wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 02:00 PM EDT

PDB ID	:	6MCK
Title	:	p97 D1D2 with CB5083 bound
Authors	:	Xia, D.; Tang, W.K.
Deposited on	:	2018-08-31
Resolution	:	3.77 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

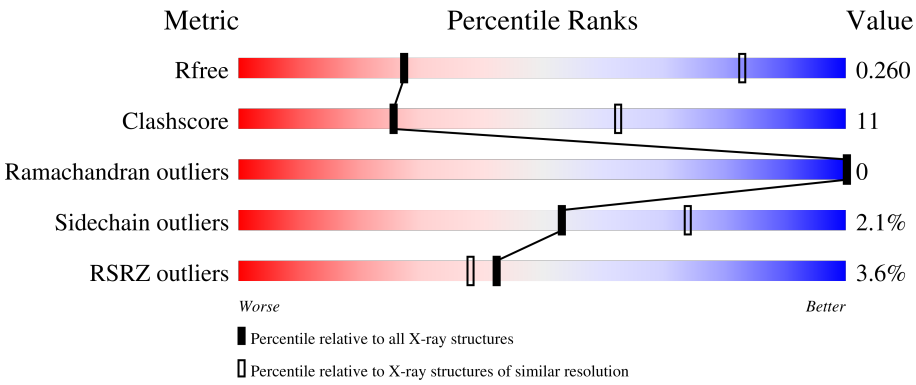
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.77 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	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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

Mol	Chain	Length	Quality of chain
1	A	606	66% 18% • 16%
1	B	606	3% 66% 17% • 16%
1	C	606	4% 66% 17% • 16%
1	D	606	2% 66% 17% • 16%
1	E	606	3% 66% 17% • 16%

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Mol	Chain	Length	Quality of chain
1	F	606	4% 66% 18% • 16%
1	G	606	2% 66% 17% • 16%
1	H	606	3% 66% 17% 16%
1	I	606	4% 66% 17% • 16%
1	J	606	2% 66% 17% • 16%
1	K	606	3% 67% 17% • 16%
1	L	606	4% 67% 16% • 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 48440 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	4003	2524	716	744	19	0	0	0
1	B	509	4003	2524	716	744	19	0	0	0
1	C	509	4003	2524	716	744	19	0	0	0
1	D	509	4003	2524	716	744	19	0	0	0
1	E	509	4003	2524	716	744	19	0	0	0
1	F	509	4003	2524	716	744	19	0	0	0
1	G	509	4003	2524	716	744	19	0	0	0
1	H	509	4003	2524	716	744	19	0	0	0
1	I	509	4003	2524	716	744	19	0	0	0
1	J	509	4003	2524	716	744	19	0	0	0
1	K	509	4003	2524	716	744	19	0	0	0
1	L	509	4003	2524	716	744	19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	MET	-	expression tag	UNP P55072
A	807	ARG	-	expression tag	UNP P55072
A	808	SER	-	expression tag	UNP P55072
A	809	HIS	-	expression tag	UNP P55072
A	810	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	811	HIS	-	expression tag	UNP P55072
A	812	HIS	-	expression tag	UNP P55072
A	813	HIS	-	expression tag	UNP P55072
A	814	HIS	-	expression tag	UNP P55072
B	209	MET	-	expression tag	UNP P55072
B	807	ARG	-	expression tag	UNP P55072
B	808	SER	-	expression tag	UNP P55072
B	809	HIS	-	expression tag	UNP P55072
B	810	HIS	-	expression tag	UNP P55072
B	811	HIS	-	expression tag	UNP P55072
B	812	HIS	-	expression tag	UNP P55072
B	813	HIS	-	expression tag	UNP P55072
B	814	HIS	-	expression tag	UNP P55072
C	209	MET	-	expression tag	UNP P55072
C	807	ARG	-	expression tag	UNP P55072
C	808	SER	-	expression tag	UNP P55072
C	809	HIS	-	expression tag	UNP P55072
C	810	HIS	-	expression tag	UNP P55072
C	811	HIS	-	expression tag	UNP P55072
C	812	HIS	-	expression tag	UNP P55072
C	813	HIS	-	expression tag	UNP P55072
C	814	HIS	-	expression tag	UNP P55072
D	209	MET	-	expression tag	UNP P55072
D	807	ARG	-	expression tag	UNP P55072
D	808	SER	-	expression tag	UNP P55072
D	809	HIS	-	expression tag	UNP P55072
D	810	HIS	-	expression tag	UNP P55072
D	811	HIS	-	expression tag	UNP P55072
D	812	HIS	-	expression tag	UNP P55072
D	813	HIS	-	expression tag	UNP P55072
D	814	HIS	-	expression tag	UNP P55072
E	209	MET	-	expression tag	UNP P55072
E	807	ARG	-	expression tag	UNP P55072
E	808	SER	-	expression tag	UNP P55072
E	809	HIS	-	expression tag	UNP P55072
E	810	HIS	-	expression tag	UNP P55072
E	811	HIS	-	expression tag	UNP P55072
E	812	HIS	-	expression tag	UNP P55072
E	813	HIS	-	expression tag	UNP P55072
E	814	HIS	-	expression tag	UNP P55072
F	209	MET	-	expression tag	UNP P55072
F	807	ARG	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	808	SER	-	expression tag	UNP P55072
F	809	HIS	-	expression tag	UNP P55072
F	810	HIS	-	expression tag	UNP P55072
F	811	HIS	-	expression tag	UNP P55072
F	812	HIS	-	expression tag	UNP P55072
F	813	HIS	-	expression tag	UNP P55072
F	814	HIS	-	expression tag	UNP P55072
G	209	MET	-	expression tag	UNP P55072
G	807	ARG	-	expression tag	UNP P55072
G	808	SER	-	expression tag	UNP P55072
G	809	HIS	-	expression tag	UNP P55072
G	810	HIS	-	expression tag	UNP P55072
G	811	HIS	-	expression tag	UNP P55072
G	812	HIS	-	expression tag	UNP P55072
G	813	HIS	-	expression tag	UNP P55072
G	814	HIS	-	expression tag	UNP P55072
H	209	MET	-	expression tag	UNP P55072
H	807	ARG	-	expression tag	UNP P55072
H	808	SER	-	expression tag	UNP P55072
H	809	HIS	-	expression tag	UNP P55072
H	810	HIS	-	expression tag	UNP P55072
H	811	HIS	-	expression tag	UNP P55072
H	812	HIS	-	expression tag	UNP P55072
H	813	HIS	-	expression tag	UNP P55072
H	814	HIS	-	expression tag	UNP P55072
I	209	MET	-	expression tag	UNP P55072
I	807	ARG	-	expression tag	UNP P55072
I	808	SER	-	expression tag	UNP P55072
I	809	HIS	-	expression tag	UNP P55072
I	810	HIS	-	expression tag	UNP P55072
I	811	HIS	-	expression tag	UNP P55072
I	812	HIS	-	expression tag	UNP P55072
I	813	HIS	-	expression tag	UNP P55072
I	814	HIS	-	expression tag	UNP P55072
J	209	MET	-	expression tag	UNP P55072
J	807	ARG	-	expression tag	UNP P55072
J	808	SER	-	expression tag	UNP P55072
J	809	HIS	-	expression tag	UNP P55072
J	810	HIS	-	expression tag	UNP P55072
J	811	HIS	-	expression tag	UNP P55072
J	812	HIS	-	expression tag	UNP P55072
J	813	HIS	-	expression tag	UNP P55072

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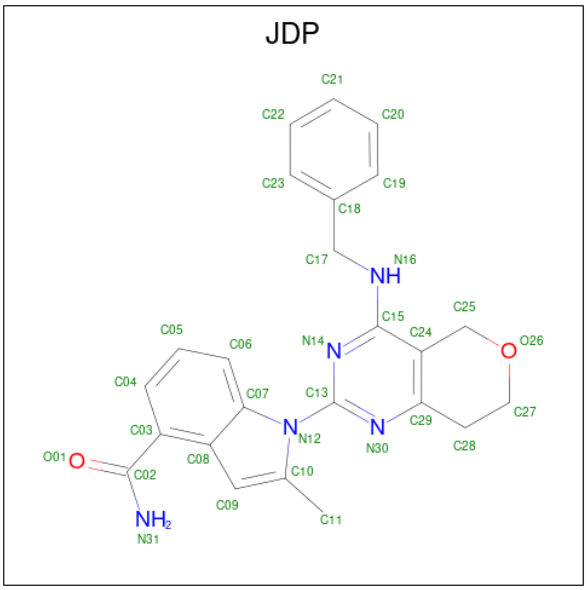
Chain	Residue	Modelled	Actual	Comment	Reference
J	814	HIS	-	expression tag	UNP P55072
K	209	MET	-	expression tag	UNP P55072
K	807	ARG	-	expression tag	UNP P55072
K	808	SER	-	expression tag	UNP P55072
K	809	HIS	-	expression tag	UNP P55072
K	810	HIS	-	expression tag	UNP P55072
K	811	HIS	-	expression tag	UNP P55072
K	812	HIS	-	expression tag	UNP P55072
K	813	HIS	-	expression tag	UNP P55072
K	814	HIS	-	expression tag	UNP P55072
L	209	MET	-	expression tag	UNP P55072
L	807	ARG	-	expression tag	UNP P55072
L	808	SER	-	expression tag	UNP P55072
L	809	HIS	-	expression tag	UNP P55072
L	810	HIS	-	expression tag	UNP P55072
L	811	HIS	-	expression tag	UNP P55072
L	812	HIS	-	expression tag	UNP P55072
L	813	HIS	-	expression tag	UNP P55072
L	814	HIS	-	expression tag	UNP P55072

- Molecule 2 is 1-[4-(benzylamino)-7,8-dihydro-5H-pyrano[4,3-d]pyrimidin-2-yl]-2-methyl-1H-indole-4-carboxamide (three-letter code: JDP) (formula: $C_{24}H_{23}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	24	5	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	31	24	5	2	0	0
2	C	1	31	24	5	2	0	0
2	D	1	31	24	5	2	0	0
2	E	1	31	24	5	2	0	0
2	F	1	31	24	5	2	0	0
2	G	1	31	24	5	2	0	0
2	H	1	31	24	5	2	0	0
2	I	1	31	24	5	2	0	0
2	J	1	31	24	5	2	0	0
2	K	1	31	24	5	2	0	0
2	L	1	31	24	5	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	3	3	3	0	0
3	B	3	3	3	0	0
3	C	3	3	3	0	0
3	D	3	3	3	0	0
3	E	2	2	2	0	0
3	F	3	3	3	0	0
3	G	3	3	3	0	0
3	H	2	2	2	0	0

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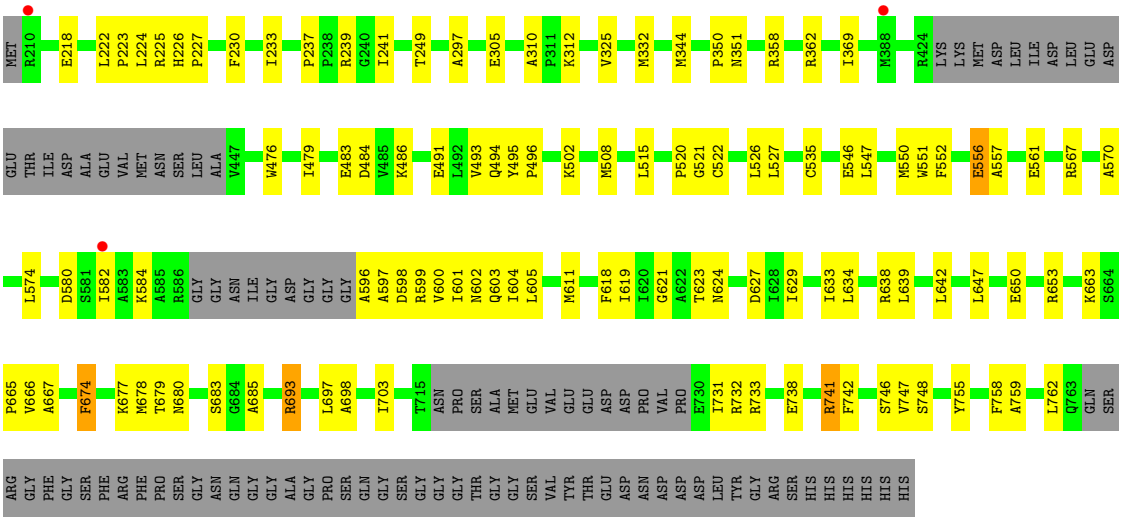
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	I	2	2	2	0	0
			Total	O		
3	J	3	3	3	0	0
			Total	O		
3	K	3	3	3	0	0
			Total	O		
3	L	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

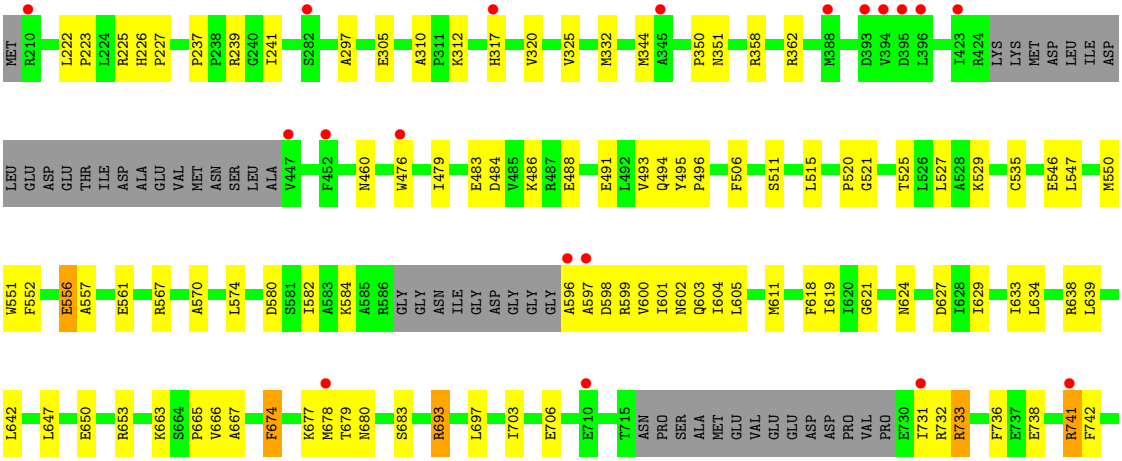
• Molecule 1: Transitional endoplasmic reticulum ATPase

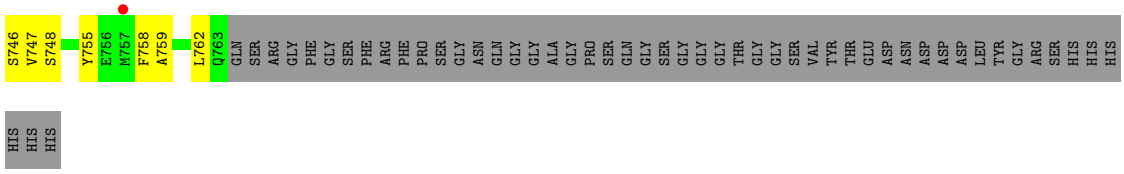
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

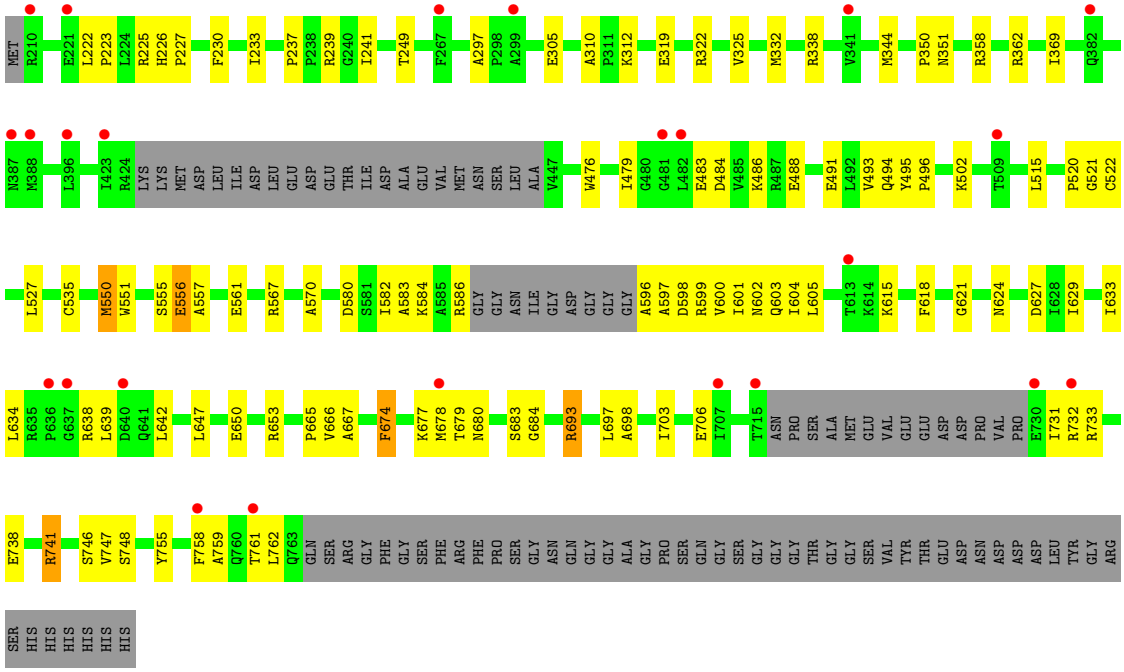
Chain B:





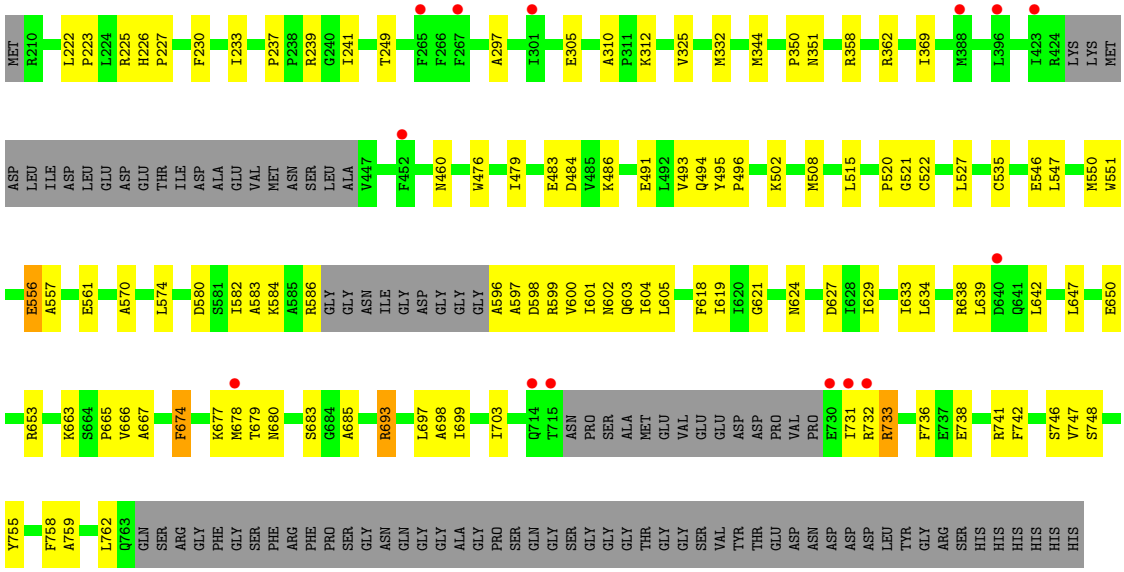
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



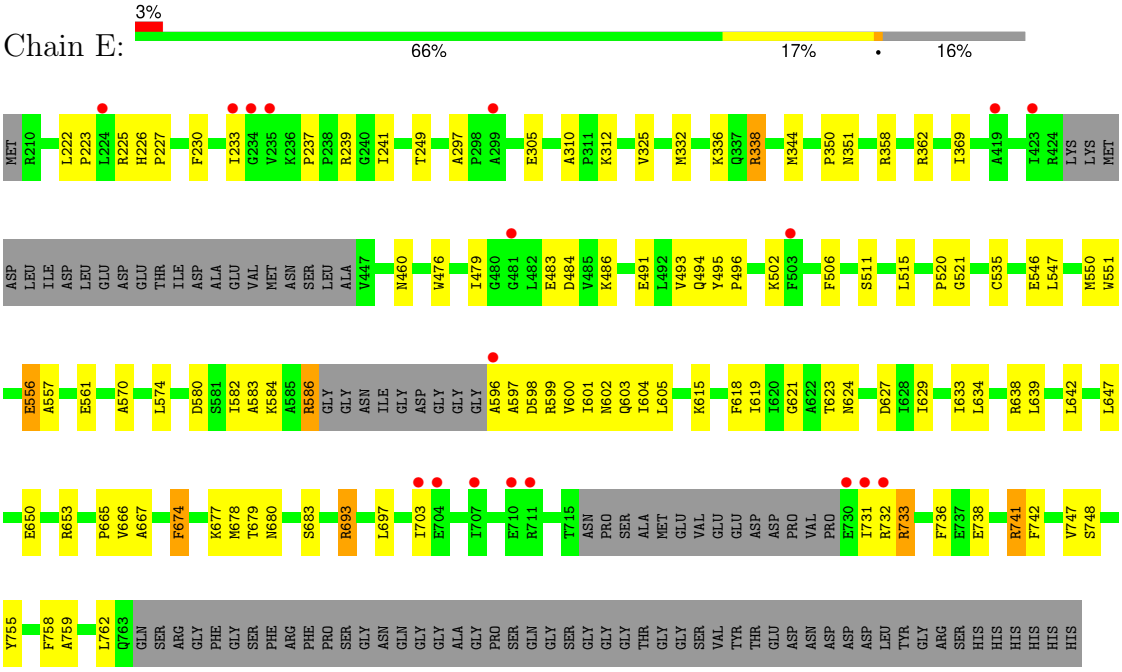
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



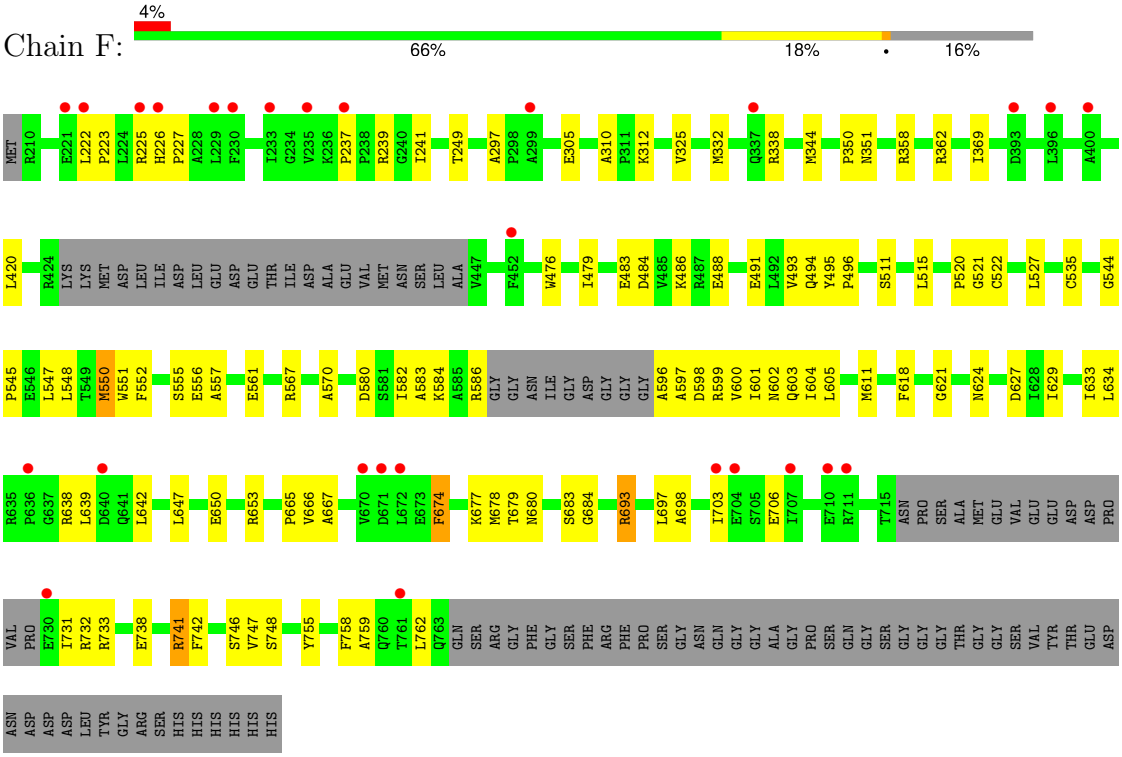
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



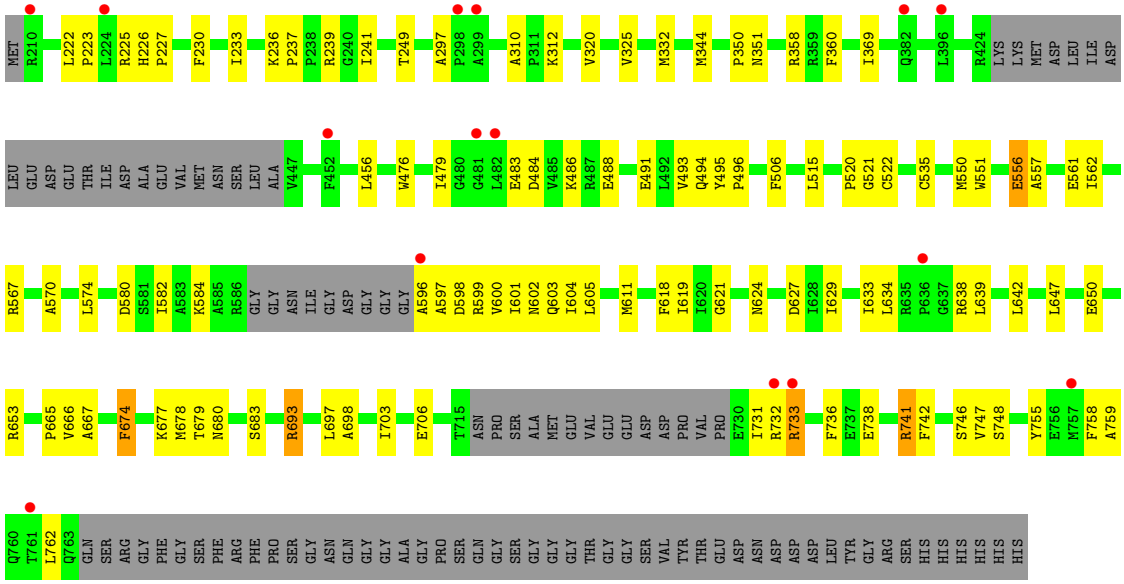
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



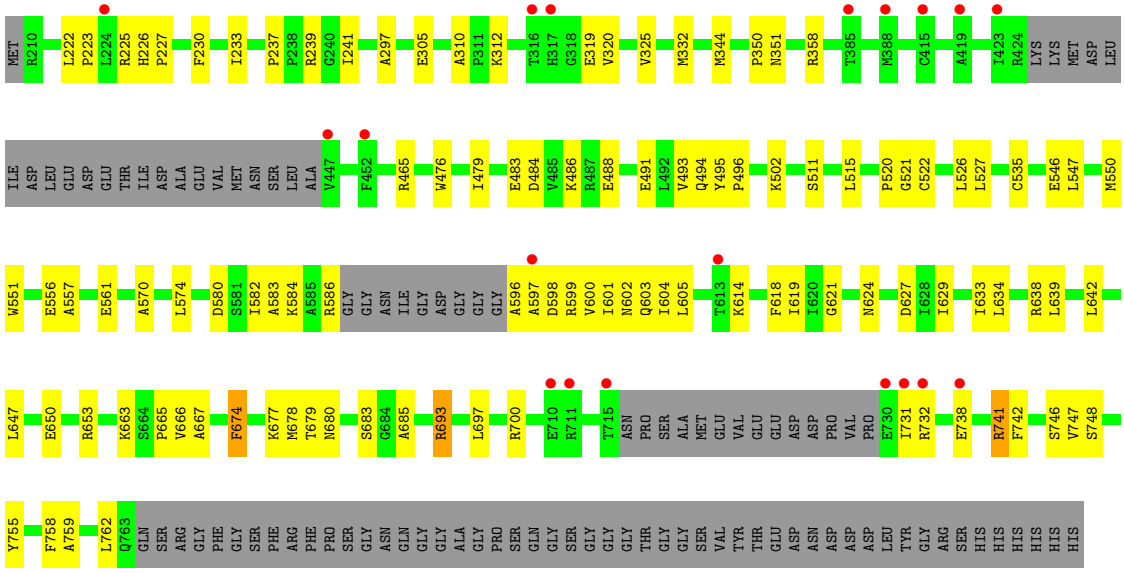
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain G:



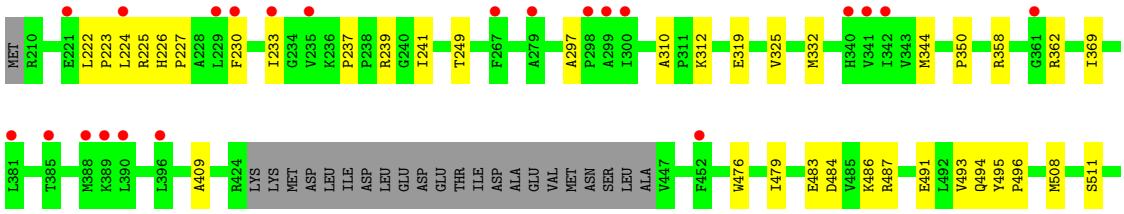
• Molecule 1: Transitional endoplasmic reticulum ATPase

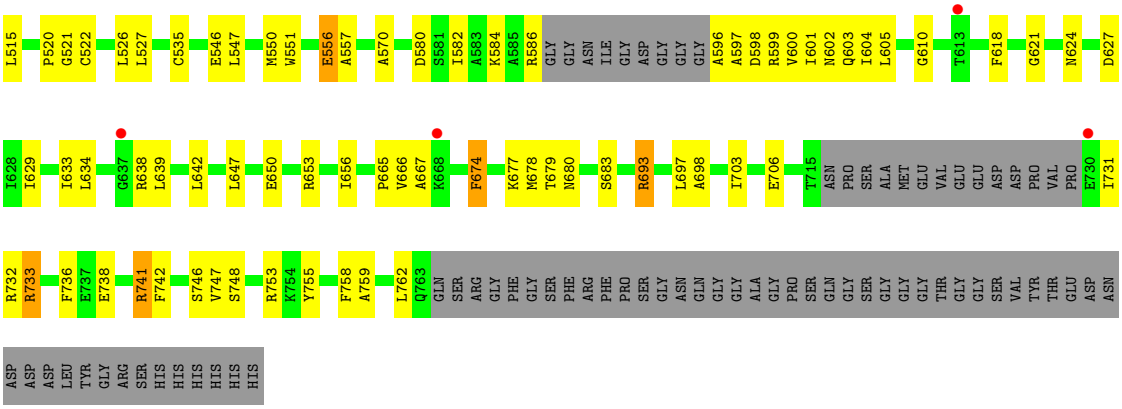
Chain H:



• Molecule 1: Transitional endoplasmic reticulum ATPase

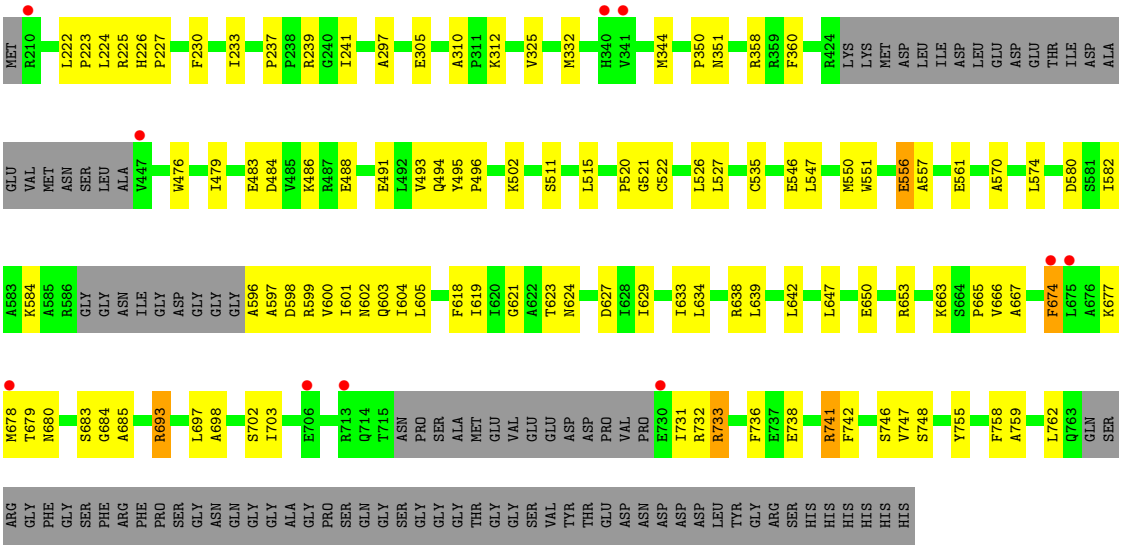
Chain I:





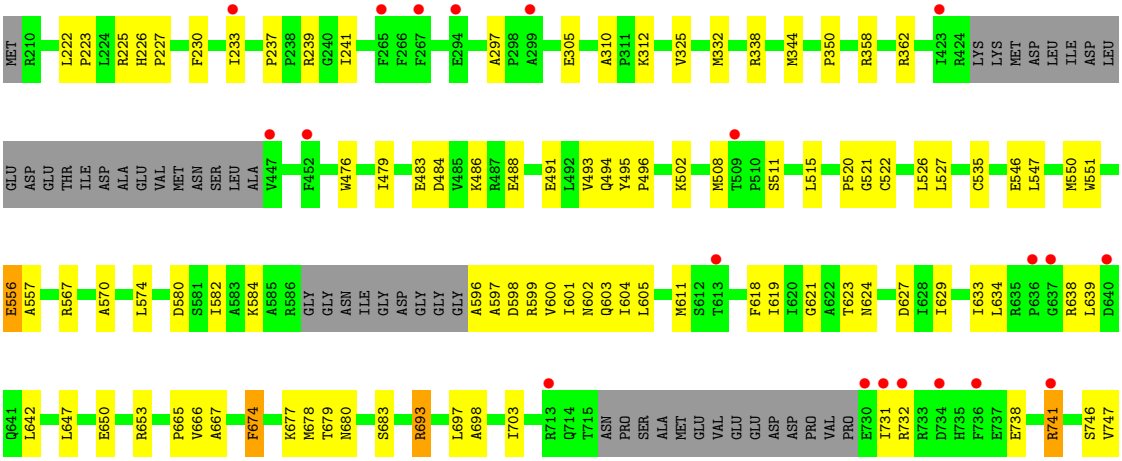
• Molecule 1: Transitional endoplasmic reticulum ATPase

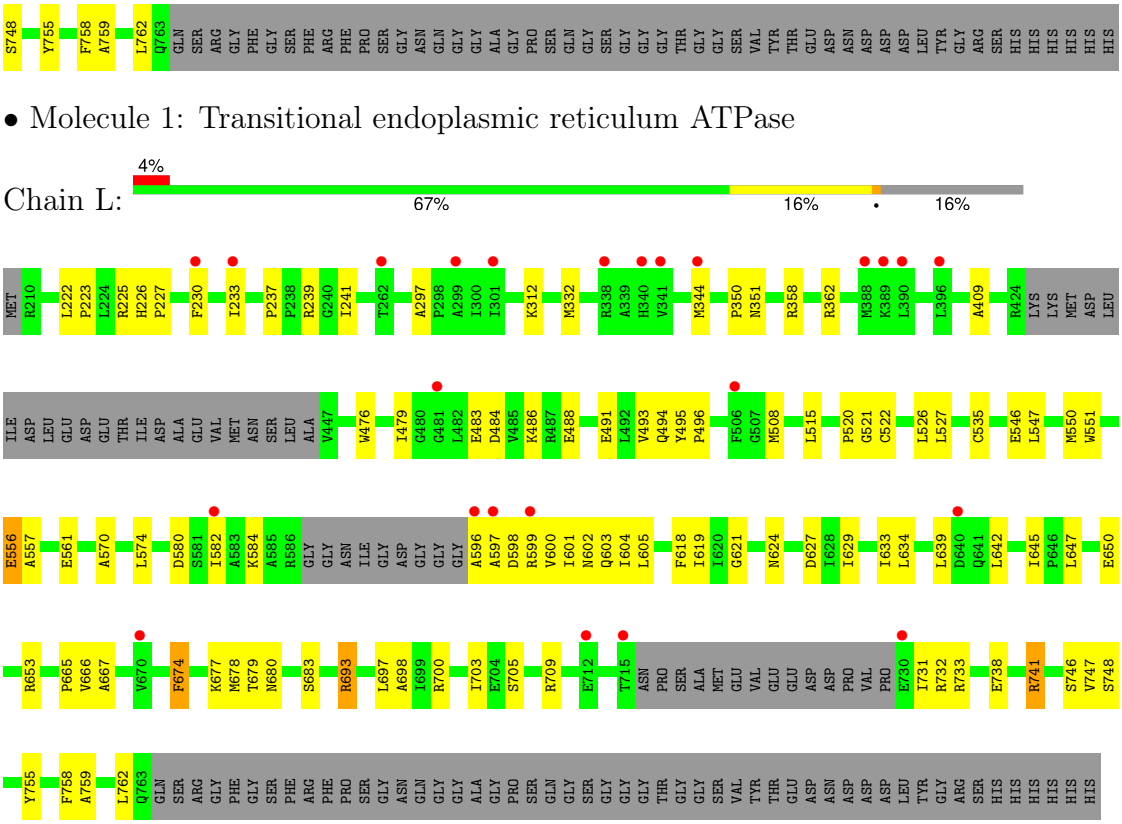
Chain J:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K:




S748 Y755 F758 A759 L762 Q763 GLN SER ARG GLY PHE GLY SER PHE ARG PHE PRO SER GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY ARG SER HIS HIS HIS HIS HIS
• Molecule 1: Transitional endoplasmic reticulum ATPase
Chain L:
4%
67%
16%
16%
MET R210 L222 P223 L224 R225 H226 P227 F230 I233 P237 P238 R239 G240 I241 T262 A297 P298 A299 I300 I301 K312 M332 R338 A339 H340 V341 M344 P350 N351 R358 R362 M388 K389 L390 L396 A409 R424 LYS LYS MET ASP LEU
ILE ASP LEU GLU ASP GLU THR ILE ASP ALA GLU VAL MET ASN SER LEU ALA V447 W476 I479 G480 G481 L482 E483 D484 V485 K486 R487 E488 E491 L492 V493 Q494 Y495 P496 F506 G507 M508 L515 P520 G521 C522 L526 L527 C535 E546 L547 M550 W551
E556 A557 E561 A570 L574 D580 S581 I582 A583 K584 A585 R586 GLY GLY ASN ILE GLY ASP GLY GLY GLY A596 A597 D598 R599 V600 I601 N602 Q603 I604 L605 F618 I619 I620 G621 N624 D627 I628 I629 I633 L634 L639 D640 Q641 L642 I645 P646 L647 E650
R653 P665 V666 A667 V670 F674 K677 M678 T679 N680 S683 R693 L697 A698 I699 R700 I703 E704 S705 R709 E712 T715 ASN PRO SER ALA MET GLU VAL GLU GLU ASP ASP PRO VAL PRO E730 I731 R732 R733 E738 R741 S746 V747 S748
Y755 F758 A759 L762 Q763 GLN SER ARG GLY PHE GLY SER PHE ARG PHE PRO SER GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY ARG SER HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.41Å 263.83Å 164.13Å 90.00° 103.67° 90.00°	Depositor
Resolution (Å)	35.03 – 3.77 35.01 – 3.77	Depositor EDS
% Data completeness (in resolution range)	71.2 (35.03-3.77) 71.3 (35.01-3.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.222 , 0.265 0.227 , 0.260	Depositor DCC
R_{free} test set	3737 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	151.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 146.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	48440	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: JDP

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	0.48	0/4068	0.67	0/5485
1	B	0.48	0/4068	0.67	0/5485
1	C	0.48	0/4068	0.67	0/5485
1	D	0.48	0/4068	0.67	0/5485
1	E	0.47	0/4068	0.67	0/5485
1	F	0.48	0/4068	0.68	0/5485
1	G	0.48	0/4068	0.67	0/5485
1	H	0.49	0/4068	0.67	0/5485
1	I	0.48	0/4068	0.67	0/5485
1	J	0.49	0/4068	0.67	0/5485
1	K	0.48	0/4068	0.67	0/5485
1	L	0.48	0/4068	0.67	0/5485
All	All	0.48	0/48816	0.67	0/65820

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	6
1	B	0	6
1	C	0	6
1	D	0	5
1	E	0	7
1	F	0	6
1	G	0	6
1	H	0	5
1	I	0	7
1	J	0	6
1	K	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	6
All	All	0	71

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	Peptide
1	A	312	LYS	Peptide
1	A	570	ALA	Peptide
1	A	693	ARG	Sidechain
1	A	733	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4003	0	4072	94	0
1	B	4003	0	4072	100	0
1	C	4003	0	4072	94	0
1	D	4003	0	4072	93	0
1	E	4003	0	4072	93	0
1	F	4003	0	4072	92	0
1	G	4003	0	4072	88	0
1	H	4003	0	4072	89	0
1	I	4003	0	4072	96	0
1	J	4003	0	4072	93	0
1	K	4003	0	4072	85	0
1	L	4003	0	4072	87	0
2	A	31	0	0	5	0
2	B	31	0	0	1	0
2	C	31	0	0	3	0
2	D	31	0	0	2	0
2	E	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	31	0	0	3	0
2	G	31	0	0	1	0
2	H	31	0	0	3	0
2	I	31	0	0	3	0
2	J	31	0	0	5	0
2	K	31	0	0	2	0
2	L	31	0	0	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	2	0	0	0	0
All	All	48440	0	48864	1034	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 11.

The worst 5 of 1034 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LYS:HE3	1:I:678:MET:SD	2.09	0.93
1:D:226:HIS:N	1:D:227:PRO:HD3	1.87	0.90
1:A:226:HIS:N	1:A:227:PRO:HD3	1.87	0.89
1:G:226:HIS:N	1:G:227:PRO:HD3	1.87	0.89
1:I:226:HIS:N	1:I:227:PRO:HD3	1.87	0.89

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	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	B	501/606 (83%)	436 (87%)	65 (13%)	0	100	100
1	C	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	D	501/606 (83%)	440 (88%)	61 (12%)	0	100	100
1	E	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	F	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	G	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	H	501/606 (83%)	436 (87%)	65 (13%)	0	100	100
1	I	501/606 (83%)	439 (88%)	62 (12%)	0	100	100
1	J	501/606 (83%)	439 (88%)	62 (12%)	0	100	100
1	K	501/606 (83%)	438 (87%)	63 (13%)	0	100	100
1	L	501/606 (83%)	439 (88%)	62 (12%)	0	100	100
All	All	6012/7272 (83%)	5257 (87%)	755 (13%)	0	100	100

There are no Ramachandran outliers to report.

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	427/501 (85%)	418 (98%)	9 (2%)	53	74
1	B	427/501 (85%)	419 (98%)	8 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	427/501 (85%)	417 (98%)	10 (2%)	50	72
1	D	427/501 (85%)	418 (98%)	9 (2%)	53	74
1	E	427/501 (85%)	420 (98%)	7 (2%)	62	80
1	F	427/501 (85%)	417 (98%)	10 (2%)	50	72
1	G	427/501 (85%)	417 (98%)	10 (2%)	50	72
1	H	427/501 (85%)	419 (98%)	8 (2%)	57	76
1	I	427/501 (85%)	418 (98%)	9 (2%)	53	74
1	J	427/501 (85%)	418 (98%)	9 (2%)	53	74
1	K	427/501 (85%)	417 (98%)	10 (2%)	50	72
1	L	427/501 (85%)	418 (98%)	9 (2%)	53	74
All	All	5124/6012 (85%)	5016 (98%)	108 (2%)	53	74

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	556	GLU
1	I	476	TRP
1	L	476	TRP
1	G	674	PHE
1	H	522	CYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	JDP	I	900	-	33,35,35	1.29	4 (12%)	32,50,50	1.85	10 (31%)
2	JDP	F	900	-	33,35,35	1.27	3 (9%)	32,50,50	2.28	8 (25%)
2	JDP	C	900	-	33,35,35	1.26	4 (12%)	32,50,50	1.72	8 (25%)
2	JDP	B	900	-	33,35,35	1.29	4 (12%)	32,50,50	1.15	4 (12%)
2	JDP	A	900	-	33,35,35	1.42	5 (15%)	32,50,50	2.11	9 (28%)
2	JDP	J	900	-	33,35,35	1.59	6 (18%)	32,50,50	2.23	9 (28%)
2	JDP	K	900	-	33,35,35	1.04	3 (9%)	32,50,50	1.66	7 (21%)
2	JDP	D	900	-	33,35,35	1.02	1 (3%)	32,50,50	1.95	8 (25%)
2	JDP	H	900	-	33,35,35	1.07	3 (9%)	32,50,50	1.10	2 (6%)
2	JDP	L	900	-	33,35,35	1.42	6 (18%)	32,50,50	2.05	7 (21%)
2	JDP	G	900	-	33,35,35	1.36	6 (18%)	32,50,50	1.89	8 (25%)
2	JDP	E	900	-	33,35,35	1.25	3 (9%)	32,50,50	1.27	3 (9%)

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	JDP	I	900	-	-	2/9/20/20	0/5/5/5
2	JDP	F	900	-	-	4/9/20/20	0/5/5/5
2	JDP	C	900	-	-	4/9/20/20	0/5/5/5
2	JDP	B	900	-	-	2/9/20/20	0/5/5/5
2	JDP	A	900	-	-	4/9/20/20	0/5/5/5
2	JDP	J	900	-	-	4/9/20/20	0/5/5/5
2	JDP	K	900	-	-	4/9/20/20	0/5/5/5
2	JDP	D	900	-	-	4/9/20/20	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JDP	H	900	-	-	4/9/20/20	0/5/5/5
2	JDP	L	900	-	-	4/9/20/20	0/5/5/5
2	JDP	G	900	-	-	2/9/20/20	0/5/5/5
2	JDP	E	900	-	-	3/9/20/20	0/5/5/5

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	900	JDP	C10-N12	4.62	1.44	1.36
2	L	900	JDP	C09-C10	-4.60	1.32	1.39
2	J	900	JDP	C09-C10	-4.02	1.32	1.39
2	A	900	JDP	C10-N12	3.90	1.43	1.36
2	F	900	JDP	C09-C10	-3.76	1.33	1.39

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	JDP	C17-N16-C15	6.52	131.51	123.08
2	D	900	JDP	C17-N16-C15	6.33	131.26	123.08
2	K	900	JDP	O01-C02-C03	5.35	126.54	120.23
2	L	900	JDP	O01-C02-C03	5.35	126.54	120.23
2	F	900	JDP	O01-C02-C03	5.34	126.53	120.23

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	JDP	N14-C15-N16-C17
2	A	900	JDP	C24-C15-N16-C17
2	B	900	JDP	N14-C15-N16-C17
2	B	900	JDP	C24-C15-N16-C17
2	C	900	JDP	N14-C15-N16-C17

There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	900	JDP	3	0
2	F	900	JDP	3	0
2	C	900	JDP	3	0

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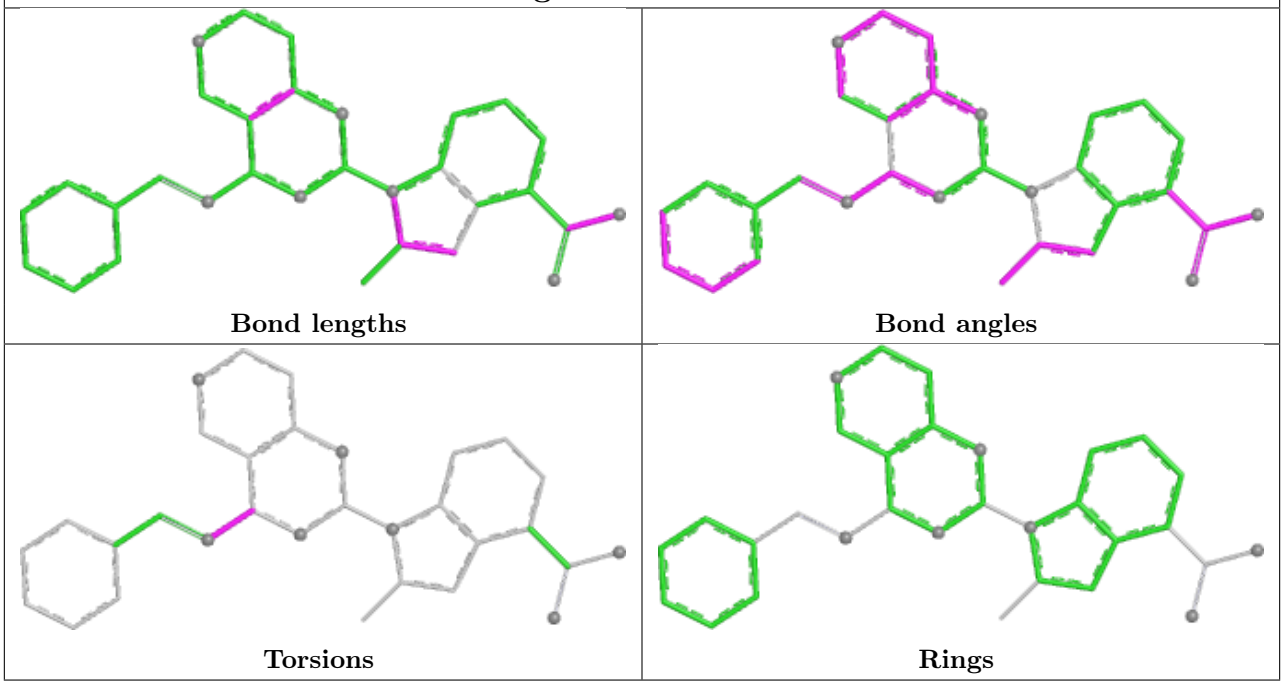
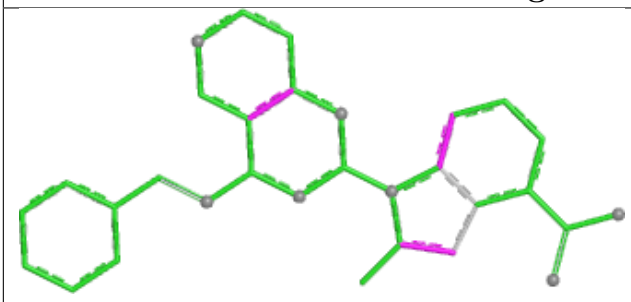
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	JDP	1	0
2	A	900	JDP	5	0
2	J	900	JDP	5	0
2	K	900	JDP	2	0
2	D	900	JDP	2	0
2	H	900	JDP	3	0
2	L	900	JDP	3	0
2	G	900	JDP	1	0
2	E	900	JDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

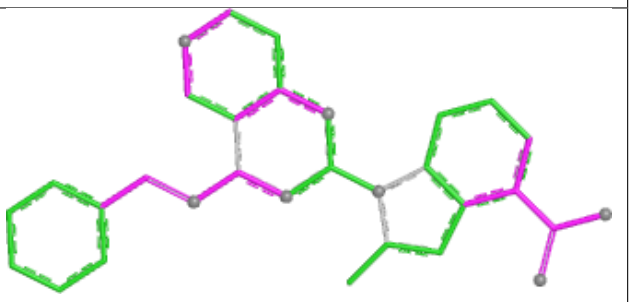
Ligand JDP I 900



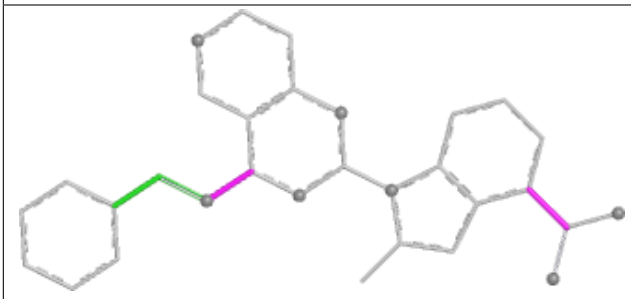
Ligand JDP F 900



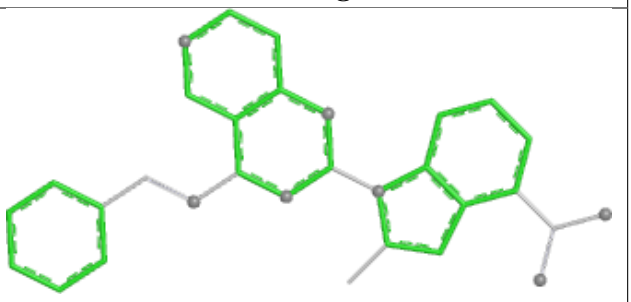
Bond lengths



Bond angles

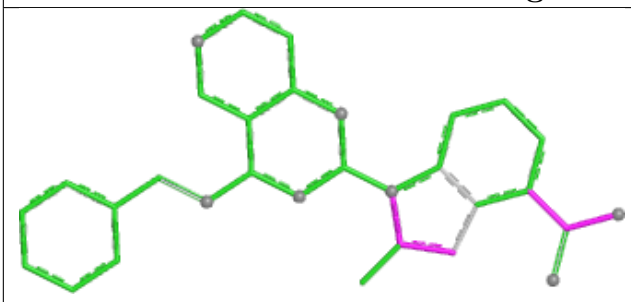


Torsions



Rings

Ligand JDP C 900



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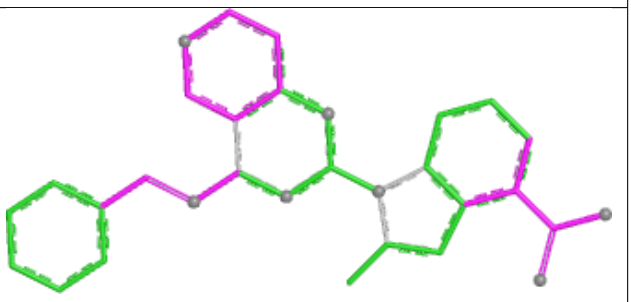
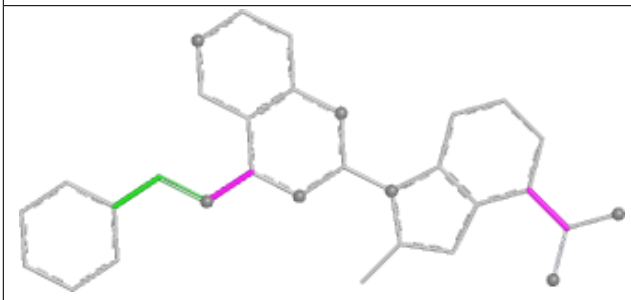
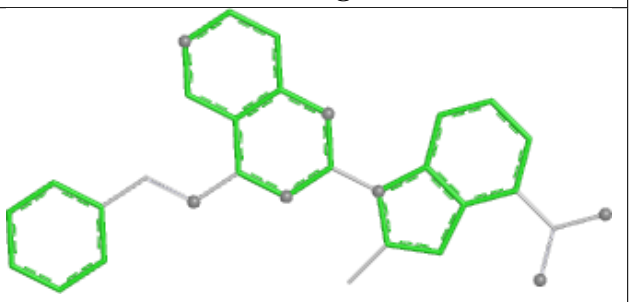


Bond angles

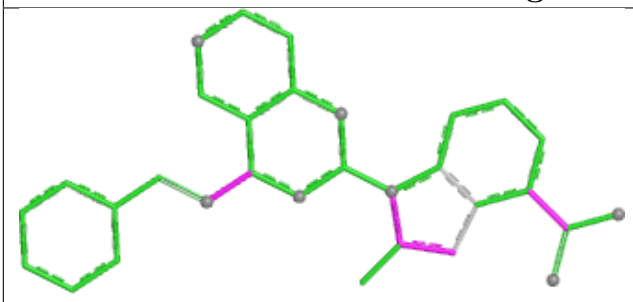


Torsions

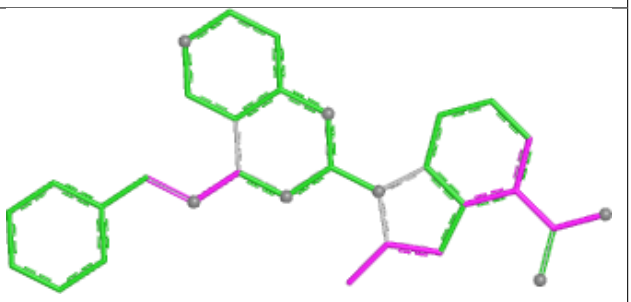


Rings

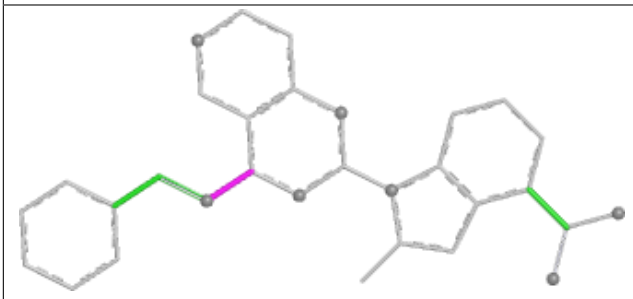
Ligand JDP B 900



Bond lengths



Bond angles



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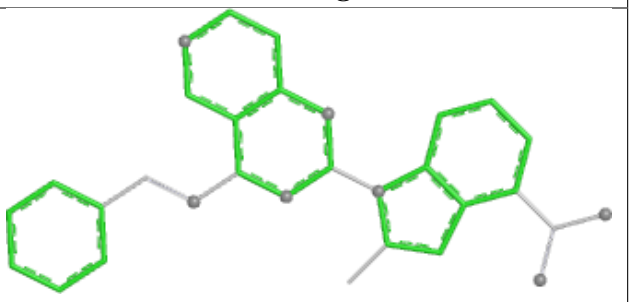
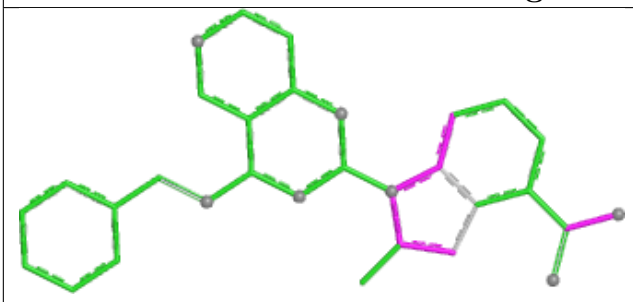
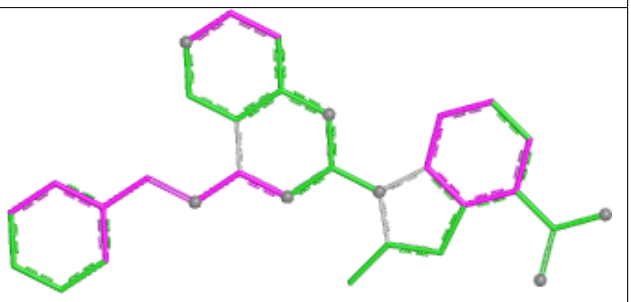


Rings

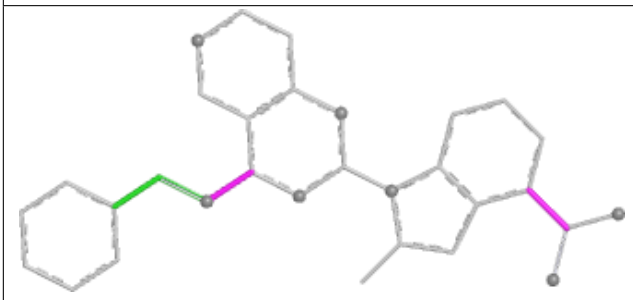
Ligand JDP A 900



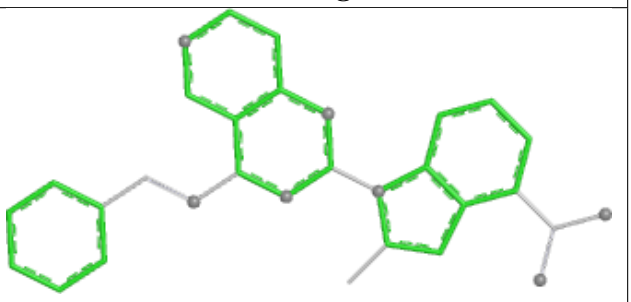
Bond lengths



Bond angles

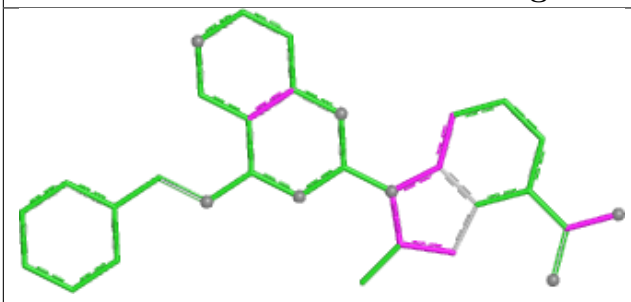


Torsions

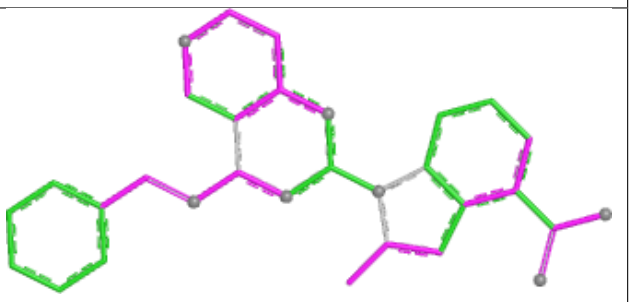


Rings

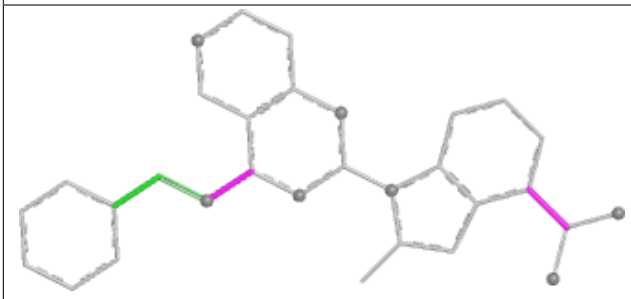
Ligand JDP J 900



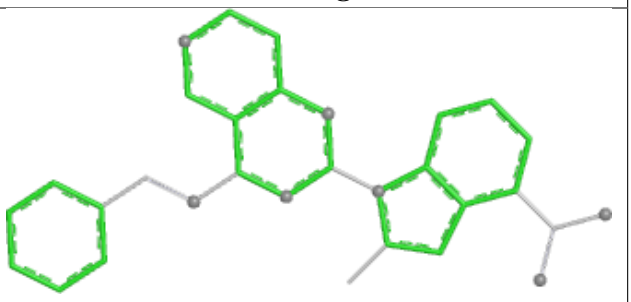
Bond lengths



Bond angles

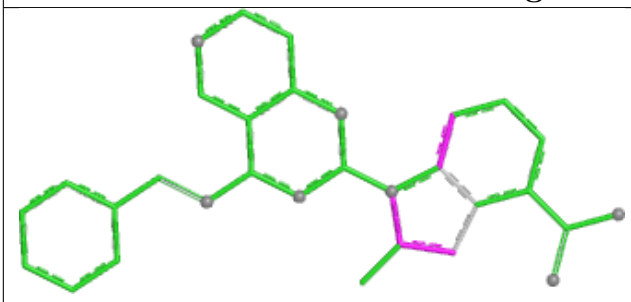


Torsions

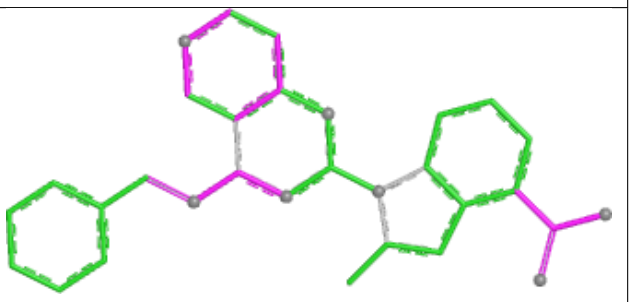


Rings

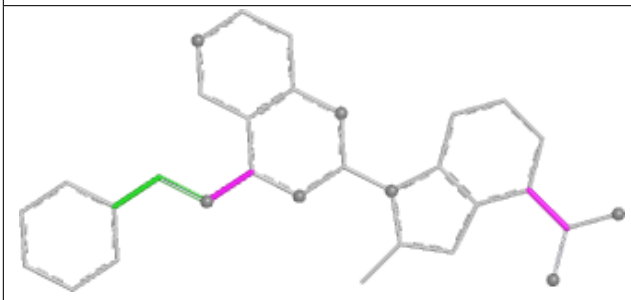
Ligand JDP K 900



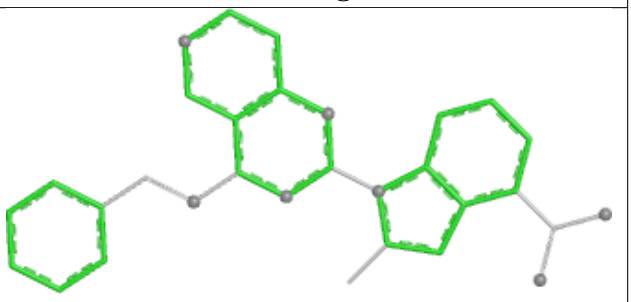
Bond lengths



Bond angles

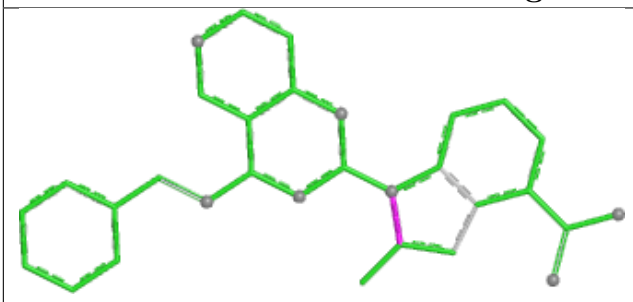


Torsions

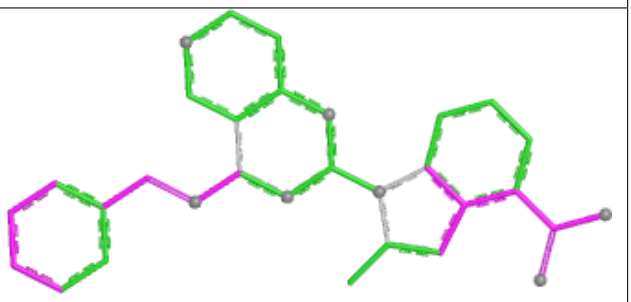


Rings

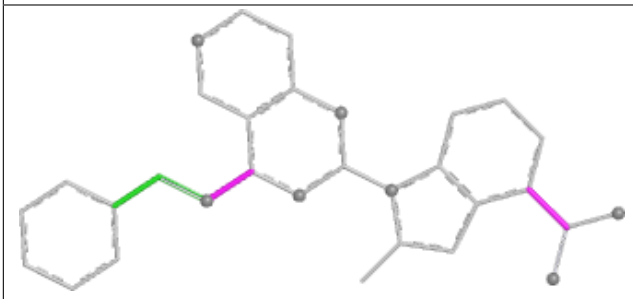
Ligand JDP D 900



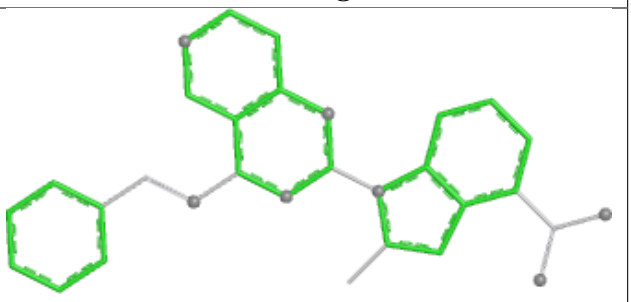
Bond lengths



Bond angles

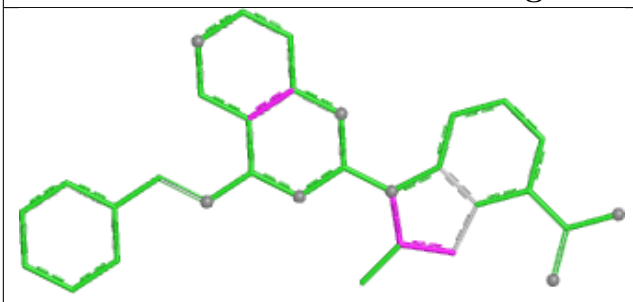


Torsions

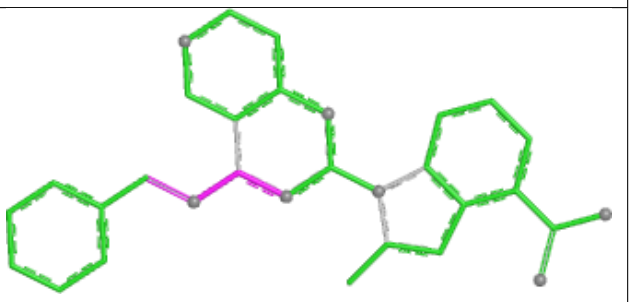


Rings

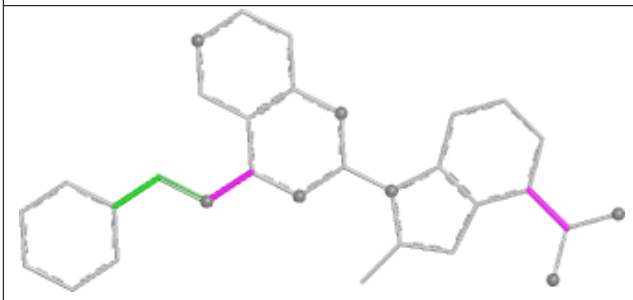
Ligand JDP H 900



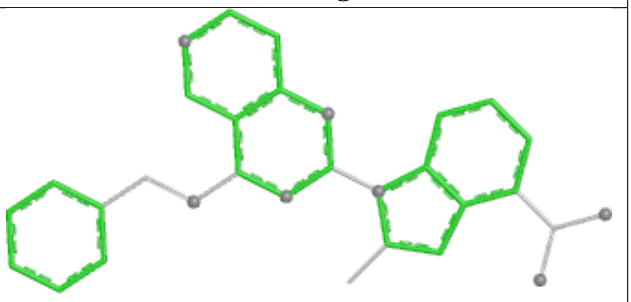
Bond lengths



Bond angles

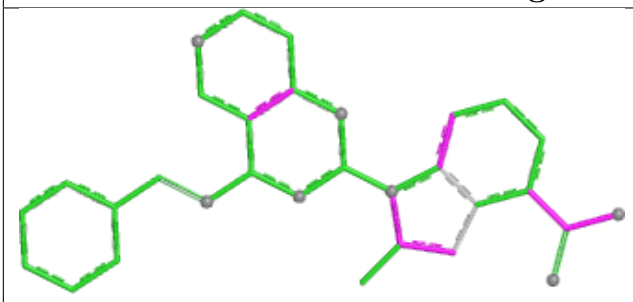


Torsions

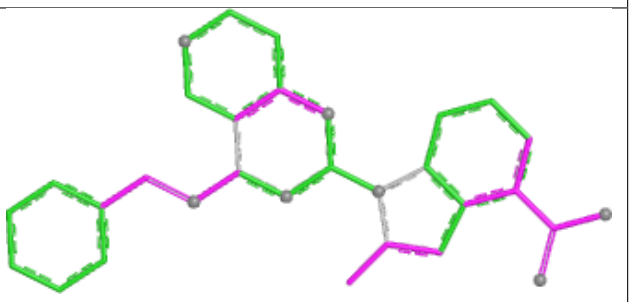


Rings

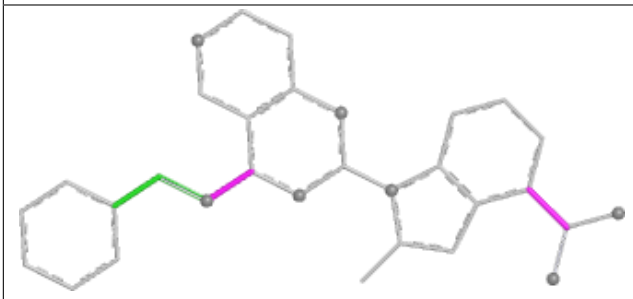
Ligand JDP L 900



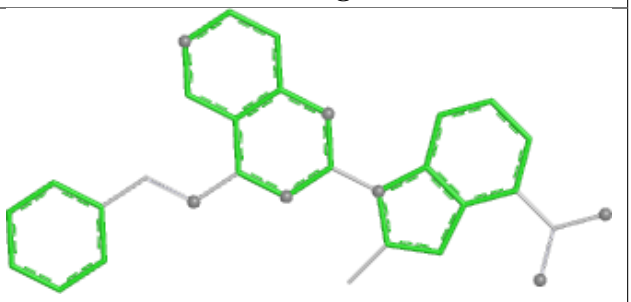
Bond lengths



Bond angles

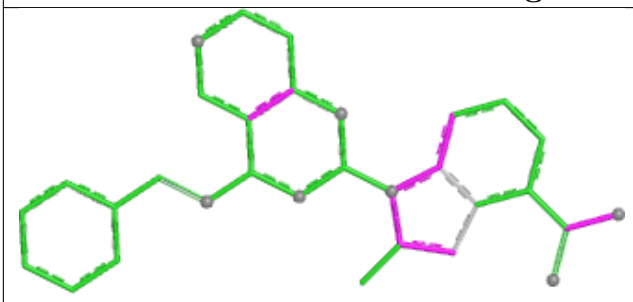


Torsions

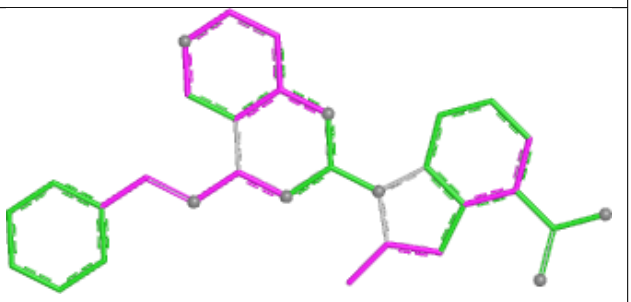


Rings

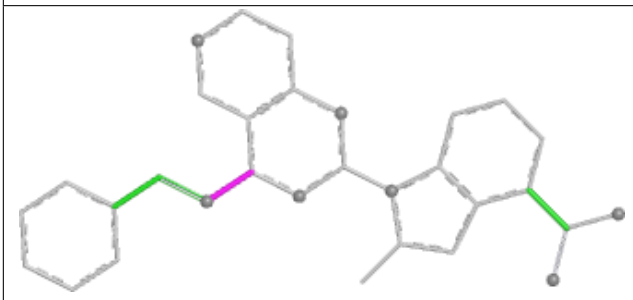
Ligand JDP G 900



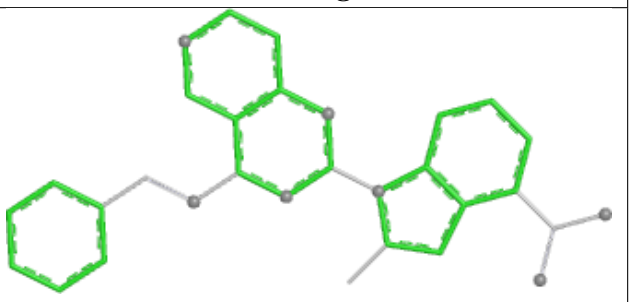
Bond lengths



Bond angles

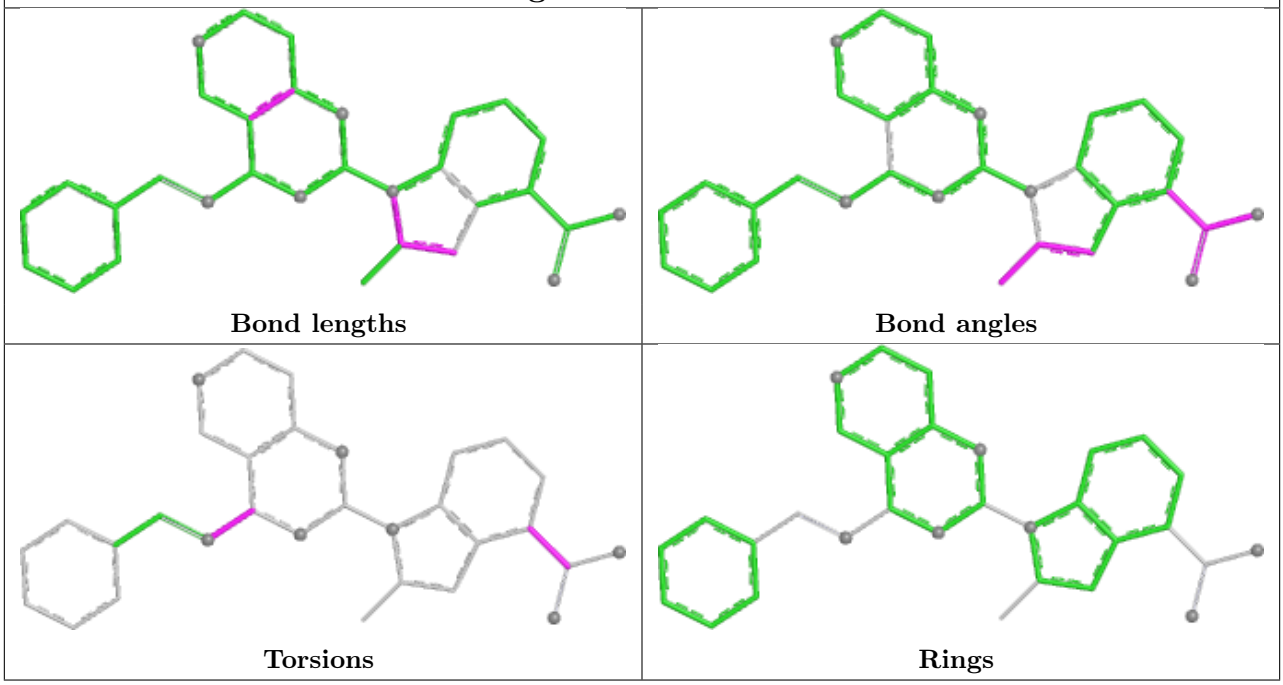


Torsions



Rings

Ligand JDP E 900



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	509/606 (83%)	-0.15	3 (0%)	89	88	110, 191, 256, 323	0
1	B	509/606 (83%)	0.07	20 (3%)	39	34	108, 197, 278, 324	0
1	C	509/606 (83%)	0.05	24 (4%)	31	29	119, 193, 267, 330	0
1	D	509/606 (83%)	-0.06	14 (2%)	53	46	102, 182, 256, 303	0
1	E	509/606 (83%)	0.02	18 (3%)	44	39	115, 194, 280, 342	0
1	F	509/606 (83%)	0.08	27 (5%)	26	25	123, 192, 278, 359	0
1	G	509/606 (83%)	0.01	15 (2%)	51	45	119, 190, 270, 363	0
1	H	509/606 (83%)	-0.01	19 (3%)	41	36	120, 204, 287, 343	0
1	I	509/606 (83%)	0.11	26 (5%)	28	26	120, 200, 276, 377	0
1	J	509/606 (83%)	-0.09	10 (1%)	65	61	98, 181, 264, 330	0
1	K	509/606 (83%)	0.02	20 (3%)	39	34	115, 192, 264, 332	0
1	L	509/606 (83%)	0.08	24 (4%)	31	29	122, 201, 271, 363	0
All	All	6108/7272 (83%)	0.01	220 (3%)	42	38	98, 193, 273, 377	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	299	ALA	9.8
1	B	396	LEU	6.7
1	I	341	VAL	5.3
1	I	388	MET	5.1
1	E	235	VAL	5.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

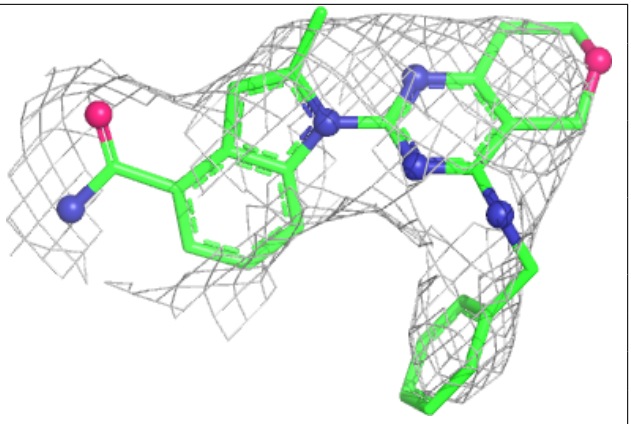
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

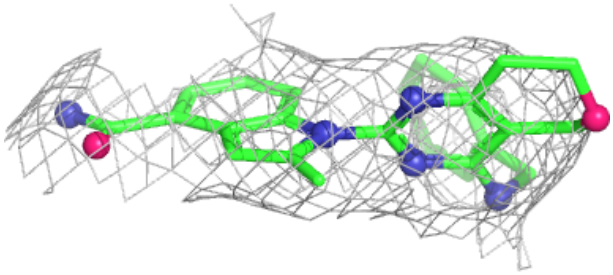
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	JDP	K	900	31/31	0.77	0.40	131,150,160,165	0
2	JDP	B	900	31/31	0.79	0.31	125,147,172,174	0
2	JDP	I	900	31/31	0.80	0.32	142,151,173,173	0
2	JDP	H	900	31/31	0.81	0.30	139,150,167,173	0
2	JDP	F	900	31/31	0.82	0.33	145,154,166,168	0
2	JDP	E	900	31/31	0.83	0.35	140,150,167,173	0
2	JDP	C	900	31/31	0.83	0.32	122,134,145,148	0
2	JDP	G	900	31/31	0.83	0.27	127,136,154,157	0
2	JDP	J	900	31/31	0.84	0.31	109,121,135,136	0
2	JDP	D	900	31/31	0.85	0.32	107,132,152,157	0
2	JDP	A	900	31/31	0.86	0.26	115,135,148,151	0
2	JDP	L	900	31/31	0.87	0.26	143,152,179,190	0

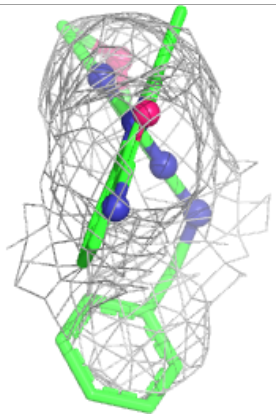
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JDP K 900:

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

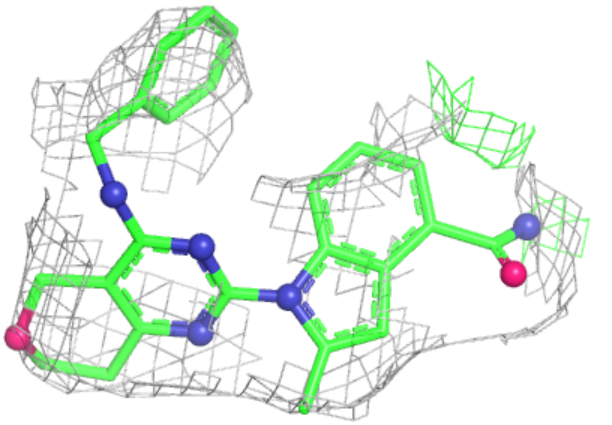


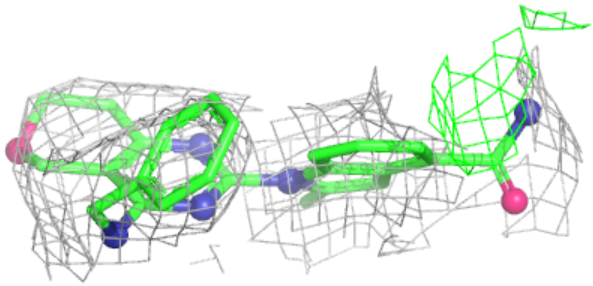


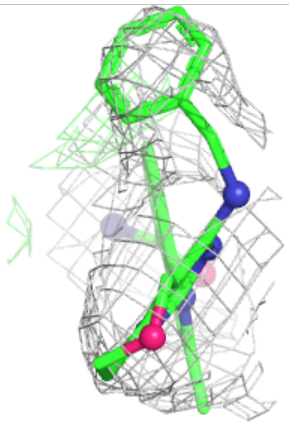


Electron density around JDP B 900:

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

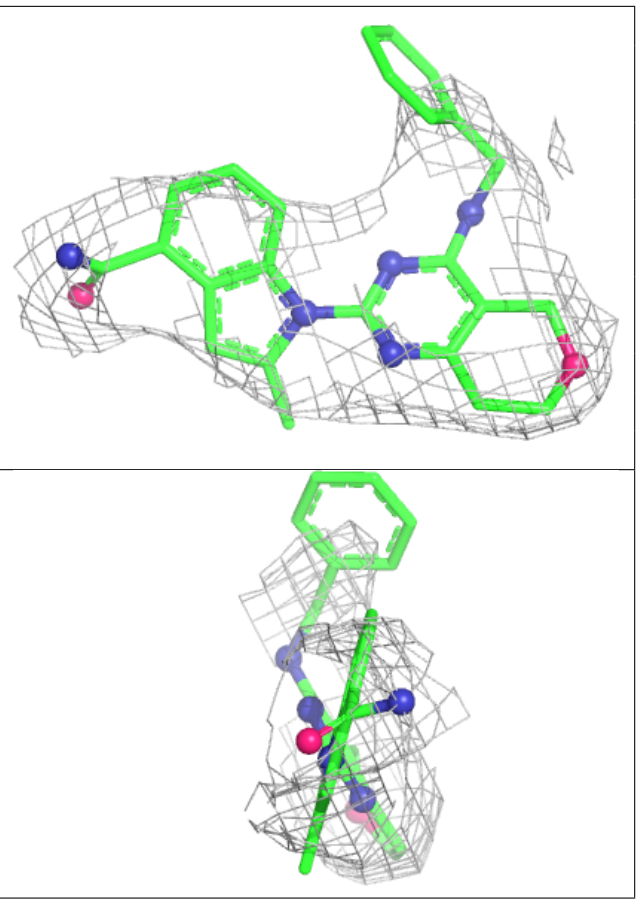






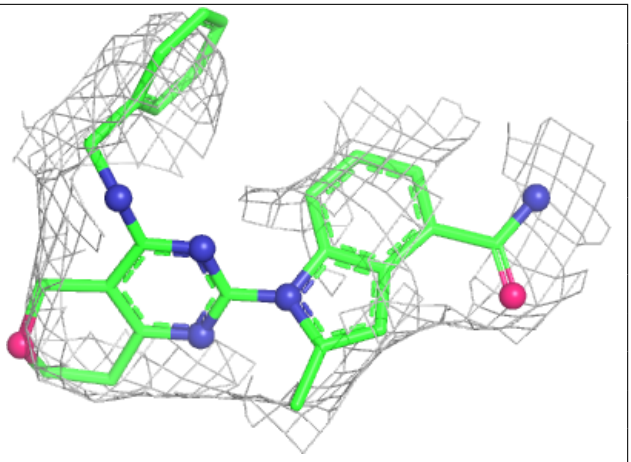
Electron density around JDP I 900:

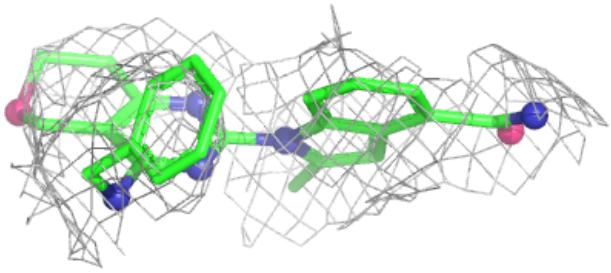
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

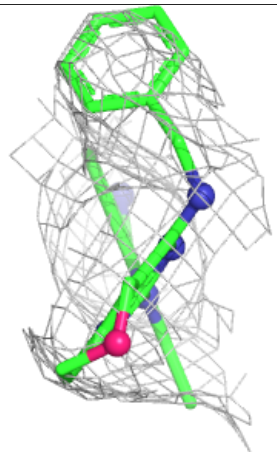


Electron density around JDP H 900:

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







Electron density around JDP F 900:

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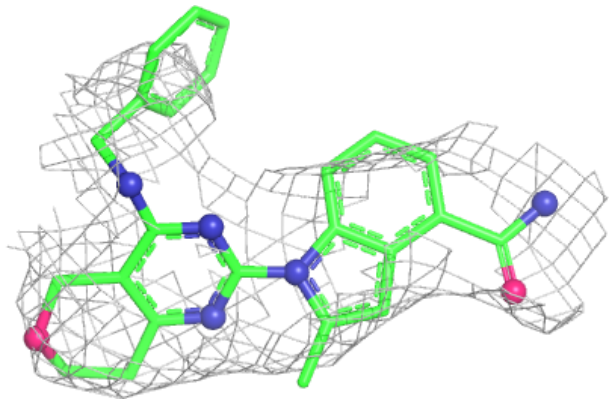
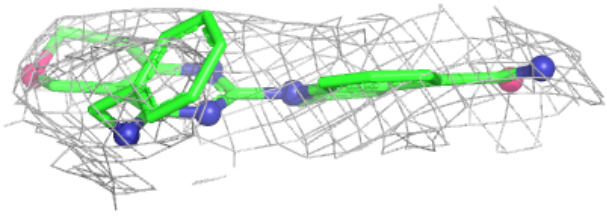
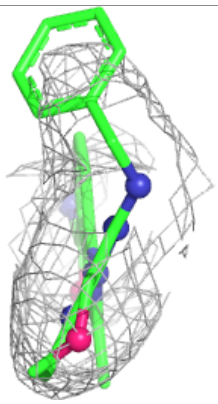
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

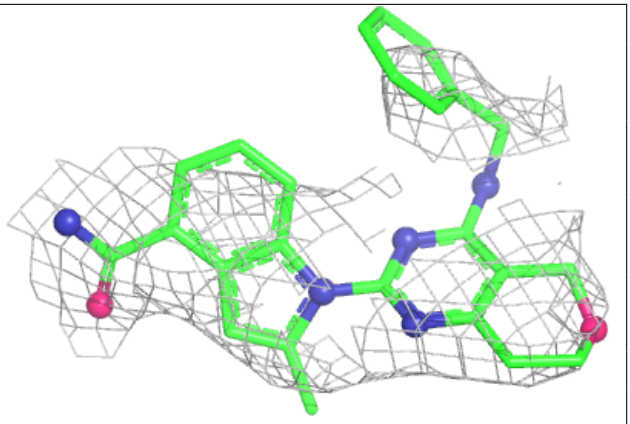


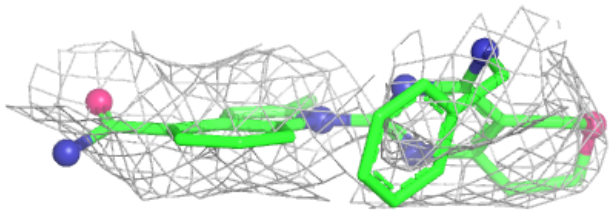


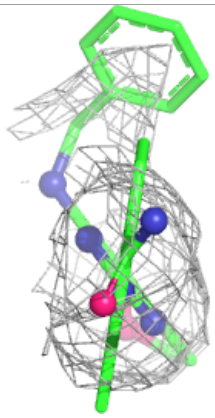


Electron density around JDP E 900:

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







Electron density around JDP C 900:

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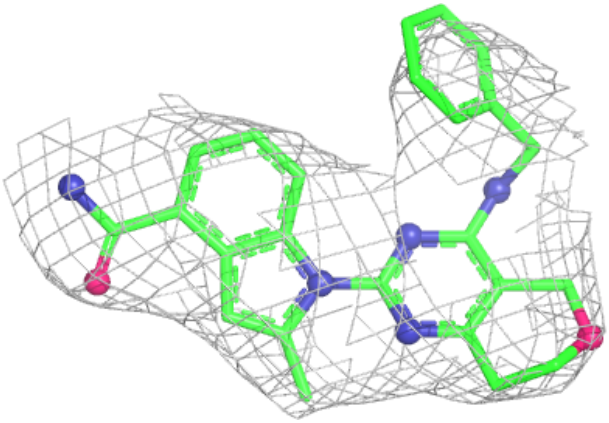
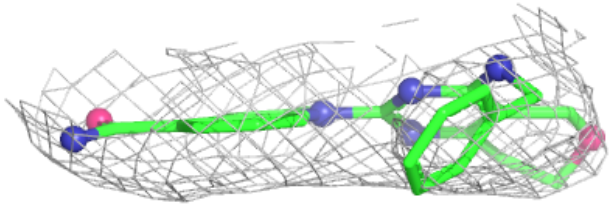
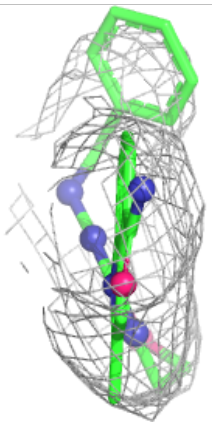
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

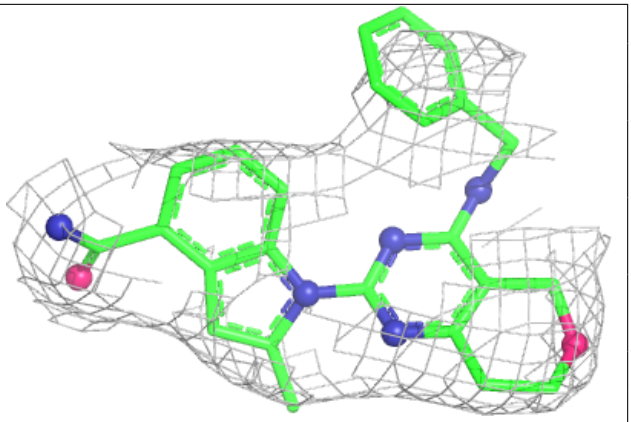


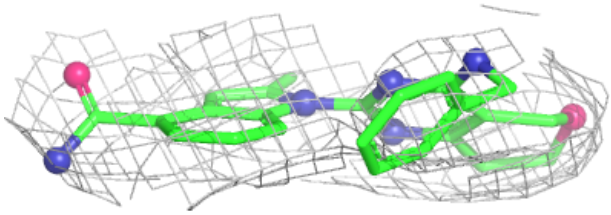


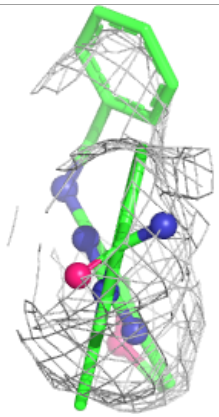


Electron density around JDP G 900:

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

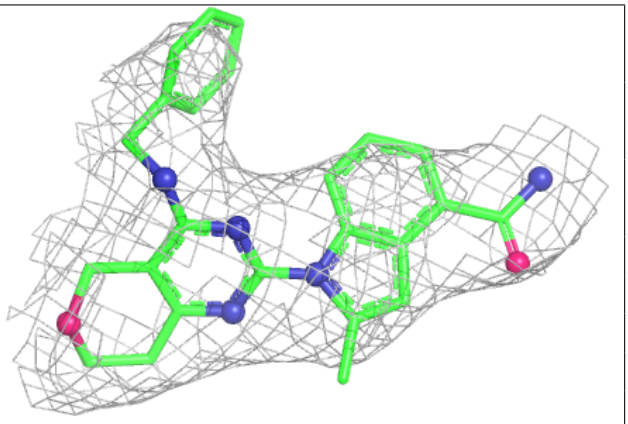


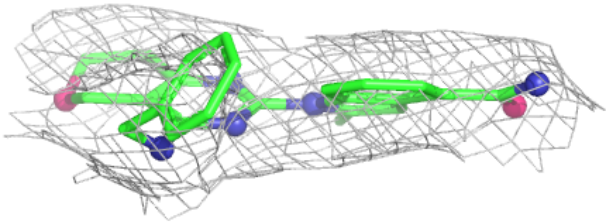


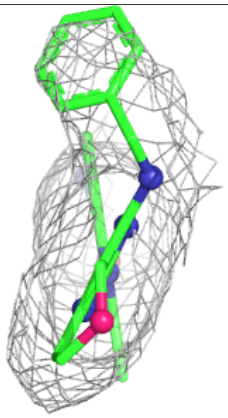


Electron density around JDP J 900:

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

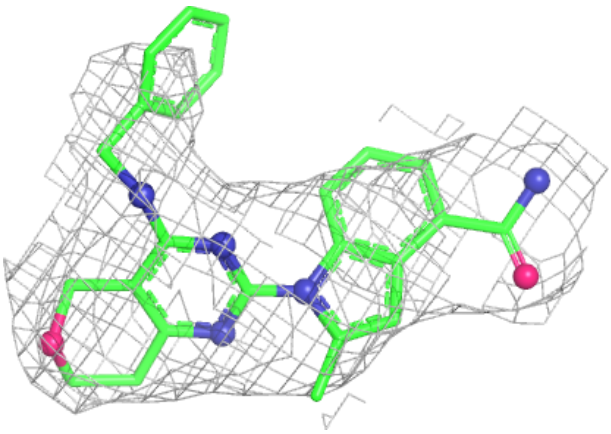


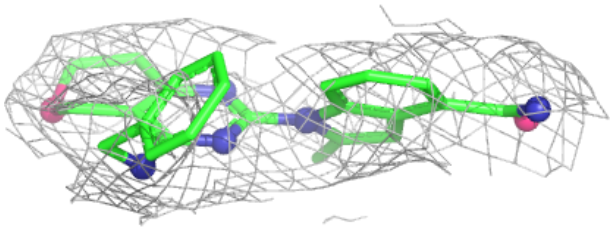


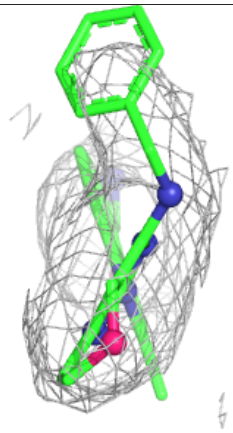


Electron density around JDP D 900:

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

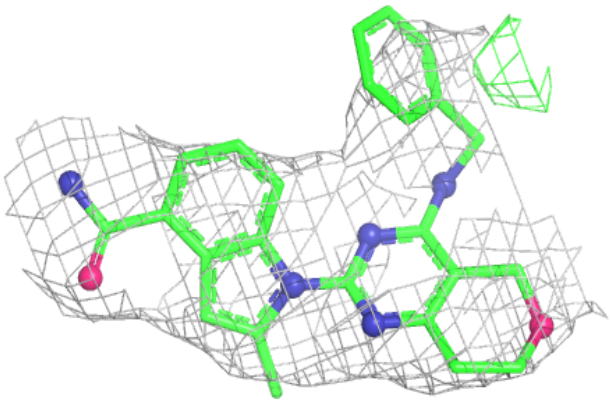


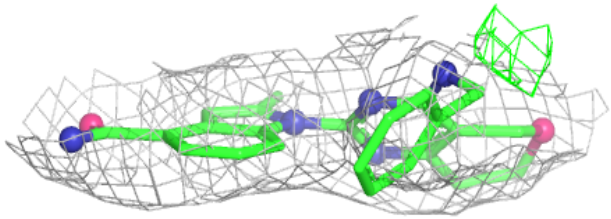


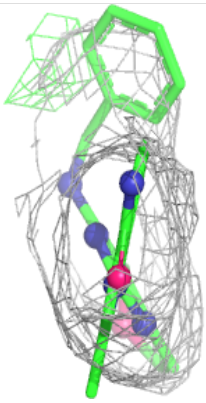


Electron density around JDP A 900:

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

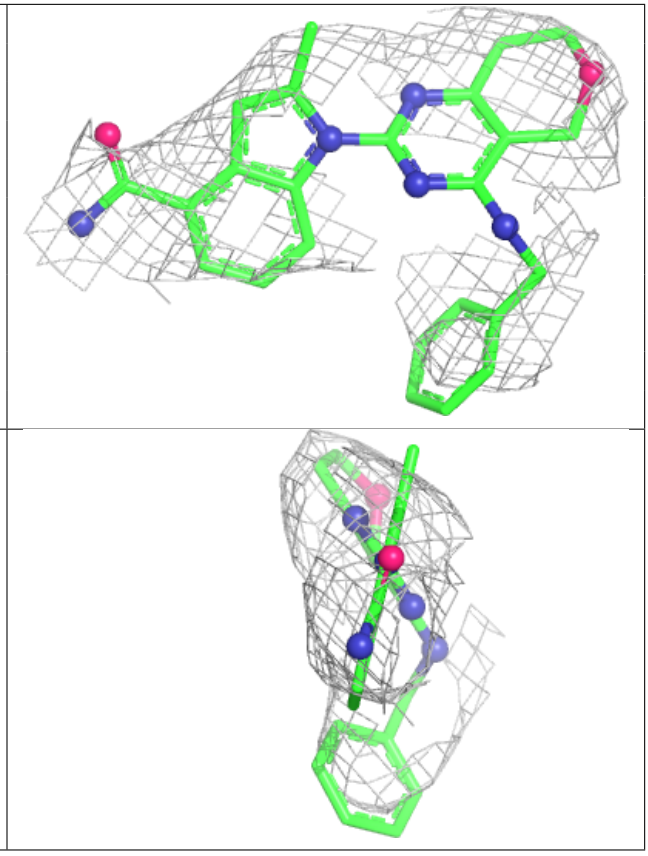






Electron density around JDP L 900:

$2mF_o$-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.