Full wwPDB X-ray Structure Validation 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 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 (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:

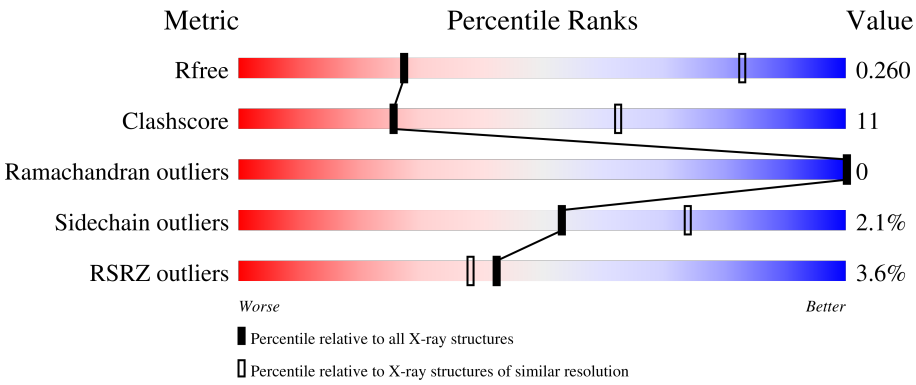
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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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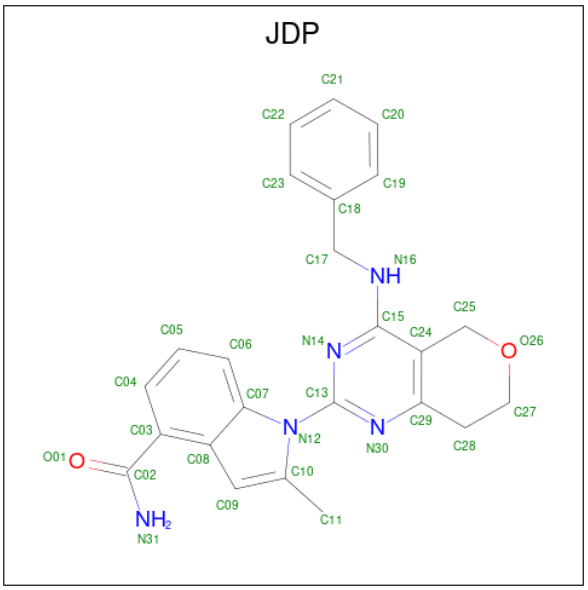
Chain	Residue	Modelled	Actual	Comment	Reference
J	814	HIS	-	expression tag	UNP P55072
K	209	MET	-	expression tag	UNP P55072
K	807	ARG	-	expression tag	UNP P55072
K	808	SER	-	expression tag	UNP P55072
K	809	HIS	-	expression tag	UNP P55072
K	810	HIS	-	expression tag	UNP P55072
K	811	HIS	-	expression tag	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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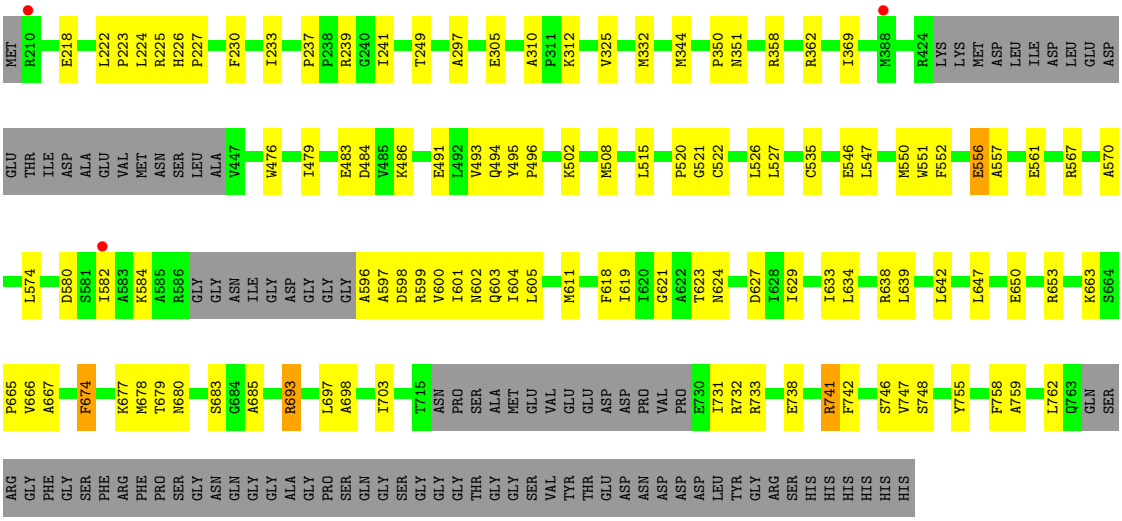
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	I	2	2	2	0	0
			Total	O		
3	J	3	3	3	0	0
			Total	O		
3	K	3	3	3	0	0
			Total	O		
3	L	2	2	2	0	0

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.

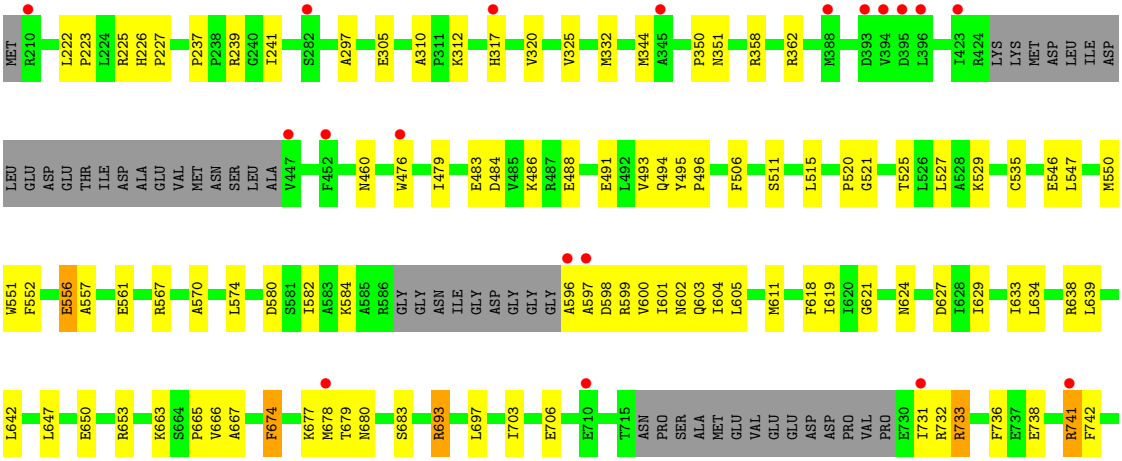
• Molecule 1: Transitional endoplasmic reticulum ATPase

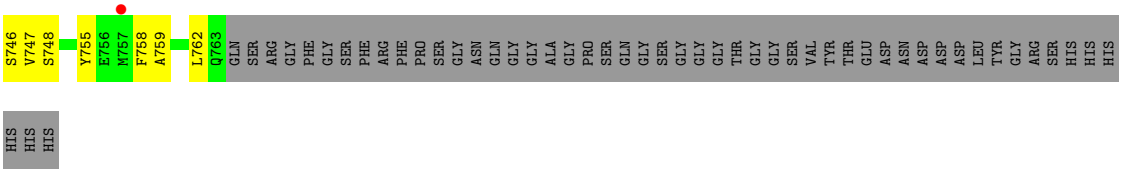
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

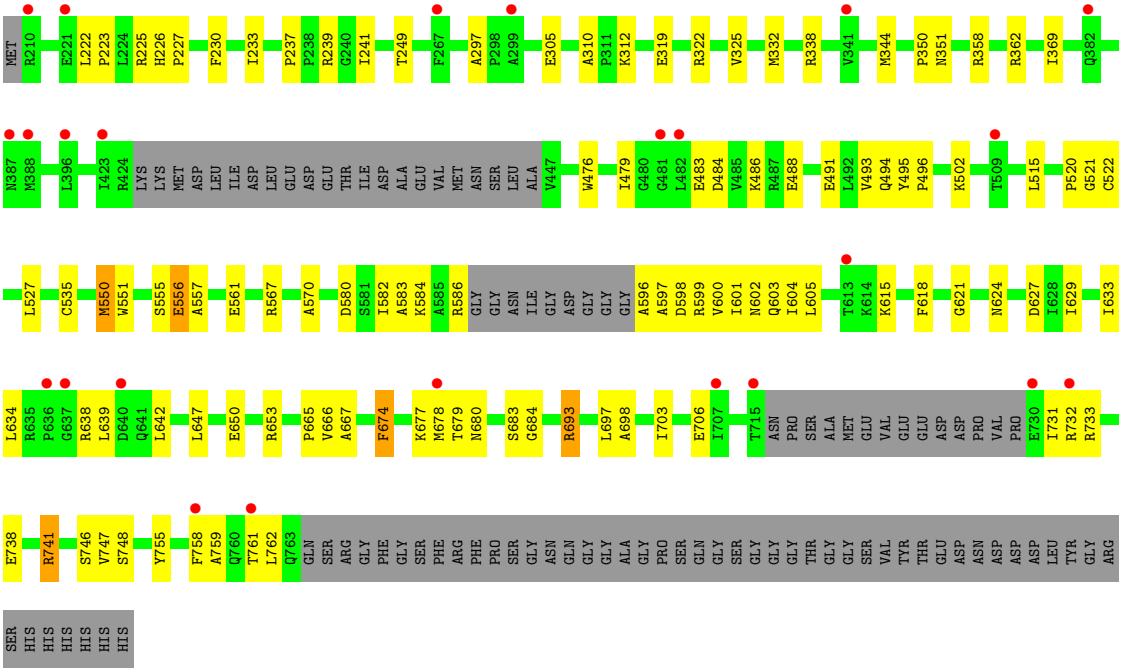
Chain B:





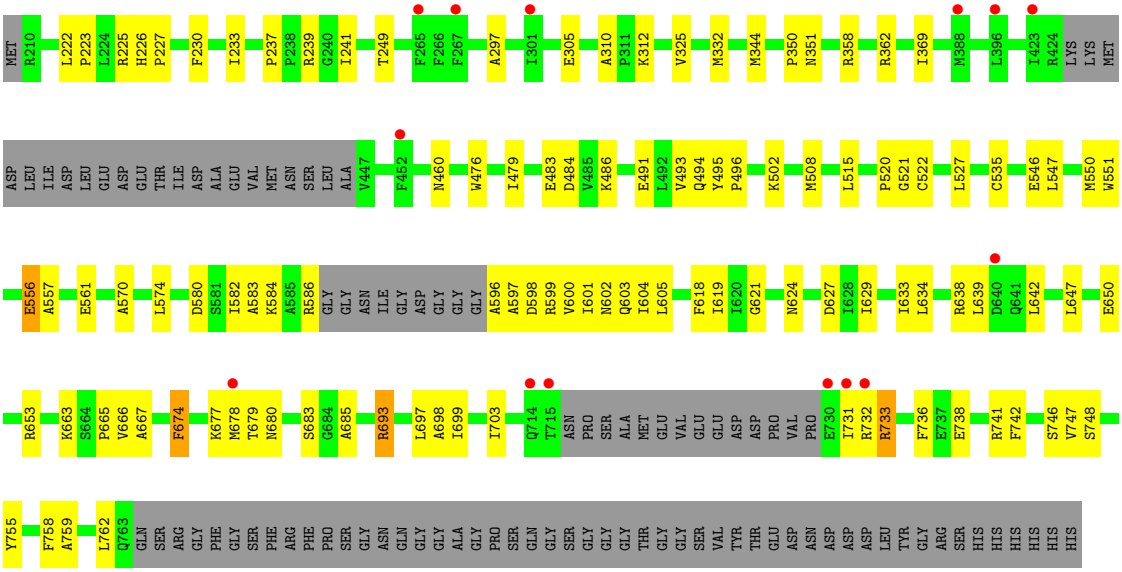
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



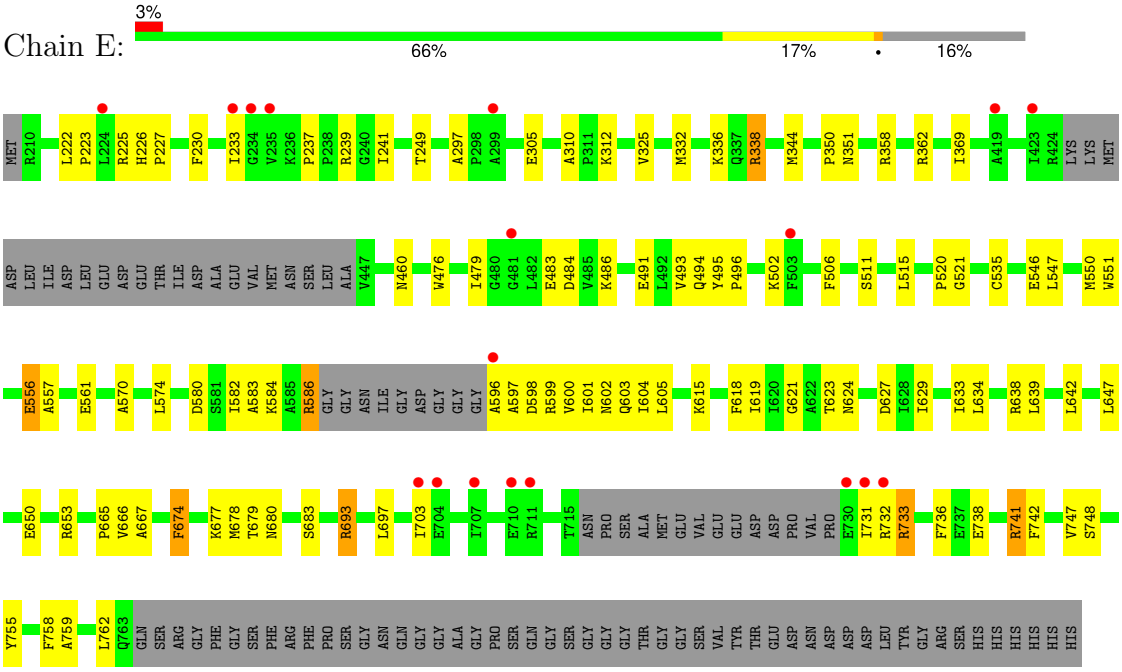
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



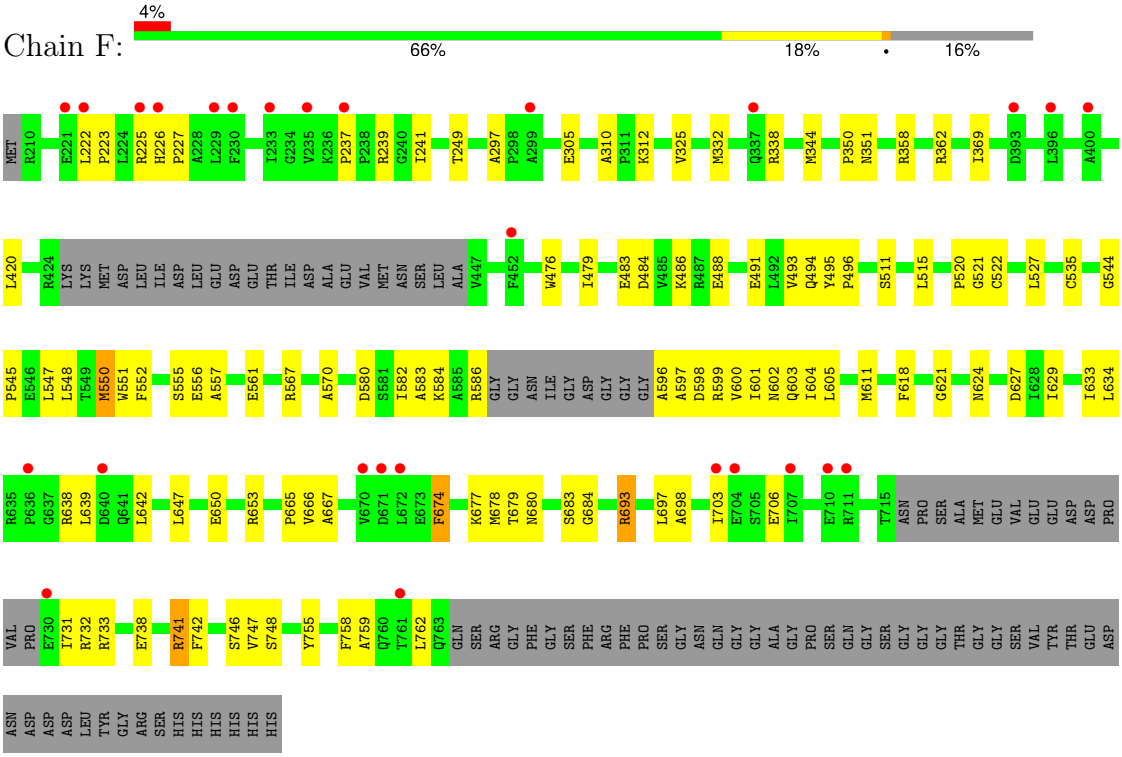
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



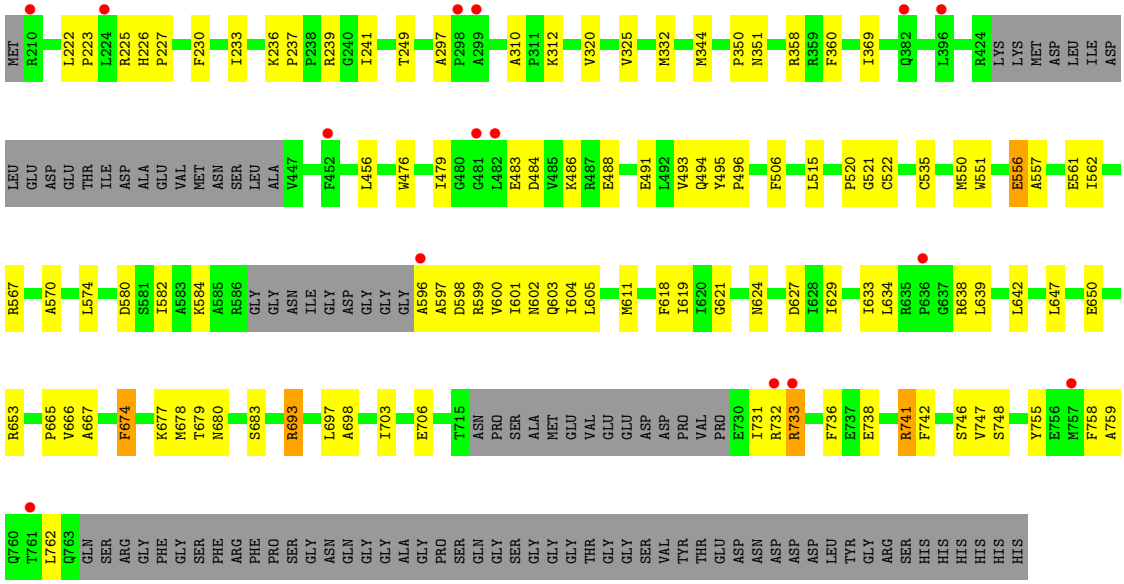
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



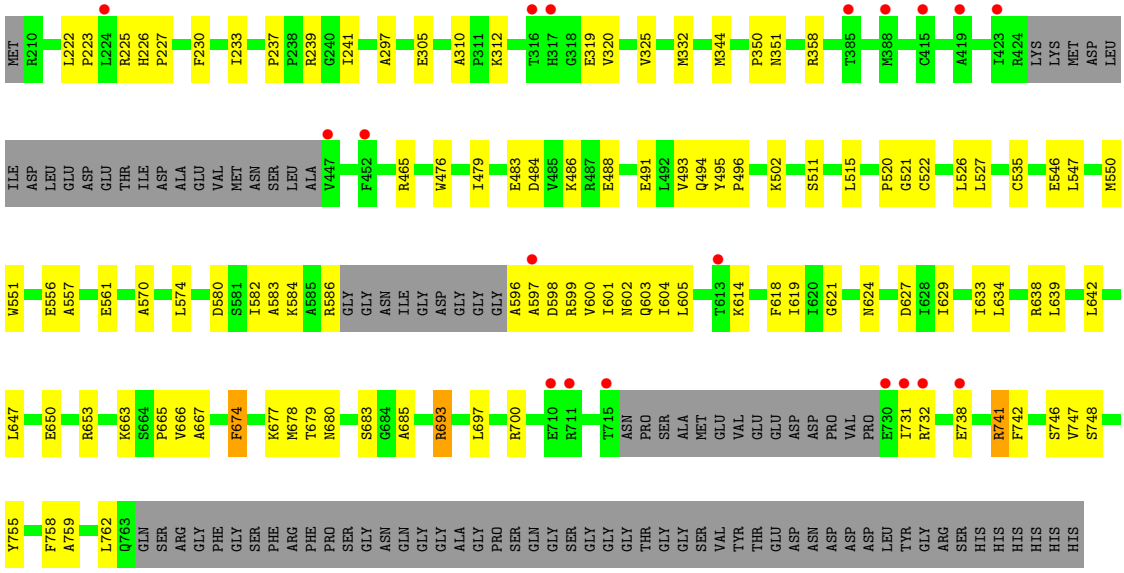
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain G:



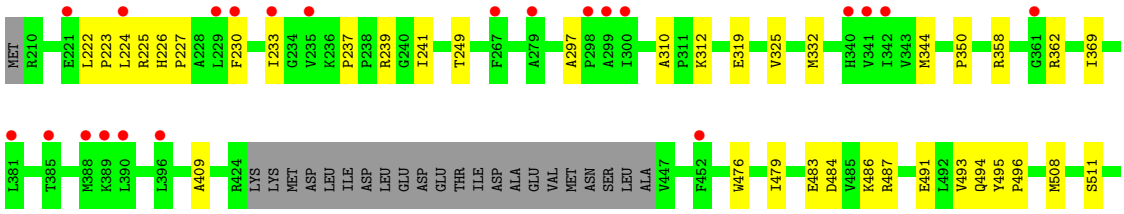
• Molecule 1: Transitional endoplasmic reticulum ATPase

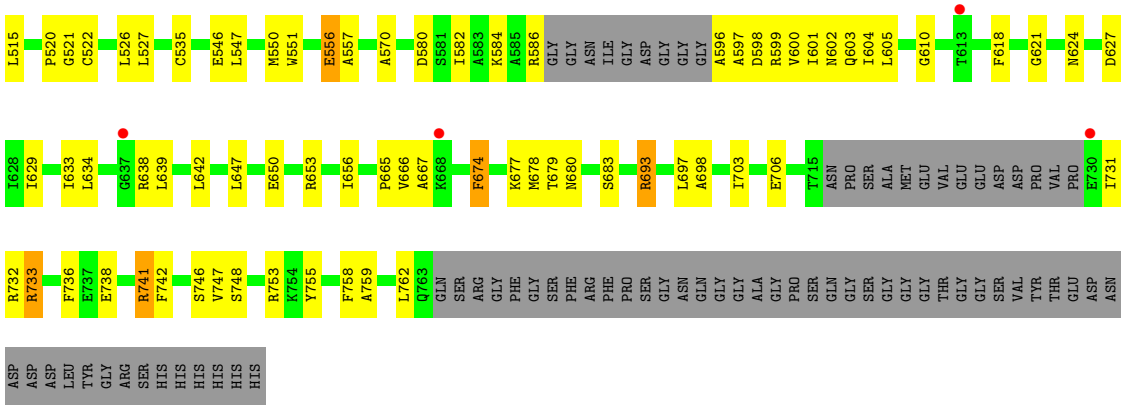
Chain H:



• Molecule 1: Transitional endoplasmic reticulum ATPase

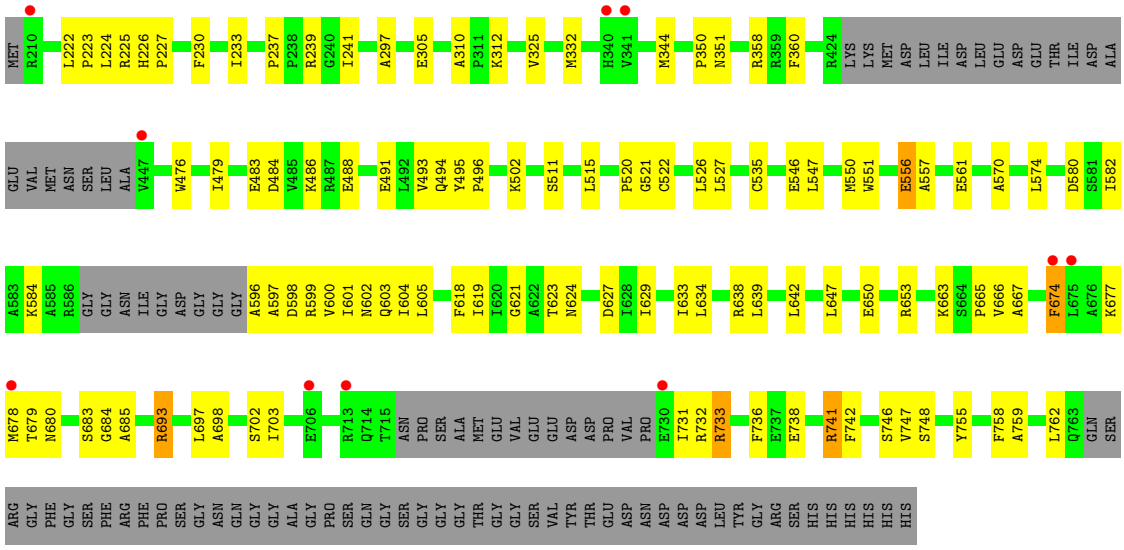
Chain I:





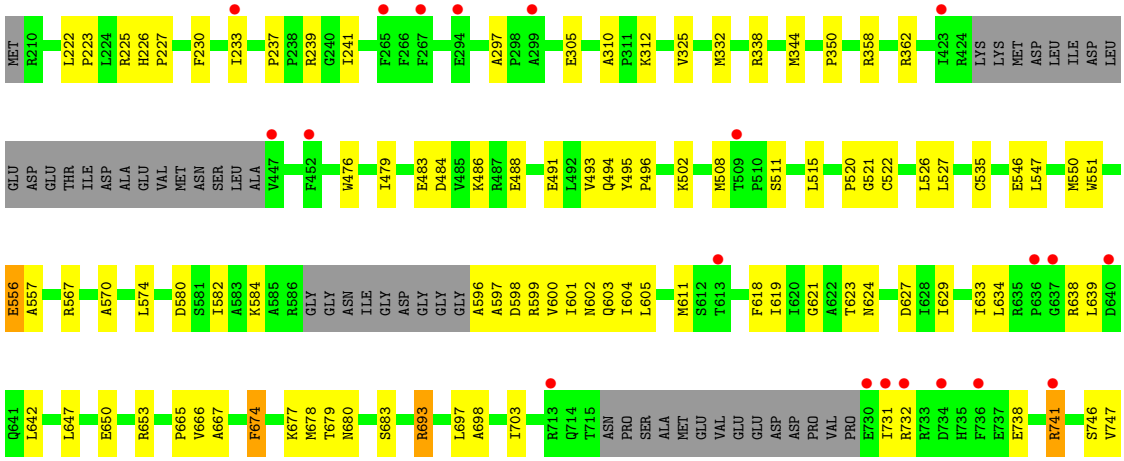
• Molecule 1: Transitional endoplasmic reticulum ATPase

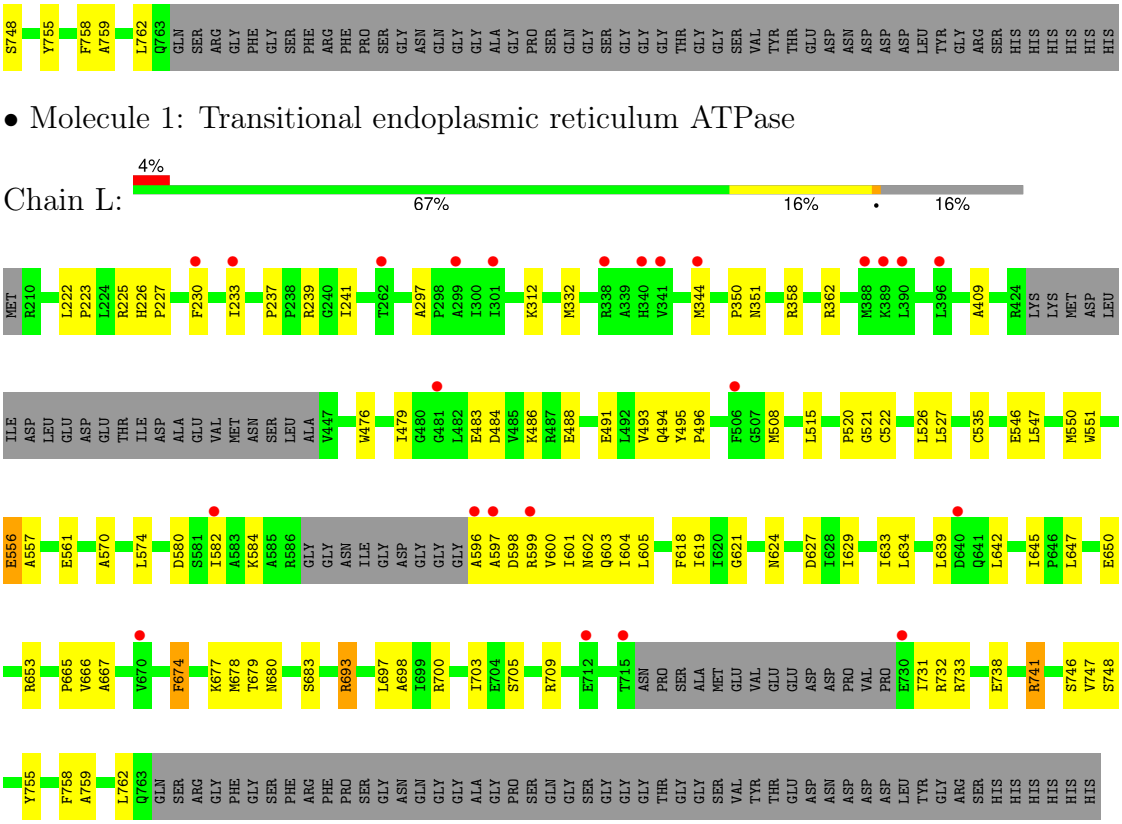
Chain J:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K:





- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L:

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.

All (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
1	A	741	ARG	Peptide
1	B	297	ALA	Peptide
1	B	312	LYS	Peptide
1	B	570	ALA	Peptide
1	B	693	ARG	Sidechain
1	B	733	ARG	Sidechain
1	B	741	ARG	Peptide
1	C	297	ALA	Peptide
1	C	312	LYS	Peptide
1	C	570	ALA	Peptide
1	C	693	ARG	Sidechain
1	C	733	ARG	Sidechain
1	C	741	ARG	Peptide
1	D	297	ALA	Peptide
1	D	312	LYS	Peptide
1	D	570	ALA	Peptide
1	D	693	ARG	Sidechain
1	D	733	ARG	Sidechain
1	E	297	ALA	Peptide
1	E	312	LYS	Peptide
1	E	570	ALA	Peptide
1	E	586	ARG	Sidechain
1	E	693	ARG	Sidechain
1	E	733	ARG	Sidechain
1	E	741	ARG	Peptide
1	F	297	ALA	Peptide
1	F	312	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	F	570	ALA	Peptide
1	F	693	ARG	Sidechain
1	F	733	ARG	Sidechain
1	F	741	ARG	Peptide
1	G	297	ALA	Peptide
1	G	312	LYS	Peptide
1	G	570	ALA	Peptide
1	G	693	ARG	Sidechain
1	G	733	ARG	Sidechain
1	G	741	ARG	Peptide
1	H	297	ALA	Peptide
1	H	312	LYS	Peptide
1	H	570	ALA	Peptide
1	H	693	ARG	Sidechain
1	H	741	ARG	Peptide
1	I	297	ALA	Peptide
1	I	312	LYS	Peptide
1	I	570	ALA	Peptide
1	I	586	ARG	Sidechain
1	I	693	ARG	Sidechain
1	I	733	ARG	Sidechain
1	I	741	ARG	Peptide
1	J	297	ALA	Peptide
1	J	312	LYS	Peptide
1	J	570	ALA	Peptide
1	J	693	ARG	Sidechain
1	J	733	ARG	Sidechain
1	J	741	ARG	Peptide
1	K	297	ALA	Peptide
1	K	312	LYS	Peptide
1	K	570	ALA	Peptide
1	K	693	ARG	Sidechain
1	K	741	ARG	Peptide
1	L	297	ALA	Peptide
1	L	312	LYS	Peptide
1	L	570	ALA	Peptide
1	L	693	ARG	Sidechain
1	L	733	ARG	Sidechain
1	L	741	ARG	Peptide

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
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.

All (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
1:B:226:HIS:N	1:B:227:PRO:HD3	1.87	0.89
1:K:226:HIS:N	1:K:227:PRO:HD3	1.87	0.89
1:E:226:HIS:N	1:E:227:PRO:HD3	1.87	0.89
1:J:226:HIS:N	1:J:227:PRO:HD3	1.87	0.88
1:L:226:HIS:N	1:L:227:PRO:HD3	1.87	0.88
1:F:226:HIS:N	1:F:227:PRO:HD3	1.87	0.88
1:H:226:HIS:N	1:H:227:PRO:HD3	1.87	0.87
1:C:226:HIS:N	1:C:227:PRO:HD3	1.87	0.87
1:H:599:ARG:HA	1:H:602:ASN:HB3	1.57	0.87
1:K:599:ARG:HA	1:K:602:ASN:HB3	1.57	0.86
1:G:599:ARG:HA	1:G:602:ASN:HB3	1.58	0.86
1:C:515:LEU:HD13	1:C:634:LEU:HD21	1.59	0.85
1:I:515:LEU:HD13	1:I:634:LEU:HD21	1.59	0.85
1:F:599:ARG:HA	1:F:602:ASN:HB3	1.57	0.85
1:D:515:LEU:HD13	1:D:634:LEU:HD21	1.59	0.84
1:I:599:ARG:HA	1:I:602:ASN:HB3	1.57	0.84
1:D:599:ARG:HA	1:D:602:ASN:HB3	1.59	0.84
1:J:599:ARG:HA	1:J:602:ASN:HB3	1.58	0.84
1:H:515:LEU:HD13	1:H:634:LEU:HD21	1.61	0.83
1:L:599:ARG:HA	1:L:602:ASN:HB3	1.58	0.83
1:E:599:ARG:HA	1:E:602:ASN:HB3	1.58	0.83
1:K:515:LEU:HD13	1:K:634:LEU:HD21	1.60	0.83
1:A:599:ARG:HA	1:A:602:ASN:HB3	1.58	0.83
1:B:515:LEU:HD13	1:B:634:LEU:HD21	1.60	0.83
1:J:515:LEU:HD13	1:J:634:LEU:HD21	1.59	0.83
1:A:515:LEU:HD13	1:A:634:LEU:HD21	1.60	0.83
1:B:599:ARG:HA	1:B:602:ASN:HB3	1.58	0.83
1:C:599:ARG:HA	1:C:602:ASN:HB3	1.58	0.83
1:F:515:LEU:HD13	1:F:634:LEU:HD21	1.60	0.82
1:C:550:MET:HG2	1:C:555:SER:O	1.78	0.82
1:L:515:LEU:HD13	1:L:634:LEU:HD21	1.60	0.82
1:F:550:MET:HG2	1:F:555:SER:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:515:LEU:HD13	1:E:634:LEU:HD21	1.60	0.81
1:G:515:LEU:HD13	1:G:634:LEU:HD21	1.60	0.81
1:C:706:GLU:OE1	1:D:502:LYS:NZ	2.16	0.79
1:B:596:ALA:HB1	1:B:599:ARG:HD3	1.67	0.77
1:F:653:ARG:NH2	1:F:680:ASN:HA	2.00	0.77
1:K:653:ARG:NH2	1:K:680:ASN:HA	2.00	0.77
1:F:596:ALA:HB1	1:F:599:ARG:HD3	1.67	0.77
1:H:653:ARG:NH2	1:H:680:ASN:HA	2.00	0.76
1:E:596:ALA:HB1	1:E:599:ARG:HD3	1.67	0.76
1:H:596:ALA:HB1	1:H:599:ARG:HD3	1.67	0.76
1:B:653:ARG:NH2	1:B:680:ASN:HA	2.00	0.76
1:K:596:ALA:HB1	1:K:599:ARG:HD3	1.67	0.76
1:C:653:ARG:NH2	1:C:680:ASN:HA	2.00	0.76
1:L:596:ALA:HB1	1:L:599:ARG:HD3	1.67	0.76
1:L:653:ARG:NH2	1:L:680:ASN:HA	2.01	0.76
1:I:653:ARG:NH2	1:I:680:ASN:HA	2.00	0.76
1:E:653:ARG:NH2	1:E:680:ASN:HA	2.00	0.76
1:J:596:ALA:HB1	1:J:599:ARG:HD3	1.67	0.76
1:G:653:ARG:NH2	1:G:680:ASN:HA	2.00	0.76
1:A:653:ARG:NH2	1:A:680:ASN:HA	2.01	0.76
1:J:653:ARG:NH2	1:J:680:ASN:HA	2.01	0.75
1:I:596:ALA:HB1	1:I:599:ARG:HD3	1.67	0.75
1:D:596:ALA:HB1	1:D:599:ARG:HD3	1.67	0.75
1:A:596:ALA:HB1	1:A:599:ARG:HD3	1.67	0.75
1:C:596:ALA:HB1	1:C:599:ARG:HD3	1.67	0.74
1:G:596:ALA:HB1	1:G:599:ARG:HD3	1.67	0.74
1:D:653:ARG:NH2	1:D:680:ASN:HA	2.01	0.74
1:B:493:VAL:HG22	1:B:618:PHE:CD2	2.23	0.74
1:F:493:VAL:HG22	1:F:618:PHE:CD2	2.23	0.73
1:C:677:LYS:HE3	1:H:678:MET:SD	2.27	0.73
1:F:479:ILE:HA	2:F:900:JDP:C17	2.18	0.73
1:J:493:VAL:HG22	1:J:618:PHE:CD2	2.24	0.73
1:C:493:VAL:HG22	1:C:618:PHE:CD2	2.23	0.73
1:H:493:VAL:HG22	1:H:618:PHE:CD2	2.24	0.73
1:D:493:VAL:HG22	1:D:618:PHE:CD2	2.24	0.73
1:E:493:VAL:HG22	1:E:618:PHE:CD2	2.24	0.72
1:K:493:VAL:HG22	1:K:618:PHE:CD2	2.24	0.72
1:I:493:VAL:HG22	1:I:618:PHE:CD2	2.24	0.72
1:L:493:VAL:HG22	1:L:618:PHE:CD2	2.24	0.71
1:G:493:VAL:HG22	1:G:618:PHE:CD2	2.24	0.71
1:L:678:MET:HE2	1:L:678:MET:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG22	1:A:618:PHE:CD2	2.24	0.71
1:E:678:MET:HE2	1:E:678:MET:HA	1.73	0.71
1:K:678:MET:HE2	1:K:678:MET:HA	1.74	0.70
1:J:678:MET:HE2	1:J:678:MET:HA	1.72	0.70
1:A:678:MET:SD	1:J:677:LYS:HE3	2.30	0.70
1:E:677:LYS:HE3	1:L:678:MET:SD	2.32	0.70
1:H:678:MET:HE2	1:H:678:MET:HA	1.74	0.70
1:L:521:GLY:HA3	1:L:683:SER:HB2	1.75	0.69
1:A:678:MET:HE2	1:A:678:MET:HA	1.73	0.69
1:C:678:MET:HE2	1:C:678:MET:HA	1.73	0.69
1:A:495:TYR:CZ	1:F:703:ILE:HD11	2.28	0.69
1:D:479:ILE:HA	2:D:900:JDP:C17	2.23	0.69
1:D:521:GLY:HA3	1:D:683:SER:HB2	1.76	0.68
1:F:521:GLY:HA3	1:F:683:SER:HB2	1.75	0.68
1:G:521:GLY:HA3	1:G:683:SER:HB2	1.76	0.68
1:E:521:GLY:HA3	1:E:683:SER:HB2	1.76	0.68
1:G:495:TYR:CZ	1:L:703:ILE:HD11	2.29	0.67
1:I:703:ILE:HD11	1:J:495:TYR:CZ	2.28	0.67
1:A:521:GLY:HA3	1:A:683:SER:HB2	1.75	0.67
1:G:703:ILE:HD11	1:H:495:TYR:CZ	2.30	0.67
1:G:758:PHE:O	1:G:762:LEU:HD12	1.95	0.67
1:H:551:TRP:HB2	1:H:582:ILE:HD12	1.77	0.67
1:B:758:PHE:O	1:B:762:LEU:HD12	1.95	0.67
1:F:758:PHE:O	1:F:762:LEU:HD12	1.95	0.67
1:K:521:GLY:HA3	1:K:683:SER:HB2	1.75	0.67
1:E:551:TRP:HB2	1:E:582:ILE:HD12	1.77	0.66
1:I:551:TRP:HB2	1:I:582:ILE:HD12	1.78	0.66
1:A:677:LYS:HE3	1:J:678:MET:SD	2.35	0.66
1:D:678:MET:SD	1:G:677:LYS:HE3	2.35	0.66
1:A:758:PHE:O	1:A:762:LEU:HD12	1.96	0.66
1:D:758:PHE:O	1:D:762:LEU:HD12	1.96	0.66
1:F:678:MET:HE2	1:F:678:MET:HA	1.77	0.66
1:L:758:PHE:O	1:L:762:LEU:HD12	1.95	0.66
1:I:521:GLY:HA3	1:I:683:SER:HB2	1.76	0.66
1:I:758:PHE:O	1:I:762:LEU:HD12	1.95	0.66
1:B:521:GLY:HA3	1:B:683:SER:HB2	1.78	0.66
1:C:758:PHE:O	1:C:762:LEU:HD12	1.95	0.66
1:J:521:GLY:HA3	1:J:683:SER:HB2	1.77	0.66
1:J:758:PHE:O	1:J:762:LEU:HD12	1.96	0.66
1:F:653:ARG:NH1	1:F:679:THR:O	2.29	0.65
1:J:653:ARG:NH1	1:J:679:THR:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:OE2	1:B:362:ARG:NH2	2.28	0.65
1:G:653:ARG:NH1	1:G:679:THR:O	2.29	0.65
1:K:650:GLU:OE1	1:K:650:GLU:N	2.30	0.65
1:L:653:ARG:NH1	1:L:679:THR:O	2.30	0.65
1:C:521:GLY:HA3	1:C:683:SER:HB2	1.77	0.65
1:H:758:PHE:O	1:H:762:LEU:HD12	1.96	0.65
1:B:653:ARG:NH1	1:B:679:THR:O	2.30	0.65
1:H:521:GLY:HA3	1:H:683:SER:HB2	1.77	0.65
1:H:650:GLU:OE1	1:H:650:GLU:N	2.30	0.65
1:K:653:ARG:NH1	1:K:679:THR:O	2.30	0.65
1:I:653:ARG:NH1	1:I:679:THR:O	2.29	0.65
1:K:551:TRP:HB2	1:K:582:ILE:HD12	1.78	0.65
1:H:653:ARG:NH1	1:H:679:THR:O	2.30	0.65
1:I:599:ARG:O	1:I:603:GLN:N	2.30	0.65
1:B:551:TRP:HB2	1:B:582:ILE:HD12	1.79	0.65
1:C:653:ARG:NH1	1:C:679:THR:O	2.30	0.65
1:J:515:LEU:HD11	1:J:629:ILE:HD13	1.79	0.65
1:A:650:GLU:OE1	1:A:650:GLU:N	2.30	0.64
1:D:599:ARG:O	1:D:603:GLN:N	2.30	0.64
1:E:678:MET:SD	1:L:677:LYS:HE3	2.36	0.64
1:I:650:GLU:N	1:I:650:GLU:OE1	2.30	0.64
1:K:758:PHE:O	1:K:762:LEU:HD12	1.95	0.64
1:L:650:GLU:N	1:L:650:GLU:OE1	2.30	0.64
1:D:650:GLU:N	1:D:650:GLU:OE1	2.30	0.64
1:D:653:ARG:NH1	1:D:679:THR:O	2.30	0.64
1:E:653:ARG:NH1	1:E:679:THR:O	2.30	0.64
1:F:551:TRP:HB2	1:F:582:ILE:HD12	1.80	0.64
1:J:226:HIS:N	1:J:227:PRO:CD	2.60	0.64
1:G:551:TRP:HB2	1:G:582:ILE:HD12	1.80	0.64
1:G:650:GLU:N	1:G:650:GLU:OE1	2.30	0.64
1:A:653:ARG:NH1	1:A:679:THR:O	2.30	0.64
1:K:674:PHE:O	1:K:678:MET:HG2	1.97	0.64
1:D:674:PHE:O	1:D:678:MET:HG2	1.98	0.64
1:E:758:PHE:O	1:E:762:LEU:HD12	1.96	0.64
1:G:599:ARG:O	1:G:603:GLN:N	2.29	0.64
1:G:674:PHE:O	1:G:678:MET:HG2	1.98	0.64
1:I:674:PHE:O	1:I:678:MET:HG2	1.98	0.64
1:D:226:HIS:N	1:D:227:PRO:CD	2.60	0.64
1:J:650:GLU:N	1:J:650:GLU:OE1	2.30	0.64
1:K:599:ARG:O	1:K:603:GLN:N	2.29	0.64
1:D:758:PHE:O	1:D:762:LEU:CG	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:674:PHE:O	1:E:678:MET:HG2	1.99	0.63
1:K:758:PHE:O	1:K:762:LEU:CG	2.46	0.63
1:L:551:TRP:HB2	1:L:582:ILE:HD12	1.80	0.63
1:D:685:ALA:N	2:D:900:JDP:N31	2.45	0.63
1:E:703:ILE:HD11	1:F:495:TYR:CZ	2.33	0.63
1:G:758:PHE:O	1:G:762:LEU:CG	2.47	0.63
1:L:599:ARG:O	1:L:603:GLN:N	2.30	0.63
1:C:599:ARG:O	1:C:603:GLN:N	2.30	0.63
1:I:226:HIS:N	1:I:227:PRO:CD	2.60	0.63
1:A:758:PHE:O	1:A:762:LEU:CG	2.46	0.63
1:B:226:HIS:N	1:B:227:PRO:CD	2.60	0.63
1:C:650:GLU:N	1:C:650:GLU:OE1	2.30	0.63
1:F:650:GLU:OE1	1:F:650:GLU:N	2.30	0.63
1:H:758:PHE:O	1:H:762:LEU:CG	2.47	0.63
1:E:650:GLU:N	1:E:650:GLU:OE1	2.30	0.63
1:F:758:PHE:O	1:F:762:LEU:CG	2.47	0.63
1:H:674:PHE:O	1:H:678:MET:HG2	1.99	0.63
1:C:226:HIS:N	1:C:227:PRO:CD	2.60	0.63
1:E:758:PHE:O	1:E:762:LEU:CG	2.47	0.63
1:L:758:PHE:O	1:L:762:LEU:CG	2.47	0.63
1:B:674:PHE:O	1:B:678:MET:HG2	1.99	0.63
1:A:599:ARG:O	1:A:603:GLN:N	2.30	0.63
1:C:738:GLU:OE2	1:C:741:ARG:NH1	2.32	0.63
1:L:738:GLU:OE2	1:L:741:ARG:NH1	2.32	0.63
1:B:650:GLU:N	1:B:650:GLU:OE1	2.30	0.62
1:B:703:ILE:HD11	1:C:495:TYR:CZ	2.33	0.62
1:G:479:ILE:HA	2:G:900:JDP:C17	2.29	0.62
1:K:515:LEU:HD11	1:K:629:ILE:HD13	1.81	0.62
1:K:738:GLU:OE2	1:K:741:ARG:NH1	2.32	0.62
1:B:706:GLU:OE1	1:C:502:LYS:NZ	2.32	0.62
1:B:758:PHE:O	1:B:762:LEU:CG	2.47	0.62
1:C:758:PHE:O	1:C:762:LEU:CG	2.47	0.62
1:F:674:PHE:O	1:F:678:MET:HG2	1.99	0.62
1:J:758:PHE:O	1:J:762:LEU:CG	2.47	0.62
1:E:599:ARG:O	1:E:603:GLN:N	2.30	0.62
1:E:738:GLU:OE2	1:E:741:ARG:NH1	2.33	0.62
1:I:738:GLU:OE2	1:I:741:ARG:NH1	2.33	0.62
1:L:226:HIS:N	1:L:227:PRO:CD	2.60	0.62
1:C:551:TRP:HB2	1:C:582:ILE:HD12	1.79	0.62
1:G:738:GLU:OE2	1:G:741:ARG:NH1	2.33	0.62
1:J:674:PHE:O	1:J:678:MET:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:PHE:O	1:A:678:MET:HG2	2.00	0.62
1:B:738:GLU:OE2	1:B:741:ARG:NH1	2.32	0.62
1:A:551:TRP:HB2	1:A:582:ILE:HD12	1.81	0.61
1:J:551:TRP:HB2	1:J:582:ILE:HD12	1.80	0.61
1:J:738:GLU:OE2	1:J:741:ARG:NH1	2.33	0.61
1:F:738:GLU:OE2	1:F:741:ARG:NH1	2.33	0.61
1:C:674:PHE:O	1:C:678:MET:HG2	1.99	0.61
1:G:226:HIS:N	1:G:227:PRO:CD	2.60	0.61
1:H:599:ARG:O	1:H:603:GLN:N	2.29	0.61
1:I:758:PHE:O	1:I:762:LEU:CG	2.47	0.61
1:L:515:LEU:HD11	1:L:629:ILE:HD13	1.83	0.61
1:A:738:GLU:OE2	1:A:741:ARG:NH1	2.33	0.61
1:D:738:GLU:OE2	1:D:741:ARG:NH1	2.33	0.61
1:F:226:HIS:N	1:F:227:PRO:CD	2.60	0.61
1:H:580:ASP:O	1:H:584:LYS:N	2.32	0.61
1:J:599:ARG:O	1:J:603:GLN:N	2.30	0.61
1:L:674:PHE:O	1:L:678:MET:HG2	2.00	0.61
1:A:515:LEU:HD11	1:A:629:ILE:HD13	1.82	0.61
1:E:226:HIS:N	1:E:227:PRO:CD	2.60	0.61
1:H:738:GLU:OE2	1:H:741:ARG:NH1	2.33	0.61
1:H:515:LEU:HD11	1:H:629:ILE:HD13	1.82	0.60
1:A:685:ALA:N	2:A:900:JDP:N31	2.49	0.60
1:H:226:HIS:N	1:H:227:PRO:CD	2.60	0.60
1:B:305:GLU:OE2	1:C:362:ARG:NH2	2.35	0.60
1:J:479:ILE:HA	2:J:900:JDP:C17	2.31	0.60
1:A:226:HIS:N	1:A:227:PRO:CD	2.60	0.60
1:A:597:ALA:C	1:A:599:ARG:N	2.55	0.60
1:I:515:LEU:HD11	1:I:629:ILE:HD13	1.82	0.60
1:C:515:LEU:HD11	1:C:629:ILE:HD13	1.82	0.60
1:D:551:TRP:HB2	1:D:582:ILE:HD12	1.82	0.60
1:B:515:LEU:HD11	1:B:629:ILE:HD13	1.83	0.59
1:E:515:LEU:HD11	1:E:629:ILE:HD13	1.83	0.59
1:G:515:LEU:HD11	1:G:629:ILE:HD13	1.85	0.59
1:B:597:ALA:C	1:B:599:ARG:N	2.55	0.59
1:I:693:ARG:HH11	1:I:693:ARG:HG2	1.68	0.59
1:H:241:ILE:O	1:H:344:MET:HA	2.03	0.59
1:L:597:ALA:C	1:L:599:ARG:N	2.55	0.59
1:C:223:PRO:HB2	1:C:237:PRO:HB3	1.85	0.59
1:D:597:ALA:C	1:D:599:ARG:N	2.55	0.59
1:E:580:ASP:O	1:E:584:LYS:N	2.32	0.59
1:K:226:HIS:N	1:K:227:PRO:CD	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ILE:O	1:E:344:MET:HA	2.03	0.59
1:F:597:ALA:C	1:F:599:ARG:N	2.55	0.59
1:I:241:ILE:O	1:I:344:MET:HA	2.03	0.58
1:I:706:GLU:OE1	1:J:502:LYS:NZ	2.36	0.58
1:B:599:ARG:O	1:B:603:GLN:N	2.30	0.58
1:G:693:ARG:HH11	1:G:693:ARG:HG2	1.68	0.58
1:L:693:ARG:HG2	1:L:693:ARG:HH11	1.68	0.58
1:A:241:ILE:O	1:A:344:MET:HA	2.04	0.58
1:C:693:ARG:HG2	1:C:693:ARG:HH11	1.68	0.58
1:F:599:ARG:O	1:F:603:GLN:N	2.29	0.58
1:H:693:ARG:HG2	1:H:693:ARG:HH11	1.68	0.58
1:J:597:ALA:C	1:J:599:ARG:N	2.55	0.58
1:G:241:ILE:O	1:G:344:MET:HA	2.03	0.58
1:B:693:ARG:HH11	1:B:693:ARG:HG2	1.68	0.58
1:D:515:LEU:HD11	1:D:629:ILE:HD13	1.84	0.58
1:F:580:ASP:O	1:F:584:LYS:N	2.32	0.58
1:I:223:PRO:HB2	1:I:237:PRO:HB3	1.86	0.58
1:K:223:PRO:HB2	1:K:237:PRO:HB3	1.86	0.58
1:E:693:ARG:HG2	1:E:693:ARG:HH11	1.68	0.58
1:F:515:LEU:HD11	1:F:629:ILE:HD13	1.85	0.58
1:K:580:ASP:O	1:K:584:LYS:N	2.31	0.58
1:A:693:ARG:HG2	1:A:693:ARG:HH11	1.68	0.58
1:D:580:ASP:O	1:D:584:LYS:N	2.31	0.58
1:J:693:ARG:HG2	1:J:693:ARG:HH11	1.68	0.58
1:L:241:ILE:O	1:L:344:MET:HA	2.03	0.58
1:C:241:ILE:O	1:C:344:MET:HA	2.03	0.58
1:K:241:ILE:O	1:K:344:MET:HA	2.03	0.58
1:D:693:ARG:HG2	1:D:693:ARG:HH11	1.68	0.57
1:E:597:ALA:C	1:E:599:ARG:N	2.55	0.57
1:B:241:ILE:O	1:B:344:MET:HA	2.03	0.57
1:K:693:ARG:HG2	1:K:693:ARG:HH11	1.69	0.57
1:C:580:ASP:O	1:C:584:LYS:N	2.32	0.57
1:H:223:PRO:HB2	1:H:237:PRO:HB3	1.86	0.57
1:J:241:ILE:O	1:J:344:MET:HA	2.03	0.57
1:D:223:PRO:HB2	1:D:237:PRO:HB3	1.87	0.57
1:F:241:ILE:O	1:F:344:MET:HA	2.04	0.57
1:K:597:ALA:C	1:K:599:ARG:N	2.55	0.57
1:A:223:PRO:HB2	1:A:237:PRO:HB3	1.86	0.57
1:D:241:ILE:O	1:D:344:MET:HA	2.04	0.57
1:F:693:ARG:HG2	1:F:693:ARG:HH11	1.69	0.57
1:A:634:LEU:HD22	1:A:642:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:597:ALA:C	1:H:599:ARG:N	2.55	0.57
1:A:552:PHE:CD2	1:B:599:ARG:HB2	2.40	0.56
1:F:684:GLY:HA3	2:F:900:JDP:C04	2.35	0.56
1:G:223:PRO:HB2	1:G:237:PRO:HB3	1.87	0.56
1:L:223:PRO:HB2	1:L:237:PRO:HB3	1.86	0.56
1:I:597:ALA:C	1:I:599:ARG:N	2.55	0.56
1:I:755:TYR:O	1:I:759:ALA:N	2.39	0.56
1:G:597:ALA:C	1:G:599:ARG:N	2.55	0.56
1:J:223:PRO:HB2	1:J:237:PRO:HB3	1.86	0.56
1:B:223:PRO:HB2	1:B:237:PRO:HB3	1.86	0.56
1:F:223:PRO:HB2	1:F:237:PRO:HB3	1.86	0.56
1:F:678:MET:SD	1:K:677:LYS:HE3	2.46	0.56
1:L:755:TYR:O	1:L:759:ALA:N	2.39	0.56
1:B:580:ASP:O	1:B:584:LYS:N	2.31	0.56
1:I:580:ASP:O	1:I:584:LYS:N	2.32	0.56
1:B:755:TYR:O	1:B:759:ALA:N	2.38	0.56
1:E:223:PRO:HB2	1:E:237:PRO:HB3	1.86	0.56
1:G:755:TYR:O	1:G:759:ALA:N	2.39	0.56
1:K:634:LEU:HD22	1:K:642:LEU:HD21	1.88	0.56
1:L:580:ASP:O	1:L:584:LYS:N	2.32	0.56
1:I:493:VAL:HG22	1:I:618:PHE:CE2	2.41	0.55
1:H:755:TYR:O	1:H:759:ALA:N	2.39	0.55
1:B:677:LYS:HD3	1:I:678:MET:HE3	1.88	0.55
1:E:755:TYR:O	1:E:759:ALA:N	2.39	0.55
1:K:755:TYR:O	1:K:759:ALA:N	2.39	0.55
1:L:479:ILE:HA	2:L:900:JDP:C17	2.37	0.55
1:C:758:PHE:O	1:C:762:LEU:CB	2.55	0.55
1:D:634:LEU:HD22	1:D:642:LEU:HD21	1.88	0.55
1:K:305:GLU:OE2	1:L:362:ARG:NH2	2.40	0.55
1:B:758:PHE:O	1:B:762:LEU:CB	2.55	0.55
1:F:758:PHE:O	1:F:762:LEU:CB	2.55	0.55
1:E:758:PHE:O	1:E:762:LEU:CB	2.55	0.55
1:J:493:VAL:HG22	1:J:618:PHE:CE2	2.42	0.55
1:J:580:ASP:O	1:J:584:LYS:N	2.31	0.55
1:K:526:LEU:HD21	2:K:900:JDP:N30	2.21	0.55
1:B:634:LEU:HD22	1:B:642:LEU:HD21	1.88	0.55
1:J:758:PHE:O	1:J:762:LEU:HB2	2.07	0.55
1:L:493:VAL:HG22	1:L:618:PHE:CE2	2.42	0.55
1:C:493:VAL:HG22	1:C:618:PHE:CE2	2.42	0.54
1:D:703:ILE:HD11	1:E:495:TYR:CZ	2.42	0.54
1:G:758:PHE:O	1:G:762:LEU:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:PHE:O	1:A:762:LEU:HB2	2.08	0.54
1:C:597:ALA:C	1:C:599:ARG:N	2.55	0.54
1:D:758:PHE:O	1:D:762:LEU:CB	2.55	0.54
1:G:634:LEU:HD22	1:G:642:LEU:HD21	1.89	0.54
1:B:678:MET:HE3	1:I:677:LYS:HD3	1.88	0.54
1:E:634:LEU:HD22	1:E:642:LEU:HD21	1.89	0.54
1:F:758:PHE:O	1:F:762:LEU:HB2	2.07	0.54
1:A:755:TYR:O	1:A:759:ALA:N	2.39	0.54
1:B:493:VAL:HG22	1:B:618:PHE:CE2	2.42	0.54
1:E:758:PHE:O	1:E:762:LEU:HB2	2.07	0.54
1:G:580:ASP:O	1:G:584:LYS:N	2.32	0.54
1:H:758:PHE:O	1:H:762:LEU:CB	2.55	0.54
1:I:634:LEU:HD22	1:I:642:LEU:HD21	1.90	0.54
1:K:758:PHE:O	1:K:762:LEU:CB	2.55	0.54
1:K:515:LEU:HD11	1:K:629:ILE:CD1	2.38	0.54
1:A:758:PHE:O	1:A:762:LEU:CB	2.55	0.54
1:E:493:VAL:HG22	1:E:618:PHE:CE2	2.41	0.54
1:H:493:VAL:HG22	1:H:618:PHE:CE2	2.41	0.54
1:L:758:PHE:O	1:L:762:LEU:CB	2.55	0.54
1:A:493:VAL:HG22	1:A:618:PHE:CE2	2.42	0.54
1:C:758:PHE:O	1:C:762:LEU:HB2	2.07	0.54
1:D:698:ALA:HB1	1:E:506:PHE:CE1	2.42	0.54
1:G:493:VAL:HG22	1:G:618:PHE:CE2	2.43	0.54
1:G:758:PHE:O	1:G:762:LEU:HB2	2.07	0.54
1:I:758:PHE:O	1:I:762:LEU:CB	2.56	0.54
1:J:755:TYR:O	1:J:759:ALA:N	2.39	0.54
1:F:493:VAL:HG22	1:F:618:PHE:CE2	2.42	0.54
1:H:515:LEU:HD11	1:H:629:ILE:CD1	2.38	0.54
1:I:758:PHE:O	1:I:762:LEU:HB2	2.08	0.54
1:J:515:LEU:HD11	1:J:629:ILE:CD1	2.38	0.54
1:J:634:LEU:HD22	1:J:642:LEU:HD21	1.89	0.54
1:J:758:PHE:O	1:J:762:LEU:CB	2.55	0.54
1:L:634:LEU:HD22	1:L:642:LEU:HD21	1.89	0.54
1:A:580:ASP:O	1:A:584:LYS:N	2.32	0.54
1:B:758:PHE:O	1:B:762:LEU:HB2	2.07	0.54
1:D:493:VAL:HG22	1:D:618:PHE:CE2	2.42	0.54
1:D:755:TYR:O	1:D:759:ALA:N	2.39	0.54
1:F:755:TYR:O	1:F:759:ALA:N	2.39	0.54
1:K:493:VAL:HG22	1:K:618:PHE:CE2	2.41	0.54
1:L:515:LEU:CD1	1:L:634:LEU:HD21	2.35	0.54
1:E:515:LEU:HD11	1:E:629:ILE:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:479:ILE:HA	2:H:900:JDP:C17	2.38	0.54
1:L:515:LEU:HD11	1:L:629:ILE:CD1	2.38	0.54
1:H:758:PHE:O	1:H:762:LEU:HB2	2.07	0.53
1:A:479:ILE:HA	2:A:900:JDP:C17	2.37	0.53
1:A:502:LYS:NZ	1:F:706:GLU:OE1	2.42	0.53
1:A:495:TYR:CE1	1:F:703:ILE:HD11	2.43	0.53
1:F:677:LYS:HE3	1:K:678:MET:SD	2.49	0.53
1:A:515:LEU:HD11	1:A:629:ILE:CD1	2.38	0.53
1:C:755:TYR:O	1:C:759:ALA:N	2.39	0.53
1:K:758:PHE:O	1:K:762:LEU:HB2	2.08	0.53
1:L:758:PHE:O	1:L:762:LEU:HB2	2.07	0.53
1:B:515:LEU:HD11	1:B:629:ILE:CD1	2.39	0.53
1:C:634:LEU:HD22	1:C:642:LEU:HD21	1.90	0.53
2:F:900:JDP:C11	2:F:900:JDP:N30	2.70	0.53
1:I:225:ARG:C	1:I:227:PRO:HD3	2.29	0.53
1:B:678:MET:SD	1:I:677:LYS:HE3	2.49	0.53
1:D:678:MET:HE3	1:G:677:LYS:HD3	1.89	0.53
1:D:758:PHE:O	1:D:762:LEU:HB2	2.07	0.53
1:G:515:LEU:HD11	1:G:629:ILE:CD1	2.39	0.53
1:I:515:LEU:HD11	1:I:629:ILE:CD1	2.38	0.53
1:K:515:LEU:CD1	1:K:634:LEU:HD21	2.36	0.53
1:H:634:LEU:HD22	1:H:642:LEU:HD21	1.89	0.53
1:D:758:PHE:O	1:D:762:LEU:CD1	2.58	0.52
1:I:758:PHE:O	1:I:762:LEU:CD1	2.57	0.52
1:A:758:PHE:O	1:A:762:LEU:CD1	2.57	0.52
1:C:515:LEU:HD11	1:C:629:ILE:CD1	2.39	0.52
1:C:758:PHE:O	1:C:762:LEU:CD1	2.57	0.52
1:F:515:LEU:HD11	1:F:629:ILE:CD1	2.40	0.52
1:F:548:LEU:HD22	1:F:552:PHE:CE2	2.45	0.52
1:B:225:ARG:C	1:B:227:PRO:HD3	2.29	0.52
1:B:758:PHE:O	1:B:762:LEU:CD1	2.57	0.52
1:D:515:LEU:HD11	1:D:629:ILE:CD1	2.39	0.52
1:H:678:MET:HE2	1:H:678:MET:CA	2.39	0.52
1:K:225:ARG:C	1:K:227:PRO:HD3	2.30	0.52
1:F:225:ARG:C	1:F:227:PRO:HD3	2.30	0.52
1:G:495:TYR:CE1	1:L:703:ILE:HD11	2.44	0.52
1:H:758:PHE:O	1:H:762:LEU:CD1	2.58	0.52
2:J:900:JDP:N14	2:J:900:JDP:C06	2.71	0.52
1:E:758:PHE:O	1:E:762:LEU:CD1	2.58	0.52
1:L:225:ARG:C	1:L:227:PRO:HD3	2.29	0.52
1:A:598:ASP:O	1:A:602:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ILE:HA	2:C:900:JDP:C17	2.40	0.52
1:D:225:ARG:C	1:D:227:PRO:HD3	2.29	0.52
1:G:678:MET:HA	1:G:678:MET:HE2	1.92	0.52
1:K:758:PHE:O	1:K:762:LEU:CD1	2.57	0.52
1:A:698:ALA:HB1	1:B:506:PHE:CE1	2.44	0.52
1:G:225:ARG:C	1:G:227:PRO:HD3	2.29	0.52
1:G:758:PHE:O	1:G:762:LEU:CD1	2.57	0.52
1:H:305:GLU:OE2	1:I:362:ARG:NH2	2.42	0.52
1:H:598:ASP:O	1:H:602:ASN:N	2.43	0.52
1:A:225:ARG:C	1:A:227:PRO:HD3	2.29	0.52
1:G:706:GLU:OE1	1:H:502:LYS:NZ	2.42	0.52
1:J:702:SER:OG	1:K:502:LYS:HE2	2.10	0.52
1:J:758:PHE:O	1:J:762:LEU:CD1	2.57	0.52
1:C:515:LEU:CD1	1:C:634:LEU:HD21	2.35	0.51
1:K:703:ILE:HD11	1:L:495:TYR:CZ	2.45	0.51
1:L:598:ASP:O	1:L:602:ASN:N	2.43	0.51
1:E:225:ARG:C	1:E:227:PRO:HD3	2.30	0.51
1:H:225:ARG:C	1:H:227:PRO:HD3	2.30	0.51
1:J:225:ARG:C	1:J:227:PRO:HD3	2.29	0.51
1:J:598:ASP:O	1:J:602:ASN:N	2.43	0.51
1:G:456:LEU:HD22	1:H:614:LYS:CE	2.39	0.51
1:E:515:LEU:CD1	1:E:634:LEU:HD21	2.36	0.51
1:E:598:ASP:O	1:E:602:ASN:N	2.43	0.51
1:D:598:ASP:O	1:D:602:ASN:N	2.43	0.51
1:F:598:ASP:O	1:F:602:ASN:N	2.44	0.51
1:I:598:ASP:O	1:I:602:ASN:N	2.43	0.51
1:L:758:PHE:O	1:L:762:LEU:CD1	2.57	0.51
1:A:515:LEU:CD1	1:A:634:LEU:HD21	2.36	0.51
1:B:596:ALA:C	1:B:599:ARG:HB3	2.31	0.51
1:C:225:ARG:C	1:C:227:PRO:HD3	2.30	0.51
1:G:515:LEU:CD1	1:G:634:LEU:HD21	2.36	0.51
1:F:634:LEU:HD22	1:F:642:LEU:HD21	1.92	0.51
1:K:598:ASP:O	1:K:602:ASN:N	2.43	0.51
1:E:624:ASN:OD1	1:E:624:ASN:N	2.44	0.51
1:F:758:PHE:O	1:F:762:LEU:CD1	2.57	0.51
1:G:598:ASP:O	1:G:602:ASN:N	2.43	0.51
1:C:665:PRO:O	1:C:731:ILE:HG22	2.12	0.50
1:D:677:LYS:HD3	1:G:678:MET:HE3	1.94	0.50
1:L:596:ALA:C	1:L:599:ARG:HB3	2.31	0.50
1:A:596:ALA:C	1:A:599:ARG:HB3	2.32	0.50
1:B:624:ASN:OD1	1:B:624:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:ALA:C	1:C:599:ARG:HB3	2.32	0.50
1:C:684:GLY:HA3	2:C:900:JDP:C04	2.42	0.50
1:E:596:ALA:C	1:E:599:ARG:HB3	2.32	0.50
1:K:596:ALA:C	1:K:599:ARG:HB3	2.32	0.50
1:A:624:ASN:N	1:A:624:ASN:OD1	2.45	0.50
1:B:598:ASP:O	1:B:602:ASN:N	2.44	0.50
1:D:665:PRO:O	1:D:731:ILE:HG22	2.12	0.50
1:F:596:ALA:C	1:F:599:ARG:HB3	2.32	0.50
1:H:515:LEU:CD1	1:H:634:LEU:HD21	2.36	0.50
1:I:665:PRO:O	1:I:731:ILE:HG22	2.11	0.50
1:B:320:VAL:HB	1:C:319:GLU:OE1	2.11	0.50
1:C:598:ASP:O	1:C:602:ASN:N	2.43	0.50
1:K:758:PHE:O	1:K:762:LEU:HG	2.12	0.50
1:F:520:PRO:HG3	1:F:624:ASN:HD22	1.77	0.50
1:H:665:PRO:O	1:H:731:ILE:HG22	2.12	0.50
1:K:624:ASN:N	1:K:624:ASN:OD1	2.45	0.50
1:L:665:PRO:O	1:L:731:ILE:HG22	2.12	0.50
1:C:239:ARG:NH2	1:C:332:MET:O	2.45	0.50
1:D:758:PHE:O	1:D:762:LEU:HG	2.13	0.49
1:F:624:ASN:N	1:F:624:ASN:OD1	2.45	0.49
1:H:596:ALA:C	1:H:599:ARG:HB3	2.32	0.49
1:I:596:ALA:C	1:I:599:ARG:HB3	2.31	0.49
1:A:239:ARG:NH2	1:A:332:MET:O	2.46	0.49
1:F:495:TYR:N	1:F:496:PRO:HD2	2.27	0.49
1:H:239:ARG:NH2	1:H:332:MET:O	2.45	0.49
1:D:239:ARG:NH2	1:D:332:MET:O	2.45	0.49
1:D:460:ASN:OD1	1:E:615:LYS:NZ	2.43	0.49
1:D:596:ALA:C	1:D:599:ARG:HB3	2.32	0.49
1:J:239:ARG:NH2	1:J:332:MET:O	2.45	0.49
1:J:665:PRO:O	1:J:731:ILE:HG22	2.12	0.49
1:A:495:TYR:N	1:A:496:PRO:HD2	2.28	0.49
1:B:665:PRO:O	1:B:731:ILE:HG22	2.12	0.49
1:B:678:MET:HA	1:B:678:MET:HE2	1.94	0.49
1:D:495:TYR:N	1:D:496:PRO:HD2	2.28	0.49
1:E:665:PRO:O	1:E:731:ILE:HG22	2.12	0.49
1:F:239:ARG:NH2	1:F:332:MET:O	2.46	0.49
1:G:350:PRO:O	1:G:358:ARG:NH1	2.46	0.49
1:G:596:ALA:C	1:G:599:ARG:HB3	2.32	0.49
1:G:624:ASN:OD1	1:G:624:ASN:N	2.45	0.49
1:H:758:PHE:O	1:H:762:LEU:HG	2.12	0.49
1:I:495:TYR:N	1:I:496:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:596:ALA:C	1:J:599:ARG:HB3	2.32	0.49
1:A:758:PHE:O	1:A:762:LEU:HG	2.13	0.49
1:G:665:PRO:O	1:G:731:ILE:HG22	2.12	0.49
1:H:350:PRO:O	1:H:358:ARG:NH1	2.45	0.49
1:I:515:LEU:CD1	1:I:634:LEU:HD21	2.35	0.49
1:L:239:ARG:NH2	1:L:332:MET:O	2.45	0.49
1:L:495:TYR:N	1:L:496:PRO:HD2	2.28	0.49
1:D:624:ASN:OD1	1:D:624:ASN:N	2.45	0.49
1:I:624:ASN:OD1	1:I:624:ASN:N	2.45	0.49
1:K:495:TYR:N	1:K:496:PRO:HD2	2.28	0.49
1:K:665:PRO:O	1:K:731:ILE:HG22	2.12	0.49
1:F:665:PRO:O	1:F:731:ILE:HG22	2.12	0.49
1:G:239:ARG:NH2	1:G:332:MET:O	2.46	0.49
1:H:495:TYR:N	1:H:496:PRO:HD2	2.28	0.49
1:I:239:ARG:NH2	1:I:332:MET:O	2.45	0.49
1:L:350:PRO:O	1:L:358:ARG:NH1	2.46	0.49
1:B:239:ARG:NH2	1:B:332:MET:O	2.46	0.49
1:C:624:ASN:N	1:C:624:ASN:OD1	2.45	0.49
1:E:350:PRO:O	1:E:358:ARG:NH1	2.46	0.49
1:G:495:TYR:N	1:G:496:PRO:HD2	2.28	0.49
1:K:350:PRO:O	1:K:358:ARG:NH1	2.46	0.49
1:A:350:PRO:O	1:A:358:ARG:NH1	2.46	0.48
1:E:239:ARG:NH2	1:E:332:MET:O	2.46	0.48
1:F:350:PRO:O	1:F:358:ARG:NH1	2.46	0.48
1:F:758:PHE:O	1:F:762:LEU:HG	2.12	0.48
1:J:495:TYR:N	1:J:496:PRO:HD2	2.28	0.48
1:B:350:PRO:O	1:B:358:ARG:NH1	2.47	0.48
1:C:350:PRO:O	1:C:358:ARG:NH1	2.46	0.48
1:I:520:PRO:HG3	1:I:624:ASN:HD22	1.79	0.48
1:C:758:PHE:O	1:C:762:LEU:HG	2.13	0.48
1:D:350:PRO:O	1:D:358:ARG:NH1	2.46	0.48
1:H:624:ASN:N	1:H:624:ASN:OD1	2.45	0.48
1:I:758:PHE:O	1:I:762:LEU:HG	2.12	0.48
1:B:495:TYR:N	1:B:496:PRO:HD2	2.28	0.48
1:C:495:TYR:N	1:C:496:PRO:HD2	2.27	0.48
1:E:758:PHE:O	1:E:762:LEU:HG	2.13	0.48
1:I:350:PRO:O	1:I:358:ARG:NH1	2.46	0.48
1:I:656:ILE:HD11	2:I:900:JDP:C20	2.43	0.48
1:L:624:ASN:OD1	1:L:624:ASN:N	2.45	0.48
1:A:665:PRO:O	1:A:731:ILE:HG22	2.13	0.48
1:J:350:PRO:O	1:J:358:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:515:LEU:CD1	1:J:634:LEU:HD21	2.36	0.48
1:J:758:PHE:O	1:J:762:LEU:HG	2.13	0.48
1:C:351:ASN:HD21	1:C:561:GLU:HG3	1.78	0.48
1:G:351:ASN:HD21	1:G:561:GLU:HG3	1.78	0.48
1:K:239:ARG:NH2	1:K:332:MET:O	2.46	0.48
1:A:520:PRO:HG3	1:A:624:ASN:HD22	1.79	0.48
1:D:596:ALA:O	1:D:599:ARG:HB3	2.14	0.48
1:C:596:ALA:O	1:C:599:ARG:HB3	2.14	0.48
1:J:520:PRO:HG3	1:J:624:ASN:HD22	1.79	0.48
1:A:491:GLU:HA	1:A:495:TYR:CD2	2.49	0.47
1:E:596:ALA:O	1:E:599:ARG:HB3	2.14	0.47
1:G:596:ALA:O	1:G:599:ARG:HB3	2.15	0.47
1:J:596:ALA:O	1:J:599:ARG:HB3	2.15	0.47
1:J:703:ILE:HD11	1:K:495:TYR:CZ	2.48	0.47
1:L:526:LEU:HD21	2:L:900:JDP:N30	2.29	0.47
1:B:491:GLU:HA	1:B:495:TYR:CD2	2.50	0.47
1:C:678:MET:SD	1:H:677:LYS:HE3	2.55	0.47
1:D:515:LEU:HB3	1:D:642:LEU:HD23	1.96	0.47
1:L:758:PHE:O	1:L:762:LEU:HG	2.12	0.47
1:A:362:ARG:NH2	1:F:305:GLU:OE2	2.47	0.47
1:C:520:PRO:HG3	1:C:624:ASN:HD22	1.79	0.47
1:F:515:LEU:CD1	1:F:634:LEU:HD21	2.36	0.47
1:F:548:LEU:HD22	1:F:552:PHE:HE2	1.79	0.47
1:J:624:ASN:OD1	1:J:624:ASN:N	2.45	0.47
1:B:515:LEU:CD1	1:B:634:LEU:HD21	2.36	0.47
1:E:520:PRO:HG3	1:E:624:ASN:HD22	1.80	0.47
1:F:596:ALA:O	1:F:599:ARG:HB3	2.14	0.47
1:G:320:VAL:HB	1:H:319:GLU:OE1	2.14	0.47
1:I:596:ALA:O	1:I:599:ARG:HB3	2.14	0.47
1:J:526:LEU:HD21	2:J:900:JDP:N30	2.29	0.47
1:L:483:GLU:O	1:L:486:LYS:HB2	2.15	0.47
1:A:552:PHE:CB	1:B:599:ARG:HD2	2.44	0.47
1:B:758:PHE:O	1:B:762:LEU:HG	2.14	0.47
1:C:305:GLU:OE2	1:D:362:ARG:NH2	2.48	0.47
1:C:491:GLU:HA	1:C:495:TYR:CD2	2.50	0.47
1:F:491:GLU:HA	1:F:495:TYR:CD2	2.50	0.47
1:B:596:ALA:O	1:B:599:ARG:HB3	2.15	0.47
1:B:678:MET:HE2	1:B:678:MET:CA	2.45	0.47
1:D:598:ASP:O	1:D:602:ASN:HB2	2.15	0.47
1:E:495:TYR:N	1:E:496:PRO:HD2	2.28	0.47
1:L:520:PRO:HG3	1:L:624:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:596:ALA:O	1:L:599:ARG:HB3	2.14	0.47
1:A:351:ASN:HD21	1:A:561:GLU:HG3	1.79	0.47
1:A:596:ALA:O	1:A:599:ARG:HB3	2.14	0.47
1:C:703:ILE:HD11	1:D:495:TYR:CZ	2.50	0.47
1:E:491:GLU:HA	1:E:495:TYR:CD2	2.50	0.47
1:H:515:LEU:HB3	1:H:642:LEU:HD23	1.97	0.47
1:J:491:GLU:HA	1:J:495:TYR:CD2	2.50	0.47
1:L:491:GLU:HA	1:L:495:TYR:CD2	2.50	0.47
1:A:678:MET:HE2	1:A:678:MET:CA	2.44	0.47
1:E:515:LEU:HG	1:E:621:GLY:O	2.15	0.47
1:H:491:GLU:HA	1:H:495:TYR:CD2	2.50	0.47
1:H:685:ALA:N	2:H:900:JDP:N31	2.63	0.47
1:B:520:PRO:HG3	1:B:624:ASN:HD22	1.80	0.47
1:D:515:LEU:CD1	1:D:634:LEU:HD21	2.36	0.47
1:F:483:GLU:O	1:F:486:LYS:HB2	2.15	0.47
1:G:491:GLU:HA	1:G:495:TYR:CD2	2.50	0.47
1:G:520:PRO:HG3	1:G:624:ASN:HD22	1.79	0.47
1:H:526:LEU:CD2	2:H:900:JDP:C29	2.92	0.47
1:H:596:ALA:O	1:H:599:ARG:HB3	2.15	0.47
1:I:491:GLU:HA	1:I:495:TYR:CD2	2.50	0.47
1:J:515:LEU:HB3	1:J:642:LEU:HD23	1.96	0.47
1:A:598:ASP:O	1:A:602:ASN:HB2	2.15	0.47
1:D:483:GLU:O	1:D:486:LYS:HB2	2.15	0.47
1:D:491:GLU:HA	1:D:495:TYR:CD2	2.50	0.47
1:E:515:LEU:HB3	1:E:642:LEU:HD23	1.97	0.47
1:J:483:GLU:O	1:J:486:LYS:HB2	2.15	0.47
1:B:483:GLU:O	1:B:486:LYS:HB2	2.15	0.46
1:K:596:ALA:O	1:K:599:ARG:HB3	2.15	0.46
1:L:515:LEU:HB3	1:L:642:LEU:HD23	1.97	0.46
1:C:556:GLU:O	1:C:557:ALA:C	2.53	0.46
1:G:678:MET:HE2	1:G:678:MET:CA	2.44	0.46
1:K:515:LEU:HB3	1:K:642:LEU:HD23	1.96	0.46
1:A:483:GLU:O	1:A:486:LYS:HB2	2.15	0.46
1:A:515:LEU:HB3	1:A:642:LEU:HD23	1.97	0.46
2:C:900:JDP:C11	2:C:900:JDP:N30	2.78	0.46
1:G:360:PHE:CD1	1:L:409:ALA:HB1	2.51	0.46
1:G:506:PHE:CE1	1:L:698:ALA:HB1	2.51	0.46
1:G:758:PHE:O	1:G:762:LEU:HG	2.13	0.46
1:H:520:PRO:HG3	1:H:624:ASN:HD22	1.80	0.46
1:K:491:GLU:HA	1:K:495:TYR:CD2	2.50	0.46
1:K:515:LEU:HG	1:K:621:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HB3	1:B:642:LEU:HD23	1.97	0.46
1:C:483:GLU:O	1:C:486:LYS:HB2	2.15	0.46
1:F:556:GLU:O	1:F:557:ALA:C	2.54	0.46
1:G:493:VAL:HG22	1:G:618:PHE:CG	2.51	0.46
1:I:483:GLU:O	1:I:486:LYS:HB2	2.15	0.46
1:J:351:ASN:HD21	1:J:561:GLU:HG3	1.80	0.46
1:K:223:PRO:CB	1:K:237:PRO:HB3	2.46	0.46
1:K:556:GLU:O	1:K:557:ALA:C	2.54	0.46
1:L:653:ARG:CZ	1:L:679:THR:O	2.64	0.46
1:E:483:GLU:O	1:E:486:LYS:HB2	2.15	0.46
1:G:598:ASP:O	1:G:602:ASN:HB2	2.15	0.46
1:H:653:ARG:CZ	1:H:679:THR:O	2.64	0.46
1:I:515:LEU:HG	1:I:621:GLY:O	2.16	0.46
1:A:515:LEU:HG	1:A:621:GLY:O	2.16	0.46
1:A:653:ARG:CZ	1:A:679:THR:O	2.64	0.46
1:B:556:GLU:O	1:B:557:ALA:C	2.53	0.46
1:D:493:VAL:HG22	1:D:618:PHE:CG	2.51	0.46
1:G:483:GLU:O	1:G:486:LYS:HB2	2.15	0.46
1:I:653:ARG:CZ	1:I:679:THR:O	2.63	0.46
1:K:483:GLU:O	1:K:486:LYS:HB2	2.15	0.46
1:L:515:LEU:HG	1:L:621:GLY:O	2.16	0.46
1:C:493:VAL:HG22	1:C:618:PHE:CG	2.51	0.46
1:D:515:LEU:HG	1:D:621:GLY:O	2.15	0.46
1:G:515:LEU:HG	1:G:621:GLY:O	2.16	0.46
1:G:703:ILE:HD11	1:H:495:TYR:CE1	2.50	0.46
1:A:693:ARG:O	1:A:697:LEU:HG	2.16	0.46
1:L:678:MET:HE2	1:L:678:MET:CA	2.43	0.46
1:A:556:GLU:O	1:A:557:ALA:C	2.53	0.46
1:D:667:ALA:HB3	1:D:732:ARG:HG2	1.98	0.46
1:G:515:LEU:HB3	1:G:642:LEU:HD23	1.98	0.46
1:H:483:GLU:O	1:H:486:LYS:HB2	2.15	0.46
1:H:515:LEU:HG	1:H:621:GLY:O	2.16	0.46
1:J:556:GLU:O	1:J:557:ALA:C	2.54	0.46
1:J:653:ARG:CZ	1:J:679:THR:O	2.64	0.46
1:B:653:ARG:CZ	1:B:679:THR:O	2.64	0.46
1:C:515:LEU:HG	1:C:621:GLY:O	2.15	0.46
1:D:647:LEU:HD21	1:D:747:VAL:HG11	1.97	0.46
1:E:633:ILE:CG2	1:E:639:LEU:HD12	2.46	0.46
1:F:493:VAL:HG22	1:F:618:PHE:CG	2.50	0.46
1:I:493:VAL:HG22	1:I:618:PHE:CG	2.51	0.46
1:J:515:LEU:HG	1:J:621:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:520:PRO:HG3	1:K:624:ASN:HD22	1.81	0.46
1:L:493:VAL:HG22	1:L:618:PHE:CG	2.51	0.46
1:L:556:GLU:O	1:L:557:ALA:C	2.54	0.46
1:A:493:VAL:HG22	1:A:618:PHE:CG	2.51	0.45
1:B:515:LEU:HG	1:B:621:GLY:O	2.16	0.45
1:F:598:ASP:O	1:F:602:ASN:HB2	2.16	0.45
1:J:493:VAL:HG22	1:J:618:PHE:CG	2.51	0.45
1:K:493:VAL:HG22	1:K:618:PHE:CG	2.51	0.45
1:B:647:LEU:HD21	1:B:747:VAL:HG11	1.98	0.45
1:D:520:PRO:HG3	1:D:624:ASN:HD22	1.81	0.45
1:E:556:GLU:O	1:E:557:ALA:C	2.54	0.45
1:E:653:ARG:CZ	1:E:679:THR:O	2.64	0.45
1:F:653:ARG:CZ	1:F:679:THR:O	2.64	0.45
1:H:493:VAL:HG22	1:H:618:PHE:CG	2.51	0.45
1:I:556:GLU:O	1:I:557:ALA:C	2.54	0.45
1:I:633:ILE:CG2	1:I:639:LEU:HD12	2.46	0.45
1:K:647:LEU:HD21	1:K:747:VAL:HG11	1.98	0.45
1:A:647:LEU:HD21	1:A:747:VAL:HG11	1.98	0.45
2:A:900:JDP:C06	2:A:900:JDP:N14	2.72	0.45
1:D:653:ARG:CZ	1:D:679:THR:O	2.64	0.45
1:H:556:GLU:O	1:H:557:ALA:C	2.54	0.45
1:K:598:ASP:O	1:K:602:ASN:HB2	2.17	0.45
1:F:515:LEU:HG	1:F:621:GLY:O	2.16	0.45
1:F:515:LEU:HB3	1:F:642:LEU:HD23	1.98	0.45
1:K:667:ALA:HB3	1:K:732:ARG:HG2	1.98	0.45
1:K:693:ARG:O	1:K:697:LEU:HG	2.17	0.45
1:L:633:ILE:CG2	1:L:639:LEU:HD12	2.47	0.45
1:L:667:ALA:HB3	1:L:732:ARG:HG2	1.99	0.45
1:D:678:MET:HA	1:D:678:MET:HE2	1.98	0.45
1:H:465:ARG:HH22	1:I:610:GLY:HA3	1.81	0.45
1:I:598:ASP:O	1:I:602:ASN:HB2	2.17	0.45
1:I:693:ARG:O	1:I:697:LEU:HG	2.16	0.45
1:J:667:ALA:HB3	1:J:732:ARG:HG2	1.98	0.45
1:K:605:LEU:HD22	1:K:638:ARG:CZ	2.47	0.45
1:L:598:ASP:O	1:L:602:ASN:HB2	2.17	0.45
1:B:552:PHE:HB3	1:C:599:ARG:HD2	1.98	0.45
1:C:653:ARG:CZ	1:C:679:THR:O	2.64	0.45
1:D:693:ARG:O	1:D:697:LEU:HG	2.16	0.45
1:G:653:ARG:CZ	1:G:679:THR:O	2.64	0.45
1:K:653:ARG:CZ	1:K:679:THR:O	2.64	0.45
1:L:351:ASN:HD21	1:L:561:GLU:HG3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:VAL:HG22	1:E:618:PHE:CG	2.51	0.45
1:E:647:LEU:HD21	1:E:747:VAL:HG11	1.99	0.45
1:G:556:GLU:O	1:G:557:ALA:C	2.53	0.45
1:J:598:ASP:O	1:J:602:ASN:HB2	2.15	0.45
1:B:460:ASN:OD1	1:C:615:LYS:HE3	2.17	0.45
1:C:667:ALA:HB3	1:C:732:ARG:HG2	1.99	0.45
1:H:700:ARG:HH12	1:I:487:ARG:HB3	1.81	0.45
1:C:598:ASP:O	1:C:602:ASN:HB2	2.17	0.45
1:B:460:ASN:OD1	1:C:615:LYS:NZ	2.47	0.45
1:B:678:MET:CE	1:I:677:LYS:HB3	2.47	0.45
1:D:547:LEU:HD23	1:D:550:MET:HE2	1.99	0.45
1:E:598:ASP:O	1:E:602:ASN:HB2	2.17	0.45
1:B:493:VAL:HG22	1:B:618:PHE:CG	2.50	0.44
1:B:598:ASP:O	1:B:602:ASN:HB2	2.17	0.44
1:B:693:ARG:O	1:B:697:LEU:HG	2.17	0.44
1:H:598:ASP:O	1:H:602:ASN:HB2	2.17	0.44
1:J:484:ASP:OD1	1:J:484:ASP:N	2.50	0.44
1:J:693:ARG:O	1:J:697:LEU:HG	2.17	0.44
1:K:633:ILE:CG2	1:K:639:LEU:HD12	2.46	0.44
1:C:223:PRO:CB	1:C:237:PRO:HB3	2.47	0.44
1:D:556:GLU:O	1:D:557:ALA:C	2.54	0.44
1:F:599:ARG:CA	1:F:602:ASN:HB3	2.40	0.44
1:G:693:ARG:O	1:G:697:LEU:HG	2.17	0.44
1:H:693:ARG:O	1:H:697:LEU:HG	2.16	0.44
1:C:647:LEU:HD21	1:C:747:VAL:HG11	1.98	0.44
1:D:484:ASP:OD1	1:D:484:ASP:N	2.50	0.44
1:E:693:ARG:O	1:E:697:LEU:HG	2.17	0.44
1:F:647:LEU:HD21	1:F:747:VAL:HG11	1.99	0.44
1:G:491:GLU:HB2	1:L:700:ARG:NH2	2.32	0.44
1:G:633:ILE:CG2	1:G:639:LEU:HD12	2.48	0.44
1:L:484:ASP:N	1:L:484:ASP:OD1	2.50	0.44
1:B:633:ILE:CG2	1:B:639:LEU:HD12	2.48	0.44
1:C:494:GLN:HA	1:C:535:CYS:SG	2.58	0.44
1:G:550:MET:HE1	1:G:562:ILE:HD12	2.00	0.44
1:G:605:LEU:HD22	1:G:638:ARG:CZ	2.48	0.44
1:I:647:LEU:HD21	1:I:747:VAL:HG11	1.98	0.44
1:K:484:ASP:OD1	1:K:484:ASP:N	2.50	0.44
1:L:693:ARG:O	1:L:697:LEU:HG	2.17	0.44
1:C:515:LEU:HB3	1:C:642:LEU:HD23	1.98	0.44
1:E:351:ASN:HD21	1:E:561:GLU:HG3	1.83	0.44
1:E:484:ASP:N	1:E:484:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:515:LEU:HB3	1:I:642:LEU:HD23	1.98	0.44
1:C:693:ARG:O	1:C:697:LEU:HG	2.17	0.44
1:E:305:GLU:OE2	1:F:362:ARG:NH2	2.51	0.44
1:H:484:ASP:OD1	1:H:484:ASP:N	2.50	0.44
1:H:633:ILE:CG2	1:H:639:LEU:HD12	2.47	0.44
1:A:484:ASP:OD1	1:A:484:ASP:N	2.50	0.44
1:B:484:ASP:OD1	1:B:484:ASP:N	2.50	0.44
1:C:633:ILE:CG2	1:C:639:LEU:HD12	2.47	0.44
1:C:678:MET:HE2	1:C:678:MET:CA	2.44	0.44
1:E:479:ILE:HA	2:E:900:JDP:C17	2.47	0.44
1:F:667:ALA:HB3	1:F:732:ARG:HG2	2.00	0.44
1:H:647:LEU:HD21	1:H:747:VAL:HG11	1.98	0.44
1:I:667:ALA:HB3	1:I:732:ARG:HG2	1.98	0.44
1:J:633:ILE:CG2	1:J:639:LEU:HD12	2.48	0.44
1:J:647:LEU:HD21	1:J:747:VAL:HG11	1.99	0.44
1:B:479:ILE:HA	2:B:900:JDP:C17	2.48	0.44
1:D:663:LYS:O	1:D:663:LYS:HG3	2.18	0.44
1:F:484:ASP:OD1	1:F:484:ASP:N	2.50	0.44
1:G:647:LEU:HD21	1:G:747:VAL:HG11	1.99	0.44
1:I:494:GLN:HA	1:I:535:CYS:SG	2.58	0.44
1:D:351:ASN:HD21	1:D:561:GLU:HG3	1.82	0.44
1:D:633:ILE:CG2	1:D:639:LEU:HD12	2.48	0.44
1:E:667:ALA:HB3	1:E:732:ARG:HG2	1.99	0.44
1:F:494:GLN:HA	1:F:535:CYS:SG	2.58	0.44
1:G:484:ASP:OD1	1:G:484:ASP:N	2.50	0.44
1:H:605:LEU:HD22	1:H:638:ARG:CZ	2.48	0.44
1:K:494:GLN:HA	1:K:535:CYS:SG	2.58	0.44
1:B:663:LYS:O	1:B:663:LYS:HG3	2.18	0.43
1:D:494:GLN:HA	1:D:535:CYS:SG	2.58	0.43
1:F:351:ASN:HD21	1:F:561:GLU:HG3	1.82	0.43
1:A:667:ALA:HB3	1:A:732:ARG:HG2	1.99	0.43
1:C:249:THR:CG2	1:C:369:ILE:HG22	2.48	0.43
1:I:484:ASP:OD1	1:I:484:ASP:N	2.51	0.43
1:A:494:GLN:HA	1:A:535:CYS:SG	2.58	0.43
1:F:693:ARG:O	1:F:697:LEU:HG	2.17	0.43
1:H:351:ASN:HD21	1:H:561:GLU:HG3	1.82	0.43
1:A:633:ILE:CG2	1:A:639:LEU:HD12	2.48	0.43
1:A:663:LYS:HG3	1:A:663:LYS:O	2.18	0.43
1:C:484:ASP:OD1	1:C:484:ASP:N	2.51	0.43
1:D:678:MET:HE2	1:D:678:MET:CA	2.47	0.43
1:F:223:PRO:CB	1:F:237:PRO:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:633:ILE:CG2	1:F:639:LEU:HD12	2.48	0.43
1:I:678:MET:CA	1:I:678:MET:HE2	2.48	0.43
1:I:703:ILE:HD11	1:J:495:TYR:CE2	2.54	0.43
1:J:678:MET:HE2	1:J:678:MET:CA	2.44	0.43
1:B:494:GLN:HA	1:B:535:CYS:SG	2.59	0.43
1:B:605:LEU:HD22	1:B:638:ARG:CZ	2.48	0.43
1:H:320:VAL:HB	1:I:319:GLU:OE1	2.19	0.43
1:J:494:GLN:HA	1:J:535:CYS:SG	2.59	0.43
1:J:546:GLU:O	1:J:550:MET:HG3	2.19	0.43
1:J:605:LEU:HD22	1:J:638:ARG:CZ	2.48	0.43
1:L:494:GLN:HA	1:L:535:CYS:SG	2.58	0.43
1:E:605:LEU:HD22	1:E:638:ARG:CZ	2.48	0.43
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.01	0.43
1:L:526:LEU:CD2	2:L:900:JDP:C29	2.97	0.43
1:I:605:LEU:HD22	1:I:638:ARG:CZ	2.48	0.43
1:J:547:LEU:HD23	1:J:550:MET:HE2	2.01	0.43
1:L:547:LEU:HD23	1:L:550:MET:HE2	2.01	0.43
1:H:663:LYS:HG3	1:H:663:LYS:O	2.19	0.43
1:C:601:ILE:O	1:C:604:ILE:HB	2.19	0.43
1:D:605:LEU:HD22	1:D:638:ARG:CZ	2.48	0.43
1:K:601:ILE:O	1:K:604:ILE:HB	2.19	0.43
1:A:552:PHE:HB2	1:B:599:ARG:HD2	2.01	0.42
1:B:525:THR:HG22	1:B:529:LYS:HE3	2.01	0.42
1:B:547:LEU:HD23	1:B:550:MET:HE2	2.01	0.42
1:B:666:VAL:HG23	1:B:666:VAL:O	2.19	0.42
1:I:409:ALA:HB1	1:J:360:PHE:CD2	2.54	0.42
1:I:601:ILE:O	1:I:604:ILE:HB	2.19	0.42
1:L:546:GLU:O	1:L:550:MET:HG3	2.19	0.42
1:L:647:LEU:HD21	1:L:747:VAL:HG11	1.99	0.42
1:G:667:ALA:HB3	1:G:732:ARG:HG2	2.01	0.42
1:I:703:ILE:HD11	1:J:495:TYR:CE1	2.55	0.42
1:J:223:PRO:CB	1:J:237:PRO:HB3	2.49	0.42
1:J:685:ALA:N	2:J:900:JDP:N31	2.67	0.42
1:C:222:LEU:O	1:C:226:HIS:HB2	2.19	0.42
1:E:494:GLN:HA	1:E:535:CYS:SG	2.59	0.42
1:G:494:GLN:HA	1:G:535:CYS:SG	2.60	0.42
1:B:601:ILE:O	1:B:604:ILE:HB	2.20	0.42
1:E:666:VAL:HG23	1:E:666:VAL:O	2.20	0.42
1:E:703:ILE:HD11	1:F:495:TYR:CE1	2.54	0.42
1:G:601:ILE:O	1:G:604:ILE:HB	2.20	0.42
1:H:602:ASN:O	1:H:605:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:666:VAL:HG23	1:H:666:VAL:O	2.19	0.42
1:I:310:ALA:HA	1:I:325:VAL:HG22	2.02	0.42
1:I:479:ILE:HA	2:I:900:JDP:C17	2.49	0.42
1:C:230:PHE:HA	1:C:233:ILE:HG22	2.01	0.42
1:C:479:ILE:HD13	1:C:527:LEU:CD2	2.50	0.42
1:E:602:ASN:O	1:E:605:LEU:HB2	2.20	0.42
1:F:547:LEU:HA	1:F:550:MET:HE2	2.01	0.42
1:H:222:LEU:O	1:H:226:HIS:HB2	2.20	0.42
1:H:667:ALA:HB3	1:H:732:ARG:HG2	2.01	0.42
1:J:601:ILE:O	1:J:604:ILE:HB	2.19	0.42
1:K:526:LEU:HD21	2:K:900:JDP:C29	2.50	0.42
1:K:546:GLU:O	1:K:550:MET:HG3	2.20	0.42
1:B:546:GLU:O	1:B:550:MET:HG3	2.20	0.42
1:B:667:ALA:HB3	1:B:732:ARG:HG2	2.01	0.42
1:C:605:LEU:HD22	1:C:638:ARG:CZ	2.49	0.42
1:E:222:LEU:O	1:E:226:HIS:HB2	2.20	0.42
1:F:601:ILE:O	1:F:604:ILE:HB	2.20	0.42
1:G:598:ASP:O	1:G:602:ASN:CB	2.68	0.42
1:I:546:GLU:O	1:I:550:MET:HG3	2.19	0.42
1:L:601:ILE:O	1:L:604:ILE:HB	2.19	0.42
1:B:479:ILE:HD13	1:B:527:LEU:CD2	2.50	0.42
1:D:601:ILE:O	1:D:604:ILE:HB	2.19	0.42
1:E:547:LEU:HD23	1:E:550:MET:HE2	2.01	0.42
1:I:249:THR:CG2	1:I:369:ILE:HG22	2.50	0.42
1:I:678:MET:HE2	1:I:678:MET:HA	2.00	0.42
1:L:222:LEU:O	1:L:226:HIS:HB2	2.20	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.92	0.42
1:A:546:GLU:O	1:A:550:MET:HG3	2.19	0.42
1:A:602:ASN:O	1:A:605:LEU:HB2	2.20	0.42
1:D:551:TRP:CD1	1:D:551:TRP:C	2.93	0.42
1:D:602:ASN:O	1:D:605:LEU:HB2	2.20	0.42
1:E:678:MET:HE2	1:E:678:MET:CA	2.46	0.42
1:G:597:ALA:O	1:G:598:ASP:C	2.58	0.42
1:I:597:ALA:O	1:I:600:VAL:N	2.53	0.42
1:K:310:ALA:HA	1:K:325:VAL:HG22	2.01	0.42
1:K:547:LEU:HD23	1:K:550:MET:HE2	2.01	0.42
1:B:597:ALA:O	1:B:600:VAL:N	2.53	0.42
1:D:249:THR:CG2	1:D:369:ILE:HG22	2.50	0.42
1:E:546:GLU:O	1:E:550:MET:HG3	2.19	0.42
1:E:601:ILE:O	1:E:604:ILE:HB	2.19	0.42
1:H:546:GLU:O	1:H:550:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:599:ARG:CA	1:K:602:ASN:HB3	2.40	0.42
1:C:666:VAL:HG23	1:C:666:VAL:O	2.20	0.42
1:D:222:LEU:O	1:D:226:HIS:HB2	2.19	0.42
1:D:546:GLU:O	1:D:550:MET:HG3	2.20	0.42
1:D:599:ARG:CA	1:D:602:ASN:HB3	2.42	0.42
1:F:602:ASN:O	1:F:605:LEU:HB2	2.20	0.42
1:I:223:PRO:CB	1:I:237:PRO:HB3	2.50	0.42
1:I:224:LEU:HD23	1:I:224:LEU:HA	1.91	0.42
1:J:224:LEU:HD23	1:J:224:LEU:HA	1.91	0.42
1:J:305:GLU:OE2	1:K:362:ARG:NH2	2.53	0.42
1:J:602:ASN:O	1:J:605:LEU:HB2	2.20	0.42
1:K:598:ASP:O	1:K:602:ASN:CB	2.68	0.42
1:L:479:ILE:HD13	1:L:527:LEU:CD2	2.50	0.42
1:L:597:ALA:O	1:L:600:VAL:N	2.53	0.42
2:A:900:JDP:C15	2:A:900:JDP:C23	2.98	0.41
1:B:222:LEU:O	1:B:226:HIS:HB2	2.20	0.41
1:B:597:ALA:O	1:B:598:ASP:C	2.59	0.41
1:D:598:ASP:O	1:D:602:ASN:CB	2.68	0.41
1:E:598:ASP:O	1:E:602:ASN:CB	2.69	0.41
1:E:599:ARG:CA	1:E:602:ASN:HB3	2.40	0.41
1:G:230:PHE:HA	1:G:233:ILE:HG22	2.03	0.41
1:G:666:VAL:HG23	1:G:666:VAL:O	2.20	0.41
1:H:494:GLN:HA	1:H:535:CYS:SG	2.59	0.41
1:H:601:ILE:O	1:H:604:ILE:HB	2.19	0.41
1:I:666:VAL:O	1:I:666:VAL:HG23	2.20	0.41
1:J:666:VAL:HG23	1:J:666:VAL:O	2.20	0.41
1:A:597:ALA:O	1:A:600:VAL:N	2.53	0.41
1:A:598:ASP:O	1:A:602:ASN:CB	2.68	0.41
1:B:552:PHE:CB	1:C:599:ARG:HD2	2.50	0.41
1:B:602:ASN:O	1:B:605:LEU:HB2	2.20	0.41
1:F:605:LEU:HD22	1:F:638:ARG:CZ	2.49	0.41
1:H:230:PHE:HA	1:H:233:ILE:HG22	2.02	0.41
1:I:698:ALA:HB2	1:I:731:ILE:HG13	2.02	0.41
1:J:222:LEU:O	1:J:226:HIS:HB2	2.20	0.41
1:J:598:ASP:O	1:J:602:ASN:CB	2.68	0.41
1:K:597:ALA:O	1:K:598:ASP:C	2.59	0.41
1:A:222:LEU:O	1:A:226:HIS:HB2	2.20	0.41
1:B:317:HIS:HB2	1:C:322:ARG:HH22	1.86	0.41
1:B:351:ASN:HD21	1:B:561:GLU:HG3	1.85	0.41
1:D:597:ALA:O	1:D:600:VAL:N	2.53	0.41
1:E:336:LYS:HB2	1:E:338:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ILE:HD13	1:F:527:LEU:CD2	2.50	0.41
1:F:598:ASP:O	1:F:602:ASN:CB	2.68	0.41
1:G:574:LEU:O	1:G:619:ILE:HA	2.21	0.41
1:H:583:ALA:O	1:H:586:ARG:HG3	2.20	0.41
1:I:222:LEU:O	1:I:226:HIS:HB2	2.20	0.41
1:I:597:ALA:O	1:I:598:ASP:C	2.59	0.41
1:I:598:ASP:O	1:I:602:ASN:CB	2.68	0.41
1:K:230:PHE:HA	1:K:233:ILE:HG22	2.02	0.41
1:B:223:PRO:CB	1:B:237:PRO:HB3	2.50	0.41
1:C:761:THR:HG22	1:I:753:ARG:HG2	2.01	0.41
1:D:597:ALA:O	1:D:598:ASP:C	2.59	0.41
1:D:666:VAL:O	1:D:666:VAL:HG23	2.20	0.41
1:I:551:TRP:CD1	1:I:551:TRP:C	2.94	0.41
1:K:602:ASN:O	1:K:605:LEU:HB2	2.20	0.41
1:L:223:PRO:CB	1:L:237:PRO:HB3	2.49	0.41
1:L:705:SER:O	1:L:709:ARG:HG2	2.21	0.41
1:C:599:ARG:CA	1:C:602:ASN:HB3	2.41	0.41
1:C:602:ASN:O	1:C:605:LEU:HB2	2.20	0.41
1:D:574:LEU:O	1:D:619:ILE:HA	2.21	0.41
1:D:703:ILE:HG23	1:E:502:LYS:HG2	2.03	0.41
1:E:310:ALA:HA	1:E:325:VAL:HG22	2.03	0.41
1:F:583:ALA:O	1:F:586:ARG:HG3	2.21	0.41
1:G:567:ARG:HH21	1:G:611:MET:HA	1.86	0.41
1:H:310:ALA:HA	1:H:325:VAL:HG22	2.03	0.41
1:I:547:LEU:HD23	1:I:550:MET:HE2	2.02	0.41
1:I:602:ASN:O	1:I:605:LEU:HB2	2.20	0.41
1:A:605:LEU:HD22	1:A:638:ARG:CZ	2.51	0.41
1:A:666:VAL:HG23	1:A:666:VAL:O	2.20	0.41
1:A:703:ILE:HD11	1:B:495:TYR:CZ	2.55	0.41
1:B:460:ASN:HD21	1:C:567:ARG:CD	2.34	0.41
1:B:574:LEU:O	1:B:619:ILE:HA	2.21	0.41
1:D:479:ILE:HD13	1:D:527:LEU:CD2	2.51	0.41
1:E:460:ASN:HD21	1:F:567:ARG:CD	2.33	0.41
1:F:222:LEU:O	1:F:226:HIS:HB2	2.20	0.41
1:G:222:LEU:O	1:G:226:HIS:HB2	2.20	0.41
1:G:698:ALA:HB2	1:G:731:ILE:HG13	2.03	0.41
1:A:223:PRO:CB	1:A:237:PRO:HB3	2.50	0.41
1:B:310:ALA:HA	1:B:325:VAL:HG22	2.03	0.41
1:B:733:ARG:HA	1:B:736:PHE:HB2	2.03	0.41
1:E:511:SER:O	1:E:618:PHE:CZ	2.74	0.41
1:E:597:ALA:O	1:E:600:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:ALA:O	1:F:600:VAL:N	2.53	0.41
1:G:597:ALA:O	1:G:600:VAL:N	2.54	0.41
1:H:511:SER:O	1:H:618:PHE:CZ	2.74	0.41
1:J:597:ALA:O	1:J:598:ASP:C	2.59	0.41
1:J:733:ARG:HA	1:J:736:PHE:HB2	2.03	0.41
1:A:230:PHE:HA	1:A:233:ILE:HG22	2.02	0.41
1:A:479:ILE:HD13	1:A:527:LEU:CD2	2.50	0.41
1:B:511:SER:O	1:B:618:PHE:CZ	2.74	0.41
1:C:310:ALA:HA	1:C:325:VAL:HG22	2.02	0.41
1:C:598:ASP:O	1:C:602:ASN:CB	2.69	0.41
1:E:223:PRO:CB	1:E:237:PRO:HB3	2.50	0.41
1:F:567:ARG:HH21	1:F:611:MET:HA	1.85	0.41
1:I:230:PHE:HA	1:I:233:ILE:HG22	2.03	0.41
1:I:479:ILE:HD13	1:I:527:LEU:CD2	2.51	0.41
1:I:599:ARG:CA	1:I:602:ASN:HB3	2.40	0.41
1:J:479:ILE:HD13	1:J:527:LEU:CD2	2.51	0.41
1:K:597:ALA:O	1:K:600:VAL:N	2.53	0.41
1:L:602:ASN:O	1:L:605:LEU:HB2	2.20	0.41
1:L:698:ALA:HB2	1:L:731:ILE:HG13	2.03	0.41
1:A:218:GLU:CG	1:F:420:LEU:HD21	2.51	0.41
1:A:547:LEU:HD23	1:A:550:MET:CE	2.50	0.41
1:A:574:LEU:O	1:A:619:ILE:HA	2.21	0.41
1:A:601:ILE:O	1:A:604:ILE:HB	2.20	0.41
1:B:598:ASP:O	1:B:602:ASN:CB	2.69	0.41
1:D:223:PRO:CB	1:D:237:PRO:HB3	2.50	0.41
1:D:230:PHE:HA	1:D:233:ILE:HG22	2.02	0.41
1:E:583:ALA:O	1:E:586:ARG:HG3	2.21	0.41
1:F:666:VAL:HG23	1:F:666:VAL:O	2.20	0.41
1:H:479:ILE:HD13	1:H:527:LEU:CD2	2.51	0.41
1:H:574:LEU:O	1:H:619:ILE:HA	2.21	0.41
1:H:597:ALA:O	1:H:598:ASP:C	2.59	0.41
1:J:310:ALA:HA	1:J:325:VAL:HG22	2.03	0.41
1:L:230:PHE:HA	1:L:233:ILE:HG22	2.02	0.41
1:L:551:TRP:CD1	1:L:551:TRP:C	2.94	0.41
1:L:598:ASP:O	1:L:602:ASN:CB	2.68	0.41
1:L:666:VAL:HG23	1:L:666:VAL:O	2.20	0.41
1:A:249:THR:CG2	1:A:369:ILE:HG22	2.51	0.41
1:A:698:ALA:HB2	1:A:731:ILE:HG13	2.03	0.41
1:B:551:TRP:CD1	1:B:551:TRP:C	2.94	0.41
1:C:551:TRP:CD1	1:C:551:TRP:C	2.94	0.41
1:C:597:ALA:O	1:C:600:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ALA:HB2	1:C:731:ILE:HG13	2.03	0.41
1:D:305:GLU:OE2	1:E:362:ARG:NH2	2.53	0.41
1:E:230:PHE:HA	1:E:233:ILE:HG22	2.03	0.41
1:E:597:ALA:O	1:E:598:ASP:C	2.59	0.41
1:F:597:ALA:O	1:F:598:ASP:C	2.59	0.41
1:G:602:ASN:O	1:G:605:LEU:HB2	2.20	0.41
1:H:598:ASP:O	1:H:602:ASN:CB	2.68	0.41
1:J:663:LYS:O	1:J:663:LYS:HG3	2.21	0.41
1:K:222:LEU:O	1:K:226:HIS:HB2	2.20	0.41
1:K:511:SER:O	1:K:618:PHE:CZ	2.74	0.41
1:K:666:VAL:O	1:K:666:VAL:HG23	2.20	0.41
1:D:733:ARG:HA	1:D:736:PHE:HB2	2.03	0.40
1:E:551:TRP:CD1	1:E:551:TRP:C	2.94	0.40
1:F:249:THR:CG2	1:F:369:ILE:HG22	2.50	0.40
1:F:511:SER:O	1:F:618:PHE:CZ	2.75	0.40
1:F:544:GLY:N	1:F:545:PRO:HD2	2.36	0.40
1:H:547:LEU:HD23	1:H:550:MET:HE2	2.03	0.40
1:I:511:SER:O	1:I:618:PHE:CZ	2.75	0.40
1:J:574:LEU:O	1:J:619:ILE:HA	2.21	0.40
1:J:597:ALA:O	1:J:600:VAL:N	2.54	0.40
1:L:574:LEU:O	1:L:619:ILE:HA	2.21	0.40
1:L:597:ALA:O	1:L:598:ASP:C	2.59	0.40
1:B:567:ARG:HH21	1:B:611:MET:HA	1.86	0.40
1:C:597:ALA:O	1:C:598:ASP:C	2.59	0.40
1:D:583:ALA:O	1:D:586:ARG:HG3	2.21	0.40
1:G:249:THR:CG2	1:G:369:ILE:HG22	2.52	0.40
1:G:733:ARG:HA	1:G:736:PHE:HB2	2.03	0.40
1:J:230:PHE:HA	1:J:233:ILE:HG22	2.02	0.40
1:K:479:ILE:HD13	1:K:527:LEU:CD2	2.52	0.40
1:D:310:ALA:HA	1:D:325:VAL:HG22	2.03	0.40
1:E:733:ARG:HA	1:E:736:PHE:HB2	2.04	0.40
1:F:698:ALA:HB2	1:F:731:ILE:HG13	2.04	0.40
1:G:310:ALA:HA	1:G:325:VAL:HG22	2.04	0.40
1:I:733:ARG:HA	1:I:736:PHE:HB2	2.03	0.40
1:J:698:ALA:HB2	1:J:731:ILE:HG13	2.03	0.40
1:K:567:ARG:HH21	1:K:611:MET:HA	1.85	0.40
1:K:574:LEU:O	1:K:619:ILE:HA	2.21	0.40
1:K:698:ALA:HB2	1:K:731:ILE:HG13	2.04	0.40
1:L:645:ILE:O	1:L:645:ILE:HG22	2.21	0.40
1:A:310:ALA:HA	1:A:325:VAL:HG22	2.03	0.40
1:A:526:LEU:HD21	2:A:900:JDP:N30	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ARG:HH21	1:A:611:MET:HA	1.86	0.40
1:A:623:THR:OG1	1:A:624:ASN:N	2.55	0.40
1:C:583:ALA:O	1:C:586:ARG:HG3	2.22	0.40
1:D:699:ILE:HG13	1:E:506:PHE:CD2	2.57	0.40
1:E:249:THR:CG2	1:E:369:ILE:HG22	2.51	0.40
1:E:574:LEU:O	1:E:619:ILE:HA	2.21	0.40
1:H:597:ALA:O	1:H:600:VAL:N	2.53	0.40
1:J:623:THR:OG1	1:J:624:ASN:N	2.55	0.40
1:J:684:GLY:HA3	2:J:900:JDP:C04	2.51	0.40
1:K:623:THR:OG1	1:K:624:ASN:N	2.55	0.40
1:E:623:THR:OG1	1:E:624:ASN:N	2.54	0.40
1:I:526:LEU:CD2	2:I:900:JDP:C29	2.99	0.40
1:J:511:SER:O	1:J:618:PHE:CZ	2.74	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	TRP
1	A	508	MET
1	A	522	CYS
1	A	556	GLU

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Mol	Chain	Res	Type
1	A	627	ASP
1	A	674	PHE
1	A	742	PHE
1	A	746	SER
1	A	748	SER
1	B	476	TRP
1	B	488	GLU
1	B	556	GLU
1	B	627	ASP
1	B	674	PHE
1	B	742	PHE
1	B	746	SER
1	B	748	SER
1	C	338	ARG
1	C	476	TRP
1	C	488	GLU
1	C	522	CYS
1	C	550	MET
1	C	556	GLU
1	C	627	ASP
1	C	674	PHE
1	C	746	SER
1	C	748	SER
1	D	476	TRP
1	D	508	MET
1	D	522	CYS
1	D	556	GLU
1	D	627	ASP
1	D	674	PHE
1	D	742	PHE
1	D	746	SER
1	D	748	SER
1	E	338	ARG
1	E	476	TRP
1	E	556	GLU
1	E	627	ASP
1	E	674	PHE
1	E	742	PHE
1	E	748	SER
1	F	338	ARG
1	F	476	TRP
1	F	488	GLU

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Mol	Chain	Res	Type
1	F	522	CYS
1	F	550	MET
1	F	627	ASP
1	F	674	PHE
1	F	742	PHE
1	F	746	SER
1	F	748	SER
1	G	236	LYS
1	G	476	TRP
1	G	488	GLU
1	G	522	CYS
1	G	556	GLU
1	G	627	ASP
1	G	674	PHE
1	G	742	PHE
1	G	746	SER
1	G	748	SER
1	H	476	TRP
1	H	488	GLU
1	H	522	CYS
1	H	627	ASP
1	H	674	PHE
1	H	742	PHE
1	H	746	SER
1	H	748	SER
1	I	476	TRP
1	I	508	MET
1	I	522	CYS
1	I	556	GLU
1	I	627	ASP
1	I	674	PHE
1	I	742	PHE
1	I	746	SER
1	I	748	SER
1	J	476	TRP
1	J	488	GLU
1	J	522	CYS
1	J	556	GLU
1	J	627	ASP
1	J	674	PHE
1	J	742	PHE
1	J	746	SER

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Mol	Chain	Res	Type
1	J	748	SER
1	K	338	ARG
1	K	476	TRP
1	K	488	GLU
1	K	508	MET
1	K	522	CYS
1	K	556	GLU
1	K	627	ASP
1	K	674	PHE
1	K	746	SER
1	K	748	SER
1	L	476	TRP
1	L	488	GLU
1	L	508	MET
1	L	522	CYS
1	L	556	GLU
1	L	627	ASP
1	L	674	PHE
1	L	746	SER
1	L	748	SER

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
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

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

All (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
2	G	900	JDP	C09-C10	-3.65	1.33	1.39
2	E	900	JDP	C09-C10	-3.45	1.33	1.39
2	B	900	JDP	C09-C10	-3.40	1.33	1.39
2	J	900	JDP	C24-C29	-3.34	1.35	1.40
2	C	900	JDP	C02-N31	3.33	1.39	1.33
2	I	900	JDP	C09-C10	-3.28	1.34	1.39
2	C	900	JDP	C09-C10	-3.19	1.34	1.39
2	E	900	JDP	C10-N12	3.18	1.41	1.36
2	C	900	JDP	C10-N12	3.01	1.41	1.36
2	G	900	JDP	C24-C29	-2.95	1.36	1.40
2	D	900	JDP	C10-N12	2.93	1.41	1.36
2	L	900	JDP	C10-N12	2.89	1.41	1.36
2	G	900	JDP	C10-N12	2.81	1.41	1.36
2	K	900	JDP	C09-C10	-2.80	1.34	1.39
2	I	900	JDP	C10-N12	2.77	1.41	1.36
2	A	900	JDP	C07-N12	-2.73	1.35	1.39
2	E	900	JDP	C24-C29	-2.73	1.36	1.40
2	G	900	JDP	C06-C07	-2.70	1.35	1.41
2	A	900	JDP	C09-C10	-2.69	1.34	1.39
2	F	900	JDP	C24-C29	-2.68	1.36	1.40
2	B	900	JDP	C10-N12	2.65	1.40	1.36
2	B	900	JDP	C15-N16	2.62	1.38	1.34
2	K	900	JDP	C06-C07	-2.55	1.36	1.41
2	F	900	JDP	C06-C07	-2.52	1.36	1.41
2	J	900	JDP	C07-N12	-2.52	1.35	1.39
2	J	900	JDP	C06-C07	-2.52	1.36	1.41
2	C	900	JDP	C03-C02	2.48	1.54	1.50
2	A	900	JDP	C06-C07	-2.46	1.36	1.41
2	G	900	JDP	C02-N31	2.41	1.37	1.33
2	G	900	JDP	C07-N12	-2.38	1.36	1.39
2	H	900	JDP	C10-N12	2.33	1.40	1.36
2	H	900	JDP	C09-C10	-2.32	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	JDP	C03-C02	-2.30	1.47	1.50
2	L	900	JDP	C02-N31	2.27	1.37	1.33
2	I	900	JDP	C02-N31	2.26	1.37	1.33
2	J	900	JDP	C02-N31	2.21	1.37	1.33
2	L	900	JDP	C24-C29	-2.19	1.37	1.40
2	A	900	JDP	C02-N31	2.14	1.36	1.33
2	I	900	JDP	C24-C29	-2.14	1.37	1.40
2	L	900	JDP	C06-C07	-2.14	1.36	1.41
2	K	900	JDP	C10-N12	2.14	1.40	1.36
2	L	900	JDP	C03-C02	2.04	1.53	1.50
2	H	900	JDP	C24-C29	-2.02	1.37	1.40

All (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
2	G	900	JDP	C18-C17-N16	-5.20	99.18	113.60
2	G	900	JDP	C17-N16-C15	5.19	129.80	123.08
2	F	900	JDP	N16-C15-N14	-5.19	111.38	118.33
2	A	900	JDP	C18-C17-N16	-5.12	99.40	113.60
2	I	900	JDP	N16-C15-N14	-5.09	111.51	118.33
2	J	900	JDP	C18-C17-N16	-4.92	99.94	113.60
2	L	900	JDP	O01-C02-N31	-4.67	115.86	122.62
2	F	900	JDP	C24-C29-N30	-4.66	119.89	123.48
2	C	900	JDP	C17-N16-C15	4.48	128.88	123.08
2	F	900	JDP	O01-C02-N31	-4.47	116.15	122.62
2	J	900	JDP	C11-C10-C09	-4.45	120.69	128.71
2	J	900	JDP	N16-C15-N14	-4.24	112.66	118.33
2	F	900	JDP	C17-N16-C15	4.18	128.49	123.08
2	C	900	JDP	C18-C17-N16	-4.09	102.27	113.60
2	D	900	JDP	C18-C17-N16	-4.05	102.37	113.60
2	J	900	JDP	C17-N16-C15	4.03	128.29	123.08
2	L	900	JDP	C04-C03-C08	-3.81	115.40	119.63
2	J	900	JDP	C04-C03-C08	-3.57	115.67	119.63
2	F	900	JDP	C18-C17-N16	-3.48	103.95	113.60
2	I	900	JDP	C03-C02-N31	-3.45	112.92	118.27
2	E	900	JDP	O01-C02-C03	3.41	124.25	120.23
2	B	900	JDP	C17-N16-C15	3.41	127.50	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	900	JDP	C24-C29-N30	-3.37	120.89	123.48
2	L	900	JDP	C11-C10-C09	-3.28	122.81	128.71
2	L	900	JDP	C18-C17-N16	-3.24	104.61	113.60
2	D	900	JDP	C08-C03-C02	3.18	125.35	120.82
2	C	900	JDP	C27-C28-C29	-3.17	105.82	111.62
2	F	900	JDP	C04-C03-C08	-3.15	116.13	119.63
2	D	900	JDP	O01-C02-C03	3.14	123.93	120.23
2	K	900	JDP	N16-C15-N14	-3.13	114.14	118.33
2	A	900	JDP	C04-C03-C08	-3.09	116.21	119.63
2	J	900	JDP	O01-C02-N31	-3.08	118.17	122.62
2	I	900	JDP	O01-C02-C03	3.07	123.85	120.23
2	A	900	JDP	C06-C07-C08	3.07	125.12	120.94
2	J	900	JDP	C24-C29-N30	-3.06	121.12	123.48
2	J	900	JDP	C27-C28-C29	3.05	117.21	111.62
2	A	900	JDP	O26-C27-C28	3.03	119.08	111.84
2	I	900	JDP	C25-O26-C27	2.96	119.58	111.08
2	D	900	JDP	C21-C20-C19	2.95	123.88	120.24
2	G	900	JDP	C24-C29-N30	-2.90	121.25	123.48
2	K	900	JDP	C03-C02-N31	-2.83	113.89	118.27
2	E	900	JDP	C11-C10-C09	-2.82	123.64	128.71
2	H	900	JDP	C17-N16-C15	2.81	126.72	123.08
2	I	900	JDP	C17-N16-C15	2.81	126.71	123.08
2	C	900	JDP	C04-C03-C08	-2.81	116.52	119.63
2	C	900	JDP	O01-C02-C03	2.80	123.53	120.23
2	I	900	JDP	C24-C29-N30	-2.79	121.33	123.48
2	L	900	JDP	C17-N16-C15	2.77	126.66	123.08
2	D	900	JDP	C20-C21-C22	-2.73	116.13	119.87
2	I	900	JDP	C27-C28-C29	2.68	116.53	111.62
2	I	900	JDP	C20-C21-C22	-2.66	116.22	119.87
2	C	900	JDP	O01-C02-N31	-2.64	118.81	122.62
2	G	900	JDP	C04-C03-C08	-2.61	116.74	119.63
2	A	900	JDP	C05-C06-C07	-2.55	114.86	119.50
2	H	900	JDP	N16-C15-N14	-2.53	114.94	118.33
2	E	900	JDP	C03-C02-N31	-2.50	114.39	118.27
2	K	900	JDP	C17-N16-C15	2.46	126.26	123.08
2	G	900	JDP	C25-O26-C27	2.44	118.08	111.08
2	J	900	JDP	C25-O26-C27	2.41	118.00	111.08
2	G	900	JDP	C11-C10-C09	-2.38	124.43	128.71
2	A	900	JDP	N16-C15-N14	-2.26	115.31	118.33
2	D	900	JDP	C09-C08-C07	-2.23	104.33	106.27
2	C	900	JDP	C25-C24-C29	2.23	123.38	119.67
2	G	900	JDP	C27-C28-C29	2.22	115.69	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	900	JDP	C03-C02-N31	-2.20	114.85	118.27
2	K	900	JDP	C28-C29-C24	2.19	123.63	121.40
2	C	900	JDP	C25-O26-C27	2.18	117.34	111.08
2	K	900	JDP	O01-C02-N31	-2.16	119.49	122.62
2	A	900	JDP	C20-C19-C18	-2.14	117.60	120.61
2	I	900	JDP	C11-C10-C09	-2.14	124.86	128.71
2	B	900	JDP	C03-C02-N31	-2.11	114.99	118.27
2	B	900	JDP	C04-C03-C08	2.11	121.97	119.63
2	K	900	JDP	C25-O26-C27	2.11	117.12	111.08
2	A	900	JDP	C23-C18-C19	2.10	121.36	118.23
2	I	900	JDP	C21-C22-C23	2.06	122.78	120.24
2	G	900	JDP	N16-C15-N14	-2.03	115.61	118.33
2	F	900	JDP	C25-O26-C27	2.02	116.87	111.08
2	B	900	JDP	C11-C10-C09	-2.02	125.08	128.71

There are no chirality outliers.

All (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
2	C	900	JDP	C24-C15-N16-C17
2	D	900	JDP	N14-C15-N16-C17
2	D	900	JDP	C24-C15-N16-C17
2	E	900	JDP	N14-C15-N16-C17
2	E	900	JDP	C24-C15-N16-C17
2	F	900	JDP	N14-C15-N16-C17
2	F	900	JDP	C24-C15-N16-C17
2	G	900	JDP	N14-C15-N16-C17
2	G	900	JDP	C24-C15-N16-C17
2	H	900	JDP	N14-C15-N16-C17
2	H	900	JDP	C24-C15-N16-C17
2	I	900	JDP	N14-C15-N16-C17
2	I	900	JDP	C24-C15-N16-C17
2	J	900	JDP	N14-C15-N16-C17
2	J	900	JDP	C24-C15-N16-C17
2	K	900	JDP	N14-C15-N16-C17
2	K	900	JDP	C24-C15-N16-C17
2	L	900	JDP	N14-C15-N16-C17

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Mol	Chain	Res	Type	Atoms
2	L	900	JDP	C24-C15-N16-C17
2	F	900	JDP	O01-C02-C03-C08
2	A	900	JDP	O01-C02-C03-C08
2	A	900	JDP	N31-C02-C03-C08
2	C	900	JDP	O01-C02-C03-C08
2	D	900	JDP	O01-C02-C03-C08
2	D	900	JDP	N31-C02-C03-C08
2	E	900	JDP	O01-C02-C03-C08
2	F	900	JDP	N31-C02-C03-C08
2	H	900	JDP	O01-C02-C03-C08
2	J	900	JDP	O01-C02-C03-C08
2	K	900	JDP	O01-C02-C03-C08
2	K	900	JDP	N31-C02-C03-C08
2	L	900	JDP	O01-C02-C03-C08
2	C	900	JDP	N31-C02-C03-C08
2	H	900	JDP	N31-C02-C03-C08
2	J	900	JDP	N31-C02-C03-C08
2	L	900	JDP	N31-C02-C03-C08

There are no ring outliers.

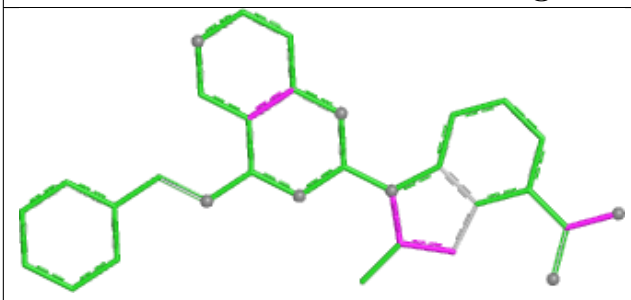
12 monomers are involved in 32 short contacts:

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
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

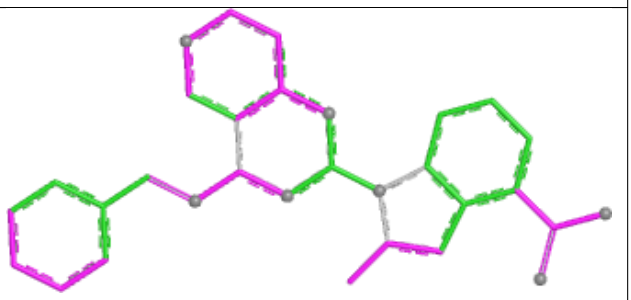
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

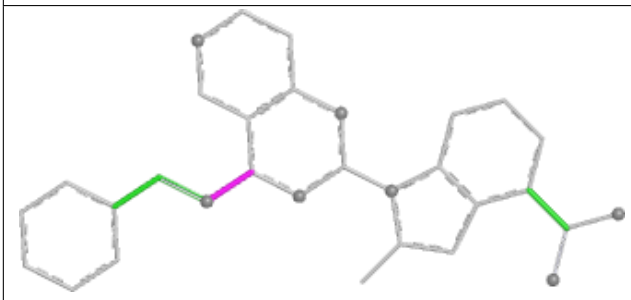
Ligand JDP I 900



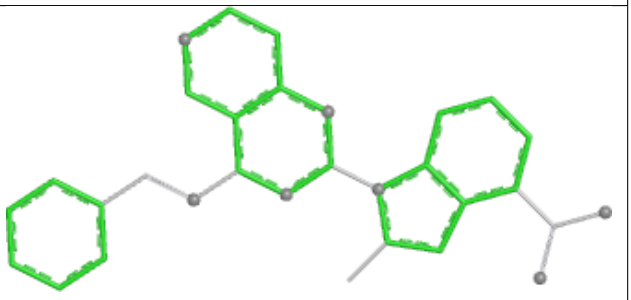
Bond lengths



Bond angles

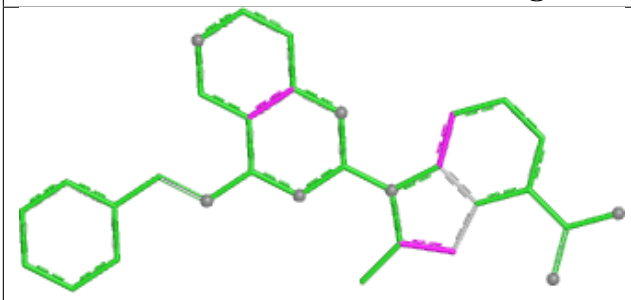


Torsions

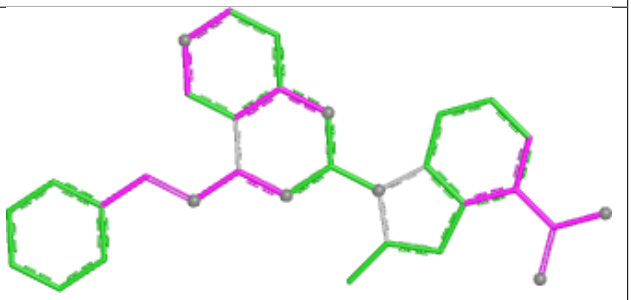


Rings

Ligand JDP F 900



Bond lengths



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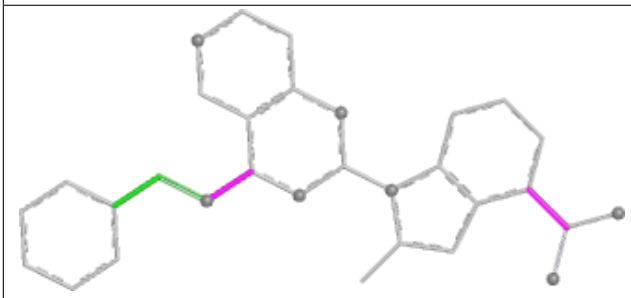
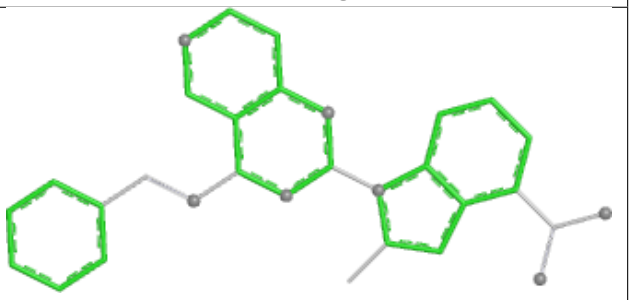
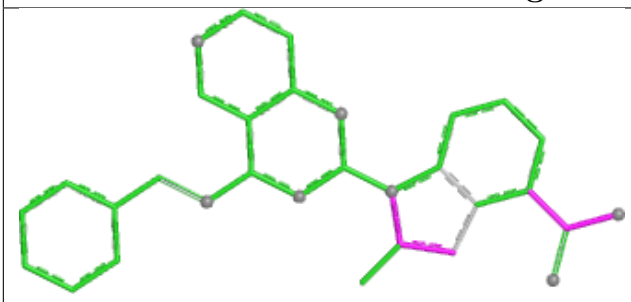
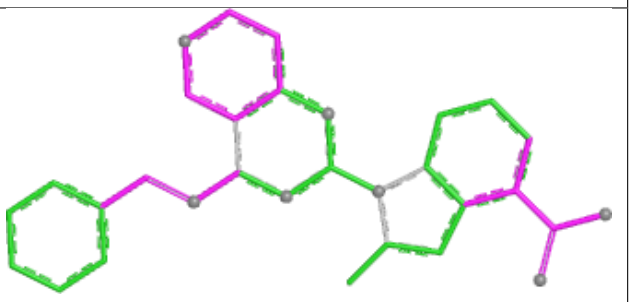
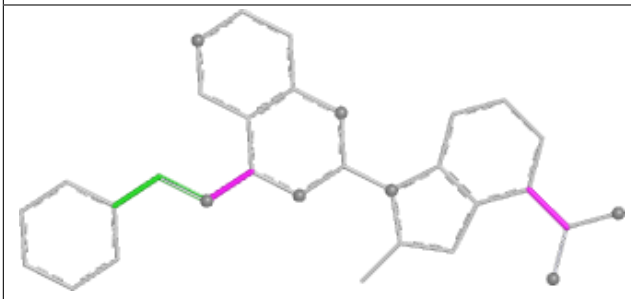
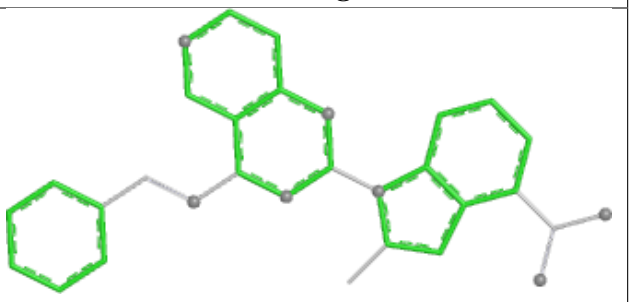


Torsions



Rings

Ligand JDP C 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

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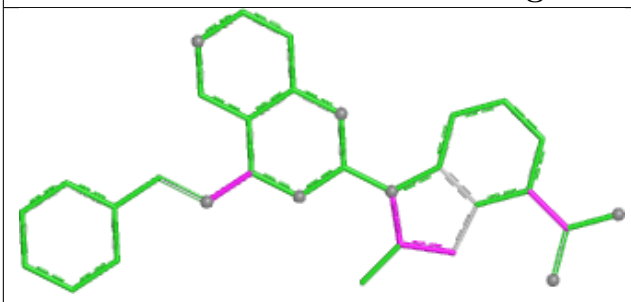
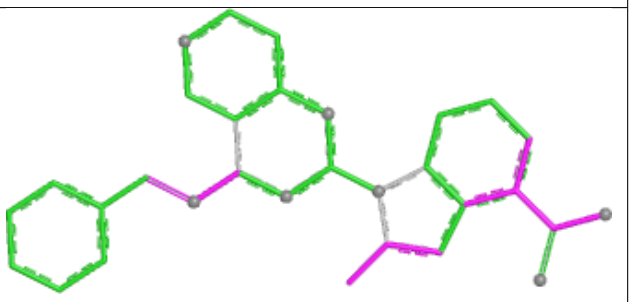
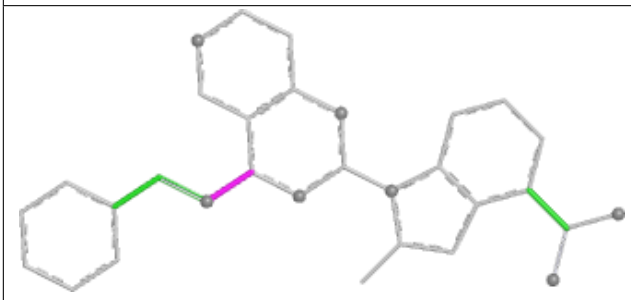
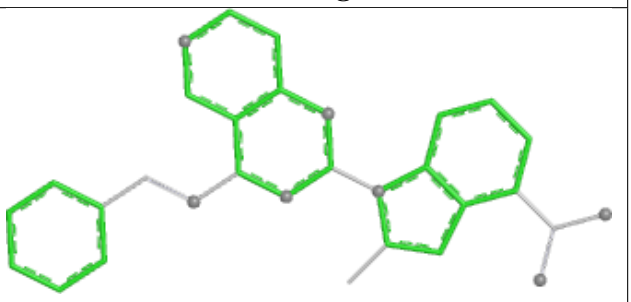
 Bond lengths	 Bond angles
 Torsions	 Rings

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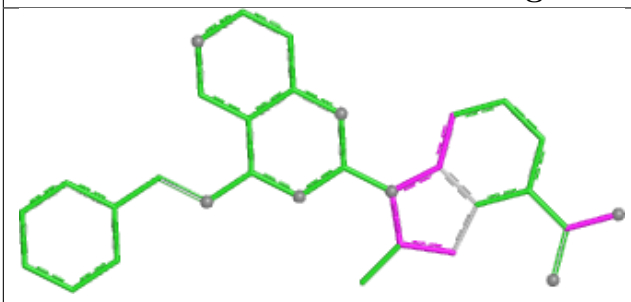
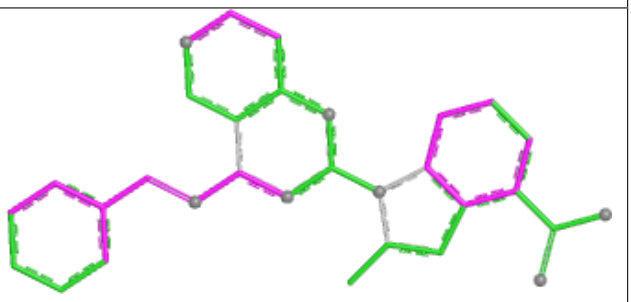
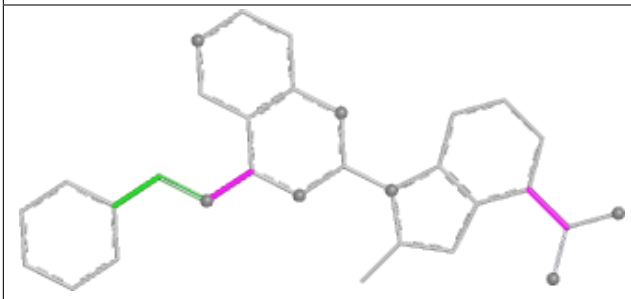
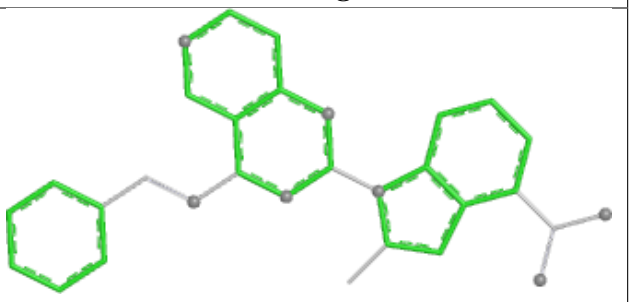
 Bond lengths	 Bond angles
 Torsions	 Rings

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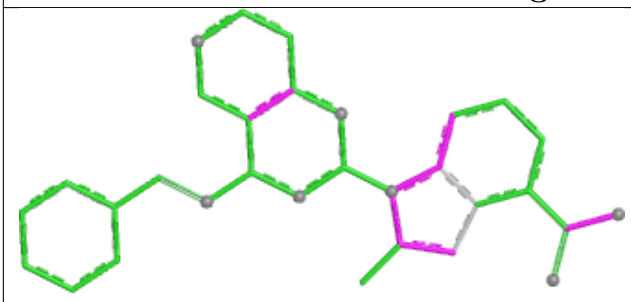
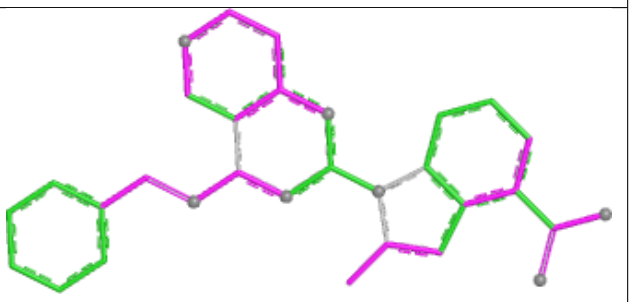
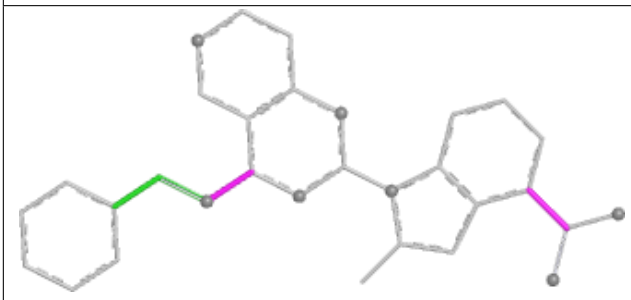
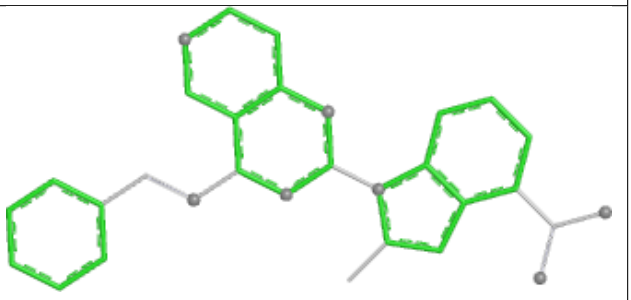
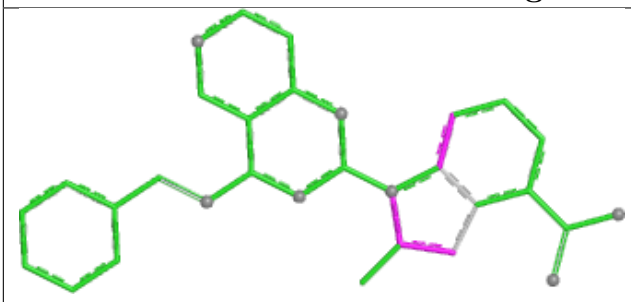
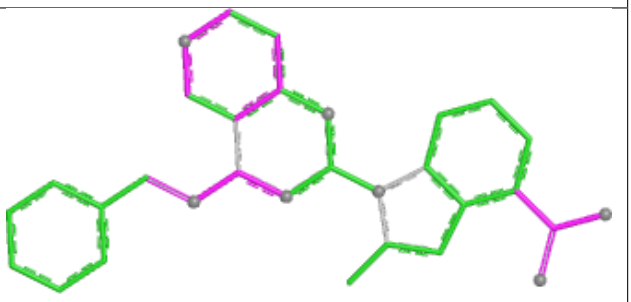
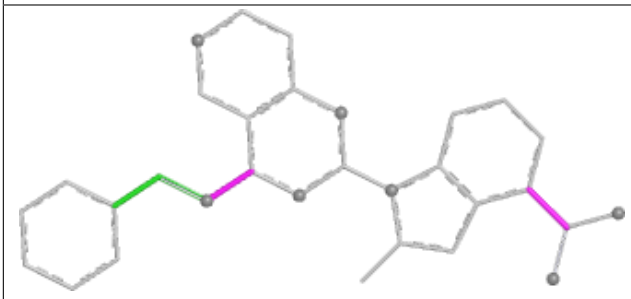
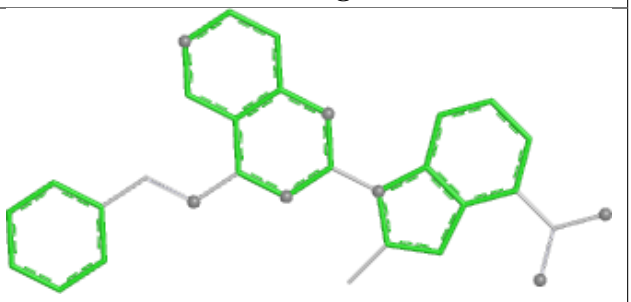
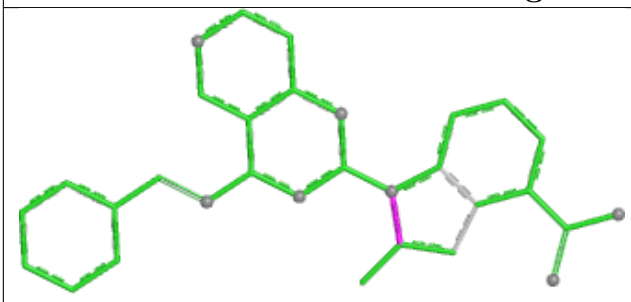
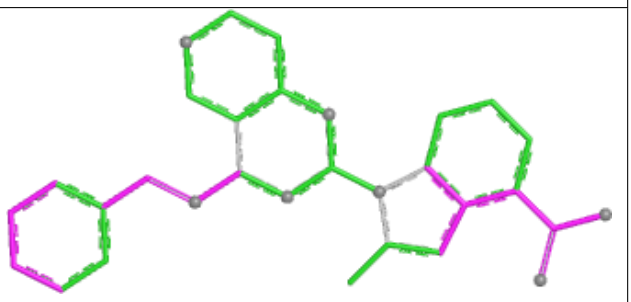
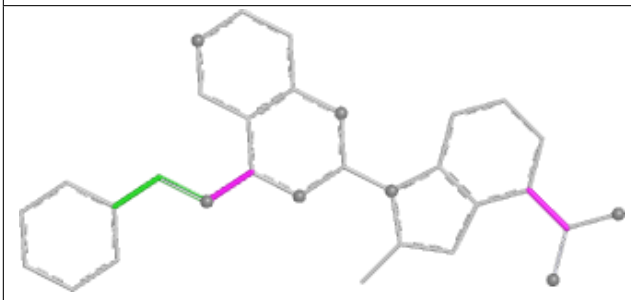
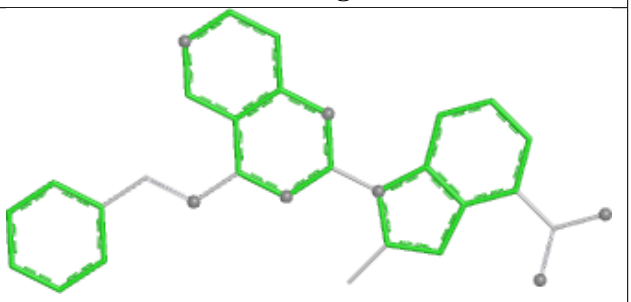
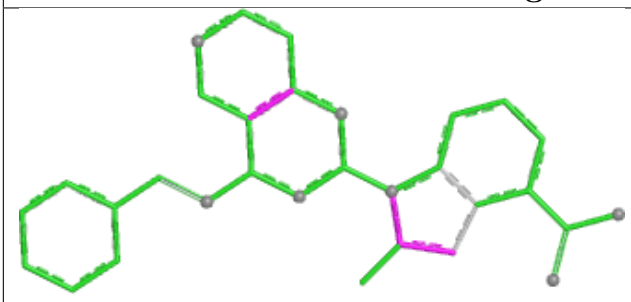
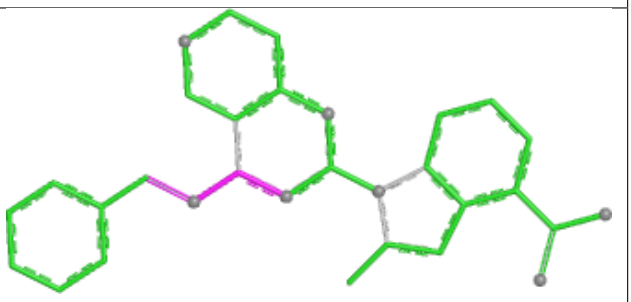
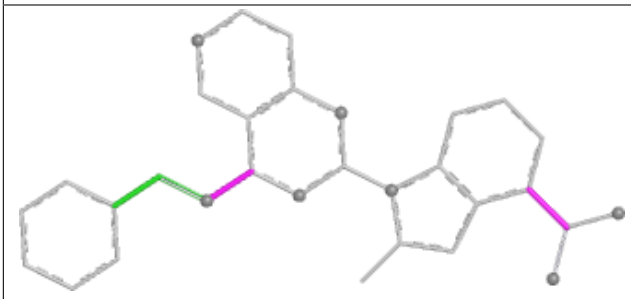
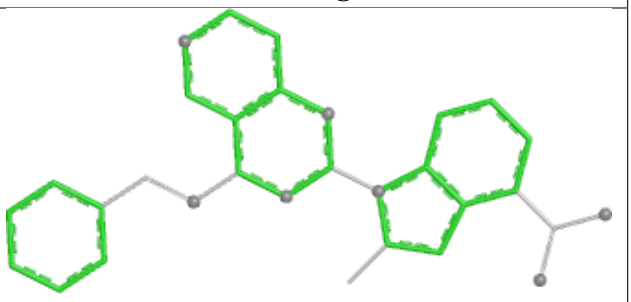
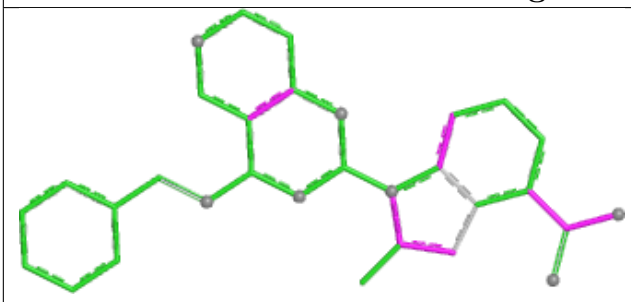
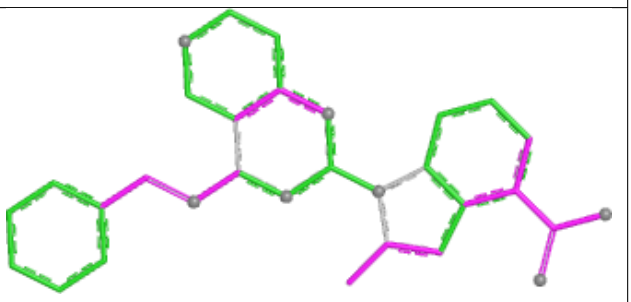
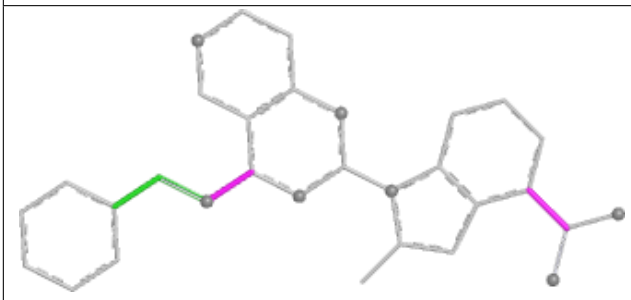
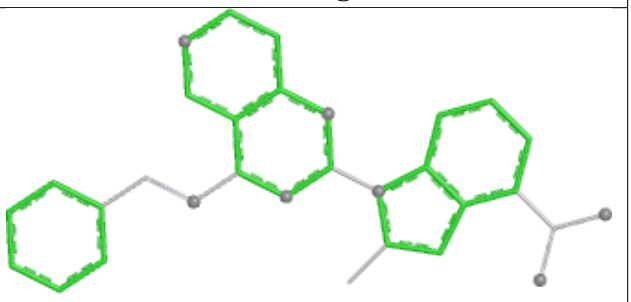
 Bond lengths	 Bond angles
 Torsions	 Rings

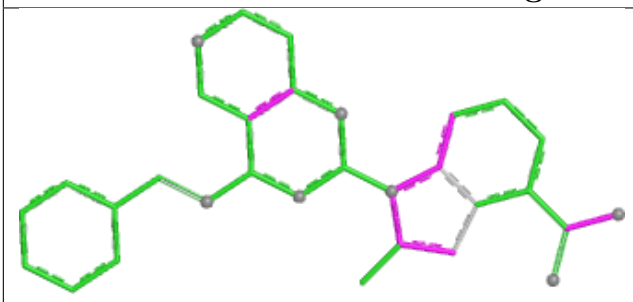
Ligand JDP K 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand JDP D 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

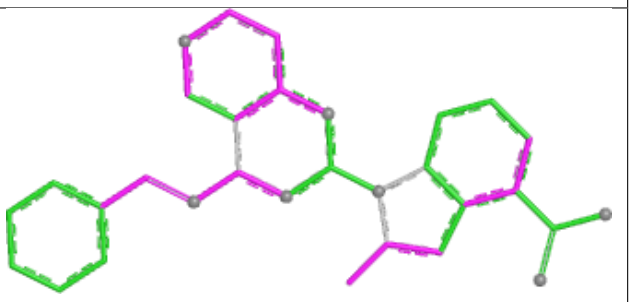
Ligand JDP H 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand JDP L 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

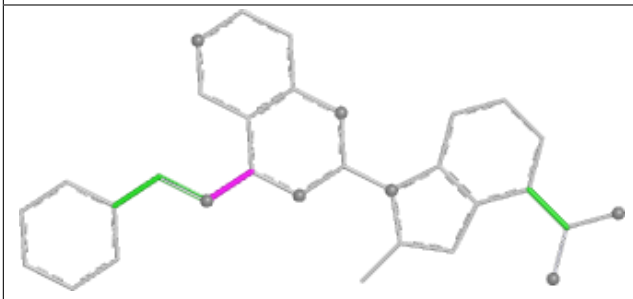
Ligand JDP G 900



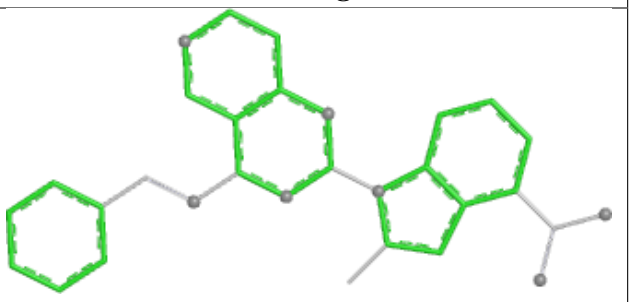
Bond lengths



Bond angles

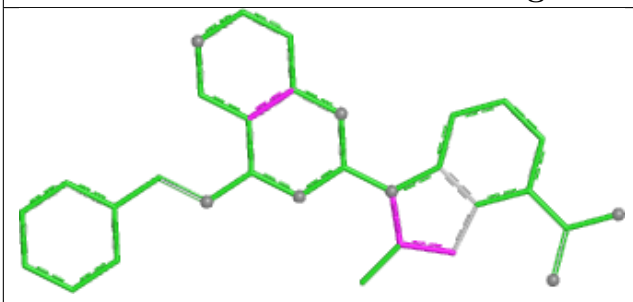


Torsions

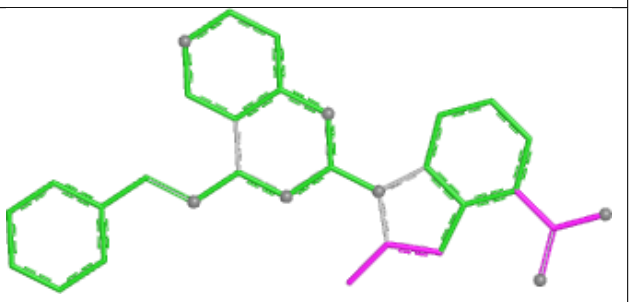


Rings

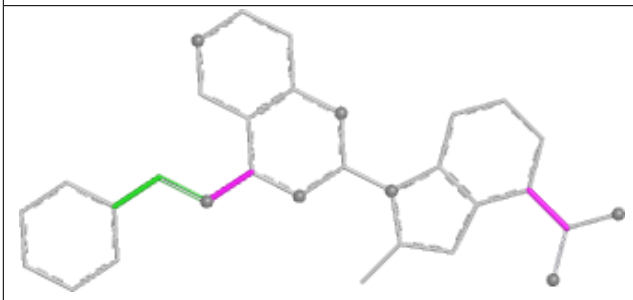
Ligand JDP E 900



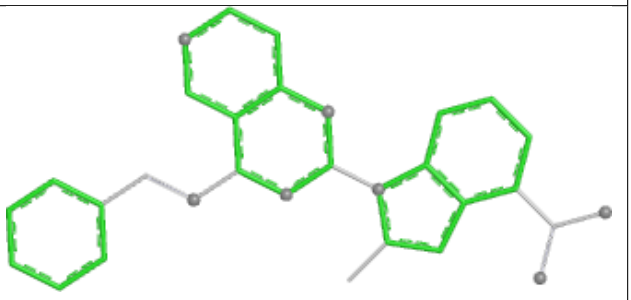
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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

All (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
1	K	447	VAL	5.1
1	I	235	VAL	4.8
1	B	447	VAL	4.8
1	B	596	ALA	4.6
1	C	396	LEU	4.4
1	L	596	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	452	PHE	4.1
1	F	226	HIS	4.1
1	C	299	ALA	4.0
1	G	636	PRO	3.9
1	F	396	LEU	3.9
1	C	509	THR	3.9
1	L	396	LEU	3.9
1	G	299	ALA	3.8
1	E	707	ILE	3.8
1	H	447	VAL	3.8
1	E	299	ALA	3.7
1	L	730	GLU	3.7
1	I	298	PRO	3.7
1	I	230	PHE	3.7
1	J	730	GLU	3.7
1	D	267	PHE	3.6
1	G	732	ARG	3.6
1	F	671	ASP	3.6
1	F	704	GLU	3.5
1	K	732	ARG	3.5
1	H	415	CYS	3.5
1	I	342	ILE	3.5
1	K	423	ILE	3.5
1	G	757	MET	3.5
1	L	715	THR	3.5
1	D	714	GLN	3.4
1	D	715	THR	3.4
1	K	730	GLU	3.4
1	C	613	THR	3.4
1	K	636	PRO	3.4
1	I	385	THR	3.4
1	H	317	HIS	3.4
1	L	390	LEU	3.3
1	H	452	PHE	3.3
1	D	452	PHE	3.3
1	H	388	MET	3.3
1	D	730	GLU	3.3
1	H	224	LEU	3.3
1	L	340	HIS	3.3
1	K	294	GLU	3.2
1	K	265	PHE	3.2
1	F	230	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	710	GLU	3.2
1	L	481	GLY	3.2
1	F	237	PRO	3.2
1	J	447	VAL	3.2
1	L	506	PHE	3.2
1	B	452	PHE	3.1
1	L	599	ARG	3.1
1	L	388	MET	3.1
1	C	715	THR	3.1
1	K	613	THR	3.1
1	C	678	MET	3.1
1	B	394	VAL	3.0
1	C	341	VAL	3.0
1	K	736	PHE	3.0
1	G	210	ARG	3.0
1	C	481	GLY	3.0
1	C	732	ARG	3.0
1	H	738	GLU	3.0
1	F	710	GLU	3.0
1	H	423	ILE	3.0
1	L	341	VAL	3.0
1	F	400	ALA	2.9
1	L	262	THR	2.9
1	D	265	PHE	2.9
1	A	388	MET	2.9
1	F	233	ILE	2.9
1	K	713	ARG	2.9
1	I	613	THR	2.9
1	G	396	LEU	2.9
1	K	267	PHE	2.9
1	H	316	THR	2.8
1	D	396	LEU	2.8
1	B	210	ARG	2.8
1	F	636	PRO	2.8
1	I	396	LEU	2.8
1	E	423	ILE	2.8
1	C	388	MET	2.8
1	A	210	ARG	2.8
1	G	452	PHE	2.8
1	I	224	LEU	2.7
1	F	640	ASP	2.7
1	G	298	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	340	HIS	2.7
1	L	712	GLU	2.7
1	F	711	ARG	2.7
1	D	731	ILE	2.7
1	C	636	PRO	2.7
1	B	317	HIS	2.7
1	B	731	ILE	2.7
1	E	730	GLU	2.7
1	I	390	LEU	2.6
1	E	596	ALA	2.6
1	E	731	ILE	2.6
1	L	299	ALA	2.6
1	I	300	ILE	2.6
1	K	637	GLY	2.6
1	H	732	ARG	2.6
1	D	640	ASP	2.6
1	E	234	GLY	2.5
1	G	382	GLN	2.5
1	I	668	LYS	2.5
1	C	640	ASP	2.5
1	J	341	VAL	2.5
1	L	389	LYS	2.5
1	I	233	ILE	2.5
1	C	637	GLY	2.5
1	B	423	ILE	2.5
1	I	389	LYS	2.5
1	K	731	ILE	2.5
1	J	678	MET	2.5
1	C	210	ARG	2.5
1	K	640	ASP	2.4
1	E	233	ILE	2.4
1	L	640	ASP	2.4
1	L	670	VAL	2.4
1	B	345	ALA	2.4
1	C	423	ILE	2.4
1	H	731	ILE	2.4
1	H	419	ALA	2.4
1	C	382	GLN	2.4
1	B	757	MET	2.4
1	F	299	ALA	2.4
1	B	282	SER	2.4
1	F	703	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	733	ARG	2.4
1	F	670	VAL	2.4
1	I	229	LEU	2.4
1	K	509	THR	2.4
1	H	730	GLU	2.4
1	D	678	MET	2.4
1	I	279	ALA	2.4
1	B	741	ARG	2.3
1	C	387	ASN	2.3
1	C	707	ILE	2.3
1	I	361	GLY	2.3
1	D	732	ARG	2.3
1	I	637	GLY	2.3
1	J	713	ARG	2.3
1	H	597	ALA	2.3
1	D	301	ILE	2.3
1	B	388	MET	2.3
1	L	582	ILE	2.3
1	C	730	GLU	2.3
1	C	761	THR	2.3
1	H	715	THR	2.3
1	I	221	GLU	2.3
1	C	267	PHE	2.3
1	D	388	MET	2.3
1	F	761	THR	2.3
1	H	385	THR	2.3
1	E	732	ARG	2.3
1	E	710	GLU	2.2
1	F	337	GLN	2.2
1	F	393	ASP	2.2
1	L	338	ARG	2.2
1	I	730	GLU	2.2
1	I	267	PHE	2.2
1	B	678	MET	2.2
1	A	582	ILE	2.2
1	E	481	GLY	2.2
1	J	706	GLU	2.2
1	B	395	ASP	2.2
1	H	613	THR	2.2
1	K	734	ASP	2.2
1	E	419	ALA	2.2
1	E	704	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	210	ARG	2.2
1	I	452	PHE	2.2
1	L	230	PHE	2.2
1	E	711	ARG	2.1
1	H	710	GLU	2.1
1	L	344	MET	2.1
1	C	221	GLU	2.1
1	F	707	ILE	2.1
1	B	393	ASP	2.1
1	I	381	LEU	2.1
1	C	482	LEU	2.1
1	B	476	TRP	2.1
1	F	225	ARG	2.1
1	J	674	PHE	2.1
1	K	233	ILE	2.1
1	L	233	ILE	2.1
1	L	301	ILE	2.1
1	B	597	ALA	2.1
1	G	482	LEU	2.1
1	F	229	LEU	2.1
1	L	597	ALA	2.1
1	F	672	LEU	2.1
1	C	758	PHE	2.1
1	F	452	PHE	2.1
1	H	711	ARG	2.1
1	J	675	LEU	2.1
1	G	224	LEU	2.1
1	G	481	GLY	2.1
1	D	423	ILE	2.0
1	E	703	ILE	2.0
1	E	503	PHE	2.0
1	K	299	ALA	2.0
1	E	224	LEU	2.0
1	F	222	LEU	2.0
1	F	235	VAL	2.0
1	G	761	THR	2.0
1	G	596	ALA	2.0
1	F	730	GLU	2.0
1	F	221	GLU	2.0
1	I	340	HIS	2.0
1	K	741	ARG	2.0

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)

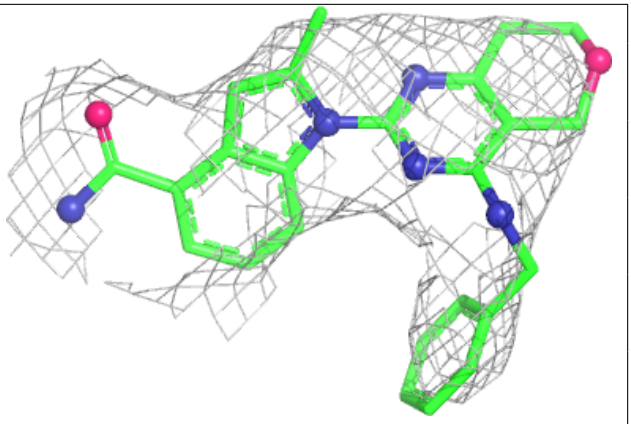
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

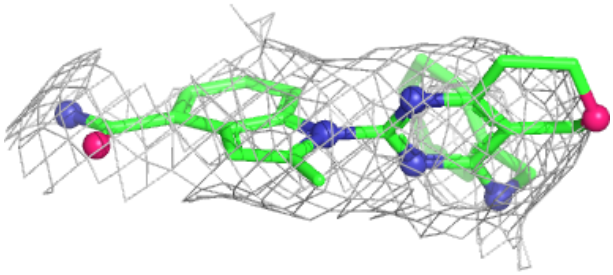
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	JDP	K	900	31/31	0.77	0.40	131,150,160,165	0
2	JDP	B	900	31/31	0.79	0.31	125,147,172,174	0
2	JDP	I	900	31/31	0.80	0.32	142,151,173,173	0
2	JDP	H	900	31/31	0.81	0.30	139,150,167,173	0
2	JDP	F	900	31/31	0.82	0.33	145,154,166,168	0
2	JDP	E	900	31/31	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

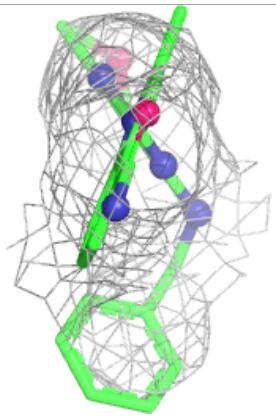
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

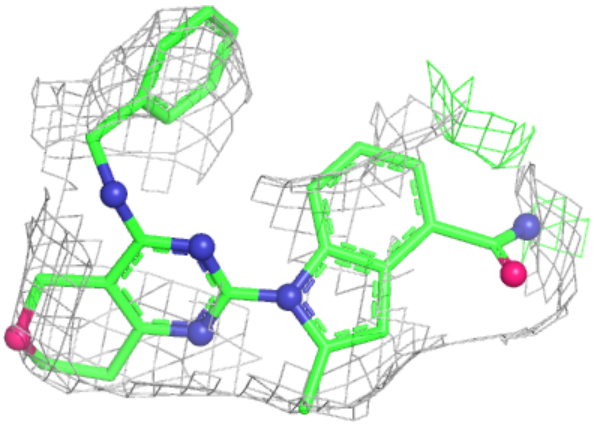


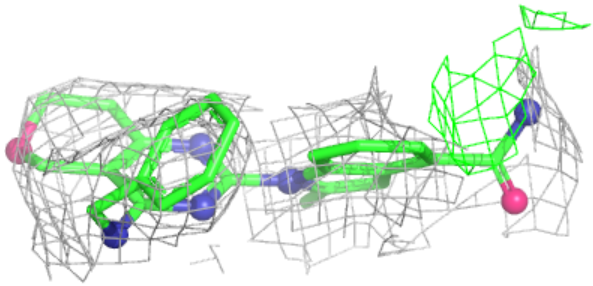


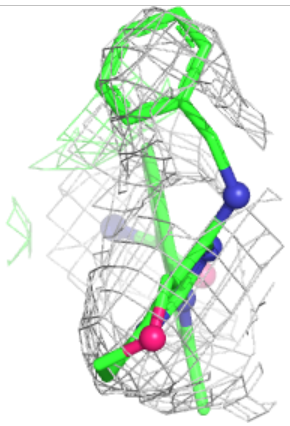


Electron density around JDP B 900:

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

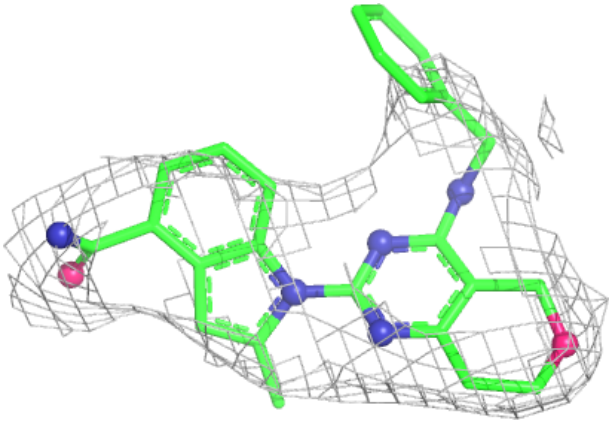


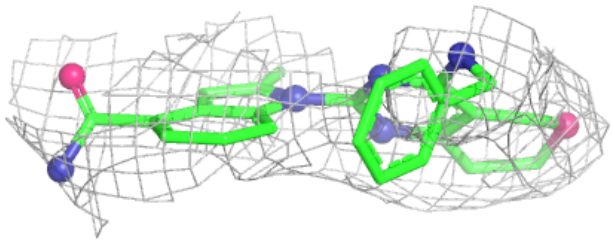


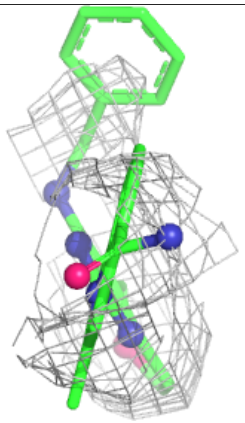


Electron density around JDP I 900:

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

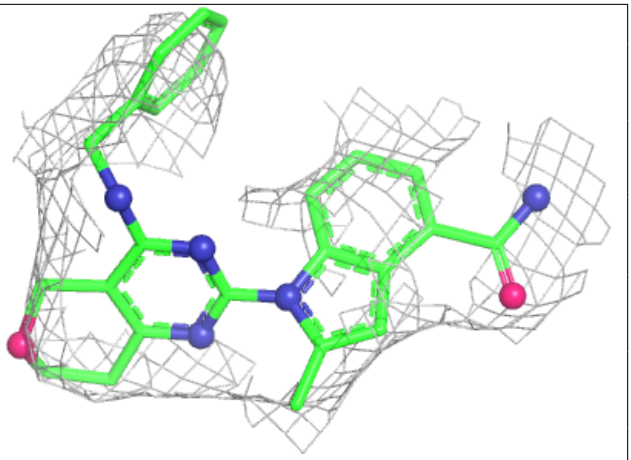


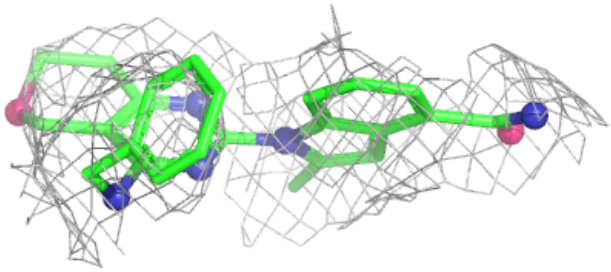


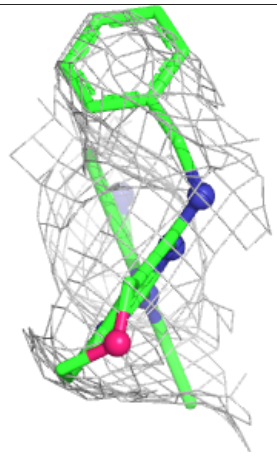


Electron density around JDP H 900:

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

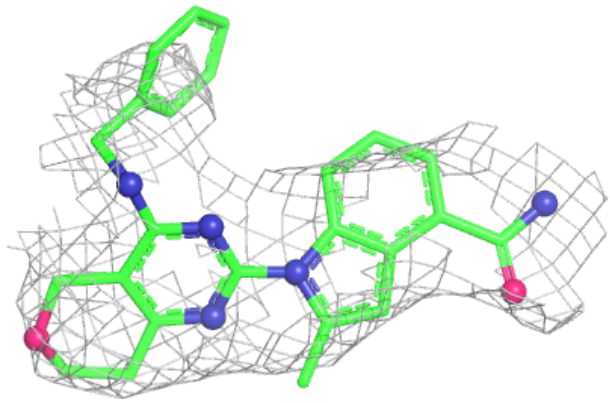


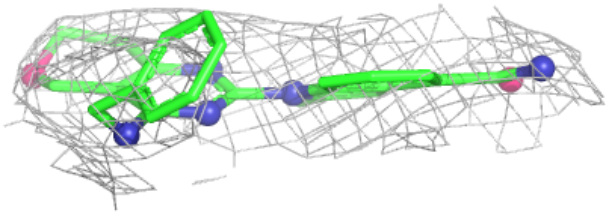


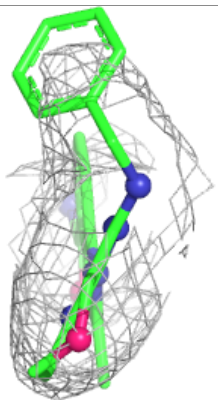


Electron density around JDP F 900:

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

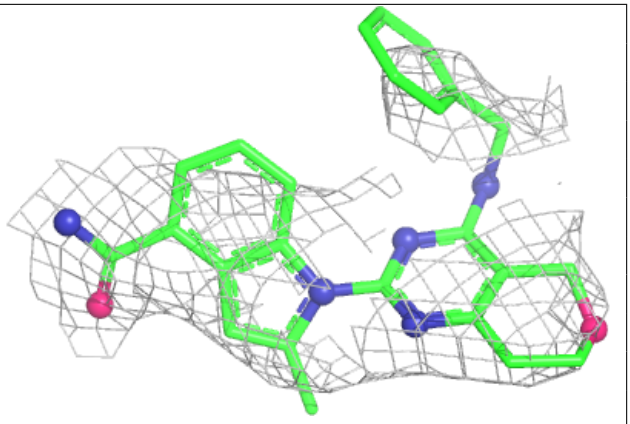


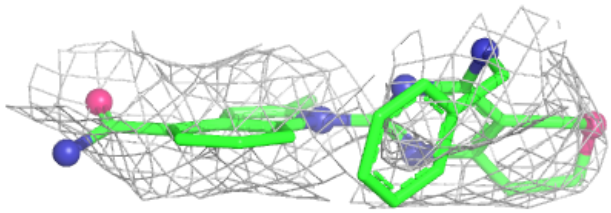


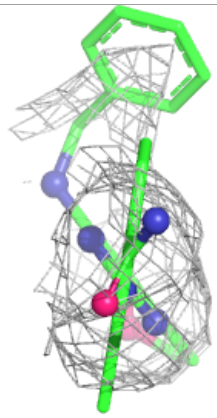


Electron density around JDP E 900:

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

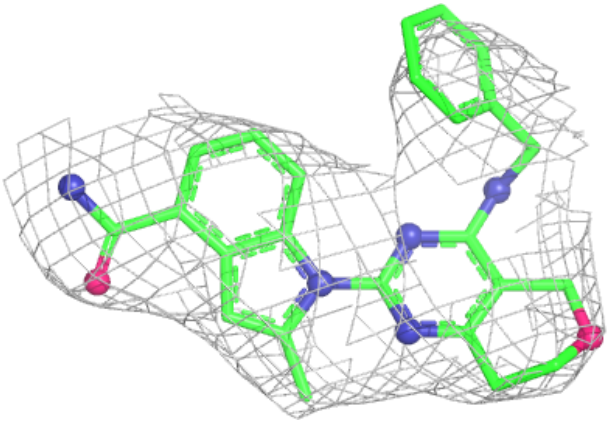


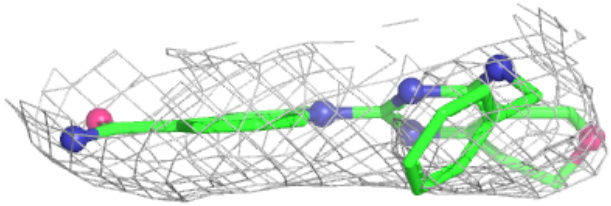


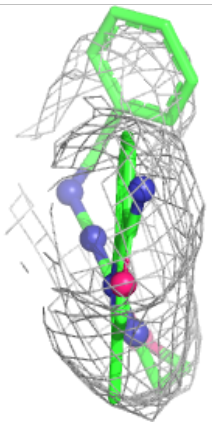


Electron density around JDP C 900:

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

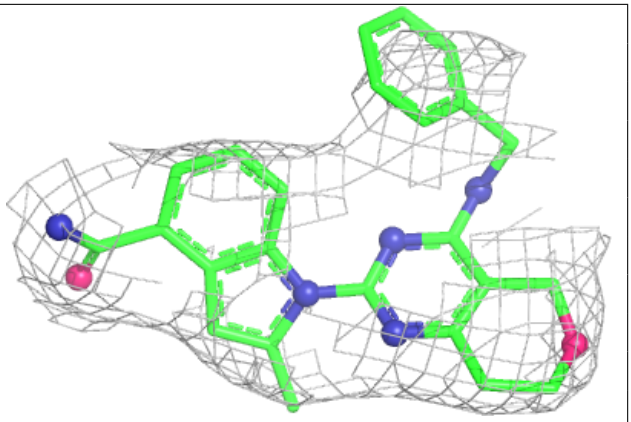


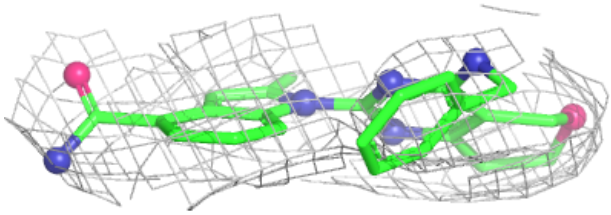


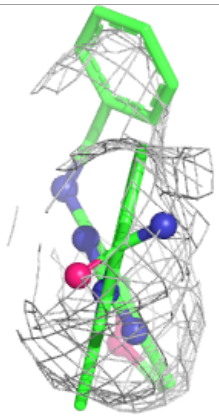


Electron density around JDP G 900:

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

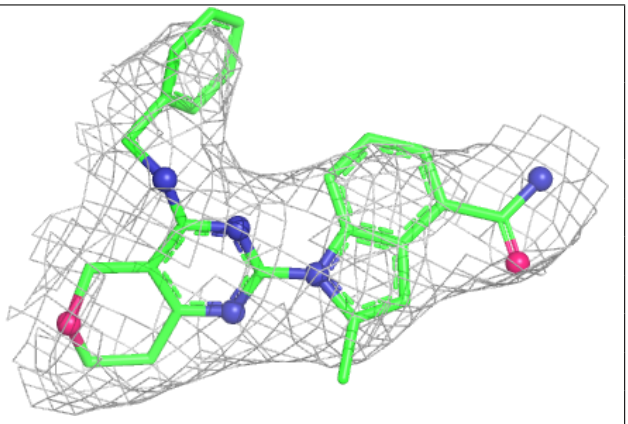


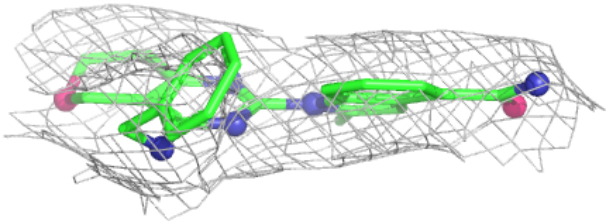


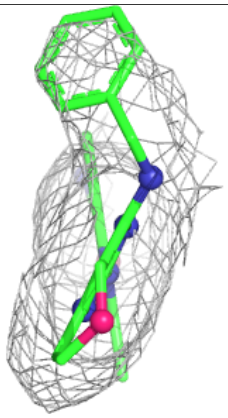


Electron density around JDP J 900:

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

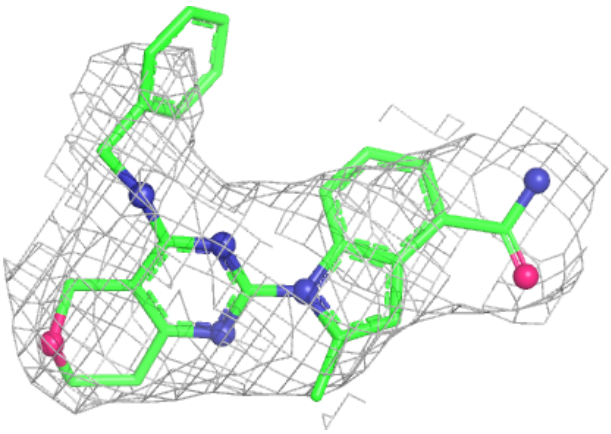


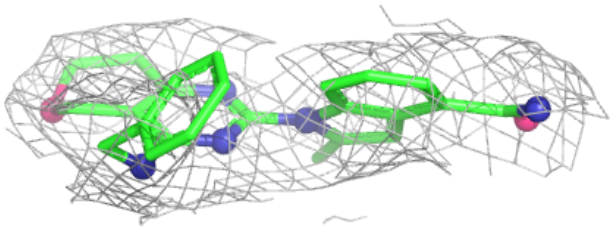


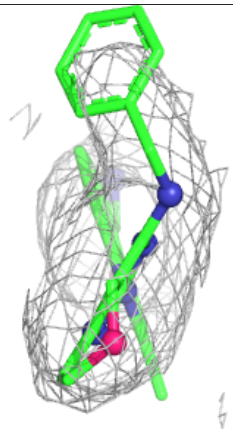


Electron density around JDP D 900:

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

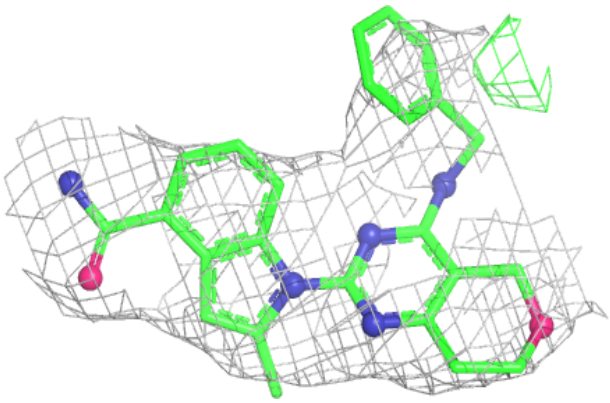


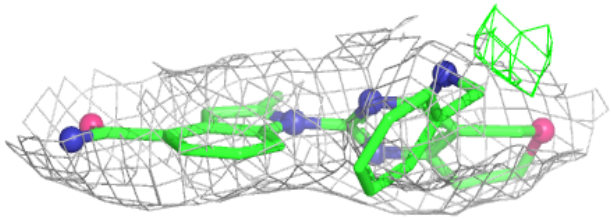


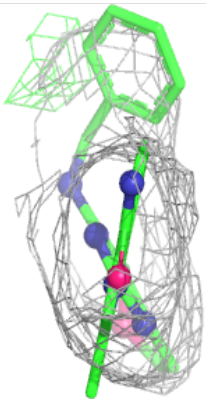


Electron density around JDP A 900:

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

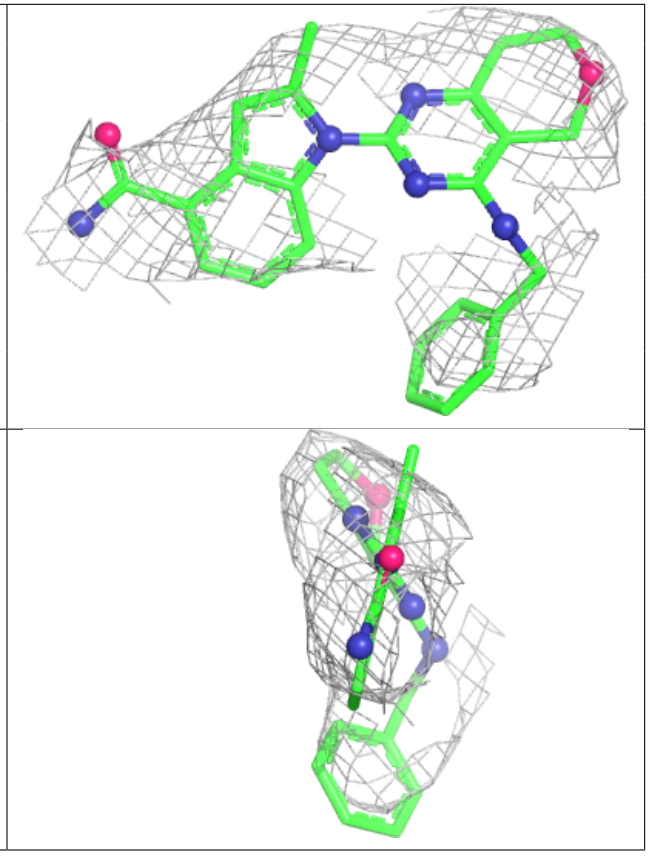






Electron density around JDP L 900:

$2mF_o$-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.