



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 02:06 PM EST

PDB ID : 6VGL  
Title : JAK2 JH1 in complex with ruxolitinib  
Authors : Davis, R.R.; Schonbrunn, E.  
Deposited on : 2020-01-08  
Resolution : 1.90 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](mailto: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.

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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 : 2.16  
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) : 2.16

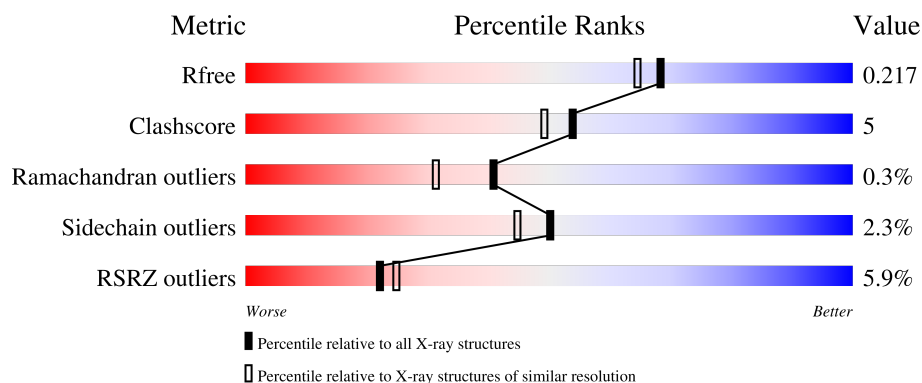
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	308	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>...</div> </div> </div>
1	B	308	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	308	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>6%</div> </div> </div>
1	D	308	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10594 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 JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	289	Total	C	N	O	P	S	0	0	0
			2395	1521	417	442	1	14			
1	B	298	Total	C	N	O	P	S	0	0	0
			2465	1567	427	456	1	14			
1	C	289	Total	C	N	O	P	S	0	0	0
			2395	1521	417	442	1	14			
1	A	305	Total	C	N	O	P	S	0	0	0
			2503	1589	435	464	1	14			

There are 60 discrepancies between the modelled and reference sequences:

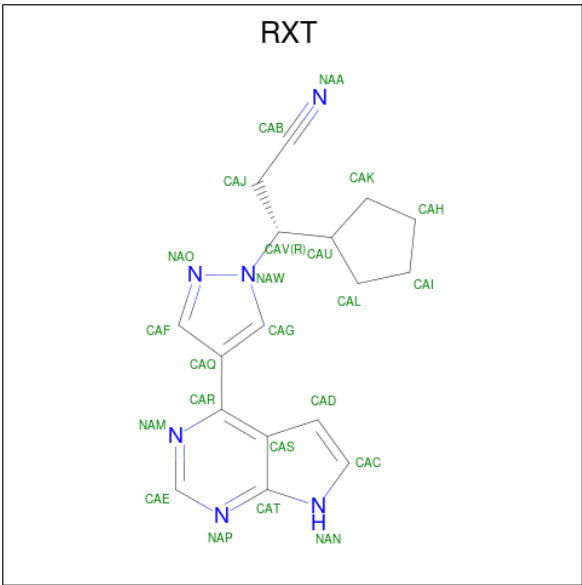
Chain	Residue	Modelled	Actual	Comment	Reference
D	825	HIS	-	expression tag	UNP O60674
D	826	HIS	-	expression tag	UNP O60674
D	827	HIS	-	expression tag	UNP O60674
D	828	HIS	-	expression tag	UNP O60674
D	829	HIS	-	expression tag	UNP O60674
D	830	HIS	-	expression tag	UNP O60674
D	831	HIS	-	expression tag	UNP O60674
D	832	HIS	-	expression tag	UNP O60674
D	833	GLU	-	expression tag	UNP O60674
D	834	ASN	-	expression tag	UNP O60674
D	835	LEU	-	expression tag	UNP O60674
D	836	TYR	-	expression tag	UNP O60674
D	837	PHE	-	expression tag	UNP O60674
D	838	GLN	-	expression tag	UNP O60674
D	839	GLY	-	expression tag	UNP O60674
B	825	HIS	-	expression tag	UNP O60674
B	826	HIS	-	expression tag	UNP O60674
B	827	HIS	-	expression tag	UNP O60674
B	828	HIS	-	expression tag	UNP O60674
B	829	HIS	-	expression tag	UNP O60674
B	830	HIS	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	831	HIS	-	expression tag	UNP O60674
B	832	HIS	-	expression tag	UNP O60674
B	833	GLU	-	expression tag	UNP O60674
B	834	ASN	-	expression tag	UNP O60674
B	835	LEU	-	expression tag	UNP O60674
B	836	TYR	-	expression tag	UNP O60674
B	837	PHE	-	expression tag	UNP O60674
B	838	GLN	-	expression tag	UNP O60674
B	839	GLY	-	expression tag	UNP O60674
C	825	HIS	-	expression tag	UNP O60674
C	826	HIS	-	expression tag	UNP O60674
C	827	HIS	-	expression tag	UNP O60674
C	828	HIS	-	expression tag	UNP O60674
C	829	HIS	-	expression tag	UNP O60674
C	830	HIS	-	expression tag	UNP O60674
C	831	HIS	-	expression tag	UNP O60674
C	832	HIS	-	expression tag	UNP O60674
C	833	GLU	-	expression tag	UNP O60674
C	834	ASN	-	expression tag	UNP O60674
C	835	LEU	-	expression tag	UNP O60674
C	836	TYR	-	expression tag	UNP O60674
C	837	PHE	-	expression tag	UNP O60674
C	838	GLN	-	expression tag	UNP O60674
C	839	GLY	-	expression tag	UNP O60674
A	825	HIS	-	expression tag	UNP O60674
A	826	HIS	-	expression tag	UNP O60674
A	827	HIS	-	expression tag	UNP O60674
A	828	HIS	-	expression tag	UNP O60674
A	829	HIS	-	expression tag	UNP O60674
A	830	HIS	-	expression tag	UNP O60674
A	831	HIS	-	expression tag	UNP O60674
A	832	HIS	-	expression tag	UNP O60674
A	833	GLU	-	expression tag	UNP O60674
A	834	ASN	-	expression tag	UNP O60674
A	835	LEU	-	expression tag	UNP O60674
A	836	TYR	-	expression tag	UNP O60674
A	837	PHE	-	expression tag	UNP O60674
A	838	GLN	-	expression tag	UNP O60674
A	839	GLY	-	expression tag	UNP O60674

- Molecule 2 is (3R)-3-cyclopentyl-3-[4-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)-1H-pyrazol-1-yl]propanenitrile (three-letter code: RXT) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	N	0	0
			23	17	6		
2	B	1	Total	C	N	0	0
			23	17	6		
2	C	1	Total	C	N	0	0
			23	17	6		
2	A	1	Total	C	N	0	0
			23	17	6		

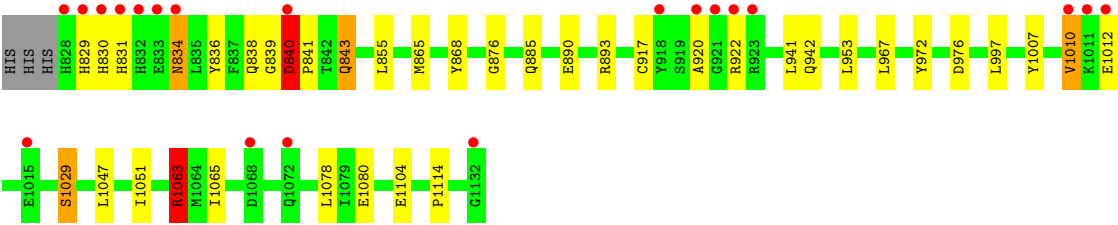
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	183	Total	O	0	0
			183	183		
3	B	187	Total	O	0	0
			187	187		
3	C	183	Total	O	0	0
			183	183		
3	A	191	Total	O	0	0
			191	191		



- Molecule 1: Tyrosine-protein kinase JAK2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.96Å 70.44Å 112.94Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	52.81 – 1.90 79.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (52.81-1.90) 99.6 (79.82-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14-3260_3260	Depositor
R, $R_{free}$	0.180 , 0.217 0.180 , 0.217	Depositor DCC
$R_{free}$ test set	6906 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.105 for l,k,-h 0.016 for h,-k,-l 0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: RXT, PTR

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	0.64	2/2540 (0.1%)	0.74	1/3420 (0.0%)
1	B	0.60	2/2502 (0.1%)	0.74	0/3367
1	C	0.68	3/2429 (0.1%)	0.73	3/3267 (0.1%)
1	D	0.58	1/2429 (0.0%)	0.71	0/3267
All	All	0.63	8/9900 (0.1%)	0.73	4/13321 (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	2
1	D	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1015	GLU	CD-OE1	8.88	1.35	1.25
1	C	1015	GLU	CD-OE2	8.13	1.34	1.25
1	A	917	CYS	CB-SG	-7.50	1.69	1.82
1	B	1015	GLU	CG-CD	-6.26	1.42	1.51
1	D	1011	LYS	C-N	6.10	1.48	1.34
1	C	1015	GLU	CG-CD	-5.85	1.43	1.51
1	A	1063	ARG	CG-CD	5.08	1.64	1.51
1	B	917	CYS	CB-SG	-5.04	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1063	ARG	CG-CD-NE	7.33	127.20	111.80
1	C	1015	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	C	947	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	C	947	ARG	CB-CG-CD	-5.63	96.95	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	839	GLY	Peptide
1	A	840	ASP	Peptide
1	D	858	GLY	Peptide
1	D	859	ASN	Peptide

## 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	2503	0	2456	33	0
1	B	2465	0	2438	32	0
1	C	2395	0	2378	27	1
1	D	2395	0	2377	19	0
2	A	23	0	18	1	0
2	B	23	0	18	0	0
2	C	23	0	18	1	0
2	D	23	0	18	1	0
3	A	191	0	0	1	1
3	B	187	0	0	3	0
3	C	183	0	0	10	1
3	D	183	0	0	5	0
All	All	10594	0	9721	103	2

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 5.

All (103) 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:C:942:GLN:HE22	1:C:1053:LYS:HE3	1.42	0.82
1:C:1072:GLN:HE21	1:C:1073:MET:H	1.27	0.79
1:C:922:ARG:O	3:C:1301:HOH:O	2.02	0.78
1:B:858:GLY:HA3	1:A:830:HIS:O	1.84	0.78
1:C:1072:GLN:NE2	1:C:1073:MET:H	1.85	0.74
1:A:1080:GLU:OE1	3:A:1301:HOH:O	2.10	0.70
1:D:943:LYS:HD3	1:D:944:HIS:CE1	2.28	0.68
1:B:1012:GLU:OE1	3:B:1301:HOH:O	2.11	0.68
1:B:859:ASN:H	1:A:831:HIS:N	1.91	0.67
1:C:942:GLN:NE2	1:C:1053:LYS:HE3	2.10	0.67
1:C:942:GLN:HE22	1:C:1053:LYS:CE	2.09	0.65
1:C:868:TYR:O	1:C:876:GLY:HA3	1.97	0.65
1:B:996:GLY:HA3	1:A:829:HIS:H	1.63	0.64
1:C:846:GLU:OE2	1:C:919:SER:HB3	1.99	0.63
1:A:1010:VAL:O	1:A:1012:GLU:N	2.31	0.63
1:D:868:TYR:O	1:D:876:GLY:HA3	1.99	0.63
1:C:890:GLU:HG3	1:C:893:ARG:NH2	2.14	0.62
1:A:1063:ARG:HG2	1:A:1063:ARG:HH11	1.64	0.62
1:D:894:ASP:OD1	1:D:897:ARG:NH2	2.33	0.62
1:B:919:SER:HB2	1:B:923:ARG:HB3	1.82	0.62
1:A:1010:VAL:HG12	1:A:1029:SER:OG	2.00	0.61
1:D:858:GLY:HA3	2:D:1201:RXT:H5	1.83	0.61
1:A:840:ASP:OD2	1:A:840:ASP:N	2.35	0.59
1:C:1072:GLN:HE21	1:C:1072:GLN:N	2.00	0.59
1:D:944:HIS:CD2	1:D:947:ARG:HD3	2.39	0.58
1:D:1127:ARG:HD2	3:D:1387:HOH:O	2.02	0.58
1:C:890:GLU:HG3	1:C:893:ARG:HH21	1.66	0.58
1:B:1072:GLN:HG3	1:B:1076:PHE:CE2	2.38	0.58
1:A:920:ALA:HA	1:A:922:ARG:H	1.69	0.57
1:C:938:ARG:NH2	3:C:1306:HOH:O	2.37	0.57
1:B:1015:GLU:HB2	1:A:836:TYR:HB3	1.85	0.57
1:C:1127:ARG:HD2	3:C:1387:HOH:O	2.05	0.55
1:B:868:TYR:O	1:B:876:GLY:HA3	2.06	0.55
1:C:889:GLU:O	1:C:893:ARG:HG3	2.06	0.55
1:A:941:LEU:HD11	1:A:953:LEU:HD21	1.89	0.55
1:C:1004:ASP:OD1	3:C:1302:HOH:O	2.18	0.54
1:D:952:LYS:NZ	1:D:988:ASN:OD1	2.41	0.54
1:C:1070:GLN:O	1:C:1072:GLN:NE2	2.40	0.54
1:B:862:SER:CB	1:B:885:GLN:HE22	2.20	0.54
1:B:841:PRO:HG2	1:B:843:GLN:HG2	1.90	0.53
1:B:994:ASP:OD1	1:A:829:HIS:CB	2.56	0.53
1:B:841:PRO:HG2	1:B:843:GLN:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:GLN:CG	1:B:1051:ILE:HB	2.40	0.52
1:A:831:HIS:HA	1:A:836:TYR:CD2	2.45	0.52
1:D:943:LYS:NZ	3:D:1309:HOH:O	2.44	0.51
1:A:840:ASP:HB3	1:A:843:GLN:HB2	1.93	0.50
1:B:840:ASP:HB3	1:B:843:GLN:H	1.77	0.50
1:C:1072:GLN:HE21	1:C:1073:MET:N	2.03	0.49
1:B:1015:GLU:HB3	1:A:838:GLN:OE1	2.11	0.49
1:A:834:ASN:OD1	1:A:834:ASN:N	2.45	0.49
1:C:1005:LYS:HE2	1:C:1007:PTR:OH	2.13	0.49
1:B:1053:LYS:HE2	1:B:1053:LYS:N	2.27	0.49
1:C:848:HIS:CG	1:C:870:PRO:HA	2.48	0.48
1:B:859:ASN:N	1:A:831:HIS:H	2.10	0.48
1:A:868:TYR:O	1:A:876:GLY:HA3	2.13	0.48
1:A:967:LEU:HG	1:A:972:TYR:HB2	1.95	0.48
1:B:996:GLY:HA3	1:A:829:HIS:N	2.28	0.48
1:A:855:LEU:HD21	1:A:865:MET:CE	2.44	0.47
1:B:859:ASN:H	1:A:831:HIS:H	1.59	0.47
1:C:985:GLU:OE1	1:C:989:ARG:NH1	2.47	0.47
1:D:848:HIS:CG	1:D:870:PRO:HA	2.49	0.47
1:A:976:ASP:HB2	1:A:997:LEU:HD12	1.95	0.47
1:C:1053:LYS:HG2	3:C:1436:HOH:O	2.14	0.47
1:A:942:GLN:CG	1:A:1051:ILE:HB	2.45	0.47
1:C:944:HIS:HE1	3:C:1462:HOH:O	1.97	0.46
1:C:857:LYS:HG3	1:C:862:SER:HB3	1.97	0.46
1:D:938:ARG:HD3	3:D:1397:HOH:O	2.16	0.46
1:B:1112:GLN:NE2	3:B:1302:HOH:O	2.14	0.45
1:A:941:LEU:HD21	1:A:1047:LEU:HA	1.98	0.45
1:B:920:ALA:HA	1:B:921:GLY:HA2	1.55	0.45
1:D:843:GLN:HE21	1:D:843:GLN:N	2.15	0.45
1:C:1045:TYR:O	1:C:1049:THR:HG23	2.17	0.45
1:B:848:HIS:HB2	1:B:868:TYR:CE2	2.51	0.45
1:B:967:LEU:HD22	1:B:972:TYR:HB2	1.99	0.45
2:C:1201:RXT:H8	2:C:1201:RXT:H12	1.71	0.44
1:D:1068:ASP:N	1:D:1068:ASP:OD1	2.48	0.44
1:B:859:ASN:HB2	1:A:831:HIS:CB	2.47	0.44
1:B:1053:LYS:H	1:B:1053:LYS:HE2	1.83	0.44
1:C:1003:GLN:NE2	3:C:1303:HOH:O	2.31	0.44
1:A:831:HIS:HA	1:A:836:TYR:CE2	2.53	0.44
1:B:912:LYS:HE2	1:B:912:LYS:HB2	1.82	0.44
1:A:1010:VAL:C	1:A:1012:GLU:H	2.21	0.44
1:D:848:HIS:HB2	1:D:868:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1201:RXT:H18	2:A:1201:RXT:H21	1.99	0.43
1:D:943:LYS:HD3	1:D:944:HIS:NE2	2.33	0.43
1:B:841:PRO:HD2	1:B:843:GLN:HG3	2.01	0.43
1:B:850:LYS:NZ	3:B:1312:HOH:O	2.51	0.43
1:D:944:HIS:HD2	1:D:947:ARG:HD3	1.82	0.43
1:A:890:GLU:H	1:A:890:GLU:CD	2.22	0.43
1:D:923:ARG:HA	3:D:1320:HOH:O	2.19	0.43
1:A:942:GLN:HG2	1:A:1051:ILE:HB	2.00	0.42
1:A:1065:ILE:HD11	1:A:1078:LEU:HA	2.00	0.42
1:D:1053:LYS:HG3	1:D:1054:SER:H	1.83	0.42
1:D:944:HIS:O	1:D:947:ARG:HG2	2.19	0.42
1:B:989:ARG:HH11	1:B:989:ARG:HD3	1.69	0.42
1:B:942:GLN:HG2	1:B:1051:ILE:HB	2.02	0.41
1:D:1003:GLN:HG2	3:D:1449:HOH:O	2.20	0.41
1:A:1104:GLU:HG2	1:A:1114:PRO:HD3	2.02	0.41
1:C:903:LYS:NZ	3:C:1305:HOH:O	2.36	0.41
1:B:1045:TYR:O	1:B:1049:THR:HG23	2.21	0.40
1:B:862:SER:HB3	1:B:885:GLN:HE22	1.85	0.40
1:C:843:GLN:HB3	3:C:1399:HOH:O	2.21	0.40
3:C:1418:HOH:O	1:A:885:GLN:HG2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:883:LYS:NZ	1:C:1007:PTR:O1P[2_645]	1.30	0.90
3:C:1462:HOH:O	3:A:1452:HOH:O[1_545]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	302/308 (98%)	290 (96%)	11 (4%)	1 (0%)	41	31
1	B	295/308 (96%)	288 (98%)	6 (2%)	1 (0%)	41	31
1	C	286/308 (93%)	281 (98%)	5 (2%)	0	100	100
1	D	286/308 (93%)	278 (97%)	7 (2%)	1 (0%)	41	31
All	All	1169/1232 (95%)	1137 (97%)	29 (2%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	920	ALA
1	A	841	PRO
1	B	841	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	271/280 (97%)	264 (97%)	7 (3%)	46	39
1	B	270/280 (96%)	263 (97%)	7 (3%)	46	39
1	C	263/280 (94%)	257 (98%)	6 (2%)	50	45
1	D	263/280 (94%)	258 (98%)	5 (2%)	57	53
All	All	1067/1120 (95%)	1042 (98%)	25 (2%)	50	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	843	GLN
1	D	918	TYR
1	D	943	LYS
1	D	1003	GLN
1	D	1080	GLU
1	B	841	PRO
1	B	857	LYS
1	B	918	TYR

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Mol	Chain	Res	Type
1	B	989	ARG
1	B	1015	GLU
1	B	1029	SER
1	B	1070	GLN
1	C	918	TYR
1	C	947	ARG
1	C	1003	GLN
1	C	1072	GLN
1	C	1073	MET
1	C	1080	GLU
1	A	834	ASN
1	A	840	ASP
1	A	843	GLN
1	A	893	ARG
1	A	1010	VAL
1	A	1029	SER
1	A	1063	ARG

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

Mol	Chain	Res	Type
1	D	843	GLN
1	D	944	HIS
1	B	843	GLN
1	B	859	ASN
1	C	854	GLN
1	C	942	GLN
1	C	1072	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PTR	C	1007	1	15,16,17	1.30	1 (6%)	19,22,24	0.70	1 (5%)
1	PTR	B	1007	1	15,16,17	1.27	1 (6%)	19,22,24	0.54	0
1	PTR	D	1007	1	15,16,17	1.27	2 (13%)	19,22,24	0.76	1 (5%)
1	PTR	A	1007	1	15,16,17	1.32	1 (6%)	19,22,24	0.52	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
1	PTR	C	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1007	PTR	OH-CZ	-4.08	1.31	1.40
1	B	1007	PTR	OH-CZ	-4.04	1.31	1.40
1	A	1007	PTR	OH-CZ	-4.03	1.31	1.40
1	D	1007	PTR	OH-CZ	-3.42	1.32	1.40
1	D	1007	PTR	P-OH	2.40	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1007	PTR	O2P-P-OH	2.18	112.06	105.24
1	D	1007	PTR	O2P-P-OH	2.02	111.57	105.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1007	PTR	1	1

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
2	RXT	D	1201	-	22,26,26	2.20	10 (45%)	20,36,36	2.35	7 (35%)
2	RXT	A	1201	-	22,26,26	2.24	12 (54%)	20,36,36	2.19	5 (25%)
2	RXT	C	1201	-	22,26,26	2.09	9 (40%)	20,36,36	2.39	6 (30%)
2	RXT	B	1201	-	22,26,26	2.28	10 (45%)	20,36,36	2.23	8 (40%)

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	RXT	D	1201	-	-	0/6/22/22	0/4/4/4
2	RXT	A	1201	-	-	0/6/22/22	0/4/4/4
2	RXT	C	1201	-	-	0/6/22/22	0/4/4/4
2	RXT	B	1201	-	-	0/6/22/22	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	RXT	CAQ-CAR	4.49	1.55	1.49
2	D	1201	RXT	CAQ-CAR	4.08	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	RXT	CAQ-CAR	3.94	1.55	1.49
2	A	1201	RXT	CAG-NAW	-3.75	1.31	1.35
2	B	1201	RXT	CAV-NAW	-3.47	1.44	1.49
2	D	1201	RXT	CAG-NAW	-3.46	1.32	1.35
2	D	1201	RXT	CAI-CAL	-3.46	1.37	1.51
2	C	1201	RXT	CAI-CAL	-3.40	1.37	1.51
2	C	1201	RXT	CAH-CAK	-3.35	1.37	1.51
2	C	1201	RXT	CAV-NAW	-3.34	1.44	1.49
2	D	1201	RXT	CAH-CAK	-3.25	1.38	1.51
2	C	1201	RXT	CAG-NAW	-3.21	1.32	1.35
2	B	1201	RXT	CAK-CAU	3.21	1.62	1.53
2	C	1201	RXT	CAQ-CAR	3.20	1.53	1.49
2	A	1201	RXT	CAJ-CAB	3.11	1.53	1.46
2	B	1201	RXT	CAH-CAK	-3.06	1.39	1.51
2	A	1201	RXT	CAR-NAM	3.04	1.35	1.32
2	B	1201	RXT	CAG-NAW	-3.03	1.32	1.35
2	B	1201	RXT	CAL-CAU	3.00	1.61	1.53
2	A	1201	RXT	CAH-CAK	-2.98	1.39	1.51
2	B	1201	RXT	CAI-CAL	-2.97	1.39	1.51
2	B	1201	RXT	CAJ-CAB	2.87	1.52	1.46
2	D	1201	RXT	CAV-NAW	-2.86	1.44	1.49
2	A	1201	RXT	CAI-CAL	-2.84	1.39	1.51
2	D	1201	RXT	CAJ-CAB	2.82	1.52	1.46
2	D	1201	RXT	CAL-CAU	2.82	1.61	1.53
2	C	1201	RXT	CAI-CAH	2.77	1.67	1.48
2	B	1201	RXT	CAI-CAH	2.76	1.67	1.48
2	A	1201	RXT	CAL-CAU	2.72	1.60	1.53
2	C	1201	RXT	CAL-CAU	2.72	1.60	1.53
2	D	1201	RXT	CAI-CAH	2.68	1.67	1.48
2	D	1201	RXT	CAK-CAU	2.61	1.60	1.53
2	A	1201	RXT	CAI-CAH	2.58	1.66	1.48
2	A	1201	RXT	CAK-CAU	2.56	1.60	1.53
2	D	1201	RXT	CAT-NAN	2.51	1.39	1.34
2	C	1201	RXT	CAJ-CAB	2.45	1.51	1.46
2	A	1201	RXT	CAT-NAN	2.45	1.39	1.34
2	C	1201	RXT	CAK-CAU	2.43	1.60	1.53
2	A	1201	RXT	CAV-NAW	-2.25	1.45	1.49
2	B	1201	RXT	CAT-NAN	2.19	1.38	1.34
2	A	1201	RXT	CAU-CAV	2.05	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	RXT	CAS-CAR-NAM	-6.56	118.72	123.04
2	C	1201	RXT	CAS-CAR-NAM	-6.03	119.07	123.04
2	B	1201	RXT	CAS-CAR-NAM	-6.00	119.09	123.04
2	C	1201	RXT	NAP-CAE-NAM	-5.53	120.03	128.68
2	A	1201	RXT	NAP-CAE-NAM	-5.48	120.12	128.68
2	D	1201	RXT	NAP-CAE-NAM	-4.84	121.11	128.68
2	B	1201	RXT	NAP-CAE-NAM	-4.58	121.52	128.68
2	A	1201	RXT	CAS-CAR-NAM	-4.42	120.13	123.04
2	A	1201	RXT	CAE-NAP-CAT	4.12	123.09	113.45
2	C	1201	RXT	CAK-CAU-CAV	-3.56	105.72	112.73
2	D	1201	RXT	CAE-NAP-CAT	3.21	120.97	113.45
2	C	1201	RXT	CAE-NAM-CAR	3.09	122.43	117.69
2	C	1201	RXT	CAE-NAP-CAT	3.03	120.55	113.45
2	C	1201	RXT	CAL-CAU-CAV	-3.01	106.81	112.73
2	B	1201	RXT	CAE-NAP-CAT	3.00	120.47	113.45
2	D	1201	RXT	CAL-CAU-CAV	-2.98	106.86	112.73
2	B	1201	RXT	CAL-CAU-CAV	-2.72	107.39	112.73
2	D	1201	RXT	CAE-NAM-CAR	2.71	121.85	117.69
2	A	1201	RXT	CAG-NAW-CAV	2.55	127.74	125.48
2	D	1201	RXT	CAK-CAU-CAV	-2.45	107.91	112.73
2	B	1201	RXT	CAG-NAW-CAV	2.26	127.48	125.48
2	B	1201	RXT	CAE-NAM-CAR	2.15	120.99	117.69
2	A	1201	RXT	CAV-CAJ-CAB	-2.12	108.89	112.12
2	B	1201	RXT	CAV-CAJ-CAB	-2.10	108.93	112.12
2	B	1201	RXT	CAQ-CAR-NAM	2.09	118.46	115.32
2	D	1201	RXT	CAL-CAU-CAK	2.01	108.04	102.91

There are no chirality outliers.

There are no torsion outliers.

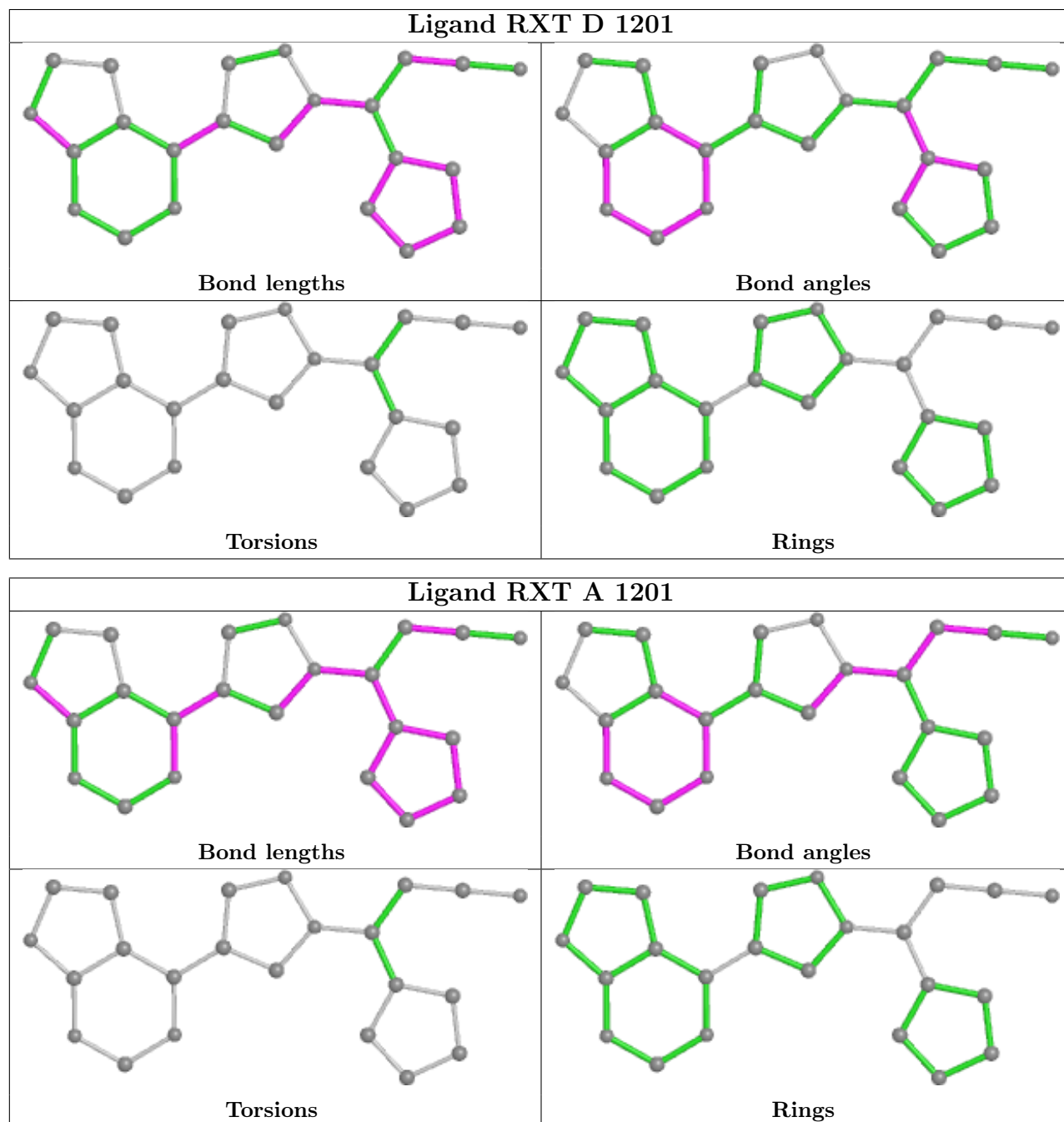
There are no ring outliers.

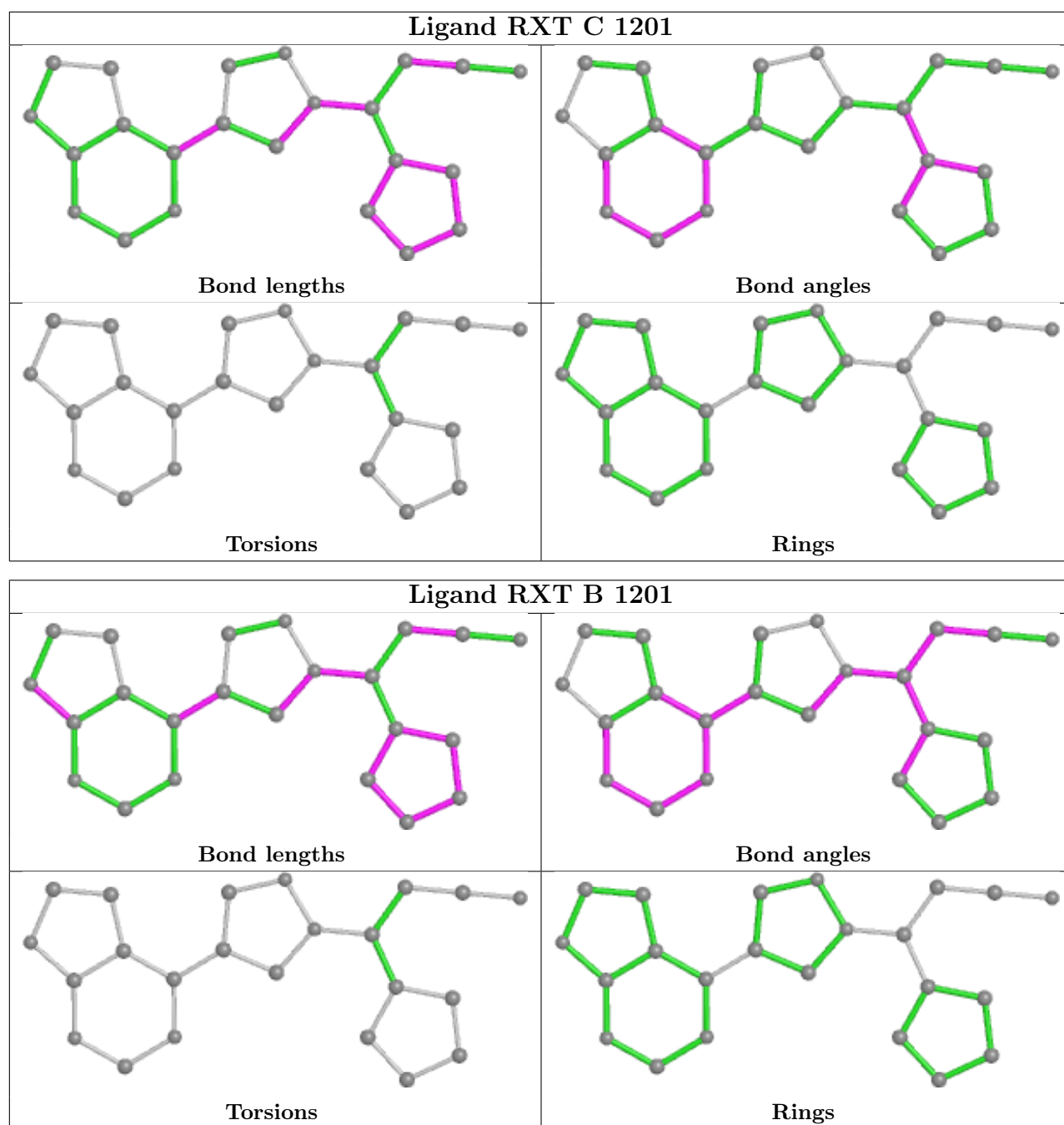
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	RXT	1	0
2	A	1201	RXT	1	0
2	C	1201	RXT	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	304/308 (98%)	0.46	20 (6%) 18 20	28, 40, 79, 105	0
1	B	297/308 (96%)	0.35	10 (3%) 45 48	29, 40, 72, 114	0
1	C	288/308 (93%)	0.44	21 (7%) 15 16	27, 38, 74, 109	0
1	D	288/308 (93%)	0.45	18 (6%) 20 22	26, 39, 76, 121	0
All	All	1177/1232 (95%)	0.43	69 (5%) 22 25	26, 39, 76, 121	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	920	ALA	10.7
1	A	832	HIS	8.9
1	C	921	GLY	8.6
1	D	921	GLY	8.5
1	A	831	HIS	7.6
1	B	922	ARG	6.4
1	C	920	ALA	6.0
1	A	833	GLU	4.8
1	A	1132	GLY	4.6
1	C	1067	ASN	4.6
1	A	834	ASN	4.5
1	D	922	ARG	4.5
1	C	859	ASN	4.5
1	D	860	PHE	4.3
1	C	1068	ASP	4.3
1	C	922	ARG	4.3
1	D	1068	ASP	4.2
1	B	921	GLY	4.1
1	A	840	ASP	4.0
1	B	1053	LYS	3.9
1	C	919	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	839	GLY	3.5
1	A	829	HIS	3.5
1	A	922	ARG	3.4
1	A	918	TYR	3.3
1	B	923	ARG	3.1
1	B	840	ASP	3.1
1	D	859	ASN	3.1
1	B	918	TYR	3.1
1	B	920	ALA	3.0
1	D	919	SER	3.0
1	D	1053	LYS	3.0
1	C	1072	GLN	3.0
1	C	860	PHE	2.9
1	C	1053	LYS	2.9
1	C	1076	PHE	2.8
1	C	918	TYR	2.8
1	C	1015	GLU	2.7
1	A	830	HIS	2.7
1	A	921	GLY	2.7
1	D	1071	GLY	2.7
1	D	923	ARG	2.7
1	D	887	SER	2.7
1	C	923	ARG	2.5
1	C	924	ASN	2.5
1	B	838	GLN	2.5
1	D	1073	MET	2.5
1	C	1014	GLY	2.5
1	C	1066	GLY	2.4
1	A	1015	GLU	2.4
1	C	1013	PRO	2.4
1	A	1010	VAL	2.4
1	A	920	ALA	2.3
1	D	1070	GLN	2.3
1	A	1011	LYS	2.3
1	D	918	TYR	2.3
1	D	1067	ASN	2.3
1	D	1069	LYS	2.2
1	D	1072	GLN	2.2
1	A	923	ARG	2.2
1	A	1072	GLN	2.2
1	A	1012	GLU	2.2
1	C	1074	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1068	ASP	2.2
1	D	843	GLN	2.1
1	C	1070	GLN	2.1
1	B	1068	ASP	2.1
1	C	886	HIS	2.1
1	A	828	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	PTR	C	1007	16/17	0.92	0.11	32,41,83,94	0
1	PTR	D	1007	16/17	0.92	0.14	33,44,78,90	0
1	PTR	A	1007	16/17	0.92	0.13	44,62,97,106	0
1	PTR	B	1007	16/17	0.93	0.12	38,54,87,93	0

## 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<sup>th</sup> 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.

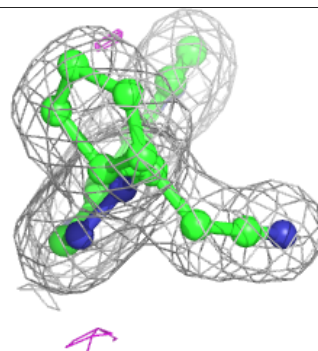
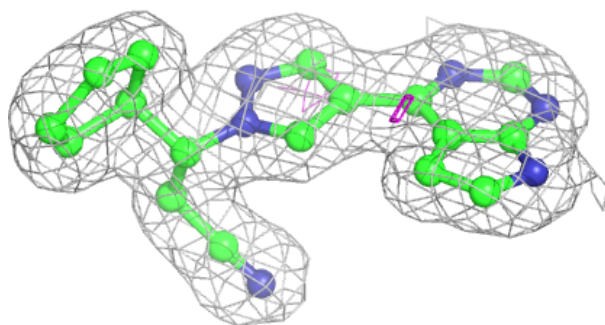
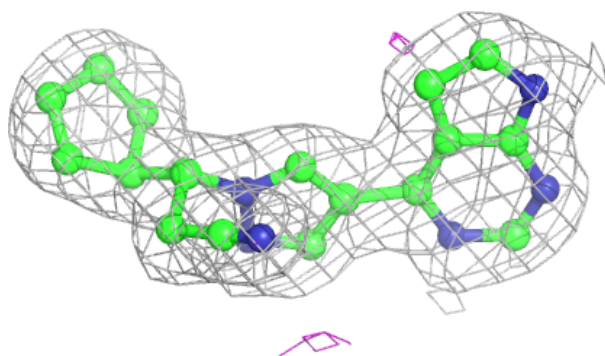
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RXT	D	1201	23/23	0.96	0.12	24,29,40,48	0
2	RXT	B	1201	23/23	0.96	0.13	27,29,36,39	0
2	RXT	A	1201	23/23	0.97	0.14	27,29,36,39	0
2	RXT	C	1201	23/23	0.98	0.12	23,29,36,50	0

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.

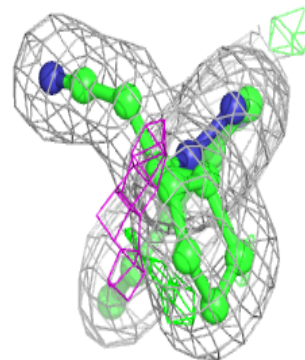
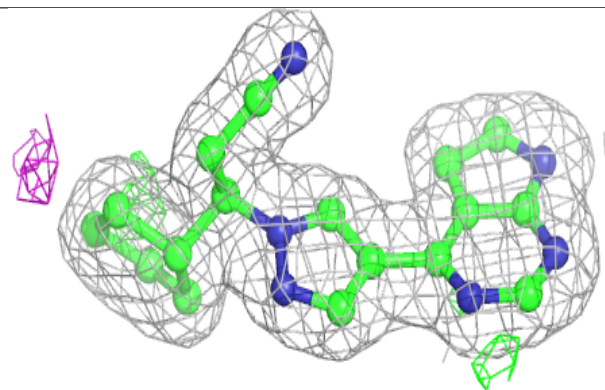
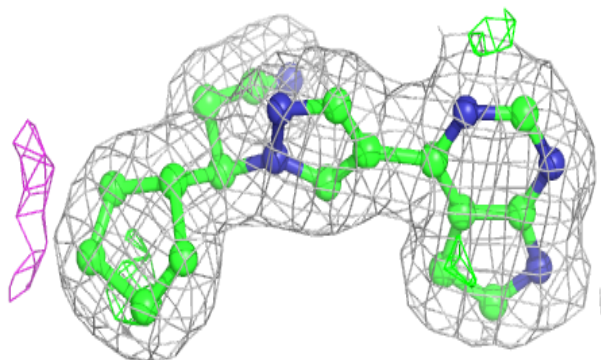


**Electron density around RXT D 1201:**

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

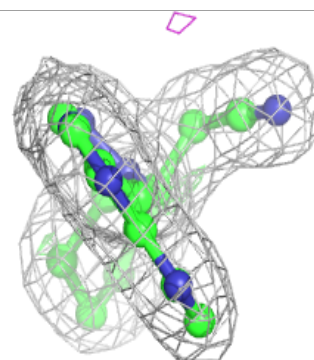
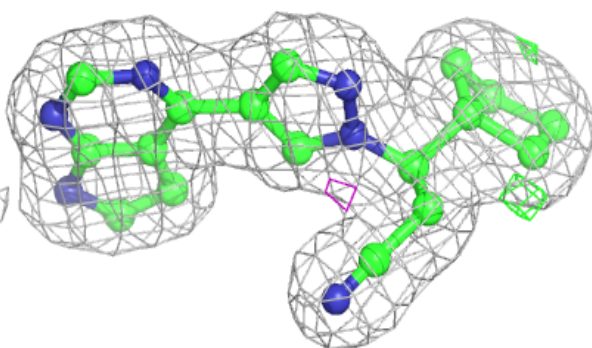
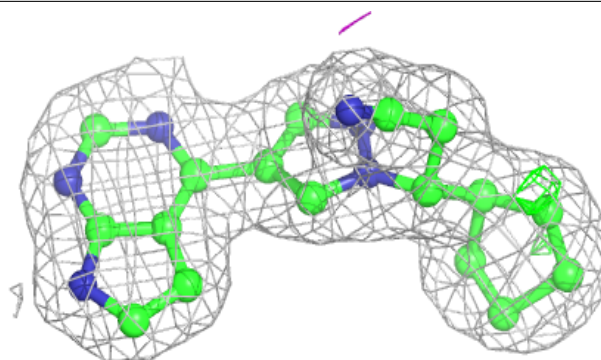
**Electron density around RXT B 1201:**

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

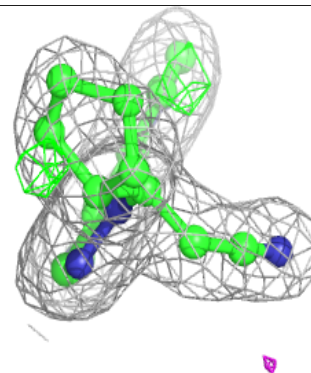
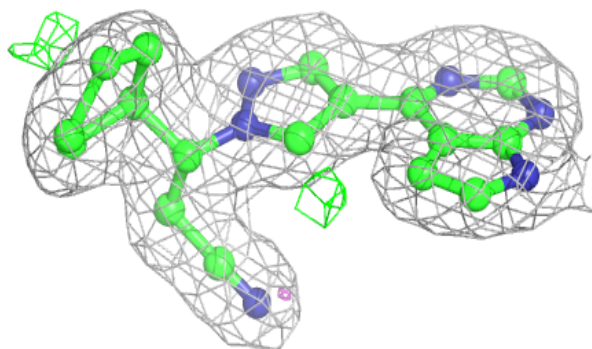
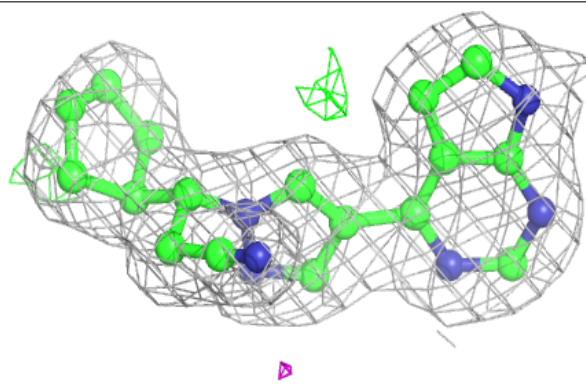


**Electron density around RXT A 1201:**

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

**Electron density around RXT 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.