



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 08:55 AM EDT

PDB ID : 7UYV / pdb_00007uyv
Title : Crystal structure of JAK3 kinase domain in complex with compound 25
Authors : Toms, A.V.; Leit, S.; Greenwood, J.R.; Mondal, S.; Carriero, S.; Dahlgren, M.; Harriman, G.C.; Kennedy-Smith, J.J.; Kapeller, R.; Lawson, J.P.; Romero, D.L.; Shelley, M.; Wester, R.T.; Westlin, W.; Mc Elwee, J.J.; Miao, W.; Edmondson, S.D.; Massee, C.E.
Deposited on : 2022-05-07
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

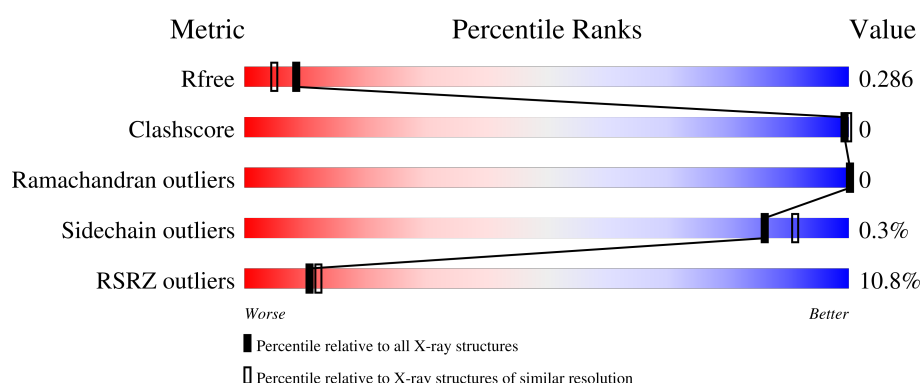
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	11% 95% • •
1	B	291	9% 97% • •
1	C	291	11% 95% • •
1	D	291	10% 91% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9659 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.

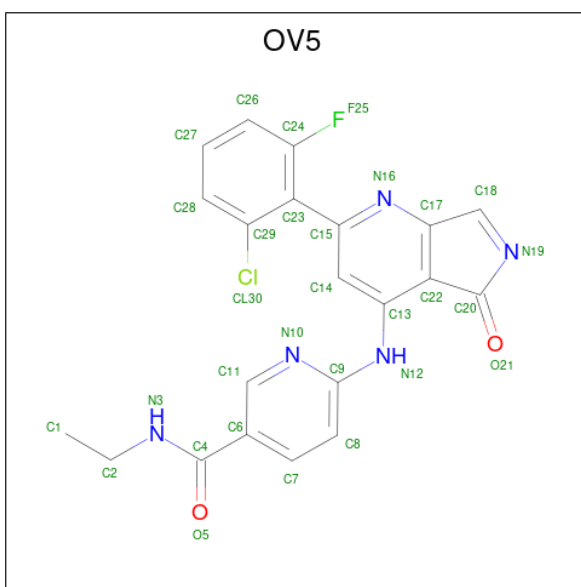
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	P	S	36	5	0
			2286	1454	399	417	2	14			
1	B	284	Total	C	N	O	P	S	45	5	0
			2335	1480	410	429	2	14			
1	C	281	Total	C	N	O	P	S	69	1	0
			2270	1440	395	419	2	14			
1	D	272	Total	C	N	O	P	S	54	2	0
			2209	1409	381	403	2	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	SER	CYS	conflict	UNP P52333
A	1048	SER	CYS	conflict	UNP P52333
B	1040	SER	CYS	conflict	UNP P52333
B	1048	SER	CYS	conflict	UNP P52333
C	1040	SER	CYS	conflict	UNP P52333
C	1048	SER	CYS	conflict	UNP P52333
D	1040	SER	CYS	conflict	UNP P52333
D	1048	SER	CYS	conflict	UNP P52333

- Molecule 2 is 6-{[(2M)-2-(2-chloro-6-fluorophenyl)-5-oxo-5H-pyrrolo[3,4-b]pyridin-4-yl]amino}-N-ethylpyridine-3-carboxamide (CCD ID: OV5) (formula: C₂₁H₁₅ClFN₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 30	C 21	Cl 1	F 1	N 5	O 2	0	0
2	B	1	Total 30	C 21	Cl 1	F 1	N 5	O 2	0	0
2	C	1	Total 30	C 21	Cl 1	F 1	N 5	O 2	3	0
2	D	1	Total 30	C 21	Cl 1	F 1	N 5	O 2	2	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		

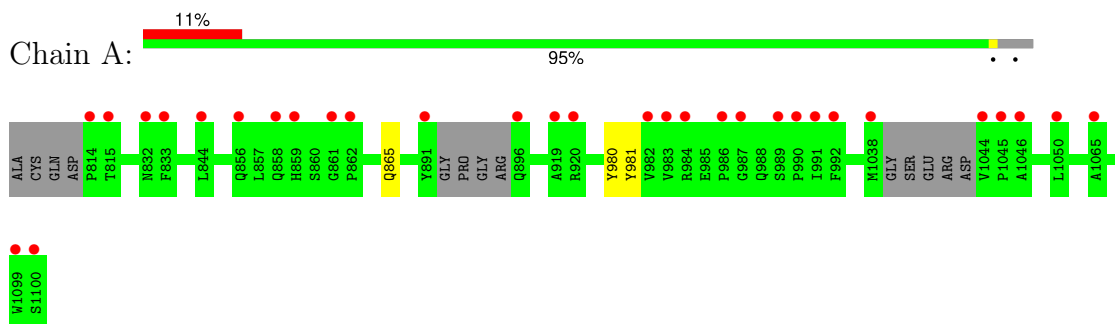
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	149	Total	O	0	0
			149	149		
4	C	84	Total	O	0	0
			84	84		
4	D	75	Total	O	0	0
			75	75		

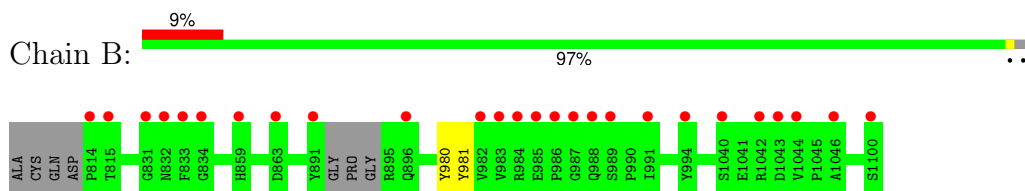
3 Residue-property plots [i](#)

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.

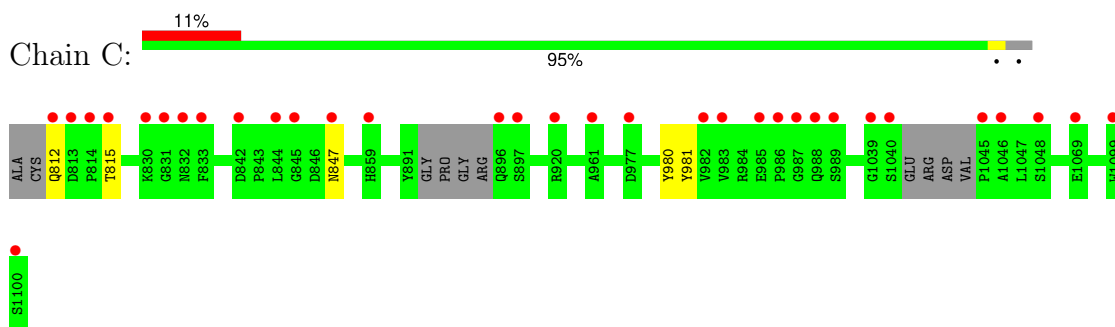
- Molecule 1: Tyrosine-protein kinase JAK3



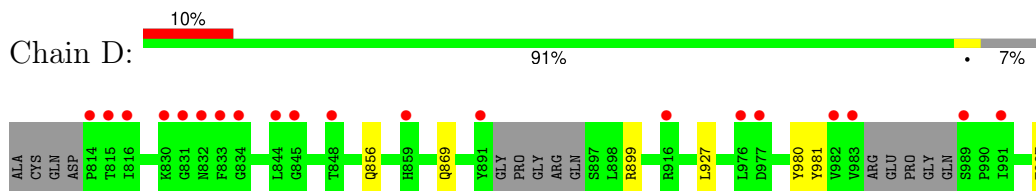
- Molecule 1: Tyrosine-protein kinase JAK3

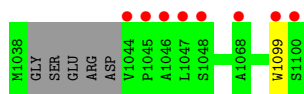


- Molecule 1: Tyrosine-protein kinase JAK3



- Molecule 1: Tyrosine-protein kinase JAK3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.07Å 114.17Å 106.09Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	105.17 – 2.15 105.17 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.0 (105.17-2.15) 96.0 (105.17-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.263 0.239 , 0.286	Depositor DCC
R_{free} test set	1558 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9659	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OV5, CL, 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	0.58	0/2305	0.81	0/3113
1	B	0.58	0/2355	0.81	0/3180
1	C	0.60	0/2289	0.80	1/3091 (0.0%)
1	D	0.59	0/2226	0.82	0/3006
All	All	0.59	0/9175	0.81	1/12390 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	847	ASN	CA-CB-CG	5.33	117.94	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2286	0	2261	0	0
1	B	2335	0	2304	0	0
1	C	2270	0	2233	1	0
1	D	2209	0	2186	2	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	D	1	0	0	0	0
4	A	130	0	0	0	0
4	B	149	0	0	0	0
4	C	84	0	0	0	0
4	D	75	0	0	0	0
All	All	9659	0	8984	3	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 0.

All (3) 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:812:GLN:N	1:C:815:THR:HG1	1.99	0.59
1:D:856:GLN:HB3	1:D:899:ARG:HG2	1.94	0.49
1:D:927:LEU:HD12	1:D:1099:TRP:CZ3	2.53	0.43

There are no symmetry-related clashes.

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	275/291 (94%)	269 (98%)	6 (2%)	0	100	100
1	B	283/291 (97%)	278 (98%)	5 (2%)	0	100	100
1	C	274/291 (94%)	265 (97%)	9 (3%)	0	100	100
1	D	264/291 (91%)	256 (97%)	8 (3%)	0	100	100
All	All	1096/1164 (94%)	1068 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	248/252 (98%)	246 (99%)	2 (1%)	73	79
1	B	253/252 (100%)	253 (100%)	0	100	100
1	C	246/252 (98%)	246 (100%)	0	100	100
1	D	240/252 (95%)	238 (99%)	2 (1%)	73	79
All	All	987/1008 (98%)	983 (100%)	4 (0%)	86	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	865[A]	GLN
1	A	865[B]	GLN
1	D	869	GLN
1	D	997	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	869	GLN
1	A	879	HIS
1	A	915	GLN
1	B	856	GLN
1	B	858	GLN
1	B	869	GLN
1	B	873	GLN
1	C	856	GLN
1	C	858	GLN
1	C	873	GLN
1	C	917	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	B	980	1	15,16,17	2.06	1 (6%)	17,22,24	0.46	0
1	PTR	C	981	1	15,16,17	2.09	1 (6%)	17,22,24	0.62	0
1	PTR	D	980	1	15,16,17	2.06	1 (6%)	17,22,24	0.47	0
1	PTR	D	981	1	15,16,17	2.05	1 (6%)	17,22,24	0.50	0
1	PTR	A	980	1	15,16,17	1.96	1 (6%)	17,22,24	0.59	0
1	PTR	C	980	1	15,16,17	2.04	1 (6%)	17,22,24	0.47	0
1	PTR	B	981	1	15,16,17	1.97	1 (6%)	17,22,24	0.53	0
1	PTR	A	981	1	15,16,17	1.98	1 (6%)	17,22,24	0.60	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	B	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	981	1	-	2/10/11/13	0/1/1/1
1	PTR	D	980	1	-	0/10/11/13	0/1/1/1
1	PTR	D	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	980	1	-	0/10/11/13	0/1/1/1
1	PTR	B	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	981	1	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	980	PTR	OH-CZ	-7.48	1.23	1.40
1	B	980	PTR	OH-CZ	-7.45	1.23	1.40
1	C	981	PTR	OH-CZ	-7.42	1.24	1.40
1	D	981	PTR	OH-CZ	-7.38	1.24	1.40
1	C	980	PTR	OH-CZ	-7.35	1.24	1.40
1	A	980	PTR	OH-CZ	-7.32	1.24	1.40
1	B	981	PTR	OH-CZ	-7.28	1.24	1.40
1	A	981	PTR	OH-CZ	-7.05	1.24	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	981	PTR	CA-CB-CG-CD2
1	C	981	PTR	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	OV5	B	1201	-	33,33,33	1.53	3 (9%)	41,47,47	1.83	9 (21%)
2	OV5	C	1201	-	33,33,33	1.52	3 (9%)	41,47,47	1.98	11 (26%)
2	OV5	D	1201	-	33,33,33	1.52	3 (9%)	41,47,47	1.85	9 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OV5	A	1201	-	33,33,33	1.52	3 (9%)	41,47,47	1.84	11 (26%)

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	OV5	B	1201	-	-	0/15/24/24	0/4/4/4
2	OV5	C	1201	-	-	0/15/24/24	0/4/4/4
2	OV5	D	1201	-	-	4/15/24/24	0/4/4/4
2	OV5	A	1201	-	-	0/15/24/24	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	OV5	C17-C18	5.53	1.51	1.42
2	D	1201	OV5	C17-C18	5.47	1.50	1.42
2	B	1201	OV5	C17-C18	5.38	1.50	1.42
2	A	1201	OV5	C17-C18	5.37	1.50	1.42
2	A	1201	OV5	C18-N19	4.36	1.46	1.33
2	C	1201	OV5	C18-N19	4.33	1.46	1.33
2	B	1201	OV5	C18-N19	4.32	1.46	1.33
2	D	1201	OV5	C18-N19	4.31	1.46	1.33
2	B	1201	OV5	C17-N16	-3.37	1.31	1.35
2	A	1201	OV5	C17-N16	-3.07	1.31	1.35
2	D	1201	OV5	C17-N16	-3.00	1.31	1.35
2	C	1201	OV5	C17-N16	-2.86	1.31	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	OV5	C11-N10-C9	6.76	124.17	117.83
2	D	1201	OV5	C11-N10-C9	6.18	123.62	117.83
2	B	1201	OV5	C11-N10-C9	5.29	122.79	117.83
2	A	1201	OV5	C11-N10-C9	5.21	122.71	117.83
2	B	1201	OV5	C22-C17-N16	-5.00	121.00	125.61
2	A	1201	OV5	C22-C17-N16	-4.89	121.10	125.61
2	C	1201	OV5	C22-C17-N16	-4.35	121.60	125.61
2	D	1201	OV5	C22-C17-N16	-4.02	121.90	125.61
2	D	1201	OV5	C13-C22-C20	4.00	133.84	129.42
2	C	1201	OV5	C13-C22-C20	3.70	133.51	129.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OV5	C17-N16-C15	3.31	121.64	117.53
2	B	1201	OV5	C17-N16-C15	3.26	121.57	117.53
2	A	1201	OV5	C26-C24-C23	-3.22	119.15	123.73
2	C	1201	OV5	C17-N16-C15	3.19	121.48	117.53
2	C	1201	OV5	C8-C9-N10	-3.05	117.96	122.61
2	B	1201	OV5	C13-C22-C20	3.04	132.78	129.42
2	D	1201	OV5	C17-N16-C15	3.03	121.28	117.53
2	B	1201	OV5	C26-C24-C23	-2.95	119.53	123.73
2	A	1201	OV5	C13-C22-C20	2.87	132.59	129.42
2	D	1201	OV5	C26-C24-C23	-2.84	119.70	123.73
2	C	1201	OV5	C14-C13-C22	-2.83	115.63	119.91
2	D	1201	OV5	C8-C9-N10	-2.74	118.44	122.61
2	C	1201	OV5	C26-C24-C23	-2.70	119.90	123.73
2	D	1201	OV5	C14-C13-C22	-2.70	115.83	119.91
2	B	1201	OV5	C14-C13-C22	-2.65	115.90	119.91
2	A	1201	OV5	C14-C13-C22	-2.55	116.05	119.91
2	C	1201	OV5	O5-C4-N3	-2.53	117.67	122.59
2	C	1201	OV5	C6-C4-N3	2.46	122.23	117.12
2	A	1201	OV5	C8-C9-N10	-2.40	118.95	122.61
2	B	1201	OV5	C8-C9-N10	-2.37	119.00	122.61
2	A	1201	OV5	C14-C13-N12	2.31	125.86	121.12
2	B	1201	OV5	C14-C13-N12	2.24	125.72	121.12
2	C	1201	OV5	C6-C11-N10	-2.21	120.34	123.59
2	B	1201	OV5	N12-C9-N10	2.20	123.68	116.78
2	C	1201	OV5	C23-C15-N16	2.17	119.24	116.02
2	A	1201	OV5	N12-C9-N10	2.12	123.43	116.78
2	D	1201	OV5	C6-C11-N10	-2.12	120.47	123.59
2	A	1201	OV5	C6-C4-N3	2.10	121.49	117.12
2	A	1201	OV5	C8-C7-C6	-2.03	118.63	120.80
2	D	1201	OV5	N12-C9-N10	2.03	123.14	116.78

There are no chirality outliers.

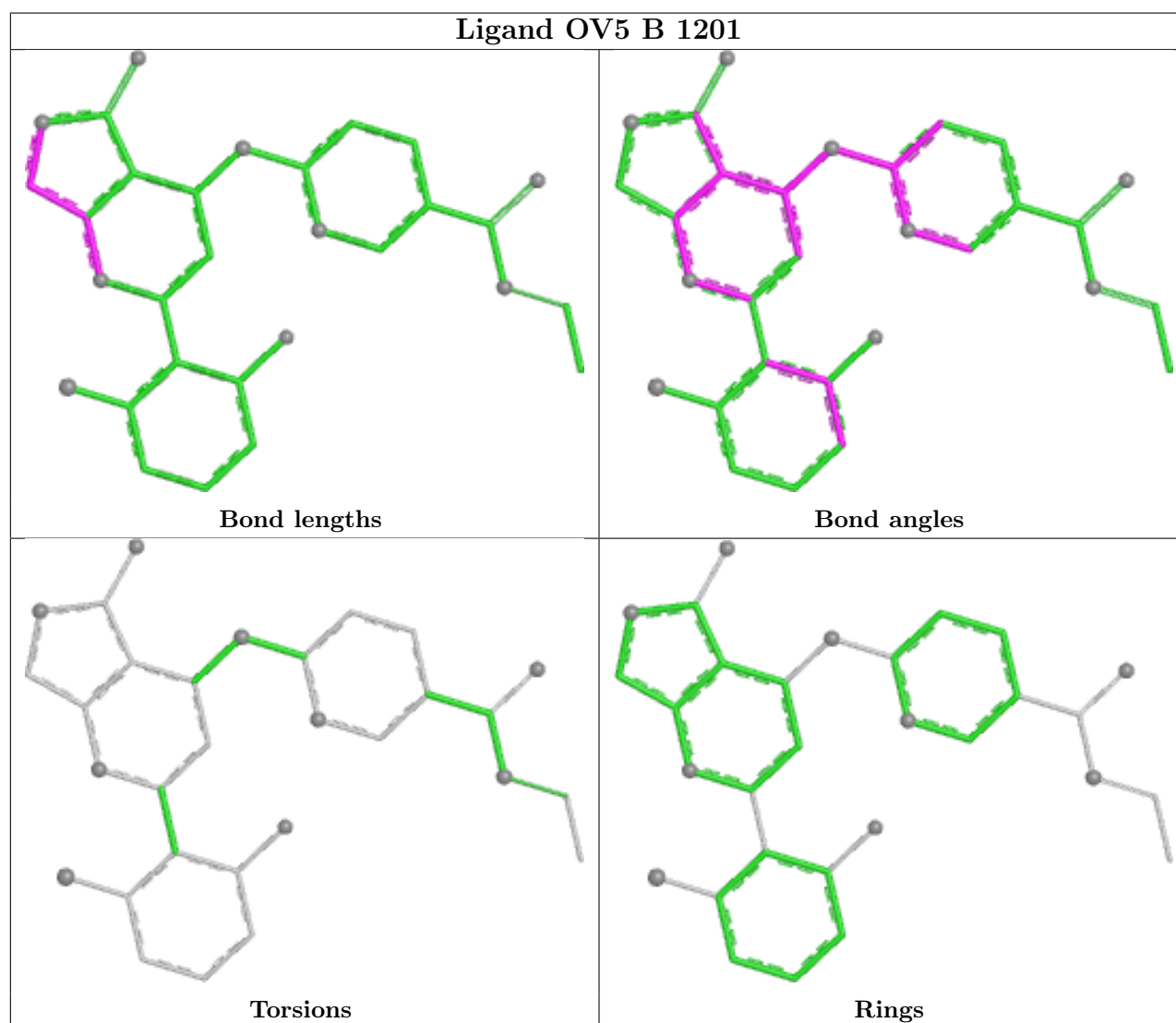
All (4) torsion outliers are listed below:

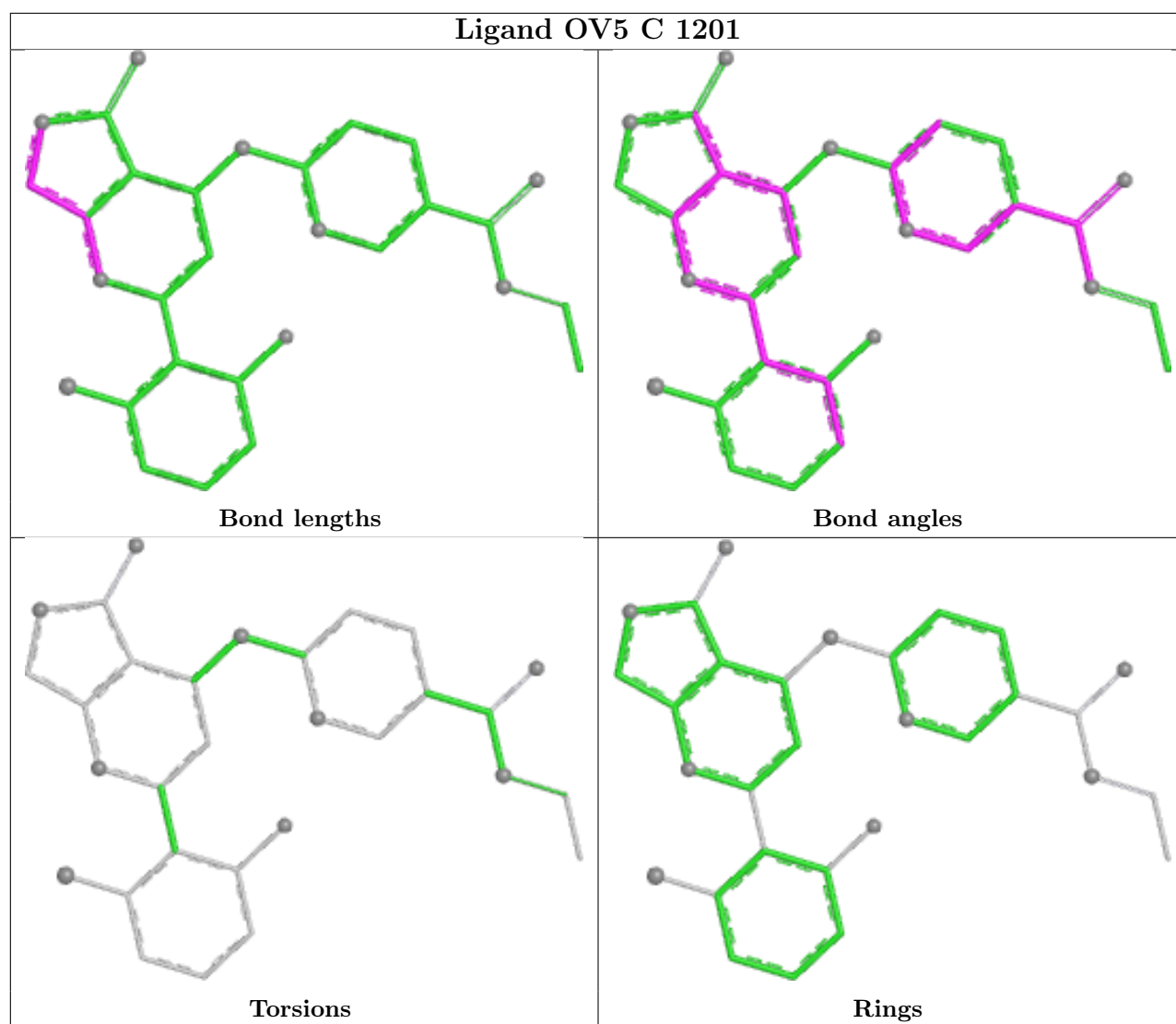
Mol	Chain	Res	Type	Atoms
2	D	1201	OV5	O5-C4-C6-C11
2	D	1201	OV5	N3-C4-C6-C11
2	D	1201	OV5	N3-C4-C6-C7
2	D	1201	OV5	O5-C4-C6-C7

There are no ring outliers.

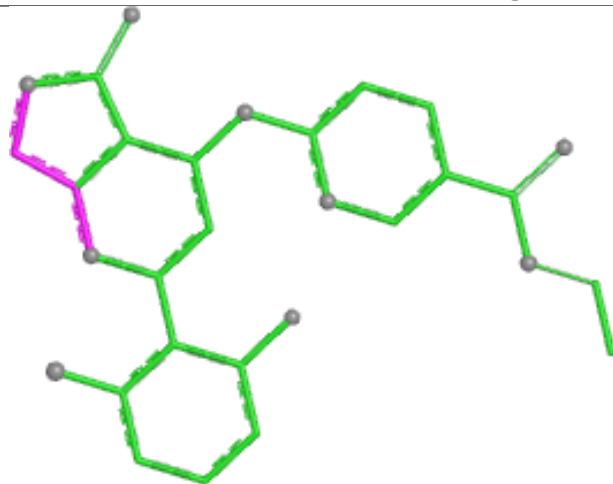
No monomer is involved in short contacts.

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.

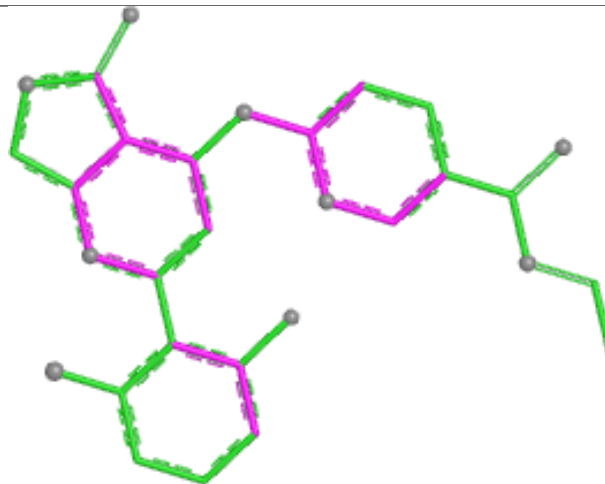




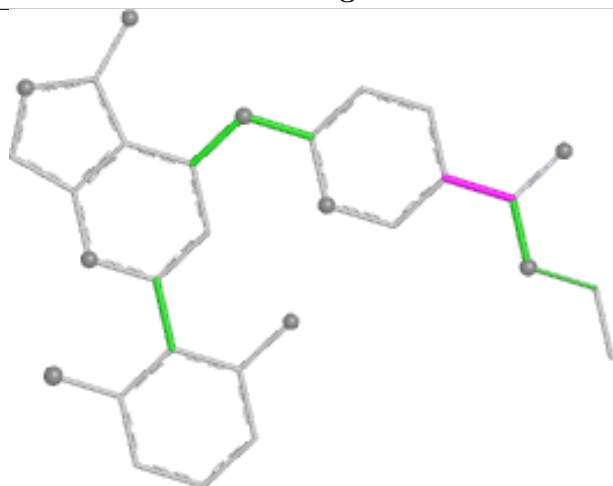
Ligand OV5 D 1201



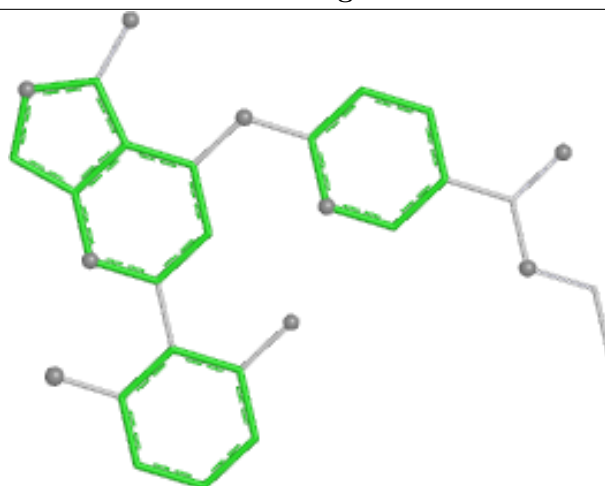
Bond lengths



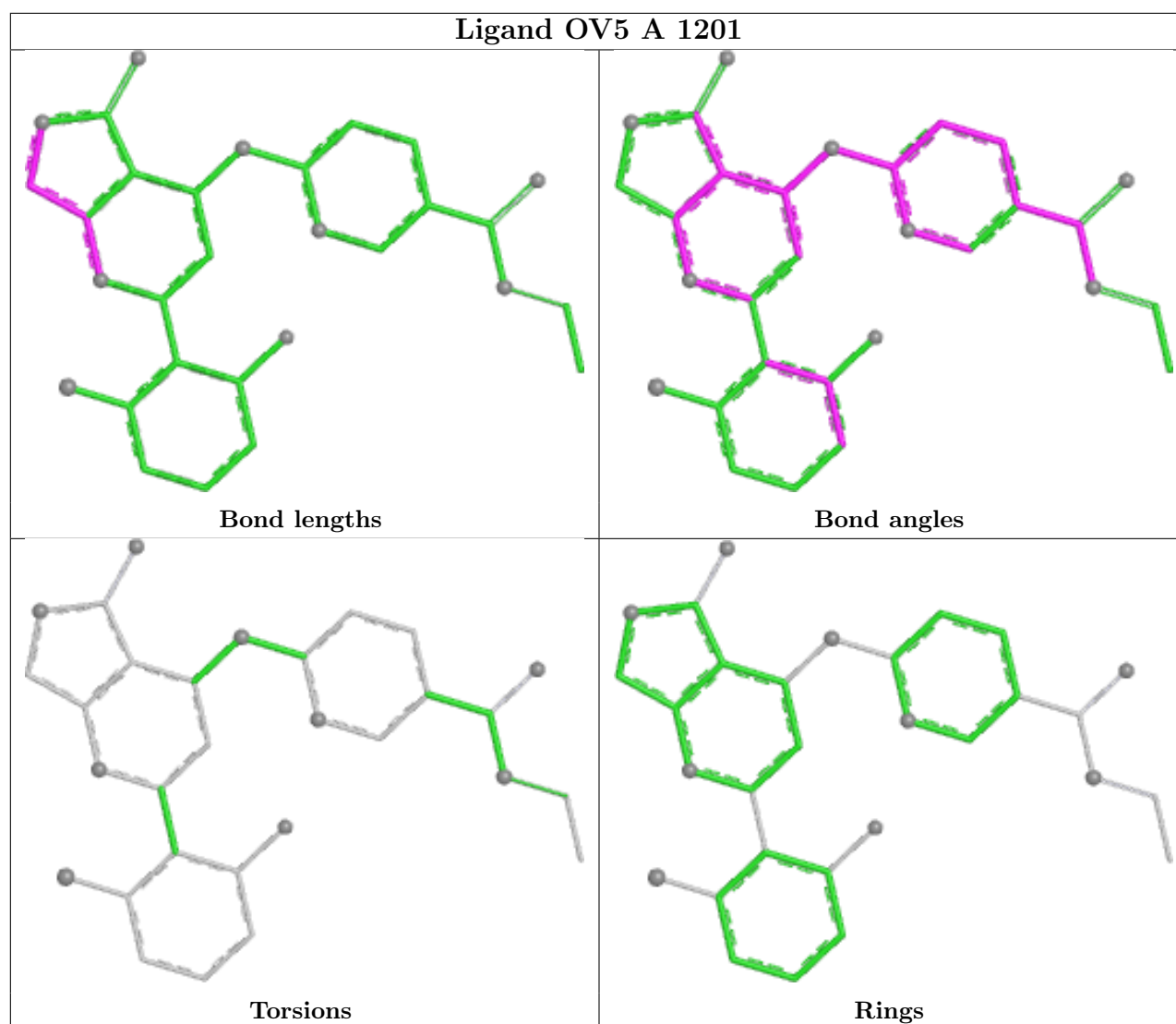
Bond angles



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/291 (94%)	0.72	31 (11%) 10 11	11, 34, 62, 84	19 (6%)
1	B	282/291 (96%)	0.67	26 (9%) 14 16	11, 33, 57, 80	20 (7%)
1	C	279/291 (95%)	0.85	33 (11%) 9 10	19, 38, 62, 74	23 (8%)
1	D	270/291 (92%)	0.99	30 (11%) 10 11	14, 41, 66, 116	21 (7%)
All	All	1107/1164 (95%)	0.81	120 (10%) 11 12	11, 37, 64, 116	83 (7%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1044	VAL	5.9
1	A	833	PHE	5.8
1	A	986	PRO	5.7
1	B	831	GLY	5.2
1	B	832	ASN	5.0
1	D	831	GLY	4.7
1	D	1100	SER	4.7
1	A	1044	VAL	4.6
1	A	987	GLY	4.6
1	D	833	PHE	4.6
1	D	1099	TRP	4.5
1	B	988	GLN	4.5
1	B	833	PHE	4.4
1	B	1042	ARG	4.4
1	D	832	ASN	4.3
1	C	815	THR	4.1
1	B	1043	ASP	4.1
1	B	896	GLN	4.0
1	C	831	GLY	3.9
1	D	1046	ALA	3.9
1	A	1099	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	833	PHE	3.9
1	B	987	GLY	3.9
1	B	814	PRO	3.9
1	C	1040	SER	3.8
1	D	1048	SER	3.8
1	C	814	PRO	3.8
1	D	844	LEU	3.8
1	C	813	ASP	3.8
1	D	859	HIS	3.7
1	B	1100	SER	3.6
1	D	815	THR	3.5
1	A	859	HIS	3.5
1	B	983	VAL	3.5
1	A	814	PRO	3.4
1	B	986	PRO	3.4
1	A	1065	ALA	3.4
1	D	989	SER	3.3
1	D	1045	PRO	3.3
1	D	1037	MET	3.3
1	C	986	PRO	3.2
1	C	1099	TRP	3.2
1	A	984	ARG	3.2
1	A	983	VAL	3.1
1	A	1100	SER	3.1
1	A	1045	PRO	3.1
1	C	859	HIS	3.1
1	B	989	SER	3.1
1	A	815	THR	3.0
1	D	814	PRO	3.0
1	A	919	ALA	3.0
1	C	812	GLN	2.9
1	C	1100	SER	2.9
1	D	1047	LEU	2.9
1	B	984	ARG	2.9
1	C	982	VAL	2.9
1	C	896	GLN	2.9
1	C	988	GLN	2.9
1	C	985	GLU	2.9
1	B	859	HIS	2.9
1	D	983	VAL	2.9
1	B	1044	VAL	2.8
1	D	982	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	832	ASN	2.8
1	C	987	GLY	2.8
1	D	816	ILE	2.8
1	C	1039	GLY	2.8
1	C	1045	PRO	2.8
1	D	845	GLY	2.7
1	A	832	ASN	2.7
1	A	989	SER	2.7
1	C	845	GLY	2.7
1	A	896	GLN	2.7
1	C	897	SER	2.7
1	C	847	ASN	2.6
1	A	991	ILE	2.6
1	B	815	THR	2.6
1	C	842	ASP	2.5
1	A	1038	MET	2.5
1	B	985	GLU	2.5
1	C	989	SER	2.5
1	D	976	LEU	2.5
1	D	891	TYR	2.4
1	A	858	GLN	2.4
1	B	982	VAL	2.4
1	C	1046	ALA	2.4
1	D	834	GLY	2.4
1	C	977	ASP	2.4
1	A	891	TYR	2.3
1	B	891	TYR	2.3
1	A	920	ARG	2.3
1	D	991	ILE	2.3
1	A	982	VAL	2.3
1	C	830	LYS	2.2
1	B	1046	ALA	2.2
1	A	856	GLN	2.2
1	C	920	ARG	2.2
1	C	983	VAL	2.2
1	B	863	ASP	2.2
1	A	861	GLY	2.2
1	D	1068	ALA	2.1
1	C	844	LEU	2.1
1	D	848	THR	2.1
1	B	991	ILE	2.1
1	A	844	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	830	LYS	2.1
1	C	1048	SER	2.1
1	B	834	GLY	2.1
1	A	1046	ALA	2.1
1	D	977	ASP	2.1
1	B	1040	SER	2.1
1	C	961	ALA	2.1
1	A	862	PRO	2.0
1	A	990	PRO	2.0
1	B	994	TYR	2.0
1	A	992	PHE	2.0
1	C	1069	GLU	2.0
1	A	1050	LEU	2.0
1	D	1035	LEU	2.0
1	D	916	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	B	981	16/17	0.67	0.21	50,62,77,78	0
1	PTR	A	981	16/17	0.74	0.20	48,59,73,74	0
1	PTR	C	981	16/17	0.80	0.16	52,58,69,72	0
1	PTR	D	981	16/17	0.80	0.16	57,65,81,83	0
1	PTR	D	980	16/17	0.82	0.14	55,63,78,81	0
1	PTR	C	980	16/17	0.83	0.13	49,56,71,74	0
1	PTR	B	980	16/17	0.83	0.13	45,51,67,70	0
1	PTR	A	980	16/17	0.86	0.12	42,49,68,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

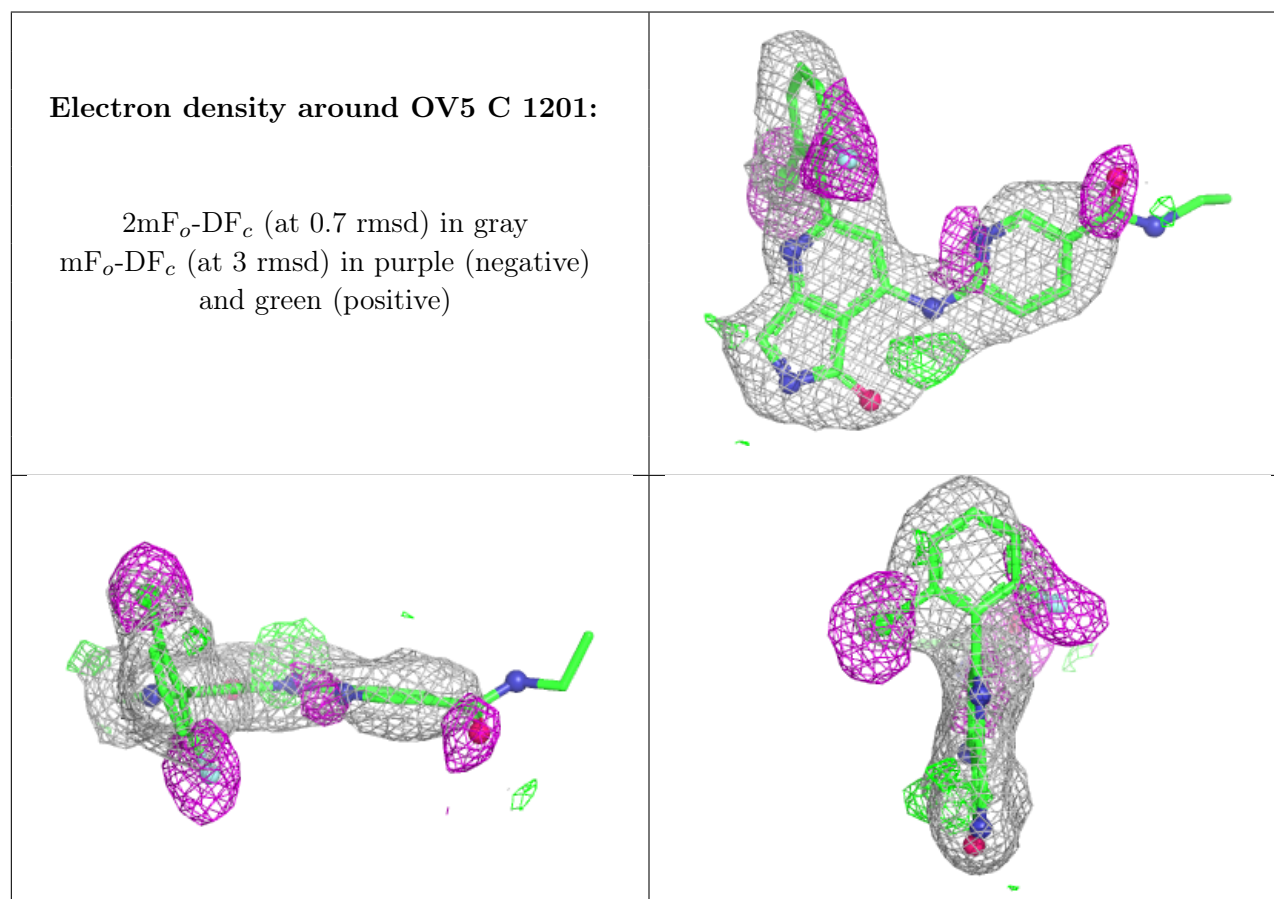
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

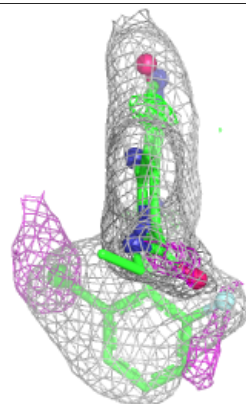
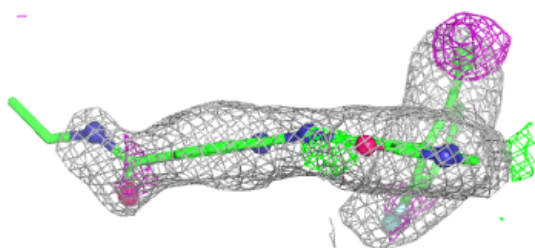
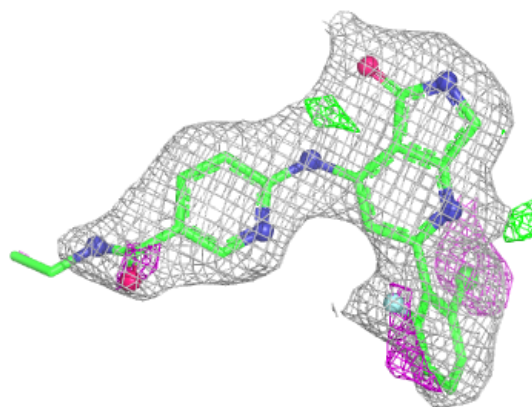
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OV5	C	1201	30/30	0.71	0.15	28,31,38,41	3
2	OV5	D	1201	30/30	0.79	0.12	26,31,37,39	2
2	OV5	A	1201	30/30	0.92	0.07	3,5,11,15	0
2	OV5	B	1201	30/30	0.93	0.07	2,8,12,16	0
3	CL	D	1202	1/1	0.97	0.20	21,21,21,21	0

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.

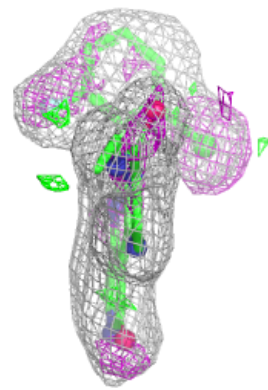
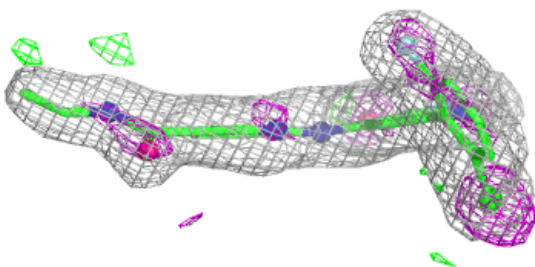
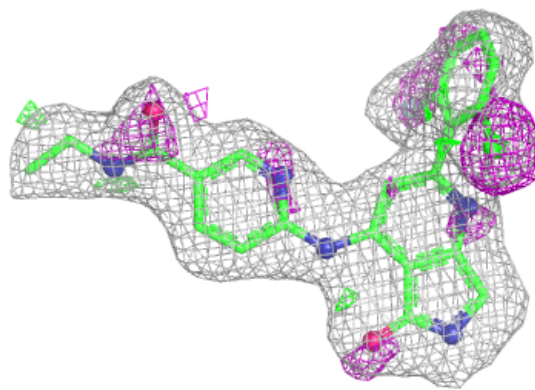


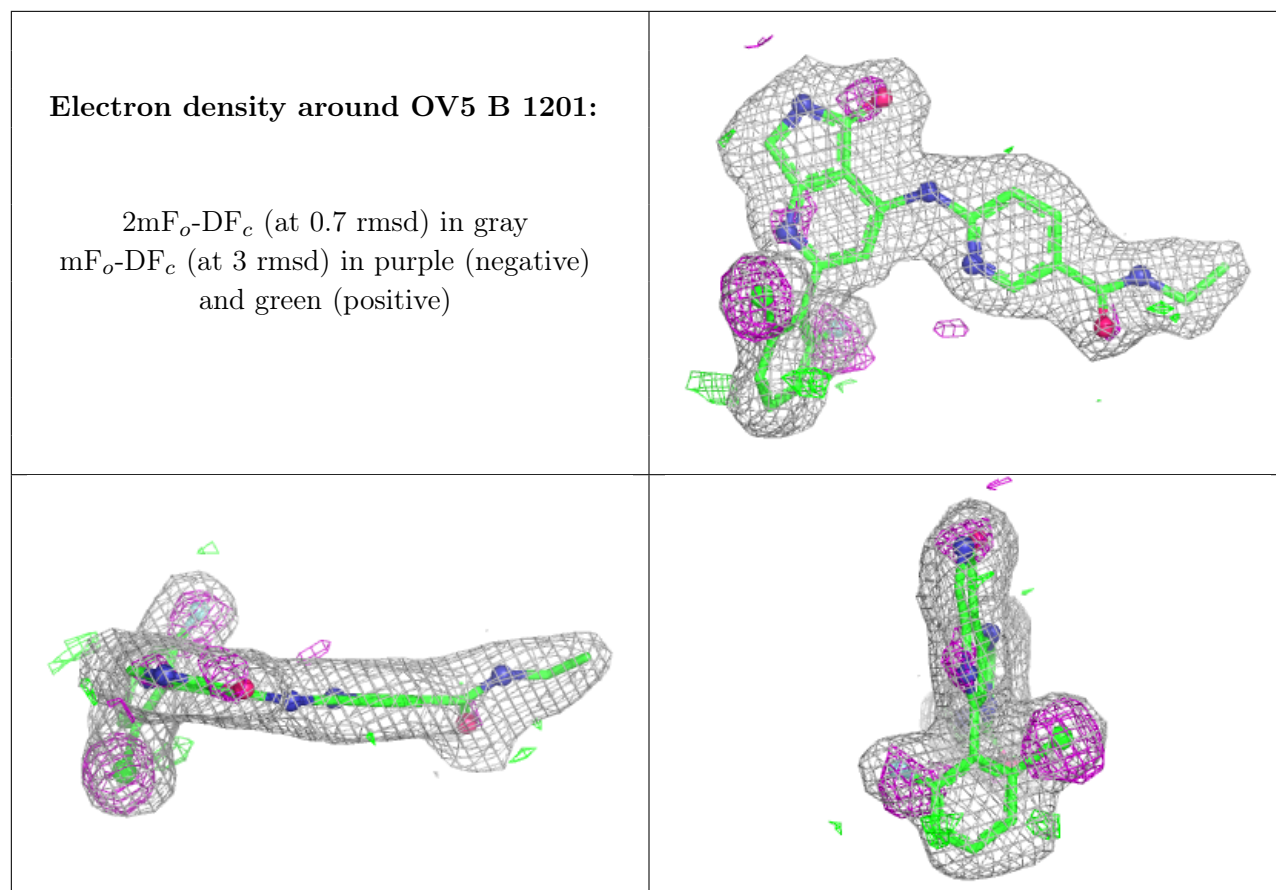
Electron density around OV5 D 1201:

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

**Electron density around OV5 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.