O 10 7 2 1	0	0
3	C	1	Total C N O 10 7 2 1	0	0
3	D	1	Total C N O 10 7 2 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	80	Total O 80 80	0	0
5	B	81	Total O 81 81	0	0

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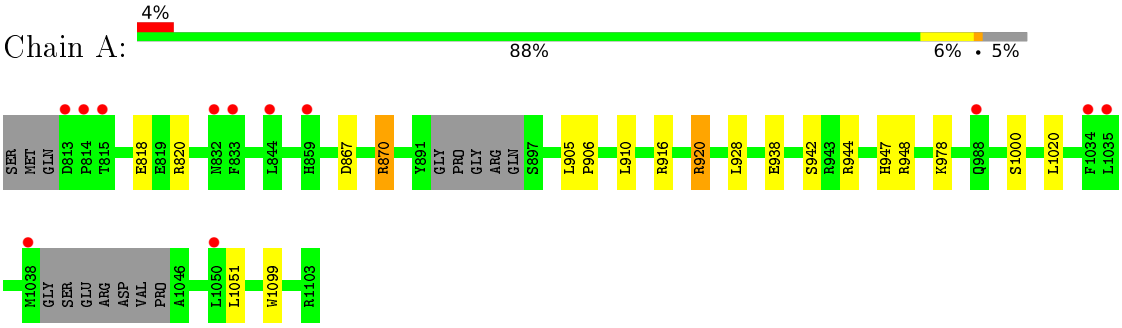
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	84	Total O 84 84	0	0
5	D	92	Total O 92 92	0	0

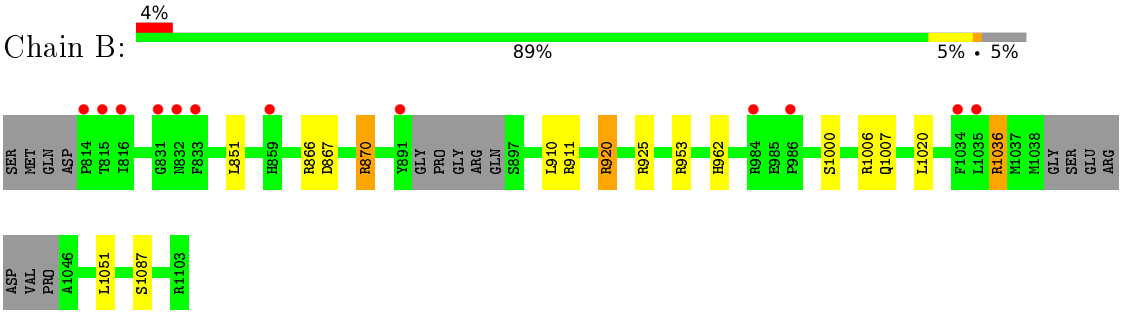
3 Residue-property plots (i)

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.

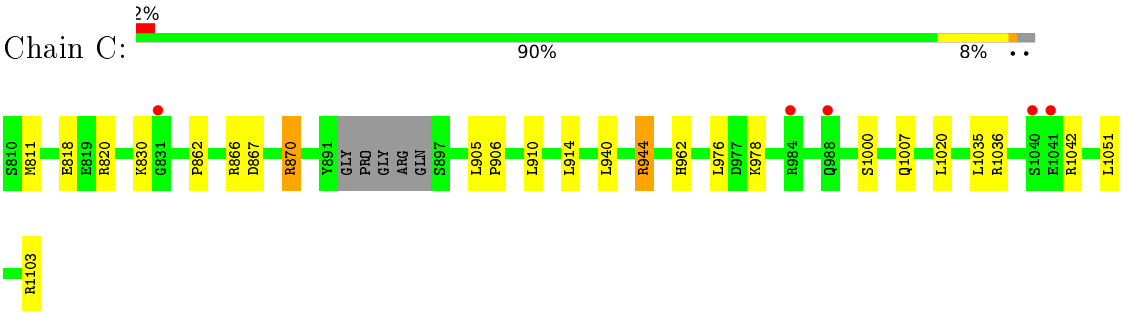
- Molecule 1: Tyrosine-protein kinase JAK3



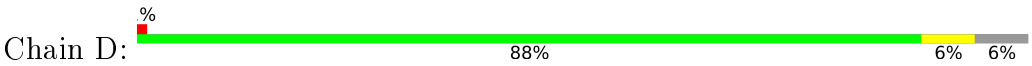
- Molecule 1: Tyrosine-protein kinase JAK3

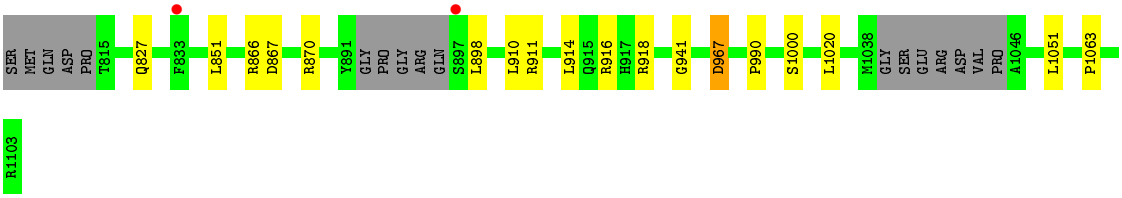


- Molecule 1: Tyrosine-protein kinase JAK3



- Molecule 1: Tyrosine-protein kinase JAK3




SER
MET
GLN
ASP
PRO
T815
Q827
F833
I851
R866
D867
R870
Y891
GLY
PRO
GLY
ARG
GLN
S897
L898
L910
R911
L914
Q915
R916
H917
R918
G941
D967
P990
S1000
L1020
M1038
GLY
SER
GLU
ARG
ASP
VAL
PRO
A1046
L1051
P1063
R1103

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.47Å 112.88Å 102.90Å 90.00° 97.21° 90.00°	Depositor
Resolution (Å)	49.39 – 2.40 49.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.39-2.40) 99.1 (49.39-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.212 , 0.256 0.216 , 0.255	Depositor DCC
R_{free} test set	2497 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9501	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0176e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: RQT, EDO, PHU

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	0.56	0/2282	0.57	0/3085
1	B	0.59	0/2276	0.60	0/3075
1	C	0.57	0/2362	0.59	1/3193 (0.0%)
1	D	0.58	0/2260	0.59	0/3054
All	All	0.57	0/9180	0.59	1/12407 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
1	C	0	3
1	D	0	1
All	All	0	12

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	944	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	870	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	916	ARG	Sidechain
1	A	920	ARG	Sidechain
1	B	1006	ARG	Sidechain
1	B	1036	ARG	Sidechain
1	B	870	ARG	Sidechain
1	B	920	ARG	Sidechain
1	B	925	ARG	Sidechain
1	C	1036	ARG	Sidechain
1	C	1103	ARG	Sidechain
1	C	870	ARG	Sidechain
1	D	916	ARG	Sidechain

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	2223	0	2196	14	0
1	B	2220	0	2200	13	0
1	C	2304	0	2274	21	0
1	D	2205	0	2176	16	0
2	A	40	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	10	0	8	0	0
3	B	10	0	8	0	0
3	C	10	0	8	0	0
3	D	10	0	8	0	0
4	A	12	0	18	0	0
4	B	16	0	24	4	0
4	C	20	0	30	0	0
4	D	24	0	36	3	0
5	A	80	0	0	0	0
5	B	81	0	0	2	0
5	C	84	0	0	2	0
5	D	92	0	0	3	0
All	All	9501	0	8986	53	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 3.

All (53) 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:867:ASP:OD1	1:A:870:ARG:NH1	2.14	0.79
1:C:867:ASP:OD1	1:C:870:ARG:NH1	2.17	0.78
1:B:867:ASP:OD1	1:B:870:ARG:NH1	2.18	0.76
1:C:811:MET:HE3	1:D:1063:PRO:HA	1.77	0.67
1:A:928:LEU:HD13	1:C:976:LEU:HB2	1.78	0.65
1:D:867:ASP:OD1	1:D:870:ARG:NH1	2.28	0.63
1:A:928:LEU:CD1	1:C:976:LEU:HB2	2.32	0.59
1:B:1007:GLN:HG3	5:B:1372:HOH:O	2.04	0.58
1:A:928:LEU:HA	1:C:976:LEU:HD12	1.86	0.57
1:B:953:ARG:HD3	4:B:1205:EDO:H21	1.85	0.57
1:D:898:LEU:N	5:D:1302:HOH:O	2.38	0.56
1:C:830:LYS:NZ	5:C:1302:HOH:O	2.34	0.55
1:A:818:GLU:OE1	1:A:820:ARG:NH1	2.41	0.54
1:C:1035:LEU:HD22	1:C:1042:ARG:HH11	1.73	0.53
1:A:910:LEU:HD21	1:A:1020:LEU:HD21	1.92	0.52
1:C:1000:SER:HB3	1:C:1051:LEU:HD21	1.90	0.52
1:C:910:LEU:HD21	1:C:1020:LEU:HD21	1.92	0.52
1:D:910:LEU:HD21	1:D:1020:LEU:HD21	1.92	0.51
1:D:941:GLY:HA3	4:D:1206:EDO:C2	2.40	0.51
1:B:1087:SER:HA	4:B:1204:EDO:O2	2.11	0.51
1:B:851:LEU:HD12	1:D:851:LEU:HD12	1.93	0.51
1:B:910:LEU:HD21	1:B:1020:LEU:HD21	1.93	0.50
1:A:1000:SER:HB3	1:A:1051:LEU:HD21	1.92	0.50
1:A:942:SER:HB2	1:C:866[A]:ARG:NH1	2.27	0.49
1:C:862:PRO:HB2	1:C:866[B]:ARG:HH12	1.77	0.49
1:B:953:ARG:HD3	4:B:1205:EDO:C2	2.43	0.48
1:D:990:PRO:O	5:D:1301:HOH:O	2.19	0.48
1:A:938:GLU:OE1	1:C:870:ARG:NH2	2.45	0.48
1:D:866:ARG:HD3	5:D:1314:HOH:O	2.15	0.47
1:D:1000:SER:HB3	1:D:1051:LEU:HD21	1.96	0.46
1:C:1035:LEU:HD22	1:C:1042:ARG:NH1	2.31	0.46
1:C:1007:GLN:HG3	5:C:1376:HOH:O	2.17	0.45
1:B:911:ARG:HH11	4:B:1205:EDO:H22	1.82	0.45
1:D:967:ASP:HB2	4:D:1203:EDO:C2	2.47	0.44
1:B:920:ARG:HH12	1:D:827:GLN:HB2	1.82	0.44
1:A:1099:TRP:CG	1:C:976:LEU:HD13	2.52	0.44
1:B:1000:SER:HB3	1:B:1051:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:ARG:NH1	1:D:827:GLN:HB2	2.33	0.44
1:A:1099:TRP:CH2	1:C:976:LEU:O	2.71	0.43
1:C:818:GLU:OE2	1:C:820:ARG:NH1	2.50	0.43
1:C:940:LEU:HA	1:C:940:LEU:HD23	1.90	0.42
1:A:905:LEU:HA	1:A:906:PRO:HD3	1.89	0.42
1:C:905:LEU:HA	1:C:906:PRO:HD3	1.87	0.42
1:C:944:ARG:NH1	1:C:978:LYS:O	2.52	0.42
1:B:866[A]:ARG:NH2	5:B:1315:HOH:O	2.53	0.41
1:A:944:ARG:NH2	1:A:978:LYS:O	2.53	0.40
1:C:914:LEU:HD11	1:C:1020:LEU:HD23	2.03	0.40
1:A:947:HIS:O	1:A:948:ARG:HB3	2.22	0.40
1:D:911:ARG:HH11	4:D:1208:EDO:H11	1.86	0.40
1:B:1036:ARG:HB3	1:B:1036:ARG:HH21	1.86	0.40
1:D:914:LEU:HD11	1:D:1020:LEU:HD23	2.04	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	275/294 (94%)	266 (97%)	9 (3%)	0	100	100
1	B	273/294 (93%)	265 (97%)	8 (3%)	0	100	100
1	C	286/294 (97%)	276 (96%)	10 (4%)	0	100	100
1	D	272/294 (92%)	265 (97%)	6 (2%)	1 (0%)	34	48
All	All	1106/1176 (94%)	1072 (97%)	33 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	967	ASP

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	241/256 (94%)	240 (100%)	1 (0%)	91 96
1	B	240/256 (94%)	239 (100%)	1 (0%)	91 96
1	C	249/256 (97%)	248 (100%)	1 (0%)	91 96
1	D	237/256 (93%)	237 (100%)	0	100 100
All	All	967/1024 (94%)	964 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	920	ARG
1	B	962	HIS
1	C	962	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

27 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	$\#\|Z\| > 2$
4	EDO	B	1203	-	3,3,3	0.62	0	2,2,2	0.29	0
4	EDO	B	1206	-	3,3,3	0.55	0	2,2,2	0.21	0
3	PHU	B	1202	-	10,10,10	0.39	0	12,12,12	0.30	0
3	PHU	A	1202	-	10,10,10	0.25	0	12,12,12	0.23	0
4	EDO	C	1206	-	3,3,3	0.58	0	2,2,2	0.10	0
4	EDO	D	1205	-	3,3,3	0.48	0	2,2,2	0.38	0
2	RQT	D	1201	1	21,22,22	0.78	1 (4%)	23,30,30	0.71	0
2	RQT	A	1201[A]	1	21,22,22	0.83	1 (4%)	23,30,30	0.56	0
2	RQT	A	1201[B]	1	21,22,22	0.82	1 (4%)	23,30,30	0.65	0
4	EDO	D	1208	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	A	1205	-	3,3,3	0.38	0	2,2,2	0.54	0
4	EDO	D	1206	-	3,3,3	0.51	0	2,2,2	0.20	0
4	EDO	A	1204	-	3,3,3	0.60	0	2,2,2	0.01	0
4	EDO	C	1205	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	C	1203	-	3,3,3	0.61	0	2,2,2	0.30	0
4	EDO	D	1207	-	3,3,3	0.91	0	2,2,2	0.14	0
4	EDO	C	1207	-	3,3,3	0.53	0	2,2,2	0.18	0
4	EDO	D	1204	-	3,3,3	0.64	0	2,2,2	0.09	0
4	EDO	B	1205	-	3,3,3	0.50	0	2,2,2	0.20	0
2	RQT	B	1201	1	21,22,22	0.79	0	23,30,30	0.71	0
2	RQT	C	1201	1	21,22,22	0.85	1 (4%)	23,30,30	0.75	0
3	PHU	C	1202	-	10,10,10	0.23	0	12,12,12	0.28	0
4	EDO	C	1204	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	A	1203	-	3,3,3	0.56	0	2,2,2	0.20	0
4	EDO	D	1203	-	3,3,3	0.33	0	2,2,2	0.43	0
4	EDO	B	1204	-	3,3,3	0.38	0	2,2,2	0.35	0
3	PHU	D	1202	-	10,10,10	0.48	0	12,12,12	0.34	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	B	1203	-	-	0/1/1/1	-
4	EDO	B	1206	-	-	1/1/1/1	-
3	PHU	B	1202	-	-	2/4/4/4	0/1/1/1
3	PHU	A	1202	-	-	2/4/4/4	0/1/1/1
4	EDO	C	1206	-	-	1/1/1/1	-
4	EDO	D	1205	-	-	1/1/1/1	-
2	RQT	D	1201	1	-	2/10/10/10	0/3/3/3
2	RQT	A	1201[A]	1	-	2/10/10/10	0/3/3/3
2	RQT	A	1201[B]	1	-	2/10/10/10	0/3/3/3
4	EDO	D	1208	-	-	1/1/1/1	-
4	EDO	A	1205	-	-	1/1/1/1	-
4	EDO	D	1206	-	-	1/1/1/1	-
4	EDO	A	1204	-	-	1/1/1/1	-
4	EDO	C	1205	-	-	0/1/1/1	-
4	EDO	C	1203	-	-	0/1/1/1	-
4	EDO	D	1207	-	-	1/1/1/1	-
4	EDO	C	1207	-	-	1/1/1/1	-
4	EDO	D	1204	-	-	1/1/1/1	-
4	EDO	B	1205	-	-	0/1/1/1	-
2	RQT	B	1201	1	-	0/10/10/10	0/3/3/3
2	RQT	C	1201	1	-	1/10/10/10	0/3/3/3
3	PHU	C	1202	-	-	3/4/4/4	0/1/1/1
4	EDO	C	1204	-	-	0/1/1/1	-
4	EDO	A	1203	-	-	0/1/1/1	-
4	EDO	D	1203	-	-	1/1/1/1	-
4	EDO	B	1204	-	-	0/1/1/1	-
3	PHU	D	1202	-	-	0/4/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201[A]	RQT	C9-N1	-2.33	1.33	1.37
2	A	1201[B]	RQT	C9-N1	-2.30	1.33	1.37
2	C	1201	RQT	C9-N1	-2.15	1.34	1.37
2	D	1201	RQT	C9-N1	-2.04	1.34	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201[B]	RQT	C2-C3-C4-C5
4	D	1205	EDO	O1-C1-C2-O2
4	D	1208	EDO	O1-C1-C2-O2
4	D	1207	EDO	O1-C1-C2-O2
4	D	1203	EDO	O1-C1-C2-O2
3	A	1202	PHU	C3-C2-N1-C1
3	A	1202	PHU	C4-C2-N1-C1
3	C	1202	PHU	C4-C2-N1-C1
4	C	1206	EDO	O1-C1-C2-O2
3	C	1202	PHU	C3-C2-N1-C1
2	D	1201	RQT	C11-C3-C4-C5
2	A	1201[B]	RQT	C11-C3-C4-C5
4	B	1206	EDO	O1-C1-C2-O2
4	C	1207	EDO	O1-C1-C2-O2
3	B	1202	PHU	C3-C2-N1-C1
3	C	1202	PHU	O1-C1-N1-C2
2	A	1201[A]	RQT	O-C-C14-C15
4	A	1205	EDO	O1-C1-C2-O2
4	D	1206	EDO	O1-C1-C2-O2
4	A	1204	EDO	O1-C1-C2-O2
4	D	1204	EDO	O1-C1-C2-O2
3	B	1202	PHU	C4-C2-N1-C1
2	A	1201[A]	RQT	N-C-C14-C15
2	D	1201	RQT	C2-C3-C4-C5
2	C	1201	RQT	C2-C3-C4-C5

There are no ring outliers.

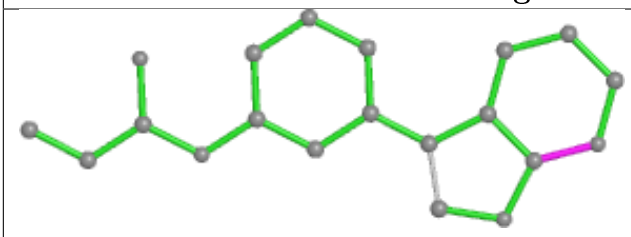
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1208	EDO	1	0
4	D	1206	EDO	1	0
4	B	1205	EDO	3	0
4	D	1203	EDO	1	0
4	B	1204	EDO	1	0

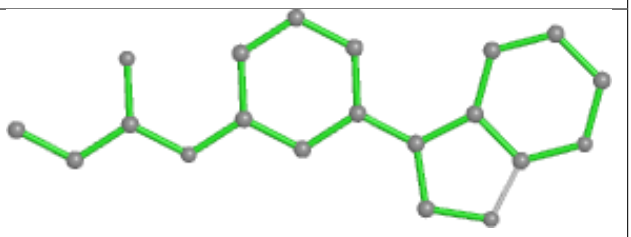
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

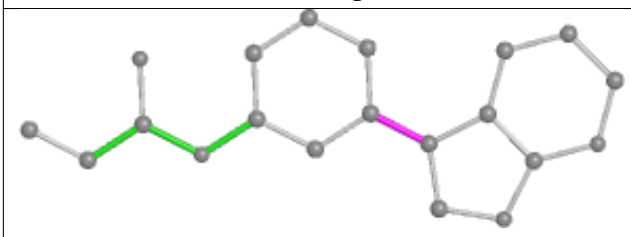
Ligand RQT D 1201



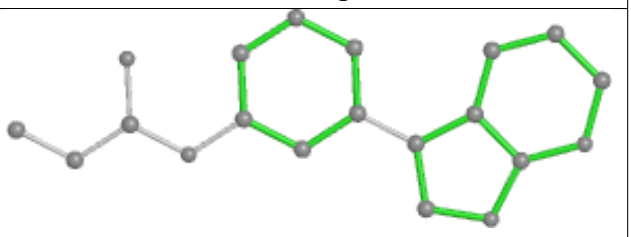
Bond lengths



Bond angles

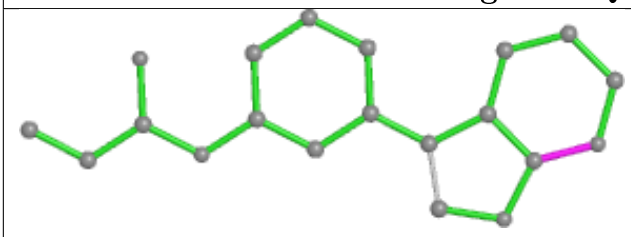


Torsions

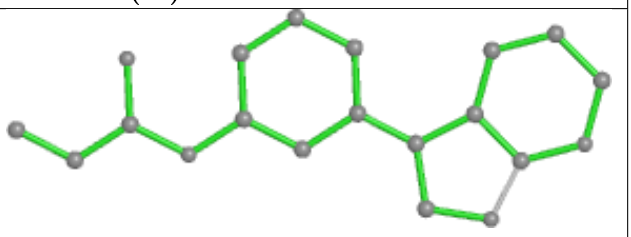


Rings

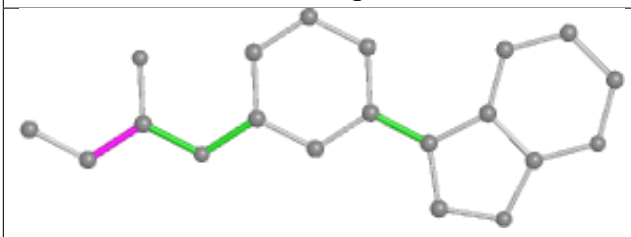
Ligand RQT A 1201 (A)



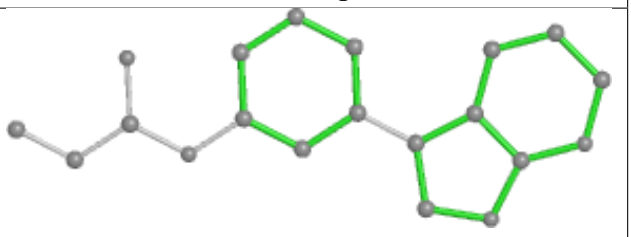
Bond lengths



Bond angles

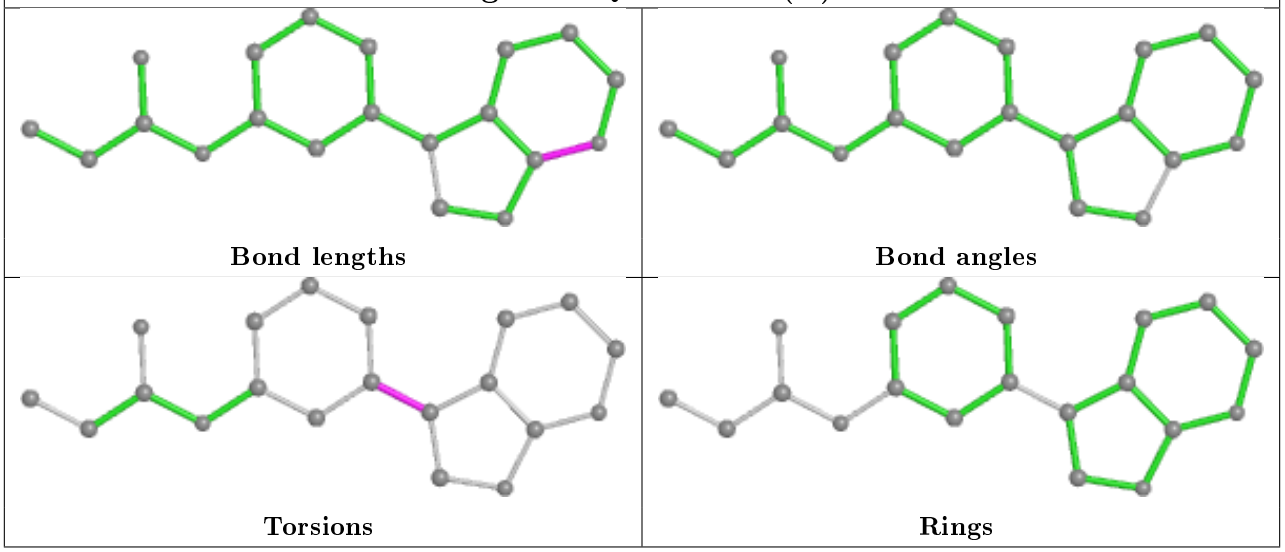


Torsions

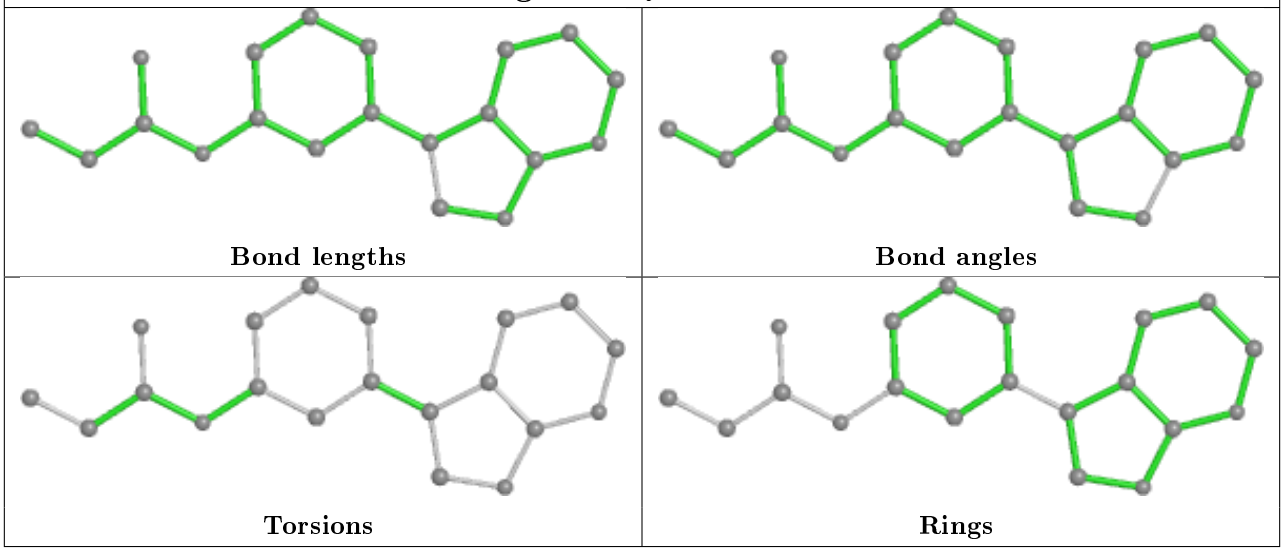


Rings

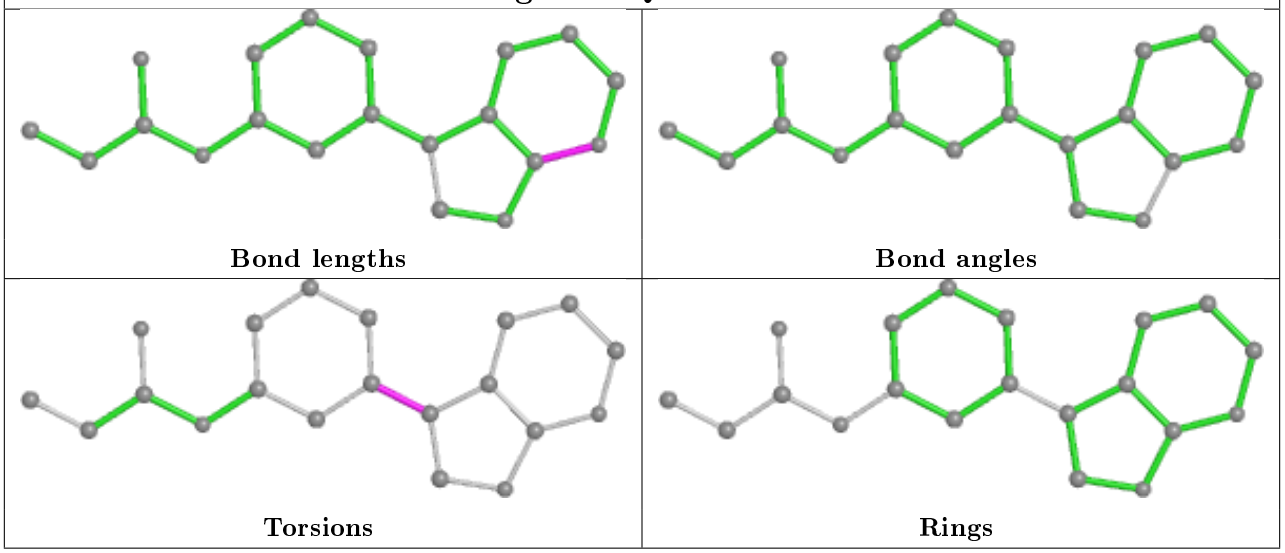
Ligand RQT A 1201 (B)



Ligand RQT B 1201



Ligand RQT C 1201



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	279/294 (94%)	-0.10	12 (4%) 35 33	20, 36, 84, 121	0
1	B	278/294 (94%)	-0.08	12 (4%) 35 33	19, 35, 73, 110	0
1	C	289/294 (98%)	-0.01	5 (1%) 70 68	20, 38, 87, 118	0
1	D	277/294 (94%)	-0.21	2 (0%) 87 86	19, 32, 66, 88	0
All	All	1123/1176 (95%)	-0.10	31 (2%) 53 51	19, 34, 78, 121	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1035	LEU	5.8
1	A	814	PRO	5.1
1	B	833	PHE	4.5
1	A	832	ASN	4.4
1	A	1038	MET	4.2
1	C	1040	SER	4.1
1	C	984	ARG	3.5
1	B	814	PRO	3.5
1	A	859	HIS	3.4
1	B	831	GLY	3.4
1	B	859	HIS	3.2
1	A	815	THR	3.2
1	B	832	ASN	3.1
1	D	833	PHE	3.1
1	B	816	ILE	3.0
1	A	1035	LEU	3.0
1	A	988	GLN	2.9
1	B	815	THR	2.9
1	A	1050	LEU	2.8
1	B	986	PRO	2.7
1	A	833	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1034	PHE	2.6
1	A	813	ASP	2.6
1	B	891	TYR	2.5
1	C	1041	GLU	2.5
1	B	984	ARG	2.4
1	B	1034	PHE	2.4
1	D	897	SER	2.2
1	C	988	GLN	2.2
1	C	831	GLY	2.2
1	A	844	LEU	2.1

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 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
3	PHU	B	1202	10/10	0.73	0.26	55,58,61,63	0
4	EDO	D	1204	4/4	0.75	0.18	49,49,50,51	0
4	EDO	B	1203	4/4	0.81	0.24	39,40,40,41	0
4	EDO	D	1205	4/4	0.84	0.23	55,55,55,56	0
4	EDO	B	1206	4/4	0.85	0.30	20,25,30,32	0
4	EDO	A	1203	4/4	0.86	0.17	40,40,41,43	0
4	EDO	C	1207	4/4	0.87	0.25	28,34,38,41	0
4	EDO	D	1208	4/4	0.87	0.26	45,45,47,49	0
4	EDO	C	1203	4/4	0.87	0.24	35,36,36,37	0
4	EDO	D	1203	4/4	0.87	0.28	43,44,44,48	0
4	EDO	A	1204	4/4	0.88	0.20	46,47,48,49	0
4	EDO	B	1205	4/4	0.88	0.31	44,47,50,52	0
4	EDO	C	1206	4/4	0.89	0.27	44,47,53,57	0

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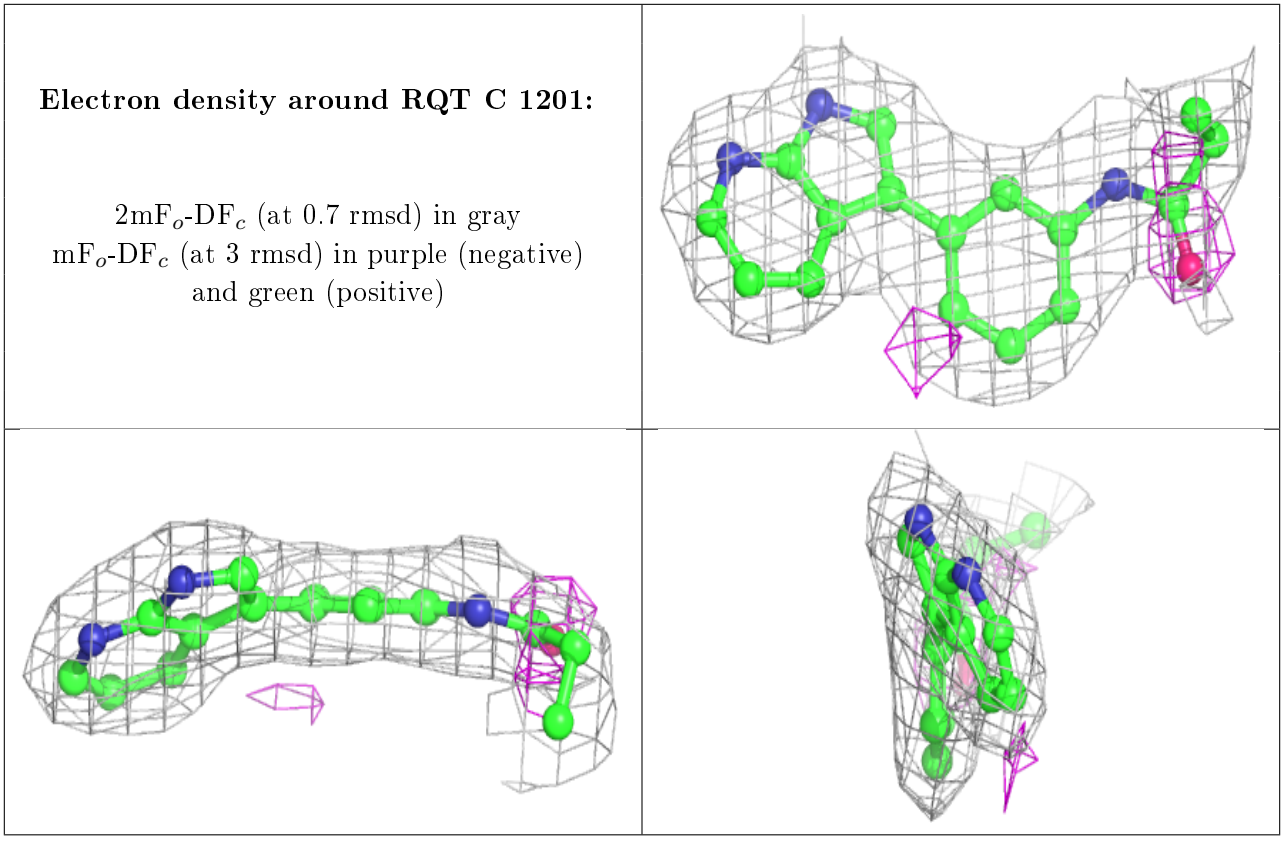
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	C	1205	4/4	0.89	0.19	63,63,65,68	0
4	EDO	D	1207	4/4	0.90	0.15	32,34,36,36	0
4	EDO	B	1204	4/4	0.90	0.30	33,33,34,35	0
3	PHU	C	1202	10/10	0.91	0.24	41,59,67,71	0
4	EDO	A	1205	4/4	0.92	0.31	35,40,45,47	0
2	RQT	C	1201	20/20	0.93	0.16	15,16,24,31	0
4	EDO	D	1206	4/4	0.94	0.22	36,37,37,40	0
2	RQT	D	1201	20/20	0.95	0.13	15,18,23,25	0
3	PHU	A	1202	10/10	0.95	0.23	46,53,56,58	0
3	PHU	D	1202	10/10	0.95	0.15	31,33,34,34	0
2	RQT	A	1201[A]	20/20	0.96	0.14	11,11,11,11	20
2	RQT	A	1201[B]	20/20	0.96	0.14	11,12,12,12	20
2	RQT	B	1201	20/20	0.96	0.12	17,18,25,28	0
4	EDO	C	1204	4/4	0.97	0.14	33,35,36,36	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.

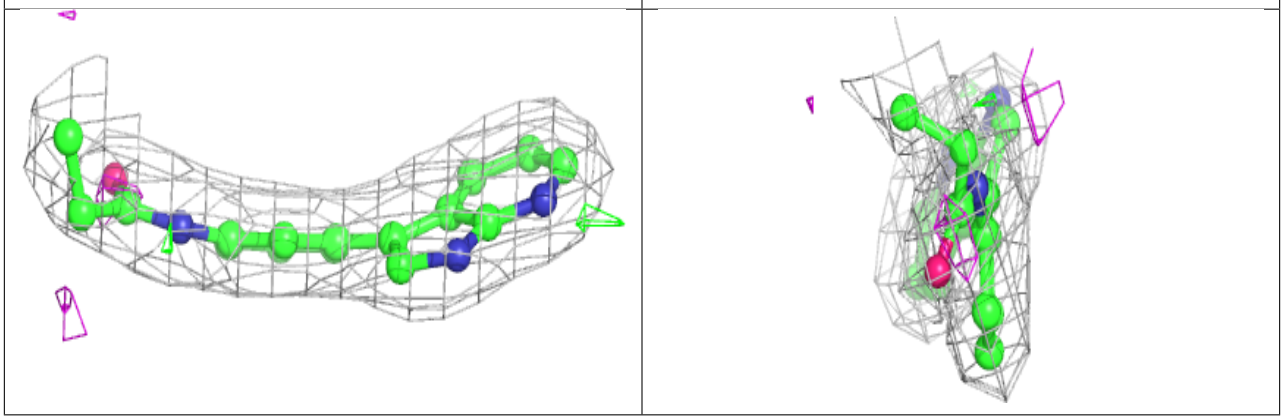
Electron density around RQT C 1201:

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



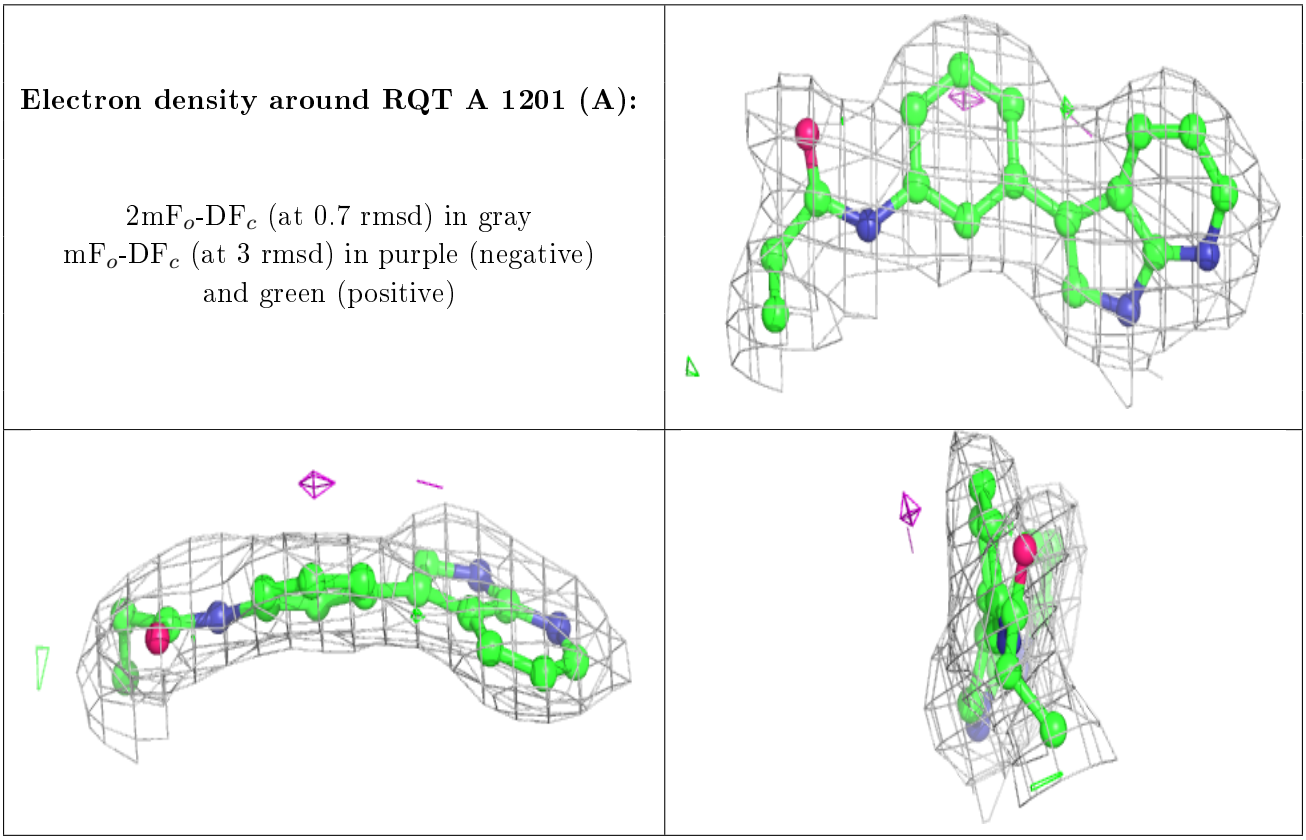
Electron density around RQT D 1201:

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



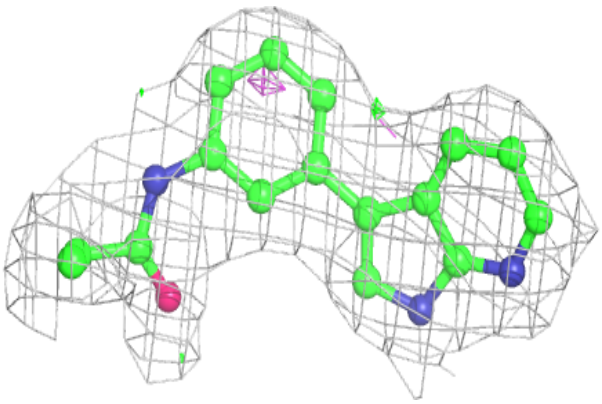
Electron density around RQT A 1201 (A):

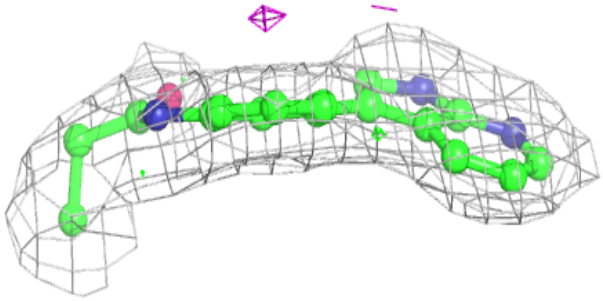
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

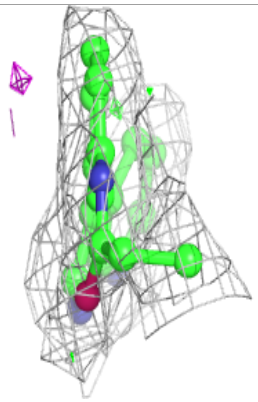


Electron density around RQT A 1201 (B):

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

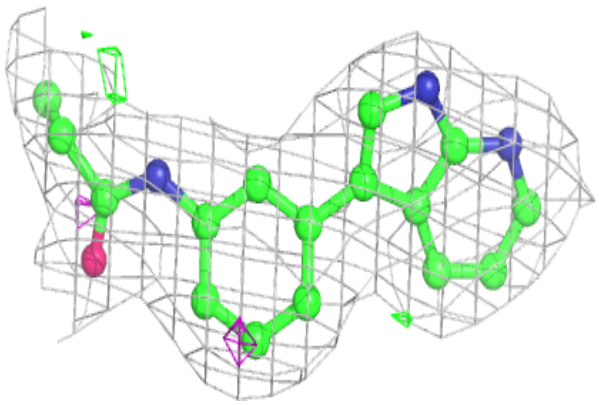


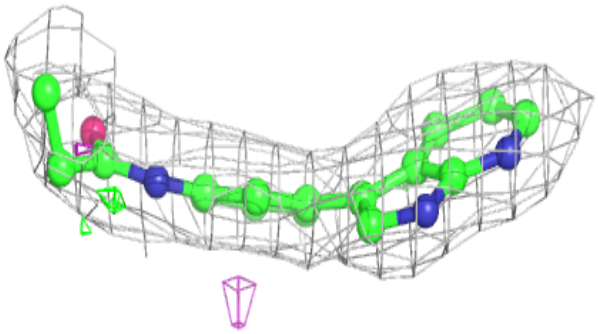


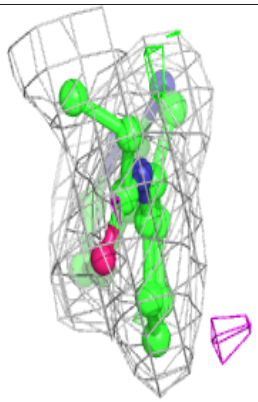


Electron density around RQT B 1201:

$2mF_o$-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.