



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:34 PM UTC

PDB ID : 7L99 / pdb_00007L99
Title : Crystal structure of BRDT bromodomain 2 in complex with CDD-1302
Authors : Sharma, R.; Yu, Z.; Ku, A.F.; Anglin, J.L.; Ucisik, M.N.; Faver, J.C.;
Sankaran, B.; Kim, C.; Matzuk, M.M.
Deposited on : 2021-01-03
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

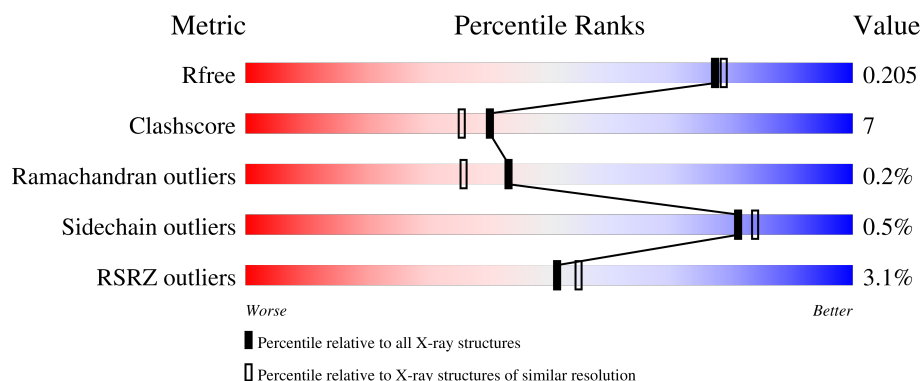
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	135	2% 78% 6% 16%
1	B	135	% 75% 7% 18%
1	C	135	3% 77% 7% 16%
1	D	135	4% 73% 11% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JEF	D	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4206 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 Bromodomain testis-specific protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	2	2	0
			915	591	150	163	11			
1	B	111	Total	C	N	O	S	0	3	0
			902	584	149	160	9			
1	C	113	Total	C	N	O	S	0	1	0
			914	592	154	159	9			
1	D	113	Total	C	N	O	S	0	3	0
			920	594	151	165	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	MET	-	initiating methionine	UNP Q58F21
A	246	GLY	-	expression tag	UNP Q58F21
A	247	SER	-	expression tag	UNP Q58F21
A	248	SER	-	expression tag	UNP Q58F21
A	249	HIS	-	expression tag	UNP Q58F21
A	250	HIS	-	expression tag	UNP Q58F21
A	251	HIS	-	expression tag	UNP Q58F21
A	252	HIS	-	expression tag	UNP Q58F21
A	253	HIS	-	expression tag	UNP Q58F21
A	254	HIS	-	expression tag	UNP Q58F21
A	255	SER	-	expression tag	UNP Q58F21
A	256	SER	-	expression tag	UNP Q58F21
A	257	GLY	-	expression tag	UNP Q58F21
A	258	LEU	-	expression tag	UNP Q58F21
A	259	VAL	-	expression tag	UNP Q58F21
A	260	PRO	-	expression tag	UNP Q58F21
A	261	ARG	-	expression tag	UNP Q58F21
A	262	GLY	-	expression tag	UNP Q58F21
A	263	SER	-	expression tag	UNP Q58F21
A	264	HIS	-	expression tag	UNP Q58F21
A	265	MET	-	expression tag	UNP Q58F21

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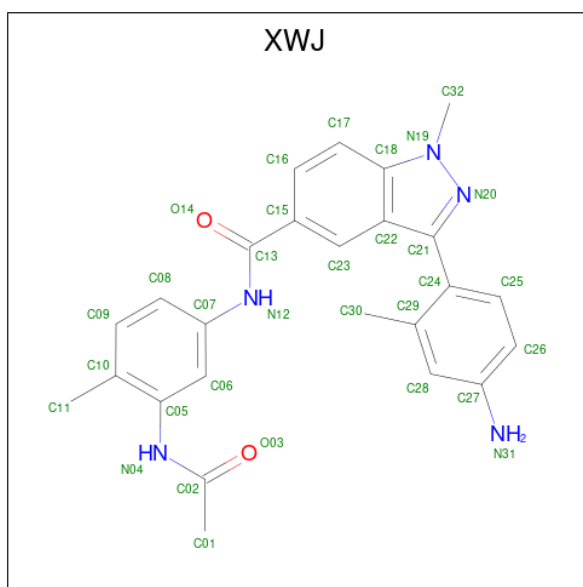
Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	-	expression tag	UNP Q58F21
A	267	SER	-	expression tag	UNP Q58F21
B	245	MET	-	initiating methionine	UNP Q58F21
B	246	GLY	-	expression tag	UNP Q58F21
B	247	SER	-	expression tag	UNP Q58F21
B	248	SER	-	expression tag	UNP Q58F21
B	249	HIS	-	expression tag	UNP Q58F21
B	250	HIS	-	expression tag	UNP Q58F21
B	251	HIS	-	expression tag	UNP Q58F21
B	252	HIS	-	expression tag	UNP Q58F21
B	253	HIS	-	expression tag	UNP Q58F21
B	254	HIS	-	expression tag	UNP Q58F21
B	255	SER	-	expression tag	UNP Q58F21
B	256	SER	-	expression tag	UNP Q58F21
B	257	GLY	-	expression tag	UNP Q58F21
B	258	LEU	-	expression tag	UNP Q58F21
B	259	VAL	-	expression tag	UNP Q58F21
B	260	PRO	-	expression tag	UNP Q58F21
B	261	ARG	-	expression tag	UNP Q58F21
B	262	GLY	-	expression tag	UNP Q58F21
B	263	SER	-	expression tag	UNP Q58F21
B	264	HIS	-	expression tag	UNP Q58F21
B	265	MET	-	expression tag	UNP Q58F21
B	266	ALA	-	expression tag	UNP Q58F21
B	267	SER	-	expression tag	UNP Q58F21
C	245	MET	-	initiating methionine	UNP Q58F21
C	246	GLY	-	expression tag	UNP Q58F21
C	247	SER	-	expression tag	UNP Q58F21
C	248	SER	-	expression tag	UNP Q58F21
C	249	HIS	-	expression tag	UNP Q58F21
C	250	HIS	-	expression tag	UNP Q58F21
C	251	HIS	-	expression tag	UNP Q58F21
C	252	HIS	-	expression tag	UNP Q58F21
C	253	HIS	-	expression tag	UNP Q58F21
C	254	HIS	-	expression tag	UNP Q58F21
C	255	SER	-	expression tag	UNP Q58F21
C	256	SER	-	expression tag	UNP Q58F21
C	257	GLY	-	expression tag	UNP Q58F21
C	258	LEU	-	expression tag	UNP Q58F21
C	259	VAL	-	expression tag	UNP Q58F21
C	260	PRO	-	expression tag	UNP Q58F21
C	261	ARG	-	expression tag	UNP Q58F21

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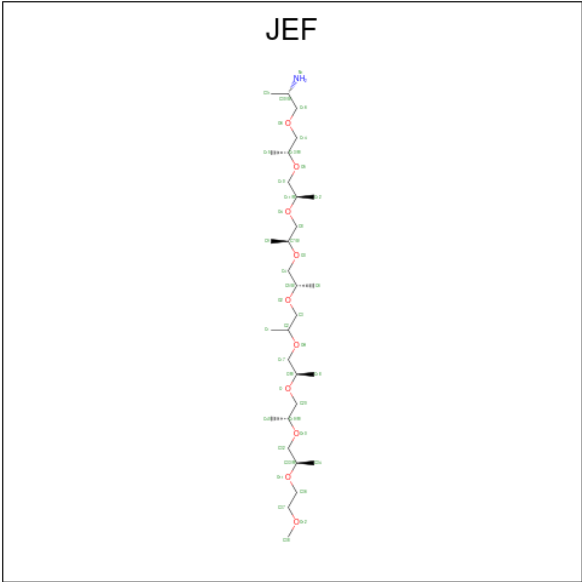
Chain	Residue	Modelled	Actual	Comment	Reference
C	262	GLY	-	expression tag	UNP Q58F21
C	263	SER	-	expression tag	UNP Q58F21
C	264	HIS	-	expression tag	UNP Q58F21
C	265	MET	-	expression tag	UNP Q58F21
C	266	ALA	-	expression tag	UNP Q58F21
C	267	SER	-	expression tag	UNP Q58F21
D	245	MET	-	initiating methionine	UNP Q58F21
D	246	GLY	-	expression tag	UNP Q58F21
D	247	SER	-	expression tag	UNP Q58F21
D	248	SER	-	expression tag	UNP Q58F21
D	249	HIS	-	expression tag	UNP Q58F21
D	250	HIS	-	expression tag	UNP Q58F21
D	251	HIS	-	expression tag	UNP Q58F21
D	252	HIS	-	expression tag	UNP Q58F21
D	253	HIS	-	expression tag	UNP Q58F21
D	254	HIS	-	expression tag	UNP Q58F21
D	255	SER	-	expression tag	UNP Q58F21
D	256	SER	-	expression tag	UNP Q58F21
D	257	GLY	-	expression tag	UNP Q58F21
D	258	LEU	-	expression tag	UNP Q58F21
D	259	VAL	-	expression tag	UNP Q58F21
D	260	PRO	-	expression tag	UNP Q58F21
D	261	ARG	-	expression tag	UNP Q58F21
D	262	GLY	-	expression tag	UNP Q58F21
D	263	SER	-	expression tag	UNP Q58F21
D	264	HIS	-	expression tag	UNP Q58F21
D	265	MET	-	expression tag	UNP Q58F21
D	266	ALA	-	expression tag	UNP Q58F21
D	267	SER	-	expression tag	UNP Q58F21

- Molecule 2 is N-[3-(acetylamino)-4-methylphenyl]-3-(4-amino-2-methylphenyl)-1-methyl-1H-indazole-5-carboxamide (CCD ID: XWJ) (formula: C₂₅H₂₅N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	25	5	2		
2	B	1	Total	C	N	O	0	0
			32	25	5	2		
2	C	1	Total	C	N	O	0	0
			32	25	5	2		
2	C	1	Total	C	N	O	0	0
			32	25	5	2		
2	D	1	Total	C	N	O	0	0
			32	25	5	2		
2	D	1	Total	C	N	O	0	0
			32	25	5	2		

- Molecule 3 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (CCD ID: JEF) (formula: C₃₀H₆₃NO₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			41	30	1	10		

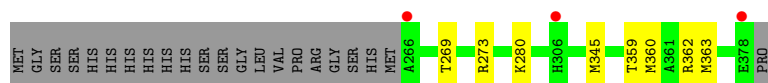
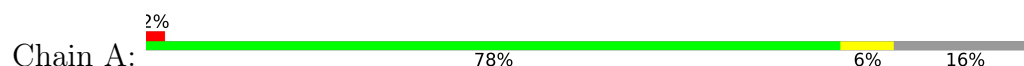
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	76	Total	O	0	0
			76	76		
4	C	79	Total	O	0	0
			79	79		
4	D	88	Total	O	0	0
			88	88		

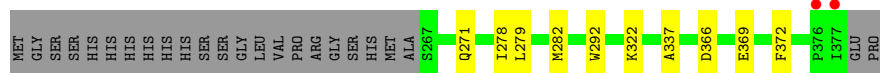
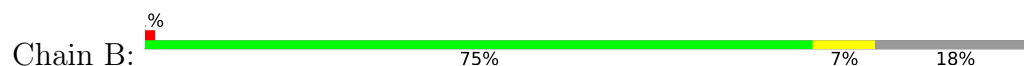
3 Residue-property plots [i](#)

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.

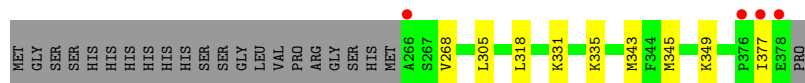
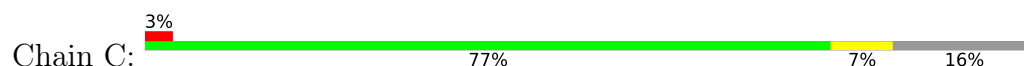
- Molecule 1: Bromodomain testis-specific protein



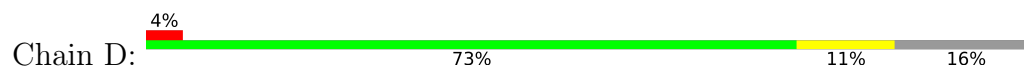
- Molecule 1: Bromodomain testis-specific protein



- Molecule 1: Bromodomain testis-specific protein



- Molecule 1: Bromodomain testis-specific protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.23Å 61.97Å 99.19Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	44.55 – 1.90 44.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.55-1.90) 98.7 (44.55-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.170 , 0.205 0.171 , 0.205	Depositor DCC
R_{free} test set	2217 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4206	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% 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: XWJ, JEF

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	0.23	0/947	0.46	0/1286
1	B	0.24	0/936	0.41	0/1269
1	C	0.24	0/944	0.46	0/1280
1	D	0.26	0/955	0.45	0/1297
All	All	0.24	0/3782	0.45	0/5132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	915	0	868	6	0
1	B	902	0	867	7	0
1	C	914	0	872	9	0
1	D	920	0	871	15	0
2	A	32	0	0	0	0
2	B	32	0	0	1	0
2	C	64	0	0	2	0
2	D	64	0	0	4	0
3	D	41	0	63	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	79	0	0	0	0
4	B	76	0	0	1	0
4	C	79	0	0	1	0
4	D	88	0	0	9	0
All	All	4206	0	3541	49	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 7.

All (49) 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)
2:D:402:XWJ:O14	4:D:501:HOH:O	2.08	0.71
2:C:801:XWJ:O14	4:D:501:HOH:O	2.12	0.66
1:C:331:LYS:H	1:C:335:LYS:HE3	1.60	0.66
2:D:402:XWJ:N04	3:D:403:JEF:H92	2.13	0.63
1:C:349:LYS:HE2	3:D:403:JEF:H313	1.80	0.62
1:A:359:THR:HG22	1:A:363:MET:HE2	1.81	0.62
3:D:403:JEF:H341	3:D:403:JEF:H403	1.82	0.62
1:A:362:ARG:NE	1:B:366:ASP:OD1	2.29	0.60
1:C:349:LYS:HE3	3:D:403:JEF:H13	1.84	0.59
1:C:305:LEU:O	4:C:901:HOH:O	2.18	0.55
1:C:331:LYS:H	1:C:335:LYS:CE	2.19	0.55
1:C:331:LYS:HD3	1:C:335:LYS:HE2	1.90	0.53
3:D:403:JEF:H	4:D:501:HOH:O	2.07	0.53
1:D:353:PRO:HG3	3:D:403:JEF:H61	1.89	0.53
1:A:345:MET:HE1	1:B:369:GLU:OE1	2.09	0.52
2:D:402:XWJ:C02	3:D:403:JEF:H92	2.41	0.50
3:D:403:JEF:H81	4:D:510:HOH:O	2.12	0.49
1:D:279:LEU:HD21	1:D:322:LYS:HA	1.94	0.49
3:D:403:JEF:H19	4:D:569:HOH:O	2.13	0.48
1:D:348:TYR:HB2	3:D:403:JEF:H402	1.95	0.48
1:A:269:THR:O	1:A:273:ARG:HG3	2.14	0.48
2:B:800:XWJ:C17	3:D:403:JEF:H153	2.44	0.46
1:D:266:ALA:N	4:D:505:HOH:O	2.49	0.45
1:D:349:LYS:HA	3:D:403:JEF:H401	1.98	0.45
1:D:349:LYS:HE2	3:D:403:JEF:H382	1.97	0.45
1:B:271:GLN:OE1	4:B:901:HOH:O	2.21	0.45
1:D:349:LYS:N	3:D:403:JEF:H401	2.32	0.45
1:C:345:MET:HB3	3:D:403:JEF:H152	1.98	0.45
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:XWJ:C30	3:D:403:JEF:H63	2.47	0.44
1:B:337:ALA:HB2	1:B:372:PHE:CZ	2.53	0.44
3:D:403:JEF:H5	4:D:501:HOH:O	2.18	0.43
2:C:801:XWJ:C02	3:D:403:JEF:H182	2.49	0.43
1:B:292:TRP:CZ3	3:D:403:JEF:H62	2.54	0.43
1:D:345:MET:HB3	3:D:403:JEF:C34	2.49	0.42
1:D:349:LYS:CA	3:D:403:JEF:H401	2.49	0.42
1:C:331:LYS:HB2	1:C:331:LYS:HE2	1.81	0.42
1:A:360:MET:HA	1:A:363:MET:HE3	2.02	0.42
1:B:279:LEU:HD21	1:B:322:LYS:HA	2.02	0.42
1:D:299:ASP:OD1	4:D:502:HOH:O	2.21	0.42
1:C:318:LEU:HD21	1:C:343:MET:HE1	2.02	0.41
1:D:327:ASN:HB3	1:D:329:GLU:HG3	2.02	0.41
3:D:403:JEF:H172	3:D:403:JEF:H201	1.52	0.41
1:D:292:TRP:NE1	1:D:360:MET:HE1	2.36	0.41
1:B:278:ILE:HG22	1:B:282:MET:HE2	2.03	0.41
3:D:403:JEF:H101	4:D:510:HOH:O	2.21	0.41
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.87	0.41
1:D:292:TRP:CG	1:D:293:PRO:HD3	2.56	0.40
1:D:348:TYR:CB	3:D:403:JEF:H402	2.52	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	113/135 (84%)	113 (100%)	0	0	100	100
1	B	112/135 (83%)	112 (100%)	0	0	100	100
1	C	112/135 (83%)	111 (99%)	0	1 (1%)	14	6
1	D	114/135 (84%)	112 (98%)	2 (2%)	0	100	100
All	All	451/540 (84%)	448 (99%)	2 (0%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	377	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/122 (80%)	98 (100%)	0	100	100
1	B	97/122 (80%)	97 (100%)	0	100	100
1	C	96/122 (79%)	95 (99%)	1 (1%)	68	70
1	D	98/122 (80%)	97 (99%)	1 (1%)	68	70
All	All	389/488 (80%)	387 (100%)	2 (0%)	81	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	VAL
1	D	325	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	271	GLN
1	D	274	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	XWJ	D	401	-	35,35,35	2.15	13 (37%)	50,51,51	1.88	14 (28%)
2	XWJ	C	800	-	35,35,35	2.17	12 (34%)	50,51,51	1.61	13 (26%)
2	XWJ	C	801	-	35,35,35	2.03	11 (31%)	50,51,51	1.57	13 (26%)
2	XWJ	B	800	-	35,35,35	2.12	12 (34%)	50,51,51	1.52	13 (26%)
2	XWJ	A	800	-	35,35,35	2.13	11 (31%)	50,51,51	1.52	11 (22%)
2	XWJ	D	402	-	35,35,35	2.08	14 (40%)	50,51,51	1.51	12 (24%)
3	JEF	D	403	-	40,40,40	1.27	6 (15%)	48,48,48	1.55	10 (20%)

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	XWJ	D	401	-	-	3/16/16/16	0/4/4/4
2	XWJ	C	800	-	-	3/16/16/16	0/4/4/4
2	XWJ	C	801	-	-	0/16/16/16	0/4/4/4
2	XWJ	B	800	-	-	4/16/16/16	0/4/4/4
2	XWJ	A	800	-	-	4/16/16/16	0/4/4/4
2	XWJ	D	402	-	-	0/16/16/16	0/4/4/4
3	JEF	D	403	-	-	26/46/46/46	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	XWJ	C02-N04	5.75	1.46	1.36
2	B	800	XWJ	C02-N04	5.66	1.46	1.36
2	C	800	XWJ	C02-N04	5.48	1.46	1.36
2	A	800	XWJ	C02-N04	5.39	1.46	1.36
2	D	401	XWJ	C02-N04	5.32	1.46	1.36
2	C	801	XWJ	C02-N04	5.31	1.46	1.36
2	C	800	XWJ	C24-C21	5.03	1.57	1.49
2	D	401	XWJ	C24-C21	4.55	1.57	1.49
2	B	800	XWJ	C24-C21	4.30	1.56	1.49
2	A	800	XWJ	C24-C21	4.15	1.56	1.49
2	A	800	XWJ	C05-N04	4.05	1.49	1.41
2	C	801	XWJ	C24-C21	3.91	1.55	1.49
2	B	800	XWJ	C05-N04	3.86	1.49	1.41
2	D	401	XWJ	C08-C07	3.83	1.45	1.39
2	A	800	XWJ	C13-N12	3.81	1.46	1.35
2	D	402	XWJ	C05-N04	3.80	1.49	1.41
2	D	401	XWJ	C05-N04	3.80	1.49	1.41
2	C	800	XWJ	C13-N12	3.79	1.46	1.35
2	D	402	XWJ	C24-C21	3.77	1.55	1.49
2	B	800	XWJ	C13-N12	3.77	1.46	1.35
2	C	801	XWJ	C05-N04	3.76	1.49	1.41
2	D	401	XWJ	C13-N12	3.69	1.46	1.35
2	C	801	XWJ	C13-N12	3.63	1.46	1.35
2	C	800	XWJ	C05-N04	3.63	1.48	1.41
2	A	800	XWJ	C08-C07	3.50	1.45	1.39
2	B	800	XWJ	C08-C07	3.50	1.45	1.39
2	D	402	XWJ	C13-N12	3.26	1.45	1.35
2	C	800	XWJ	C07-N12	3.17	1.48	1.41
2	C	801	XWJ	O03-C02	-3.03	1.16	1.23
2	C	800	XWJ	C08-C07	3.02	1.44	1.39
2	D	402	XWJ	C16-C15	3.02	1.44	1.39
2	C	800	XWJ	C16-C15	2.90	1.43	1.39
2	C	801	XWJ	C16-C15	2.89	1.43	1.39
3	D	403	JEF	O4-C11	-2.89	1.39	1.44
2	B	800	XWJ	O14-C13	-2.82	1.16	1.23
2	A	800	XWJ	O03-C02	-2.79	1.17	1.23
2	C	800	XWJ	O14-C13	-2.78	1.16	1.23
2	C	801	XWJ	O14-C13	-2.78	1.16	1.23
2	A	800	XWJ	C16-C15	2.71	1.43	1.39
2	D	401	XWJ	O14-C13	-2.70	1.17	1.23
2	B	800	XWJ	C32-N19	2.69	1.50	1.46
2	D	402	XWJ	O03-C02	-2.62	1.17	1.23
2	D	401	XWJ	C32-N19	2.60	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	XWJ	O03-C02	-2.56	1.17	1.23
2	D	401	XWJ	C16-C15	2.52	1.43	1.39
2	D	402	XWJ	O14-C13	-2.49	1.17	1.23
2	D	402	XWJ	C08-C07	2.48	1.43	1.39
2	C	800	XWJ	C32-N19	2.48	1.49	1.46
2	A	800	XWJ	C07-N12	2.47	1.46	1.41
2	B	800	XWJ	C07-N12	2.44	1.46	1.41
3	D	403	JEF	O4-C8	-2.38	1.39	1.43
2	D	401	XWJ	C27-N31	2.37	1.46	1.38
2	B	800	XWJ	O03-C02	-2.37	1.17	1.23
2	B	800	XWJ	C30-C29	2.36	1.55	1.51
2	A	800	XWJ	O14-C13	-2.35	1.17	1.23
2	C	801	XWJ	C08-C07	2.34	1.43	1.39
2	D	402	XWJ	C32-N19	2.33	1.49	1.46
2	C	800	XWJ	C30-C29	2.33	1.55	1.51
2	D	401	XWJ	C07-N12	2.33	1.46	1.41
2	C	801	XWJ	C07-N12	2.33	1.46	1.41
2	B	800	XWJ	C27-N31	2.31	1.46	1.38
3	D	403	JEF	O11-C33	-2.31	1.40	1.44
2	D	401	XWJ	C30-C29	2.26	1.55	1.51
2	A	800	XWJ	C30-C29	2.23	1.55	1.51
2	C	800	XWJ	O03-C02	-2.22	1.18	1.23
3	D	403	JEF	O10-C19	-2.20	1.40	1.44
2	C	801	XWJ	C27-N31	2.19	1.45	1.38
3	D	403	JEF	O2-C3	-2.16	1.40	1.43
2	C	801	XWJ	C32-N19	2.14	1.49	1.46
2	D	402	XWJ	C17-C18	2.09	1.42	1.39
2	C	800	XWJ	C27-N31	2.09	1.45	1.38
3	D	403	JEF	O3-C4	-2.07	1.40	1.43
2	D	402	XWJ	C21-N20	-2.05	1.30	1.33
2	D	402	XWJ	C07-N12	2.05	1.45	1.41
2	B	800	XWJ	C11-C10	2.04	1.54	1.51
2	D	402	XWJ	C11-C10	2.04	1.54	1.51
2	D	402	XWJ	C30-C29	2.02	1.54	1.51
2	D	401	XWJ	C09-C10	2.01	1.43	1.39
2	A	800	XWJ	C27-N31	2.00	1.45	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	XWJ	C22-C21-N20	-4.73	106.60	110.60
3	D	403	JEF	C32-O10-C19	4.51	121.71	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	XWJ	C22-C21-N20	-4.44	106.84	110.60
2	D	401	XWJ	C32-N19-N20	4.28	125.79	119.97
2	D	401	XWJ	C10-C05-N04	4.23	125.58	118.82
2	C	800	XWJ	C10-C05-N04	4.01	125.22	118.82
2	D	401	XWJ	C32-N19-C18	-3.95	123.49	128.36
2	C	801	XWJ	C22-C21-N20	-3.61	107.54	110.60
3	D	403	JEF	O10-C32-C33	3.42	119.14	110.82
2	B	800	XWJ	C22-C21-N20	-3.37	107.75	110.60
2	D	401	XWJ	C16-C15-C23	3.29	123.05	119.25
2	B	800	XWJ	C09-C10-C05	3.21	120.51	117.50
2	C	801	XWJ	C05-N04-C02	-3.21	119.75	127.50
2	D	402	XWJ	C05-N04-C02	-3.20	119.78	127.50
3	D	403	JEF	C8-O4-C11	3.16	119.71	115.05
2	D	401	XWJ	C05-N04-C02	-3.13	119.93	127.50
2	A	800	XWJ	C09-C10-C05	3.13	120.43	117.50
2	D	402	XWJ	C01-C02-N04	3.09	119.60	114.95
2	A	800	XWJ	C22-C21-N20	-3.08	107.99	110.60
2	A	800	XWJ	O03-C02-N04	-3.03	118.90	123.06
2	D	401	XWJ	O03-C02-N04	-3.03	118.91	123.06
2	A	800	XWJ	C32-N19-N20	3.00	124.05	119.97
2	C	801	XWJ	C16-C15-C23	2.98	122.69	119.25
2	C	801	XWJ	C09-C10-C05	2.93	120.24	117.50
2	C	801	XWJ	C01-C02-N04	2.92	119.35	114.95
2	D	401	XWJ	C17-C16-C15	-2.91	117.69	120.80
3	D	403	JEF	C40-C19-C20	-2.89	104.55	112.69
2	D	401	XWJ	C06-C05-N04	-2.88	114.40	121.95
2	B	800	XWJ	C16-C15-C23	2.88	122.58	119.25
2	C	800	XWJ	C32-N19-N20	2.87	123.88	119.97
2	D	401	XWJ	C28-C29-C24	2.87	120.17	117.97
2	C	800	XWJ	C09-C10-C05	2.85	120.17	117.50
2	B	800	XWJ	C32-N19-N20	2.83	123.81	119.97
2	A	800	XWJ	C32-N19-C18	-2.81	124.89	128.36
2	C	800	XWJ	C06-C05-N04	-2.80	114.62	121.95
2	D	402	XWJ	C09-C10-C05	2.78	120.10	117.50
2	A	800	XWJ	C16-C15-C23	2.76	122.45	119.25
2	C	801	XWJ	C32-N19-N20	2.72	123.67	119.97
2	D	401	XWJ	C24-C21-N20	2.70	125.13	119.32
2	C	800	XWJ	C24-C21-N20	2.68	125.09	119.32
2	C	800	XWJ	C16-C15-C23	2.67	122.34	119.25
2	A	800	XWJ	C05-N04-C02	-2.57	121.30	127.50
2	C	801	XWJ	C24-C21-N20	2.55	124.82	119.32
2	D	401	XWJ	C09-C10-C05	2.53	119.87	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	XWJ	C32-N19-C18	-2.53	125.24	128.36
2	D	402	XWJ	C22-C21-N20	-2.50	108.49	110.60
2	D	402	XWJ	C27-C28-C29	-2.44	118.65	121.80
2	C	801	XWJ	C30-C29-C24	-2.43	119.21	122.81
2	D	402	XWJ	C24-C21-N20	2.42	124.53	119.32
2	C	800	XWJ	C05-N04-C02	-2.41	121.69	127.50
2	D	401	XWJ	C01-C02-N04	2.37	118.51	114.95
2	D	402	XWJ	C30-C29-C24	-2.34	119.35	122.81
2	B	800	XWJ	C07-N12-C13	-2.34	120.46	126.61
2	B	800	XWJ	C24-C21-N20	2.33	124.34	119.32
3	D	403	JEF	C10-O5-C13	-2.33	111.61	115.05
2	C	800	XWJ	C32-N19-C18	-2.31	125.50	128.36
2	D	402	XWJ	C11-C10-C05	-2.31	118.61	121.23
2	A	800	XWJ	C28-C29-C24	2.29	119.73	117.97
2	C	801	XWJ	C28-C29-C24	2.28	119.72	117.97
2	B	800	XWJ	C10-C05-N04	2.28	122.45	118.82
2	A	800	XWJ	C10-C05-N04	2.26	122.43	118.82
2	A	800	XWJ	C01-C02-N04	2.25	118.34	114.95
2	A	800	XWJ	C24-C21-N20	2.25	124.17	119.32
3	D	403	JEF	C9-C7-C8	-2.25	106.38	112.69
3	D	403	JEF	C1-C2-C3	-2.24	106.39	112.69
2	B	800	XWJ	C17-C16-C15	-2.23	118.41	120.80
2	C	801	XWJ	C22-C23-C15	-2.23	117.02	120.70
2	B	800	XWJ	C32-N19-C18	-2.22	125.62	128.36
2	C	800	XWJ	C07-N12-C13	-2.20	120.83	126.61
2	D	402	XWJ	O03-C02-N04	-2.19	120.06	123.06
2	D	401	XWJ	C07-N12-C13	-2.18	120.87	126.61
2	C	800	XWJ	O03-C02-N04	-2.18	120.08	123.06
2	D	402	XWJ	C16-C15-C23	2.16	121.75	119.25
2	B	800	XWJ	O03-C02-N04	-2.13	120.14	123.06
2	C	801	XWJ	O03-C02-N04	-2.13	120.14	123.06
2	C	800	XWJ	C28-C29-C24	2.13	119.60	117.97
2	C	801	XWJ	C11-C10-C05	-2.11	118.84	121.23
3	D	403	JEF	O4-C8-C7	-2.11	105.70	110.82
2	B	800	XWJ	C28-C29-C24	2.10	119.58	117.97
2	C	800	XWJ	C17-C16-C15	-2.07	118.59	120.80
2	D	402	XWJ	C28-C29-C24	2.05	119.55	117.97
3	D	403	JEF	C18-C-C17	-2.05	106.93	112.69
2	B	800	XWJ	C09-C08-C07	-2.04	117.96	120.30
2	D	402	XWJ	C26-C27-C28	2.03	121.23	118.62
2	B	800	XWJ	C08-C07-C06	2.02	122.10	119.66
3	D	403	JEF	O3-C7-C8	2.01	115.37	108.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

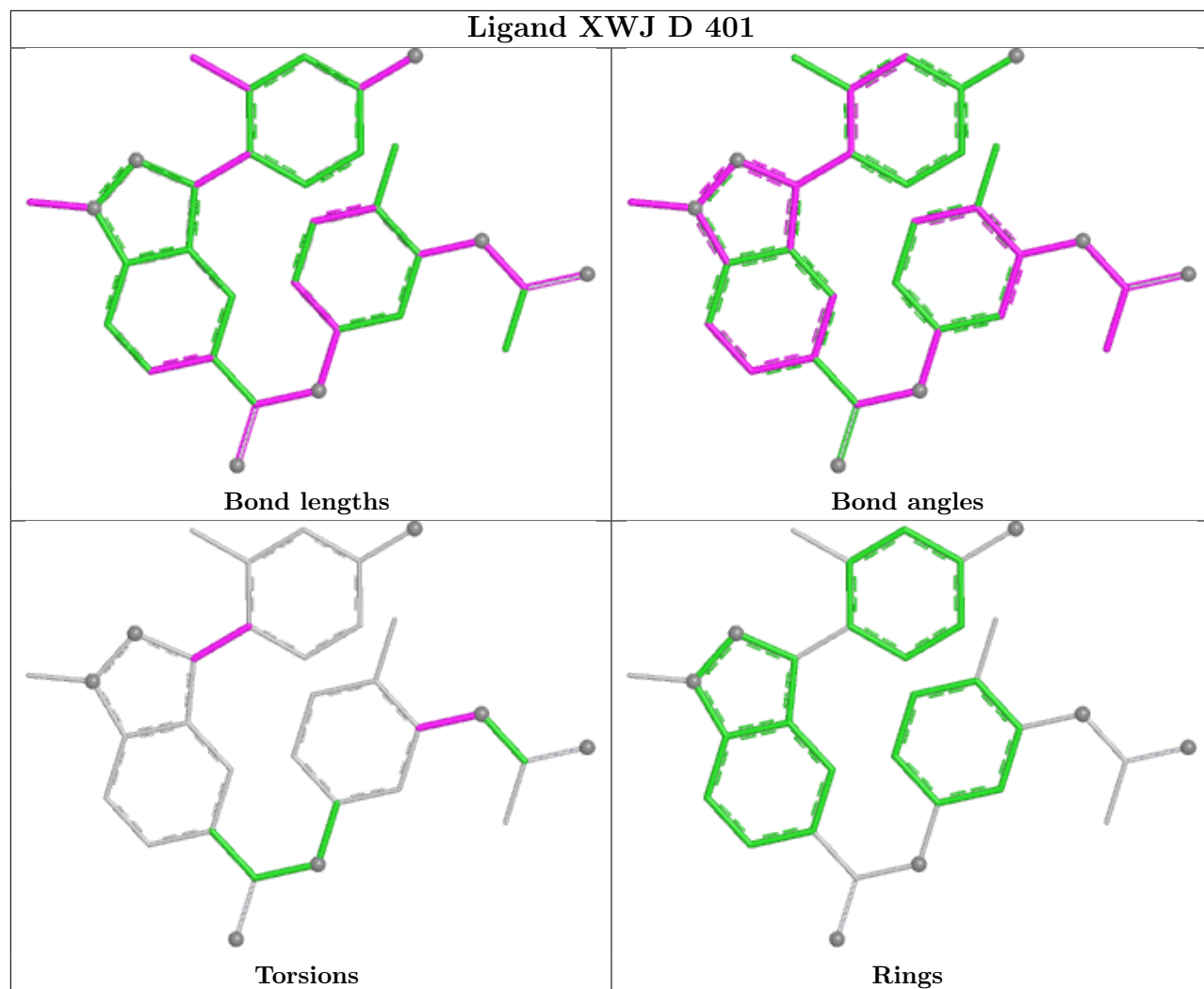
Mol	Chain	Res	Type	Atoms
3	D	403	JEF	C33-C32-O10-C19
3	D	403	JEF	C17-C-O-C20
3	D	403	JEF	OH-C2-C3-O2
3	D	403	JEF	C1-C2-C3-O2
3	D	403	JEF	O3-C4-C5-O2
3	D	403	JEF	O5-C10-C11-C12
3	D	403	JEF	O6-C16-C30-C31
3	D	403	JEF	O11-C36-C37-O12
3	D	403	JEF	C2-C3-O2-C5
3	D	403	JEF	C5-C4-O3-C7
3	D	403	JEF	O10-C32-C33-C34
3	D	403	JEF	C40-C19-C20-O
3	D	403	JEF	O3-C4-C5-C6
3	D	403	JEF	C15-C13-C14-O6
3	D	403	JEF	O10-C32-C33-O11
3	D	403	JEF	O10-C19-C20-O
3	D	403	JEF	O5-C10-C11-O4
3	D	403	JEF	O5-C13-C14-O6
3	D	403	JEF	C36-C37-O12-C38
3	D	403	JEF	C15-C13-O5-C10
2	C	800	XWJ	C22-C21-C24-C29
2	D	401	XWJ	C22-C21-C24-C29
2	A	800	XWJ	N20-C21-C24-C29
2	B	800	XWJ	N20-C21-C24-C29
2	C	800	XWJ	N20-C21-C24-C29
3	D	403	JEF	C19-C20-O-C
3	D	403	JEF	C37-C36-O11-C33
3	D	403	JEF	O-C-C17-OH
3	D	403	JEF	C12-C11-O4-C8
2	A	800	XWJ	C06-C05-N04-C02
2	D	401	XWJ	C06-C05-N04-C02
2	B	800	XWJ	C06-C05-N04-C02
2	C	800	XWJ	C06-C05-N04-C02
3	D	403	JEF	C6-C5-O2-C3
2	A	800	XWJ	C22-C21-C24-C29
2	B	800	XWJ	C22-C21-C24-C29
3	D	403	JEF	C30-C16-O6-C14
2	B	800	XWJ	C10-C05-N04-C02
2	A	800	XWJ	C10-C05-N04-C02
2	D	401	XWJ	C10-C05-N04-C02

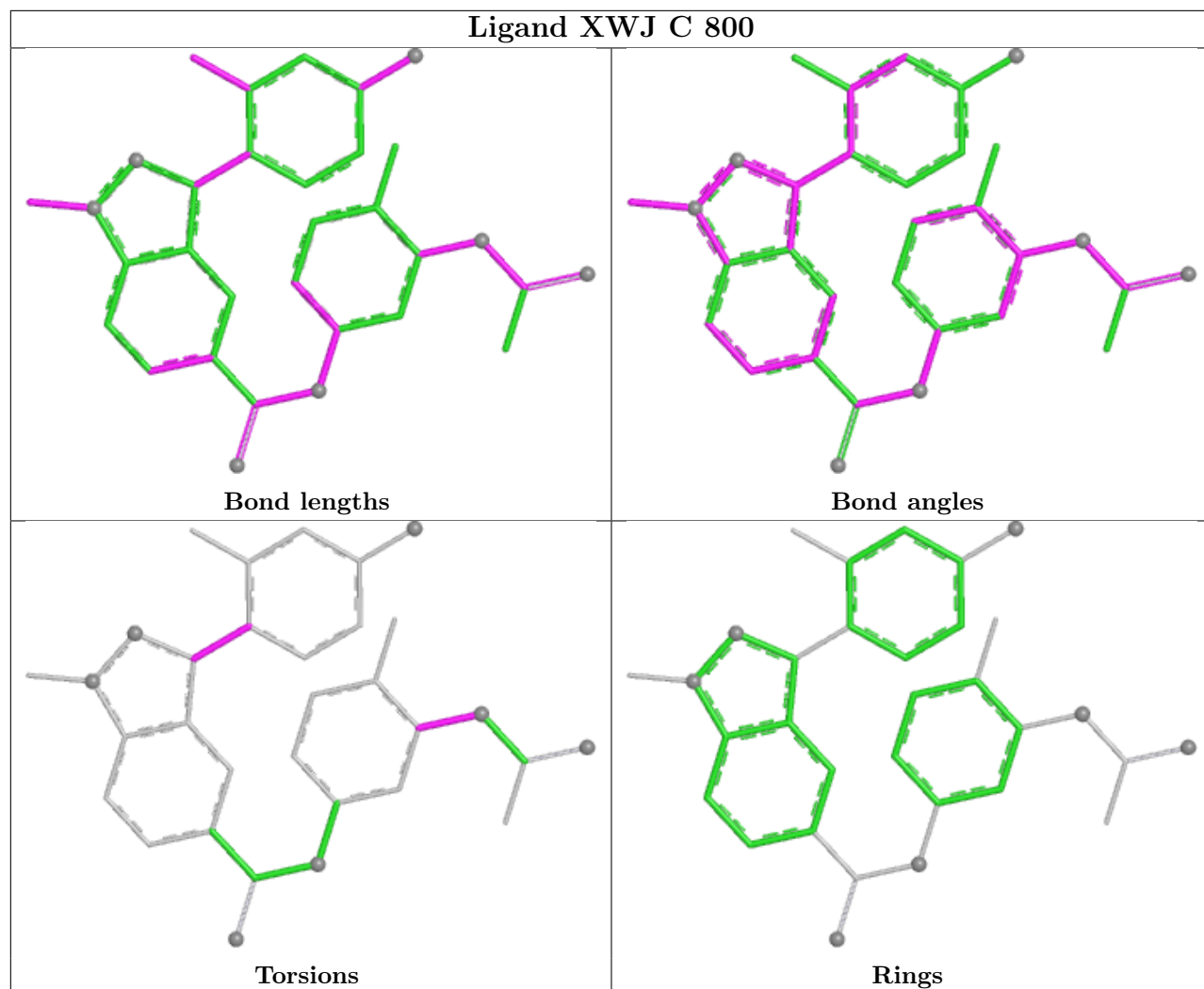
There are no ring outliers.

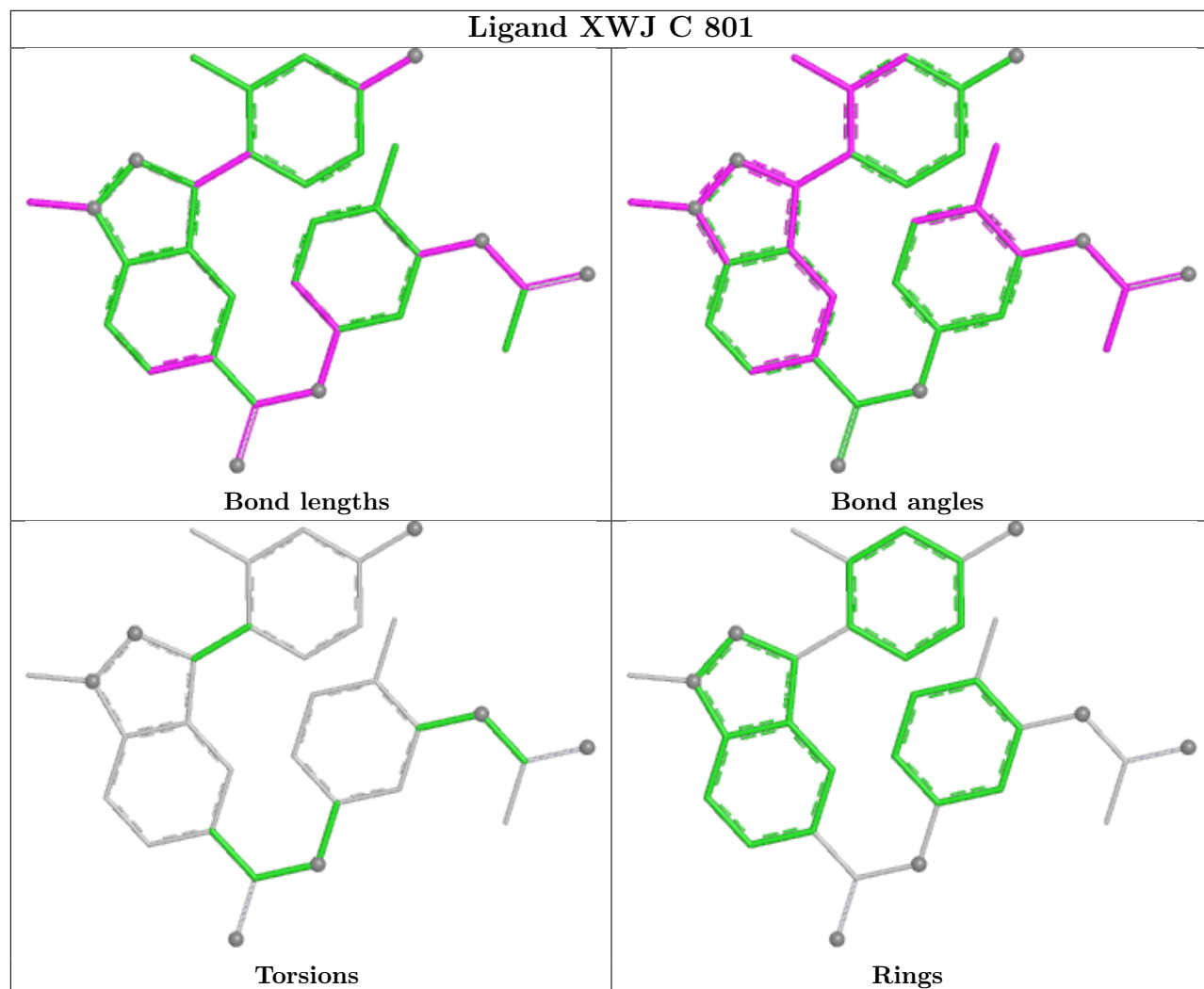
4 monomers are involved in 26 short contacts:

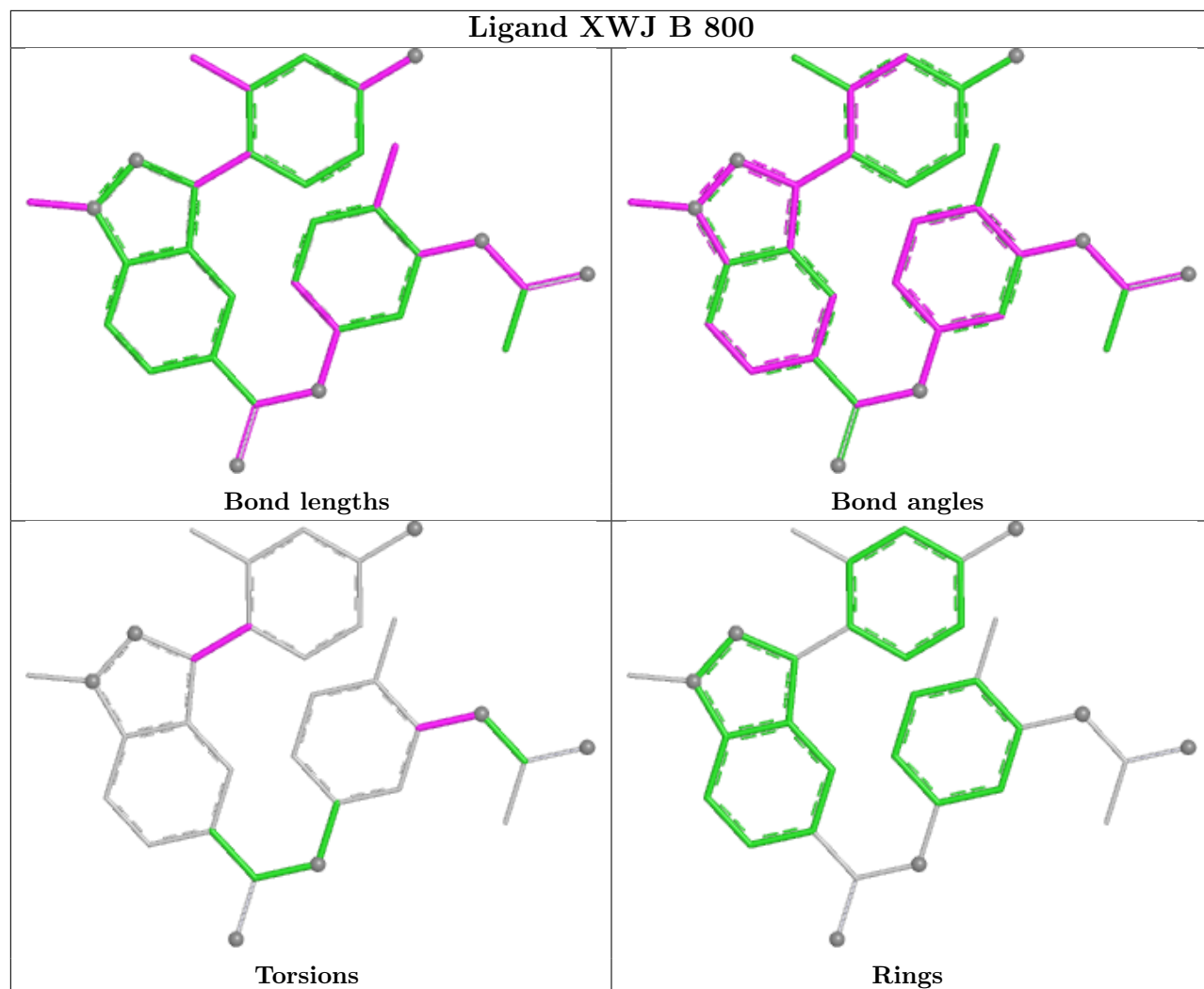
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	XWJ	2	0
2	B	800	XWJ	1	0
2	D	402	XWJ	4	0
3	D	403	JEF	24	0

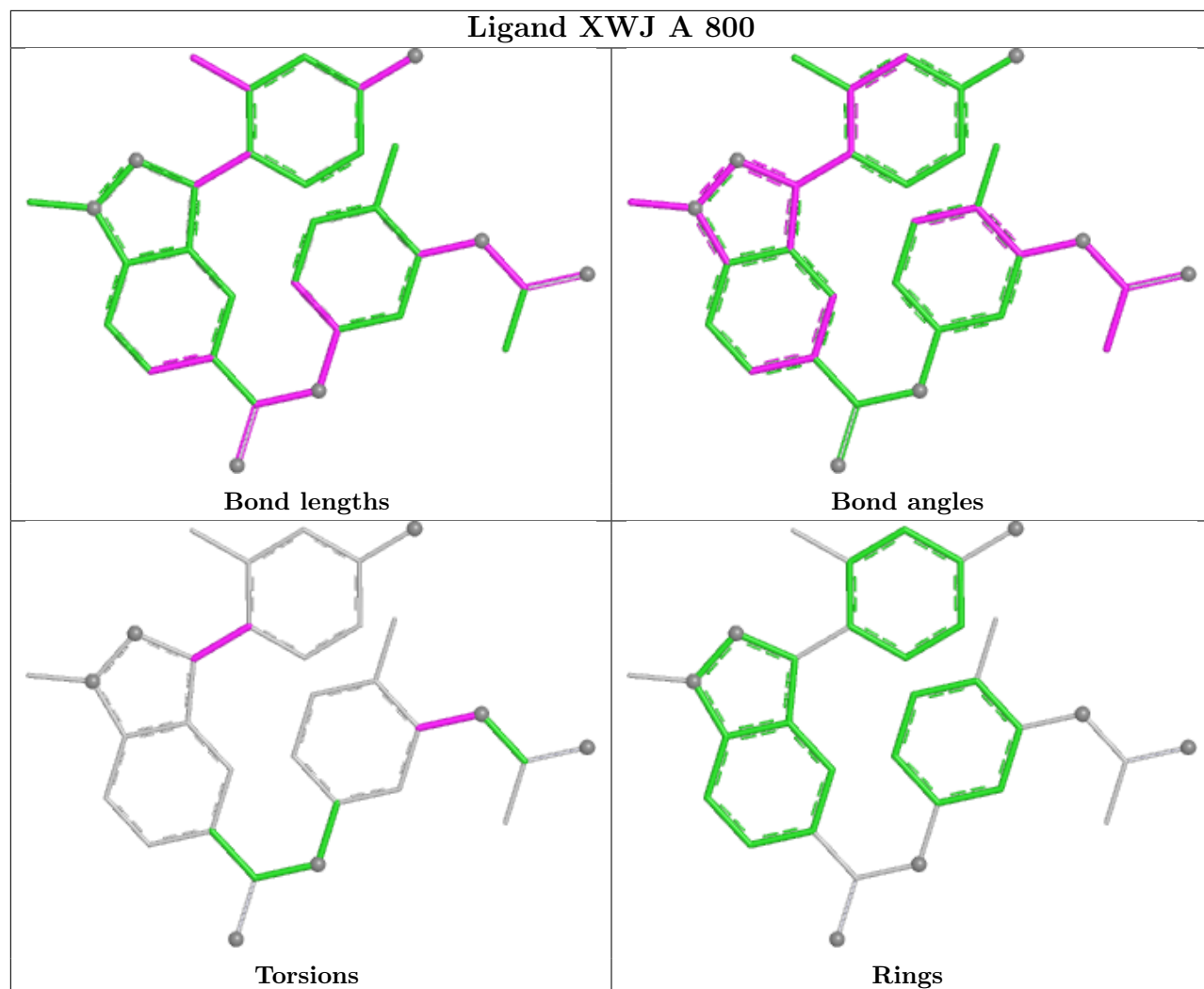
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

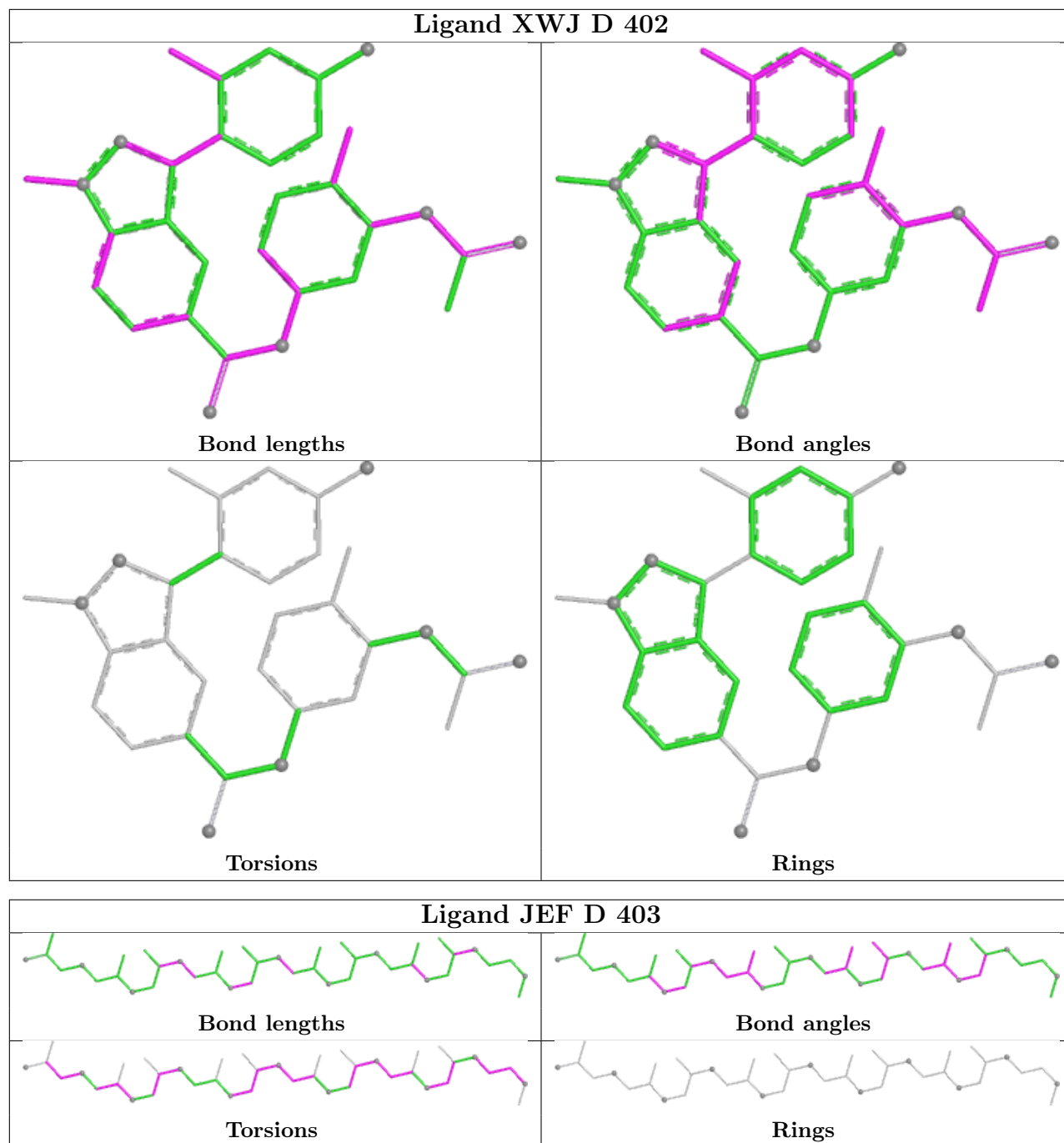












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	113/135 (83%)	0.08	3 (2%) 56 60	13, 31, 51, 68	3 (2%)
1	B	111/135 (82%)	0.11	2 (1%) 67 71	19, 31, 60, 74	3 (2%)
1	C	113/135 (83%)	0.14	4 (3%) 47 50	18, 33, 56, 85	1 (0%)
1	D	113/135 (83%)	0.11	5 (4%) 39 41	12, 33, 55, 68	3 (2%)
All	All	450/540 (83%)	0.11	14 (3%) 51 55	12, 32, 56, 85	10 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	266	ALA	4.1
1	A	266	ALA	3.9
1	C	266	ALA	3.8
1	C	377	ILE	3.7
1	C	378	GLU	3.6
1	C	376	PRO	3.5
1	D	377	ILE	3.5
1	B	377	ILE	2.9
1	D	376	PRO	2.6
1	B	376	PRO	2.5
1	A	378	GLU	2.3
1	D	326	ASP	2.3
1	D	378	GLU	2.2
1	A	306	HIS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

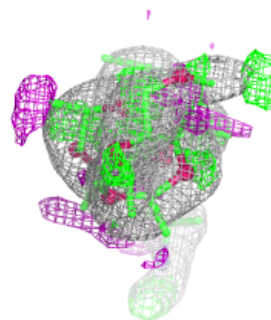
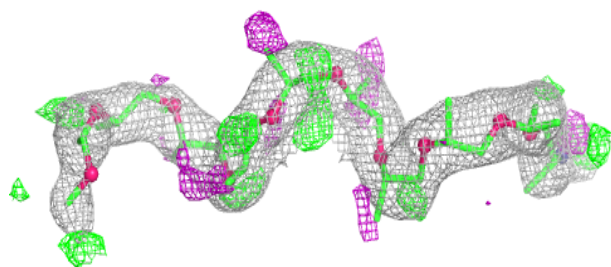
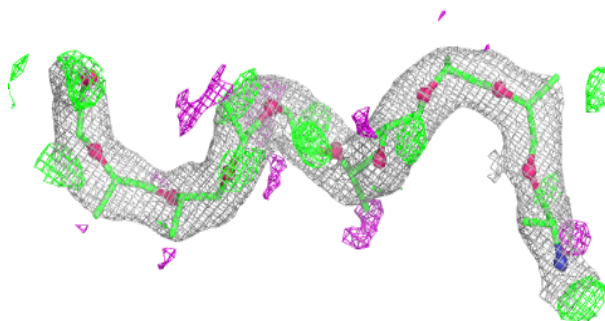
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	JEF	D	403	41/41	0.90	0.17	16,37,54,76	0
2	XWJ	B	800	32/32	0.96	0.06	16,19,22,25	0
2	XWJ	C	800	32/32	0.96	0.06	16,24,30,34	0
2	XWJ	D	402	32/32	0.96	0.06	13,18,27,32	0
2	XWJ	A	800	32/32	0.96	0.05	14,18,25,26	0
2	XWJ	C	801	32/32	0.97	0.07	13,18,36,43	0
2	XWJ	D	401	32/32	0.97	0.06	16,23,28,29	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.

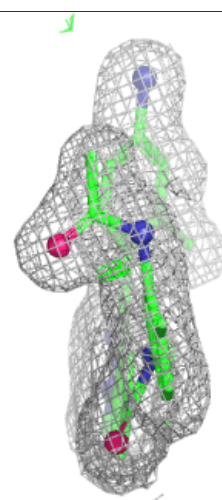
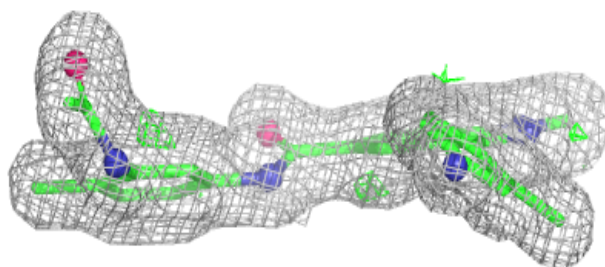
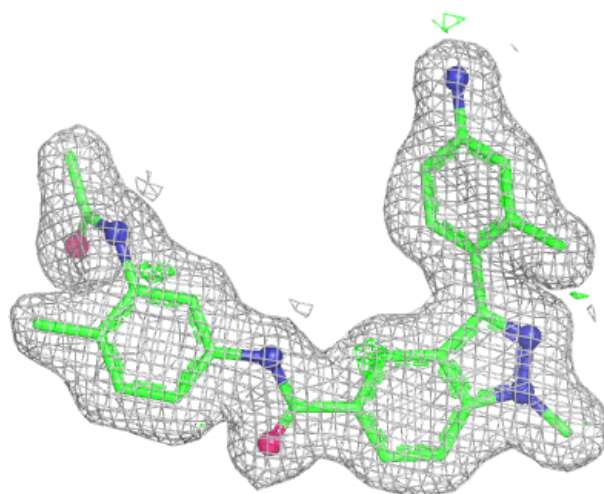
Electron density around JEF D 403:

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



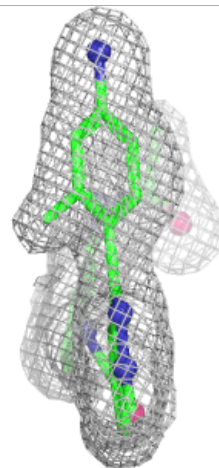
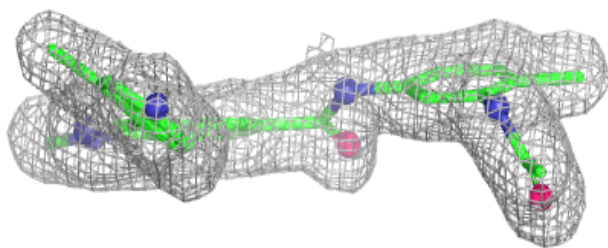
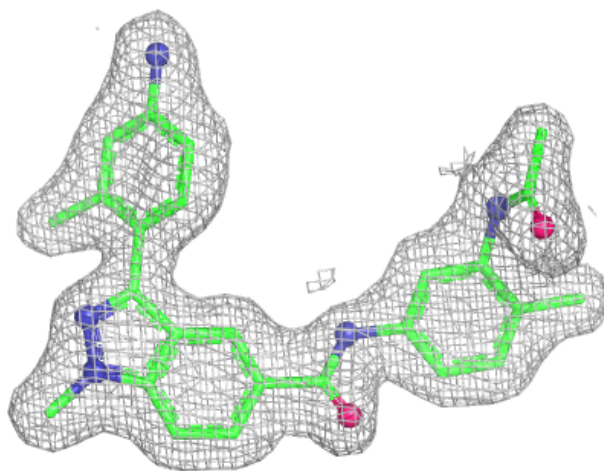
Electron density around XWJ B 800:

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



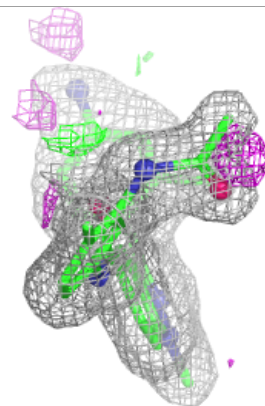
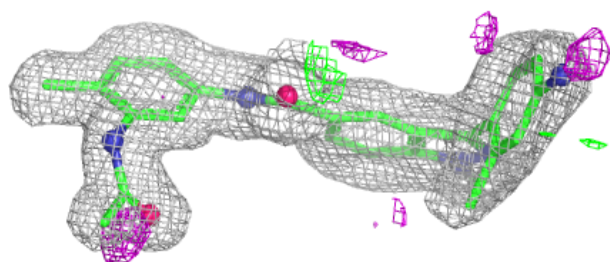
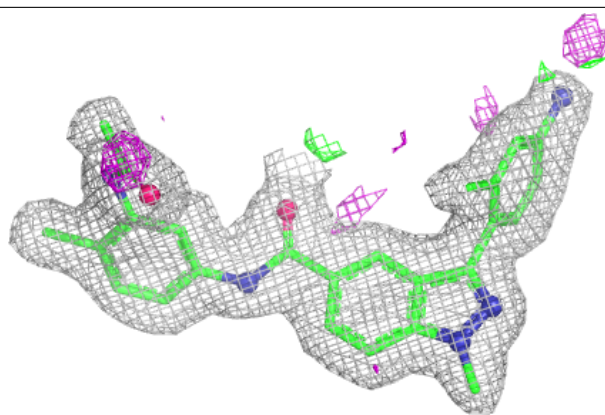
Electron density around XWJ C 800:

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



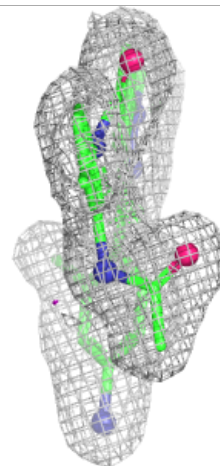
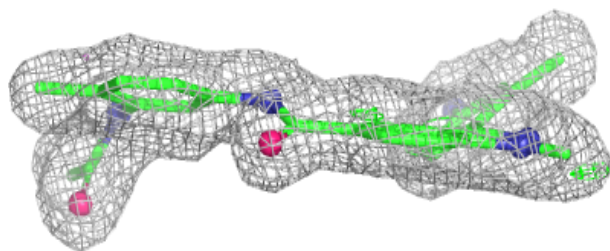
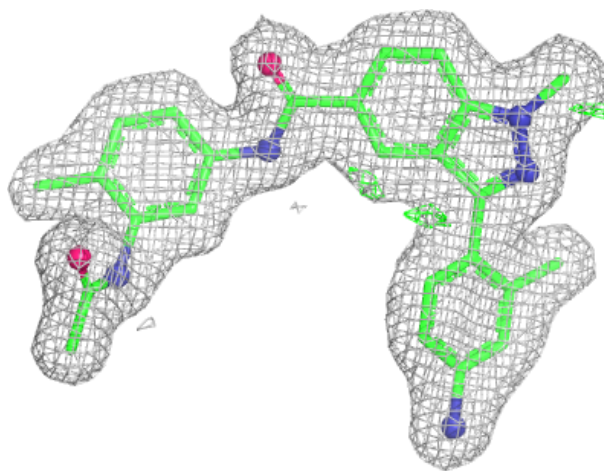
Electron density around XWJ D 402:

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



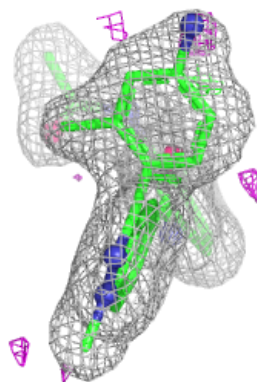
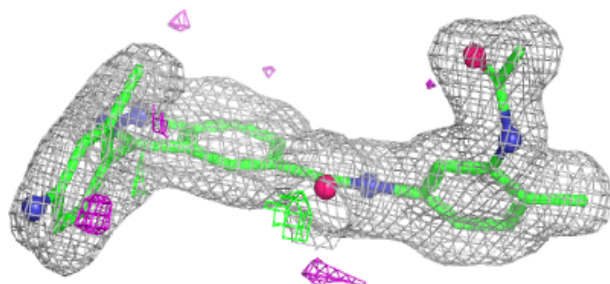
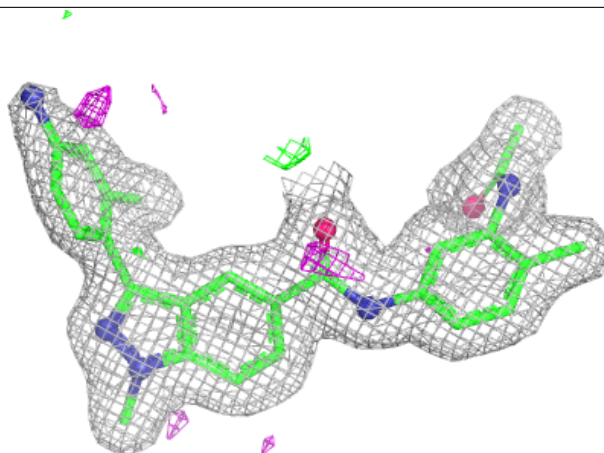
Electron density around XWJ A 800:

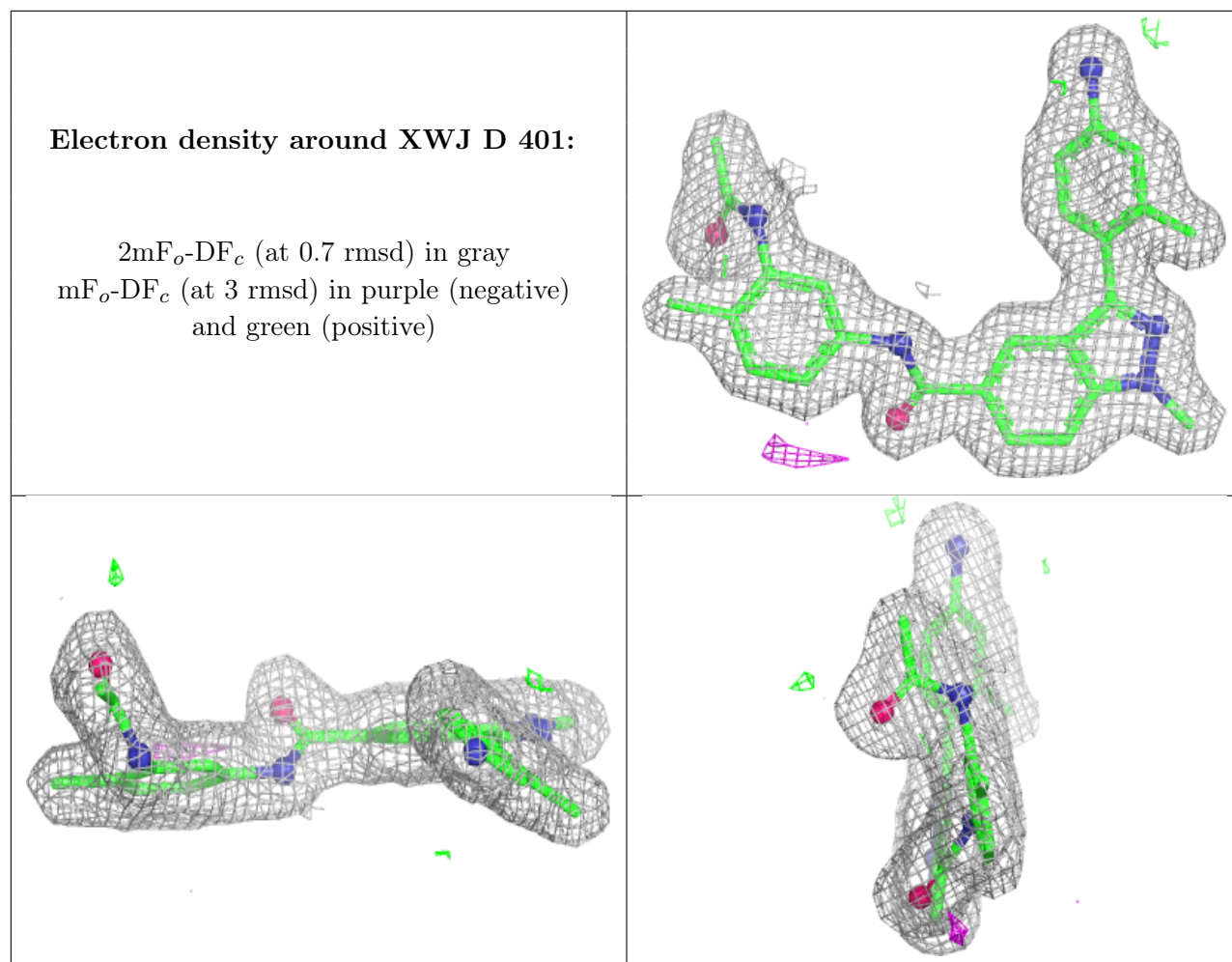
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XWJ C 801:

$2mF_o-DF_c$ (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.