



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:24 pm BST

PDB ID : 5DYI  
Title : Structure of p97 N-D1 wild-type in complex with ADP  
Authors : Tang, W.K.; Xia, D.  
Deposited on : 2015-09-24  
Resolution : 3.71 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

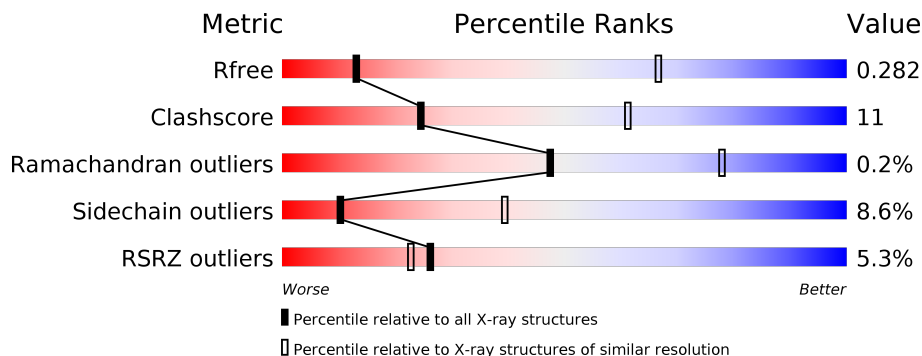
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.71 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.



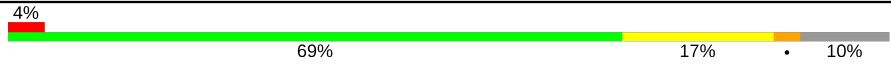

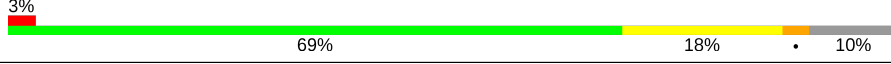
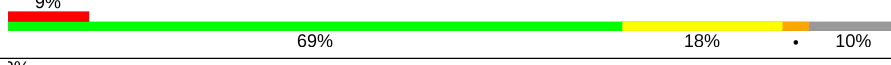

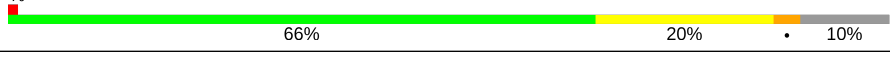
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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

Mol	Chain	Length	Quality of chain
1	A	489	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">69% 17% • 10%</p>
1	B	489	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">69% 17% • 10%</p>
1	C	489	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">69% 16% • 10%</p>
1	D	489	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">69% 18% • 10%</p>
1	E	489	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">66% 19% • 10%</p>
1	F	489	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">70% 17% • 10%</p>

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Mol	Chain	Length	Quality of chain
1	G	489	
1	H	489	
1	I	489	
1	J	489	
1	K	489	
1	L	489	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41579 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	440	3447	2162	612	655	18	0	0	0
1	B	438	3433	2155	609	651	18	0	0	0
1	C	438	3433	2155	609	651	18	0	0	0
1	D	439	3439	2158	610	653	18	0	0	0
1	E	438	3433	2155	609	651	18	0	0	0
1	F	438	3433	2155	609	651	18	0	0	0
1	G	438	3433	2155	609	651	18	0	0	0
1	H	439	3439	2158	610	653	18	0	0	0
1	I	439	3439	2158	610	653	18	0	0	0
1	J	441	3454	2167	613	656	18	0	0	0
1	K	439	3439	2158	610	653	18	0	0	0
1	L	438	3433	2155	609	651	18	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	482	ARG	-	expression tag	UNP P55072
A	483	SER	-	expression tag	UNP P55072
A	484	HIS	-	expression tag	UNP P55072
A	485	HIS	-	expression tag	UNP P55072
A	486	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	487	HIS	-	expression tag	UNP P55072
A	488	HIS	-	expression tag	UNP P55072
A	489	HIS	-	expression tag	UNP P55072
B	482	ARG	-	expression tag	UNP P55072
B	483	SER	-	expression tag	UNP P55072
B	484	HIS	-	expression tag	UNP P55072
B	485	HIS	-	expression tag	UNP P55072
B	486	HIS	-	expression tag	UNP P55072
B	487	HIS	-	expression tag	UNP P55072
B	488	HIS	-	expression tag	UNP P55072
B	489	HIS	-	expression tag	UNP P55072
C	482	ARG	-	expression tag	UNP P55072
C	483	SER	-	expression tag	UNP P55072
C	484	HIS	-	expression tag	UNP P55072
C	485	HIS	-	expression tag	UNP P55072
C	486	HIS	-	expression tag	UNP P55072
C	487	HIS	-	expression tag	UNP P55072
C	488	HIS	-	expression tag	UNP P55072
C	489	HIS	-	expression tag	UNP P55072
D	482	ARG	-	expression tag	UNP P55072
D	483	SER	-	expression tag	UNP P55072
D	484	HIS	-	expression tag	UNP P55072
D	485	HIS	-	expression tag	UNP P55072
D	486	HIS	-	expression tag	UNP P55072
D	487	HIS	-	expression tag	UNP P55072
D	488	HIS	-	expression tag	UNP P55072
D	489	HIS	-	expression tag	UNP P55072
E	482	ARG	-	expression tag	UNP P55072
E	483	SER	-	expression tag	UNP P55072
E	484	HIS	-	expression tag	UNP P55072
E	485	HIS	-	expression tag	UNP P55072
E	486	HIS	-	expression tag	UNP P55072
E	487	HIS	-	expression tag	UNP P55072
E	488	HIS	-	expression tag	UNP P55072
E	489	HIS	-	expression tag	UNP P55072
F	482	ARG	-	expression tag	UNP P55072
F	483	SER	-	expression tag	UNP P55072
F	484	HIS	-	expression tag	UNP P55072
F	485	HIS	-	expression tag	UNP P55072
F	486	HIS	-	expression tag	UNP P55072
F	487	HIS	-	expression tag	UNP P55072
F	488	HIS	-	expression tag	UNP P55072

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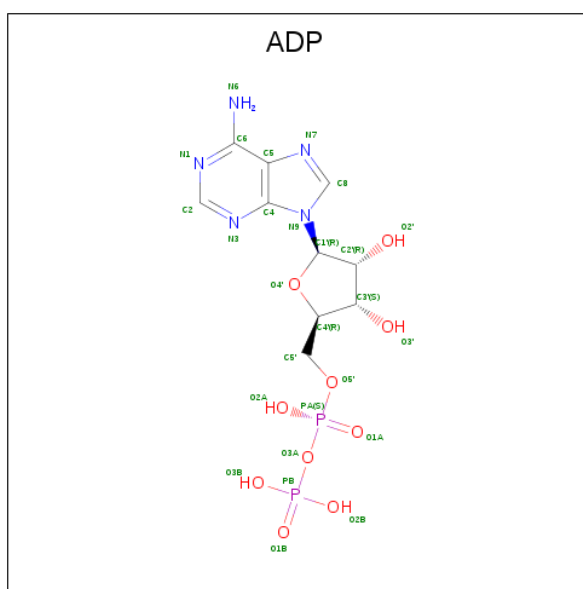
Chain	Residue	Modelled	Actual	Comment	Reference
F	489	HIS	-	expression tag	UNP P55072
G	482	ARG	-	expression tag	UNP P55072
G	483	SER	-	expression tag	UNP P55072
G	484	HIS	-	expression tag	UNP P55072
G	485	HIS	-	expression tag	UNP P55072
G	486	HIS	-	expression tag	UNP P55072
G	487	HIS	-	expression tag	UNP P55072
G	488	HIS	-	expression tag	UNP P55072
G	489	HIS	-	expression tag	UNP P55072
H	482	ARG	-	expression tag	UNP P55072
H	483	SER	-	expression tag	UNP P55072
H	484	HIS	-	expression tag	UNP P55072
H	485	HIS	-	expression tag	UNP P55072
H	486	HIS	-	expression tag	UNP P55072
H	487	HIS	-	expression tag	UNP P55072
H	488	HIS	-	expression tag	UNP P55072
H	489	HIS	-	expression tag	UNP P55072
I	482	ARG	-	expression tag	UNP P55072
I	483	SER	-	expression tag	UNP P55072
I	484	HIS	-	expression tag	UNP P55072
I	485	HIS	-	expression tag	UNP P55072
I	486	HIS	-	expression tag	UNP P55072
I	487	HIS	-	expression tag	UNP P55072
I	488	HIS	-	expression tag	UNP P55072
I	489	HIS	-	expression tag	UNP P55072
J	482	ARG	-	expression tag	UNP P55072
J	483	SER	-	expression tag	UNP P55072
J	484	HIS	-	expression tag	UNP P55072
J	485	HIS	-	expression tag	UNP P55072
J	486	HIS	-	expression tag	UNP P55072
J	487	HIS	-	expression tag	UNP P55072
J	488	HIS	-	expression tag	UNP P55072
J	489	HIS	-	expression tag	UNP P55072
K	482	ARG	-	expression tag	UNP P55072
K	483	SER	-	expression tag	UNP P55072
K	484	HIS	-	expression tag	UNP P55072
K	485	HIS	-	expression tag	UNP P55072
K	486	HIS	-	expression tag	UNP P55072
K	487	HIS	-	expression tag	UNP P55072
K	488	HIS	-	expression tag	UNP P55072
K	489	HIS	-	expression tag	UNP P55072
L	482	ARG	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
L	483	SER	-	expression tag	UNP P55072
L	484	HIS	-	expression tag	UNP P55072
L	485	HIS	-	expression tag	UNP P55072
L	486	HIS	-	expression tag	UNP P55072
L	487	HIS	-	expression tag	UNP P55072
L	488	HIS	-	expression tag	UNP P55072
L	489	HIS	-	expression tag	UNP P55072

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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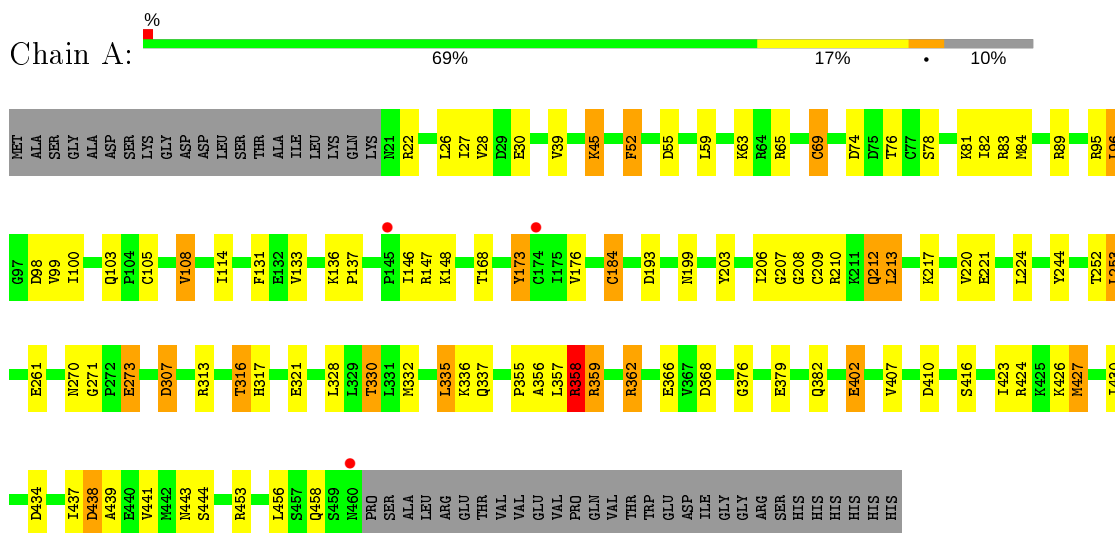
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	H	1	Total 27	10	5	10	2	0	0
2	I	1	Total 27	10	5	10	2	0	0
2	J	1	Total 27	10	5	10	2	0	0
2	K	1	Total 27	10	5	10	2	0	0
2	L	1	Total 27	10	5	10	2	0	0



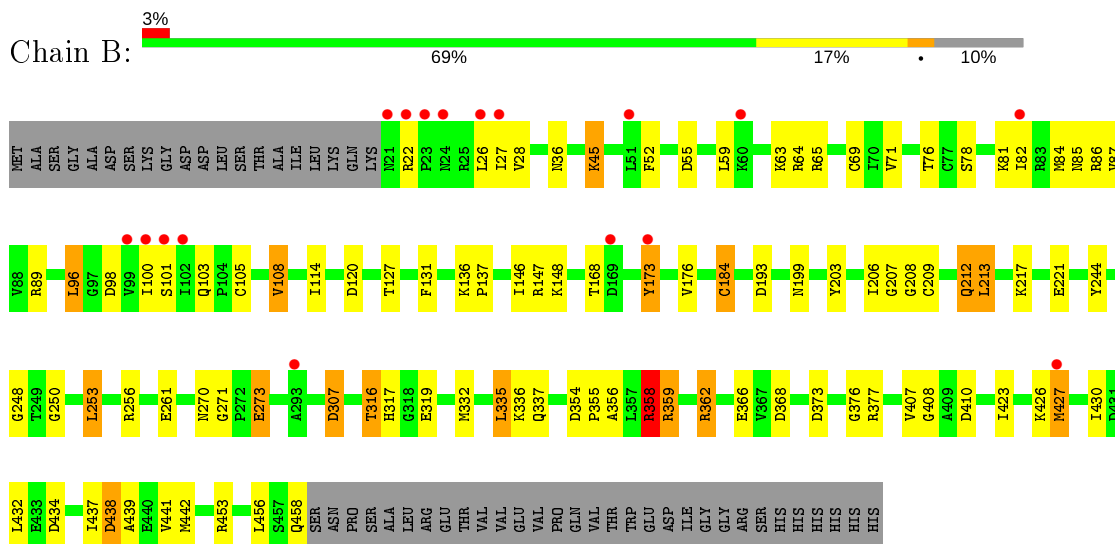
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Transitional endoplasmic reticulum ATPase



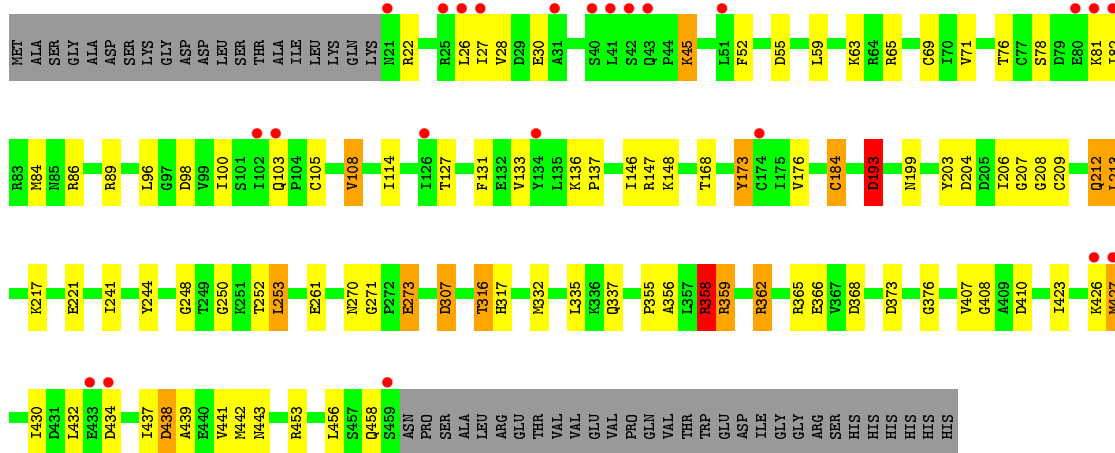
- Molecule 1: Transitional endoplasmic reticulum ATPase





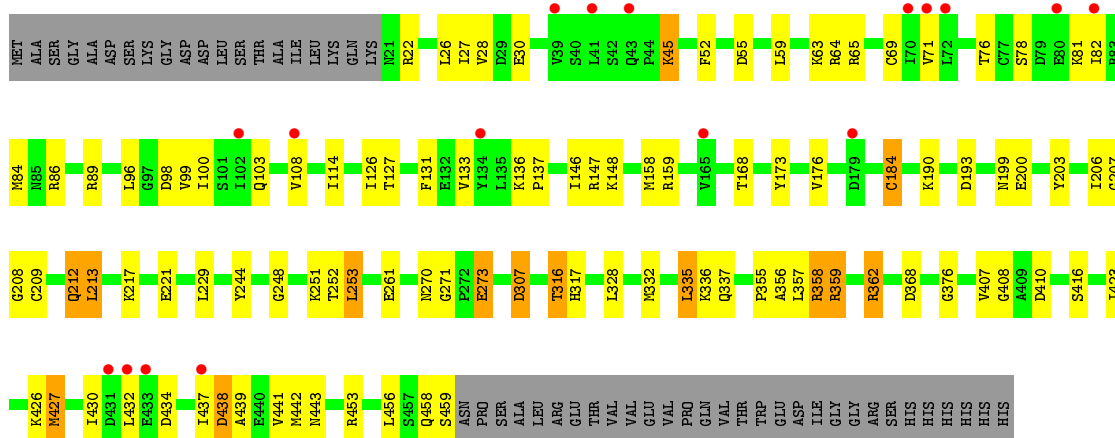


Chain H: 5% 70% 16% 10%



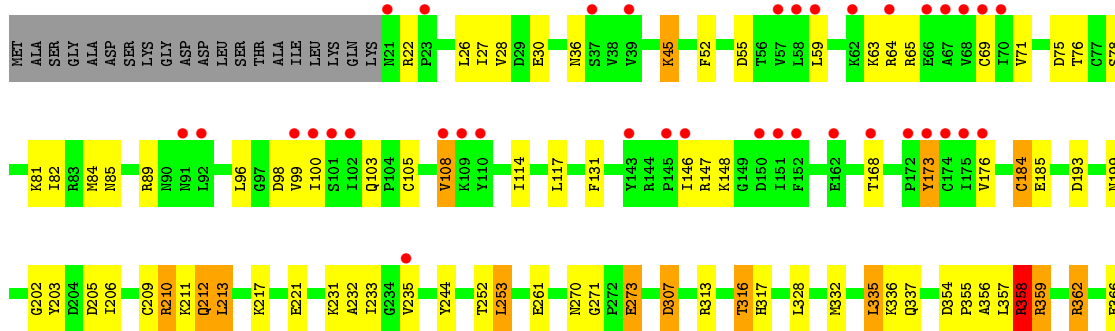
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain I: 3% 69% 18% 10%



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain J: 9% 69% 18% 10%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.44Å 176.21Å 256.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.71 48.91 – 3.71	Depositor EDS
% Data completeness (in resolution range)	68.1 (50.00-3.71) 68.2 (48.91-3.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 3.67Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.249 , 0.285 0.249 , 0.282	Depositor DCC
$R_{free}$ test set	2448 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.7	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 92.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	41579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.59	1/3500 (0.0%)	0.84	2/4729 (0.0%)
1	B	0.59	0/3486	0.84	2/4710 (0.0%)
1	C	0.57	0/3486	0.82	1/4710 (0.0%)
1	D	0.58	0/3492	0.84	0/4718
1	E	0.60	1/3486 (0.0%)	0.85	3/4710 (0.1%)
1	F	0.57	0/3486	0.82	1/4710 (0.0%)
1	G	0.56	0/3486	0.82	0/4710
1	H	0.56	0/3492	0.82	2/4718 (0.0%)
1	I	0.57	0/3492	0.84	0/4718
1	J	0.58	0/3508	0.83	2/4741 (0.0%)
1	K	0.62	0/3492	0.86	3/4718 (0.1%)
1	L	0.60	0/3486	0.85	2/4710 (0.0%)
All	All	0.58	2/41892 (0.0%)	0.84	18/56602 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	398	GLN	CD-NE2	-7.20	1.14	1.32
1	A	402	GLU	CD-OE1	-5.38	1.19	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	402	GLU	OE1-CD-OE2	-8.23	113.42	123.30
1	E	398	GLN	CG-CD-OE1	5.97	133.54	121.60
1	B	358	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	H	193	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	K	191	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	K	358	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	358	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	358	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	H	358	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	256	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	J	371	ILE	C-N-CD	-5.26	109.02	120.60
1	E	358	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	K	167	GLU	CG-CD-OE1	5.18	128.67	118.30
1	L	256	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	358	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	L	354	ASP	CB-CG-OD1	5.10	122.89	118.30
1	F	358	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	424	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3498	75	1
1	B	3433	0	3487	76	0
1	C	3433	0	3487	78	0
1	D	3439	0	3492	89	0
1	E	3433	0	3487	86	2
1	F	3433	0	3487	74	0
1	G	3433	0	3487	70	0
1	H	3439	0	3492	75	1
1	I	3439	0	3492	93	0
1	J	3454	0	3505	81	1
1	K	3439	0	3492	85	2
1	L	3433	0	3487	78	1
2	A	27	0	12	3	0
2	B	27	0	12	6	0
2	C	27	0	12	4	0
2	D	27	0	12	2	0
2	E	27	0	12	3	0
2	F	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	27	0	12	3	0
2	H	27	0	12	6	0
2	I	27	0	12	6	0
2	J	27	0	12	2	0
2	K	27	0	12	4	0
2	L	27	0	12	4	0
All	All	41579	0	42037	911	4

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 (911) 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:K:127:THR:HG23	1:K:438:ASP:HA	1.31	1.12
1:L:127:THR:HG23	1:L:438:ASP:HA	1.19	1.08
2:H:800:ADP:O3B	1:I:359:ARG:NH1	1.97	0.97
1:I:432:LEU:HD21	1:J:27:ILE:HD11	1.46	0.95
1:I:458:GLN:N	1:I:458:GLN:OE1	2.03	0.91
1:E:427:MET:HA	1:E:427:MET:HE2	1.56	0.88
2:B:800:ADP:O3B	1:C:359:ARG:NH1	2.07	0.87
1:F:427:MET:HE2	1:F:427:MET:HA	1.56	0.87
1:E:356:ALA:O	1:E:359:ARG:HB2	1.75	0.87
1:D:458:GLN:OE1	1:D:458:GLN:N	2.08	0.86
1:L:127:THR:HG23	1:L:438:ASP:CA	2.06	0.86
1:F:356:ALA:O	1:F:359:ARG:HB2	1.76	0.85
1:K:167:GLU:OE2	1:K:168:THR:N	2.09	0.85
1:L:127:THR:CG2	1:L:438:ASP:HA	2.04	0.85
1:C:427:MET:HA	1:C:427:MET:HE2	1.56	0.84
1:H:356:ALA:O	1:H:359:ARG:HB2	1.77	0.84
1:K:427:MET:HE2	1:K:430:ILE:HB	1.59	0.84
1:E:127:THR:HG23	1:E:438:ASP:HA	1.59	0.84
1:D:295:LYS:CD	1:H:193:ASP:OD1	2.25	0.84
1:J:427:MET:HA	1:J:427:MET:HE2	1.60	0.83
1:D:427:MET:HA	1:D:427:MET:HE2	1.59	0.83
1:C:356:ALA:O	1:C:359:ARG:HB2	1.79	0.82
1:L:427:MET:HE2	1:L:430:ILE:HB	1.58	0.82
1:L:356:ALA:O	1:L:359:ARG:HB2	1.78	0.82
1:I:427:MET:HE2	1:I:427:MET:HA	1.61	0.82
1:K:356:ALA:O	1:K:359:ARG:HB2	1.80	0.82
1:A:356:ALA:O	1:A:359:ARG:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:ALA:O	1:G:359:ARG:HB2	1.80	0.81
1:B:427:MET:HA	1:B:427:MET:HE2	1.61	0.81
1:D:356:ALA:O	1:D:359:ARG:HB2	1.79	0.81
1:G:427:MET:HA	1:G:427:MET:HE2	1.61	0.81
1:H:427:MET:HA	1:H:427:MET:HE2	1.63	0.81
1:I:356:ALA:O	1:I:359:ARG:HB2	1.81	0.81
1:A:437:ILE:HG23	1:A:441:VAL:HB	1.63	0.80
1:G:359:ARG:NH1	2:L:800:ADP:O3B	2.14	0.80
1:I:432:LEU:CD2	1:J:27:ILE:HD11	2.12	0.80
1:J:356:ALA:O	1:J:359:ARG:HB2	1.80	0.80
1:A:427:MET:HE2	1:A:430:ILE:HB	1.64	0.79
1:B:356:ALA:O	1:B:359:ARG:HB2	1.82	0.79
1:H:427:MET:HE2	1:H:430:ILE:HB	1.65	0.79
1:J:427:MET:HE2	1:J:430:ILE:HB	1.64	0.79
1:C:127:THR:HG23	1:C:438:ASP:HA	1.65	0.79
1:A:427:MET:HE2	1:A:427:MET:HA	1.65	0.78
1:D:275:MET:HB3	1:E:322:ARG:HH12	1.47	0.78
1:G:427:MET:HE2	1:G:430:ILE:HB	1.64	0.78
1:B:427:MET:HE2	1:B:430:ILE:HB	1.65	0.77
1:C:427:MET:HE2	1:C:430:ILE:HB	1.66	0.77
1:D:209:CYS:HB2	1:D:212:GLN:CG	2.14	0.77
1:I:427:MET:HE2	1:I:430:ILE:HB	1.66	0.76
1:F:427:MET:HE2	1:F:430:ILE:HB	1.66	0.76
1:D:133:VAL:HG11	1:D:439:ALA:HB1	1.68	0.76
1:D:427:MET:HE2	1:D:430:ILE:HB	1.66	0.76
1:I:209:CYS:HB2	1:I:212:GLN:CG	2.16	0.75
1:A:427:MET:CE	1:A:427:MET:HA	2.17	0.75
1:K:113:ARG:NH2	1:K:115:HIS:NE2	2.34	0.75
1:L:209:CYS:HB2	1:L:212:GLN:CG	2.16	0.75
1:A:209:CYS:HB2	1:A:212:GLN:CG	2.16	0.75
1:E:427:MET:HA	1:E:427:MET:CE	2.17	0.74
1:E:427:MET:HE2	1:E:430:ILE:HB	1.68	0.74
1:B:120:ASP:HB2	1:I:190:LYS:NZ	2.02	0.74
1:H:209:CYS:HB2	1:H:212:GLN:CG	2.16	0.74
1:E:209:CYS:HB2	1:E:212:GLN:CG	2.17	0.74
1:K:427:MET:HA	1:K:427:MET:CE	2.18	0.74
1:J:209:CYS:HB2	1:J:212:GLN:CG	2.17	0.74
1:J:427:MET:CE	1:J:427:MET:HA	2.18	0.74
1:I:427:MET:HA	1:I:427:MET:CE	2.18	0.74
1:K:209:CYS:HB2	1:K:212:GLN:CG	2.16	0.74
1:L:427:MET:CE	1:L:427:MET:HA	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:427:MET:CE	1:H:427:MET:HA	2.18	0.73
1:B:209:CYS:HB2	1:B:212:GLN:CG	2.18	0.73
1:D:427:MET:HA	1:D:427:MET:CE	2.18	0.73
1:K:113:ARG:NH2	1:K:115:HIS:CE1	2.56	0.73
1:F:209:CYS:HB2	1:F:212:GLN:CG	2.18	0.73
1:G:427:MET:HA	1:G:427:MET:CE	2.18	0.73
1:C:427:MET:HA	1:C:427:MET:CE	2.18	0.72
1:G:209:CYS:HB2	1:G:212:GLN:CG	2.19	0.72
1:F:427:MET:HA	1:F:427:MET:CE	2.18	0.72
1:G:127:THR:HG23	1:G:438:ASP:HA	1.71	0.72
1:B:427:MET:HA	1:B:427:MET:CE	2.18	0.72
1:C:209:CYS:HB2	1:C:212:GLN:CG	2.18	0.72
1:I:127:THR:HG23	1:I:438:ASP:HA	1.72	0.70
1:A:458:GLN:N	1:A:458:GLN:OE1	2.25	0.70
1:B:127:THR:HG23	1:B:438:ASP:HA	1.71	0.70
1:L:427:MET:HE2	1:L:427:MET:HA	1.72	0.70
1:B:206:ILE:HG21	1:B:213:LEU:HD21	1.73	0.70
1:J:206:ILE:HD11	1:J:253:LEU:HD22	1.74	0.69
1:F:206:ILE:HD11	1:F:253:LEU:HD22	1.75	0.68
1:I:206:ILE:HG21	1:I:213:LEU:HD21	1.75	0.68
1:F:206:ILE:HG21	1:F:213:LEU:HD21	1.76	0.68
1:E:206:ILE:HG21	1:E:213:LEU:HD21	1.76	0.68
2:I:800:ADP:O1B	1:J:359:ARG:NH1	2.24	0.68
1:B:438:ASP:OD1	1:B:438:ASP:N	2.27	0.68
1:K:427:MET:HA	1:K:427:MET:HE2	1.75	0.67
1:H:206:ILE:HG21	1:H:213:LEU:HD21	1.76	0.67
1:K:133:VAL:HG13	1:K:443:ASN:HB2	1.76	0.67
1:A:206:ILE:HD11	1:A:253:LEU:HD22	1.77	0.67
1:E:438:ASP:N	1:E:438:ASP:OD1	2.27	0.67
1:F:438:ASP:OD1	1:F:438:ASP:N	2.28	0.67
1:A:359:ARG:NH1	2:F:800:ADP:O3B	2.28	0.67
1:J:438:ASP:N	1:J:438:ASP:OD1	2.28	0.67
1:A:438:ASP:OD1	1:A:438:ASP:N	2.28	0.67
1:G:206:ILE:HG21	1:G:213:LEU:HD21	1.77	0.67
1:D:206:ILE:HG21	1:D:213:LEU:HD21	1.76	0.67
1:A:206:ILE:HG21	1:A:213:LEU:HD21	1.76	0.66
1:K:206:ILE:HG21	1:K:213:LEU:HD21	1.75	0.66
1:L:127:THR:O	1:L:439:ALA:N	2.21	0.66
1:E:208:GLY:HA2	1:E:376:GLY:HA2	1.78	0.66
1:G:438:ASP:N	1:G:438:ASP:OD1	2.27	0.66
1:D:295:LYS:HD3	1:H:193:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:458:GLN:N	1:H:458:GLN:OE1	2.28	0.66
1:F:426:LYS:O	1:F:430:ILE:HG13	1.96	0.66
1:L:206:ILE:HG21	1:L:213:LEU:HD21	1.76	0.66
1:E:426:LYS:O	1:E:430:ILE:HG13	1.96	0.66
1:L:426:LYS:O	1:L:430:ILE:HG13	1.96	0.66
1:D:206:ILE:HD11	1:D:253:LEU:HD22	1.78	0.66
1:I:426:LYS:O	1:I:430:ILE:HG13	1.96	0.66
1:I:438:ASP:OD1	1:I:438:ASP:N	2.27	0.66
1:K:426:LYS:O	1:K:430:ILE:HG13	1.96	0.66
1:A:426:LYS:O	1:A:430:ILE:HG13	1.96	0.65
1:C:206:ILE:HD11	1:C:253:LEU:HD22	1.77	0.65
1:D:275:MET:HB3	1:E:322:ARG:NH1	2.10	0.65
1:G:426:LYS:O	1:G:430:ILE:HG13	1.96	0.65
1:I:206:ILE:HD11	1:I:253:LEU:HD22	1.78	0.65
1:L:438:ASP:N	1:L:438:ASP:OD1	2.28	0.65
1:C:206:ILE:HG21	1:C:213:LEU:HD21	1.77	0.65
1:D:438:ASP:OD1	1:D:438:ASP:N	2.28	0.65
1:D:426:LYS:O	1:D:430:ILE:HG13	1.96	0.65
1:C:426:LYS:O	1:C:430:ILE:HG13	1.96	0.65
1:J:206:ILE:HG21	1:J:213:LEU:HD21	1.76	0.65
1:H:206:ILE:HD11	1:H:253:LEU:HD22	1.78	0.65
1:G:206:ILE:HD11	1:G:253:LEU:HD22	1.78	0.65
1:H:426:LYS:O	1:H:430:ILE:HG13	1.96	0.65
1:J:426:LYS:O	1:J:430:ILE:HG13	1.96	0.65
2:C:800:ADP:O1B	1:D:359:ARG:NH1	2.29	0.65
1:K:438:ASP:N	1:K:438:ASP:OD1	2.28	0.65
1:C:438:ASP:OD1	1:C:438:ASP:N	2.28	0.64
1:H:438:ASP:N	1:H:438:ASP:OD1	2.28	0.64
1:B:206:ILE:HD11	1:B:253:LEU:HD22	1.79	0.64
1:K:28:VAL:HG13	1:K:98:ASP:O	1.97	0.64
1:D:133:VAL:HG21	1:D:439:ALA:HB3	1.80	0.64
1:E:206:ILE:HD11	1:E:253:LEU:HD22	1.78	0.64
1:D:217:LYS:O	1:D:221:GLU:N	2.30	0.64
1:K:206:ILE:HD11	1:K:253:LEU:HD22	1.78	0.64
1:L:206:ILE:HD11	1:L:253:LEU:HD22	1.80	0.64
1:A:427:MET:CE	1:A:430:ILE:HD12	2.28	0.64
1:E:275:MET:HB3	1:F:322:ARG:NH1	2.12	0.64
1:D:295:LYS:HD2	1:H:193:ASP:OD1	1.97	0.64
1:B:426:LYS:O	1:B:430:ILE:HG13	1.97	0.63
1:F:127:THR:HG23	1:F:438:ASP:HA	1.80	0.63
1:J:374:ALA:HA	1:J:377:ARG:CZ	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HE3	1:A:430:ILE:HD12	1.81	0.63
1:K:27:ILE:O	1:K:82:ILE:HG22	1.99	0.63
1:G:437:ILE:HG23	1:G:441:VAL:HB	1.81	0.63
1:C:432:LEU:CD2	1:D:27:ILE:HD11	2.28	0.63
1:G:252:THR:HB	2:G:800:ADP:O2A	1.98	0.62
1:K:458:GLN:OE1	1:K:458:GLN:N	2.33	0.62
1:A:252:THR:HB	2:A:800:ADP:O2A	2.00	0.62
1:E:217:LYS:O	1:E:221:GLU:N	2.32	0.62
1:F:437:ILE:HG23	1:F:441:VAL:HB	1.82	0.62
1:B:120:ASP:HB2	1:I:190:LYS:HZ1	1.64	0.62
1:L:427:MET:CE	1:L:430:ILE:HD12	2.30	0.62
1:E:27:ILE:O	1:E:82:ILE:HG22	2.00	0.62
1:C:217:LYS:O	1:C:221:GLU:N	2.33	0.62
1:L:27:ILE:O	1:L:82:ILE:HG22	1.99	0.62
1:L:63:LYS:O	1:L:65:ARG:HG2	2.00	0.62
1:I:27:ILE:O	1:I:82:ILE:HG22	1.99	0.62
1:I:437:ILE:HG23	1:I:441:VAL:HB	1.82	0.62
1:D:437:ILE:HG23	1:D:441:VAL:HB	1.82	0.61
1:J:437:ILE:HG23	1:J:441:VAL:HB	1.82	0.61
1:G:27:ILE:O	1:G:82:ILE:HG22	2.00	0.61
1:B:27:ILE:O	1:B:82:ILE:HG22	2.00	0.61
1:F:27:ILE:O	1:F:82:ILE:HG22	1.99	0.61
1:D:27:ILE:O	1:D:82:ILE:HG22	2.00	0.61
1:H:252:THR:HB	2:H:800:ADP:O2A	2.00	0.61
2:A:800:ADP:O3B	1:B:359:ARG:NH1	2.33	0.61
1:E:437:ILE:HG23	1:E:441:VAL:HB	1.81	0.61
1:H:27:ILE:O	1:H:82:ILE:HG22	1.99	0.61
1:K:427:MET:CE	1:K:430:ILE:HD12	2.30	0.61
1:K:437:ILE:HG23	1:K:441:VAL:HB	1.82	0.61
1:A:27:ILE:O	1:A:82:ILE:HG22	2.00	0.61
1:E:276:SER:HB3	1:F:326:SER:HB3	1.83	0.61
1:K:63:LYS:O	1:K:65:ARG:HG2	2.01	0.61
1:J:27:ILE:O	1:J:82:ILE:HG22	2.00	0.61
1:C:27:ILE:O	1:C:82:ILE:HG22	2.00	0.60
1:E:432:LEU:O	1:F:25:ARG:NH1	2.32	0.60
1:F:63:LYS:O	1:F:65:ARG:HG2	2.01	0.60
1:E:28:VAL:HG13	1:E:98:ASP:O	2.01	0.60
1:L:28:VAL:HG13	1:L:98:ASP:O	2.02	0.60
1:F:217:LYS:O	1:F:221:GLU:N	2.34	0.60
1:C:437:ILE:HG23	1:C:441:VAL:HB	1.83	0.60
1:I:427:MET:CE	1:I:430:ILE:HD12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:MET:CE	1:C:430:ILE:HD12	2.32	0.60
1:J:427:MET:CE	1:J:430:ILE:HD12	2.32	0.60
1:E:275:MET:HB3	1:F:322:ARG:HH12	1.66	0.60
1:E:427:MET:CE	1:E:430:ILE:HD12	2.32	0.60
1:G:217:LYS:O	1:G:221:GLU:N	2.33	0.60
1:J:217:LYS:O	1:J:221:GLU:N	2.34	0.60
1:B:307:ASP:OD1	1:B:307:ASP:N	2.35	0.60
1:H:28:VAL:HG13	1:H:98:ASP:O	2.01	0.59
1:I:432:LEU:HA	1:J:99:VAL:HG11	1.84	0.59
1:B:120:ASP:CB	1:I:190:LYS:NZ	2.65	0.59
1:B:427:MET:CE	1:B:430:ILE:HD12	2.32	0.59
1:H:437:ILE:HG23	1:H:441:VAL:HB	1.83	0.59
1:J:28:VAL:HG13	1:J:98:ASP:O	2.02	0.59
1:D:427:MET:CE	1:D:430:ILE:HD12	2.33	0.59
1:H:427:MET:CE	1:H:430:ILE:HD12	2.31	0.59
1:D:63:LYS:O	1:D:65:ARG:HG2	2.03	0.59
1:B:437:ILE:HG23	1:B:441:VAL:HB	1.82	0.59
1:B:28:VAL:HG13	1:B:98:ASP:O	2.03	0.59
1:L:437:ILE:HG23	1:L:441:VAL:HB	1.85	0.59
1:G:427:MET:CE	1:G:430:ILE:HD12	2.32	0.59
1:C:63:LYS:O	1:C:65:ARG:HG2	2.01	0.59
1:E:252:THR:HB	2:E:800:ADP:O1A	2.02	0.59
1:I:251:LYS:N	2:I:800:ADP:O2A	2.36	0.58
1:F:427:MET:CE	1:F:430:ILE:HD12	2.33	0.58
1:B:217:LYS:O	1:B:221:GLU:N	2.36	0.58
1:D:147:ARG:HG2	1:D:148:LYS:N	2.17	0.58
1:D:295:LYS:HB3	1:H:193:ASP:OD1	2.03	0.58
1:L:147:ARG:HG2	1:L:148:LYS:N	2.17	0.58
1:E:131:PHE:HB2	1:E:184:CYS:SG	2.44	0.58
1:C:432:LEU:HD21	1:D:27:ILE:HD11	1.86	0.58
1:D:457:SER:HB2	1:D:458:GLN:OE1	2.03	0.58
1:J:252:THR:HB	2:J:800:ADP:O1A	2.03	0.58
1:K:427:MET:HE3	1:K:430:ILE:HD12	1.86	0.58
1:A:63:LYS:O	1:A:65:ARG:HG2	2.04	0.58
1:I:63:LYS:O	1:I:65:ARG:HG2	2.02	0.58
1:A:217:LYS:O	1:A:221:GLU:N	2.36	0.58
1:I:159:ARG:NH2	1:J:231:LYS:O	2.37	0.58
1:H:209:CYS:HB2	1:H:212:GLN:CD	2.24	0.58
1:D:28:VAL:HG13	1:D:98:ASP:O	2.04	0.57
1:E:427:MET:HE3	1:E:430:ILE:HD12	1.86	0.57
1:H:217:LYS:O	1:H:221:GLU:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:MET:HE3	1:L:430:ILE:HD12	1.85	0.57
1:I:28:VAL:HG13	1:I:98:ASP:O	2.03	0.57
1:K:209:CYS:HB2	1:K:212:GLN:CD	2.23	0.57
1:A:28:VAL:HG23	1:A:96:LEU:HA	1.86	0.57
1:H:427:MET:HE3	1:H:430:ILE:HD12	1.87	0.57
1:I:217:LYS:O	1:I:221:GLU:N	2.37	0.57
1:B:206:ILE:HG21	1:B:213:LEU:CD2	2.34	0.57
1:H:127:THR:HG23	1:H:438:ASP:HA	1.85	0.57
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.86	0.57
1:E:307:ASP:N	1:E:307:ASP:OD1	2.38	0.57
1:L:126:ILE:HB	1:L:439:ALA:HB2	1.85	0.57
1:B:131:PHE:HB2	1:B:184:CYS:SG	2.45	0.57
1:I:427:MET:HE3	1:I:430:ILE:HD12	1.86	0.57
1:A:28:VAL:HG13	1:A:98:ASP:O	2.05	0.56
1:F:131:PHE:HB2	1:F:184:CYS:SG	2.45	0.56
1:F:28:VAL:HG13	1:F:98:ASP:O	2.05	0.56
1:H:206:ILE:HG21	1:H:213:LEU:CD2	2.36	0.56
1:C:28:VAL:HG13	1:C:98:ASP:O	2.05	0.56
1:L:206:ILE:HG21	1:L:213:LEU:CD2	2.36	0.56
1:D:427:MET:HE3	1:D:430:ILE:HD12	1.88	0.56
1:F:307:ASP:N	1:F:307:ASP:OD1	2.38	0.56
1:G:427:MET:HE3	1:G:430:ILE:HD12	1.88	0.56
2:K:800:ADP:O1B	1:L:359:ARG:NH1	2.39	0.56
1:K:206:ILE:HG21	1:K:213:LEU:CD2	2.36	0.56
1:B:120:ASP:OD2	1:I:190:LYS:HE2	2.05	0.56
1:C:427:MET:HE3	1:C:430:ILE:HD12	1.88	0.56
1:D:206:ILE:HG21	1:D:213:LEU:CD2	2.36	0.56
1:B:427:MET:HE3	1:B:430:ILE:HD12	1.88	0.56
1:H:63:LYS:O	1:H:65:ARG:HG2	2.06	0.56
1:E:206:ILE:HG21	1:E:213:LEU:CD2	2.35	0.56
1:L:217:LYS:O	1:L:221:GLU:N	2.38	0.56
1:B:244:TYR:HB2	1:B:368:ASP:HA	1.89	0.55
1:F:206:ILE:HG21	1:F:213:LEU:CD2	2.35	0.55
1:I:133:VAL:HG13	1:I:443:ASN:HB2	1.87	0.55
1:I:206:ILE:HG21	1:I:213:LEU:CD2	2.36	0.55
1:A:423:ILE:O	1:A:427:MET:HB2	2.07	0.55
1:J:203:TYR:CD2	1:J:261:GLU:HG2	2.42	0.55
1:A:206:ILE:HG21	1:A:213:LEU:CD2	2.35	0.55
1:B:120:ASP:HB2	1:I:190:LYS:HZ3	1.72	0.55
1:H:131:PHE:HB2	1:H:184:CYS:SG	2.45	0.55
1:K:244:TYR:HB2	1:K:368:ASP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:PHE:HB2	1:J:184:CYS:SG	2.47	0.55
1:K:147:ARG:O	1:K:148:LYS:C	2.44	0.55
1:K:217:LYS:O	1:K:221:GLU:N	2.39	0.55
1:L:158:MET:HA	1:L:387:ASN:O	2.07	0.55
1:G:307:ASP:OD1	1:G:307:ASP:N	2.40	0.55
1:E:275:MET:CB	1:F:322:ARG:HH12	2.20	0.55
1:J:427:MET:HE3	1:J:430:ILE:HD12	1.89	0.55
1:C:206:ILE:HG21	1:C:213:LEU:CD2	2.37	0.55
1:C:321:GLU:HG3	1:D:319:GLU:HG2	1.89	0.55
1:F:203:TYR:CD2	1:F:261:GLU:HG2	2.42	0.54
1:I:244:TYR:HB2	1:I:368:ASP:HA	1.88	0.54
1:A:203:TYR:CD2	1:A:261:GLU:HG2	2.42	0.54
1:B:63:LYS:O	1:B:65:ARG:HG2	2.07	0.54
1:D:275:MET:CB	1:E:322:ARG:HH12	2.18	0.54
1:G:63:LYS:O	1:G:65:ARG:HG2	2.06	0.54
1:I:432:LEU:CD2	1:J:27:ILE:CD1	2.84	0.54
1:I:208:GLY:HA2	1:I:376:GLY:HA2	1.89	0.54
1:A:209:CYS:HB2	1:A:212:GLN:CD	2.27	0.54
1:G:206:ILE:HG21	1:G:213:LEU:CD2	2.36	0.54
1:H:248:GLY:N	2:H:800:ADP:O2B	2.41	0.54
1:A:131:PHE:HB2	1:A:184:CYS:SG	2.47	0.54
1:D:28:VAL:HG23	1:D:96:LEU:HA	1.90	0.54
1:J:206:ILE:HG21	1:J:213:LEU:CD2	2.37	0.54
1:J:423:ILE:O	1:J:427:MET:HB2	2.07	0.54
1:J:63:LYS:O	1:J:65:ARG:HG2	2.07	0.54
1:F:147:ARG:HG2	1:F:148:LYS:N	2.22	0.54
1:F:208:GLY:HA2	1:F:376:GLY:HA2	1.89	0.54
1:K:113:ARG:HH21	1:K:115:HIS:CE1	2.26	0.54
1:C:273:GLU:HA	1:D:330:THR:OG1	2.07	0.54
1:G:28:VAL:HG13	1:G:98:ASP:O	2.07	0.54
1:J:354:ASP:OD1	1:J:355:PRO:HD2	2.07	0.54
1:F:427:MET:HE3	1:F:430:ILE:HD12	1.90	0.54
1:D:173:TYR:HD1	1:D:173:TYR:O	1.91	0.53
1:E:332:MET:HB3	1:E:362:ARG:HG2	1.91	0.53
1:H:423:ILE:HG21	1:I:229:LEU:HD21	1.90	0.53
1:J:307:ASP:N	1:J:307:ASP:OD1	2.41	0.53
1:L:147:ARG:HG3	1:L:173:TYR:HB3	1.90	0.53
1:B:120:ASP:OD2	1:I:190:LYS:CE	2.57	0.53
1:L:423:ILE:O	1:L:427:MET:HB2	2.09	0.53
1:A:321:GLU:HG3	1:B:319:GLU:HG2	1.90	0.53
1:K:147:ARG:HG2	1:K:148:LYS:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:CYS:HB2	1:D:212:GLN:CD	2.29	0.53
1:E:244:TYR:HB2	1:E:368:ASP:HA	1.91	0.53
1:G:244:TYR:HB2	1:G:368:ASP:HA	1.91	0.53
1:H:28:VAL:HG23	1:H:96:LEU:HA	1.91	0.53
1:I:209:CYS:HB2	1:I:212:GLN:CD	2.28	0.53
1:I:158:MET:HB2	1:J:233:ILE:HG22	1.90	0.53
1:D:147:ARG:HG3	1:D:173:TYR:HB3	1.90	0.53
1:H:244:TYR:HB2	1:H:368:ASP:HA	1.91	0.53
1:K:208:GLY:HA2	1:K:376:GLY:HA2	1.91	0.53
1:D:307:ASP:N	1:D:307:ASP:OD1	2.39	0.53
1:D:276:SER:HA	1:E:326:SER:HB2	1.91	0.53
1:I:307:ASP:OD1	1:I:307:ASP:N	2.42	0.53
1:A:307:ASP:OD1	1:A:307:ASP:N	2.42	0.53
1:D:203:TYR:CD2	1:D:261:GLU:HG2	2.44	0.53
1:D:423:ILE:O	1:D:427:MET:HB2	2.08	0.53
1:C:244:TYR:HB2	1:C:368:ASP:HA	1.91	0.52
1:L:209:CYS:HB2	1:L:212:GLN:CD	2.28	0.52
1:F:209:CYS:HB2	1:F:212:GLN:CD	2.30	0.52
1:K:423:ILE:O	1:K:427:MET:HB2	2.08	0.52
1:B:147:ARG:HG2	1:B:148:LYS:N	2.25	0.52
1:F:423:ILE:O	1:F:427:MET:HB2	2.10	0.52
1:H:307:ASP:OD1	1:H:307:ASP:N	2.43	0.52
1:L:307:ASP:N	1:L:307:ASP:OD1	2.42	0.52
1:C:332:MET:HB3	1:C:362:ARG:HG2	1.91	0.52
2:G:800:ADP:O3B	1:H:359:ARG:NH1	2.42	0.52
1:G:25:ARG:NH1	1:L:434:ASP:OD2	2.42	0.52
1:B:423:ILE:O	1:B:427:MET:HB2	2.10	0.52
1:I:131:PHE:HB2	1:I:184:CYS:SG	2.50	0.52
1:F:252:THR:HB	2:F:800:ADP:O2A	2.10	0.52
1:I:86:ARG:NH2	1:I:200:GLU:O	2.38	0.52
1:I:147:ARG:HG2	1:I:148:LYS:N	2.25	0.52
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.92	0.52
1:C:147:ARG:HG2	1:C:148:LYS:N	2.25	0.52
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.45	0.52
1:I:28:VAL:HG23	1:I:96:LEU:HA	1.92	0.52
1:C:423:ILE:O	1:C:427:MET:HB2	2.10	0.51
1:I:423:ILE:O	1:I:427:MET:HB2	2.09	0.51
1:J:332:MET:HB3	1:J:362:ARG:HG2	1.92	0.51
1:K:250:GLY:N	2:K:800:ADP:O2A	2.34	0.51
1:J:244:TYR:HB2	1:J:368:ASP:HA	1.92	0.51
1:E:30:GLU:HG2	1:E:96:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:MET:HB3	1:F:362:ARG:HG2	1.92	0.51
1:J:373:ASP:OD1	1:J:373:ASP:N	2.40	0.51
1:K:28:VAL:HG23	1:K:96:LEU:HA	1.92	0.51
1:E:208:GLY:HA2	1:E:376:GLY:CA	2.41	0.51
1:F:244:TYR:HB2	1:F:368:ASP:HA	1.92	0.51
1:C:203:TYR:CD2	1:C:261:GLU:HG2	2.46	0.51
1:D:244:TYR:HB2	1:D:368:ASP:HA	1.92	0.51
1:L:244:TYR:HB2	1:L:368:ASP:HA	1.92	0.51
1:A:147:ARG:HG2	1:A:148:LYS:N	2.26	0.51
1:B:203:TYR:CD2	1:B:261:GLU:HG2	2.45	0.51
1:C:355:PRO:O	1:C:358:ARG:HG2	2.10	0.51
1:L:209:CYS:HB2	1:L:212:GLN:HG2	1.92	0.51
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.93	0.51
1:J:28:VAL:HG23	1:J:96:LEU:HA	1.93	0.51
1:A:147:ARG:HG3	1:A:173:TYR:HB3	1.92	0.51
1:G:30:GLU:HG2	1:G:96:LEU:HD21	1.93	0.50
1:H:203:TYR:CD2	1:H:261:GLU:HG2	2.46	0.50
1:K:332:MET:HB3	1:K:362:ARG:HG2	1.93	0.50
1:A:244:TYR:HB2	1:A:368:ASP:HA	1.93	0.50
1:G:147:ARG:HG2	1:G:148:LYS:N	2.25	0.50
1:I:26:LEU:HD21	1:I:45:LYS:HE2	1.93	0.50
1:H:147:ARG:HG2	1:H:148:LYS:N	2.25	0.50
1:L:26:LEU:HD21	1:L:45:LYS:HE2	1.94	0.50
1:A:209:CYS:HB2	1:A:212:GLN:HG2	1.94	0.50
1:C:131:PHE:HB2	1:C:184:CYS:SG	2.52	0.50
1:H:209:CYS:HB2	1:H:212:GLN:HG2	1.92	0.50
1:J:30:GLU:HG2	1:J:96:LEU:HD21	1.93	0.50
1:K:408:GLY:C	2:K:800:ADP:C8	2.85	0.50
1:B:147:ARG:HG3	1:B:173:TYR:HB3	1.93	0.50
1:E:158:MET:HA	1:E:387:ASN:O	2.11	0.50
1:G:28:VAL:HG23	1:G:96:LEU:HA	1.94	0.50
1:I:30:GLU:HG2	1:I:96:LEU:HD21	1.93	0.50
1:H:30:GLU:HG2	1:H:96:LEU:HD21	1.93	0.50
1:J:209:CYS:HB2	1:J:212:GLN:HG2	1.92	0.50
1:L:203:TYR:CD2	1:L:261:GLU:HG2	2.45	0.50
1:D:105:CYS:O	1:D:108:VAL:HG23	2.12	0.50
1:E:203:TYR:CD2	1:E:261:GLU:HG2	2.47	0.50
1:F:427:MET:CE	1:F:430:ILE:HB	2.39	0.50
1:J:206:ILE:CD1	1:J:253:LEU:HD22	2.42	0.50
1:F:30:GLU:HG2	1:F:96:LEU:HD21	1.93	0.50
1:J:26:LEU:HD21	1:J:45:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:ARG:HG3	1:K:173:TYR:HB3	1.93	0.50
1:B:354:ASP:OD1	1:B:355:PRO:HD2	2.12	0.50
1:H:209:CYS:HB2	1:H:212:GLN:NE2	2.27	0.50
1:L:332:MET:HB3	1:L:362:ARG:HG2	1.94	0.50
1:H:423:ILE:O	1:H:427:MET:HB2	2.12	0.49
1:I:203:TYR:CD2	1:I:261:GLU:HG2	2.47	0.49
1:J:147:ARG:HG2	1:J:148:LYS:N	2.27	0.49
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.46	0.49
1:C:30:GLU:HG2	1:C:96:LEU:HD21	1.94	0.49
1:D:30:GLU:HG2	1:D:96:LEU:HD21	1.93	0.49
1:E:147:ARG:HG2	1:E:148:LYS:N	2.27	0.49
1:H:332:MET:HB3	1:H:362:ARG:HG2	1.93	0.49
1:A:332:MET:HB3	1:A:362:ARG:HG2	1.93	0.49
1:B:209:CYS:HB2	1:B:212:GLN:CD	2.32	0.49
1:B:212:GLN:CD	1:B:212:GLN:H	2.15	0.49
1:F:209:CYS:HB2	1:F:212:GLN:HG2	1.94	0.49
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.93	0.49
1:I:126:ILE:HG23	1:J:232:ALA:O	2.12	0.49
1:B:120:ASP:CB	1:I:190:LYS:HZ3	2.25	0.49
1:K:126:ILE:HB	1:K:439:ALA:HB2	1.94	0.49
1:E:209:CYS:HB2	1:E:212:GLN:CD	2.33	0.49
1:E:423:ILE:O	1:E:427:MET:HB2	2.11	0.49
1:G:332:MET:HB3	1:G:362:ARG:HG2	1.94	0.49
1:K:113:ARG:HB2	1:K:169:ASP:HB2	1.95	0.49
1:I:332:MET:HB3	1:I:362:ARG:HG2	1.94	0.49
1:K:423:ILE:HG21	1:L:229:LEU:HD21	1.93	0.49
1:A:437:ILE:HG23	1:A:441:VAL:CB	2.40	0.49
1:C:427:MET:CE	1:C:430:ILE:HB	2.40	0.49
1:F:26:LEU:HD21	1:F:45:LYS:HE2	1.95	0.49
1:F:251:LYS:N	2:F:800:ADP:O1A	2.46	0.49
1:B:332:MET:HB3	1:B:362:ARG:HG2	1.93	0.49
1:C:307:ASP:N	1:C:307:ASP:OD1	2.46	0.49
1:D:209:CYS:HB2	1:D:212:GLN:HG2	1.92	0.49
1:D:332:MET:HB3	1:D:362:ARG:HG2	1.94	0.49
1:E:212:GLN:H	1:E:212:GLN:CD	2.16	0.49
1:K:408:GLY:HA3	2:K:800:ADP:N7	2.28	0.49
1:D:133:VAL:HG11	1:D:439:ALA:CB	2.38	0.49
1:B:209:CYS:HB2	1:B:212:GLN:HG2	1.94	0.49
1:C:209:CYS:HB2	1:C:212:GLN:CD	2.32	0.49
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.94	0.49
1:E:408:GLY:HA3	2:E:800:ADP:N7	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:TYR:CD2	1:G:261:GLU:HG2	2.48	0.49
1:K:30:GLU:HG2	1:K:96:LEU:HD21	1.93	0.49
1:B:248:GLY:HA2	2:B:800:ADP:O3A	2.13	0.48
1:B:26:LEU:HD21	1:B:45:LYS:HE2	1.95	0.48
1:D:276:SER:HB3	1:E:326:SER:HB3	1.94	0.48
1:K:173:TYR:HD1	1:K:173:TYR:O	1.96	0.48
1:C:453:ARG:HA	1:C:456:LEU:HD12	1.95	0.48
1:H:26:LEU:HD21	1:H:45:LYS:HE2	1.95	0.48
1:J:355:PRO:O	1:J:358:ARG:HG2	2.13	0.48
1:C:84:MET:HG3	1:C:89:ARG:HG3	1.95	0.48
1:F:84:MET:HG3	1:F:89:ARG:HG3	1.95	0.48
1:G:147:ARG:HG3	1:G:173:TYR:HB3	1.95	0.48
1:G:209:CYS:HB2	1:G:212:GLN:CD	2.32	0.48
1:I:82:ILE:HG21	1:I:100:ILE:HD11	1.94	0.48
1:L:28:VAL:HG23	1:L:96:LEU:HA	1.94	0.48
1:A:133:VAL:HG11	1:A:439:ALA:HB1	1.95	0.48
1:C:26:LEU:HD21	1:C:45:LYS:HE2	1.96	0.48
1:E:84:MET:HG3	1:E:89:ARG:HG3	1.95	0.48
1:I:212:GLN:CD	1:I:212:GLN:H	2.16	0.48
1:G:423:ILE:O	1:G:427:MET:HB2	2.14	0.48
1:K:203:TYR:CD2	1:K:261:GLU:HG2	2.48	0.48
1:C:133:VAL:HG13	1:C:443:ASN:HB2	1.96	0.48
1:J:209:CYS:HB2	1:J:212:GLN:CD	2.33	0.48
1:G:427:MET:CE	1:G:430:ILE:HB	2.41	0.48
1:J:427:MET:CE	1:J:430:ILE:HB	2.41	0.48
1:I:209:CYS:HB2	1:I:212:GLN:HG2	1.91	0.48
1:J:374:ALA:HB2	1:J:377:ARG:NH2	2.29	0.48
1:A:330:THR:OG1	1:F:273:GLU:HA	2.14	0.48
1:D:439:ALA:O	1:D:442:MET:HB2	2.14	0.48
1:A:270:ASN:HB3	1:A:273:GLU:HG2	1.96	0.48
1:J:203:TYR:CE2	1:J:261:GLU:HG2	2.49	0.48
1:J:36:ASN:HA	1:J:85:ASN:HD21	1.79	0.48
1:L:30:GLU:HG2	1:L:96:LEU:HD21	1.95	0.48
1:I:84:MET:HG3	1:I:89:ARG:HG3	1.95	0.47
1:L:206:ILE:HG22	1:L:207:GLY:N	2.29	0.47
1:L:458:GLN:N	1:L:458:GLN:OE1	2.47	0.47
1:C:316:THR:O	1:C:316:THR:HG23	2.14	0.47
1:E:193:ASP:OD2	1:G:194:GLU:OE2	2.32	0.47
1:C:146:ILE:HD11	1:C:168:THR:HG21	1.96	0.47
1:E:408:GLY:C	2:E:800:ADP:C8	2.88	0.47
1:H:133:VAL:HG13	1:H:443:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:355:PRO:O	1:K:358:ARG:HG2	2.14	0.47
1:A:453:ARG:HA	1:A:456:LEU:HD12	1.97	0.47
1:D:146:ILE:HD11	1:D:168:THR:HG21	1.96	0.47
1:D:84:MET:HG3	1:D:89:ARG:HG3	1.96	0.47
1:F:206:ILE:CD1	1:F:253:LEU:HD22	2.44	0.47
1:G:453:ARG:HA	1:G:456:LEU:HD12	1.97	0.47
1:K:113:ARG:CZ	1:K:115:HIS:NE2	2.77	0.47
1:A:39:VAL:HG13	1:A:69:CYS:SG	2.55	0.47
1:C:270:ASN:HB3	1:C:273:GLU:HG2	1.97	0.47
1:C:439:ALA:O	1:C:442:MET:HB2	2.14	0.47
1:A:146:ILE:HD11	1:A:168:THR:HG21	1.96	0.47
1:G:84:MET:HG3	1:G:89:ARG:HG3	1.95	0.47
1:H:250:GLY:N	2:H:800:ADP:O1A	2.47	0.47
1:K:209:CYS:HB2	1:K:212:GLN:NE2	2.29	0.47
1:A:206:ILE:HG22	1:A:207:GLY:N	2.29	0.47
1:D:427:MET:CE	1:D:430:ILE:HB	2.42	0.47
1:A:212:GLN:H	1:A:212:GLN:CD	2.18	0.47
1:A:26:LEU:HD21	1:A:45:LYS:HE2	1.96	0.47
1:G:26:LEU:HD21	1:G:45:LYS:HE2	1.96	0.47
1:I:209:CYS:HB2	1:I:212:GLN:NE2	2.29	0.47
1:A:52:PHE:N	1:A:55:ASP:OD2	2.41	0.47
1:A:84:MET:HG3	1:A:89:ARG:HG3	1.97	0.47
1:F:355:PRO:O	1:F:358:ARG:HG2	2.15	0.47
1:F:453:ARG:HA	1:F:456:LEU:HD12	1.97	0.47
1:J:210:ARG:HG2	1:J:210:ARG:HH11	1.80	0.47
1:B:146:ILE:HD11	1:B:168:THR:HG21	1.97	0.47
1:J:458:GLN:OE1	1:J:458:GLN:N	2.48	0.47
1:K:27:ILE:O	1:K:82:ILE:CG2	2.63	0.47
1:D:26:LEU:HD21	1:D:45:LYS:HE2	1.97	0.47
1:E:82:ILE:HG21	1:E:100:ILE:HD11	1.97	0.47
1:H:147:ARG:HG3	1:H:173:TYR:HB3	1.97	0.47
1:H:208:GLY:HA2	1:H:376:GLY:HA2	1.97	0.47
1:I:206:ILE:CD1	1:I:253:LEU:HD22	2.45	0.47
1:B:355:PRO:O	1:B:358:ARG:HG2	2.15	0.46
1:C:212:GLN:CD	1:C:212:GLN:H	2.18	0.46
1:C:458:GLN:OE1	1:C:458:GLN:N	2.48	0.46
1:E:26:LEU:HD21	1:E:45:LYS:HE2	1.97	0.46
1:E:316:THR:O	1:E:316:THR:HG23	2.14	0.46
1:G:358:ARG:HB3	1:G:366:GLU:OE2	2.14	0.46
1:J:332:MET:HE2	1:J:362:ARG:HB3	1.97	0.46
1:J:82:ILE:HG21	1:J:100:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:GLN:CD	1:L:212:GLN:H	2.19	0.46
1:E:355:PRO:O	1:E:358:ARG:HG2	2.16	0.46
1:F:358:ARG:HB3	1:F:366:GLU:OE2	2.15	0.46
1:H:82:ILE:HG21	1:H:100:ILE:HD11	1.97	0.46
1:H:84:MET:HG3	1:H:89:ARG:HG3	1.95	0.46
1:B:82:ILE:HG21	1:B:100:ILE:HD11	1.97	0.46
1:B:439:ALA:O	1:B:442:MET:HB2	2.16	0.46
1:C:206:ILE:CD1	1:C:253:LEU:HD22	2.45	0.46
1:C:250:GLY:N	2:C:800:ADP:O1A	2.42	0.46
1:G:173:TYR:O	1:G:173:TYR:HD1	1.99	0.46
1:J:147:ARG:HG3	1:J:173:TYR:HB3	1.97	0.46
1:A:355:PRO:O	1:A:358:ARG:HG2	2.16	0.46
1:B:84:MET:HG3	1:B:89:ARG:HG3	1.97	0.46
1:C:209:CYS:HB2	1:C:212:GLN:HG2	1.94	0.46
1:C:82:ILE:HG21	1:C:100:ILE:HD11	1.97	0.46
1:D:131:PHE:HB2	1:D:184:CYS:SG	2.55	0.46
1:E:209:CYS:HB2	1:E:212:GLN:HG2	1.93	0.46
1:F:208:GLY:HA2	1:F:376:GLY:CA	2.45	0.46
1:G:131:PHE:HB2	1:G:184:CYS:SG	2.55	0.46
1:G:458:GLN:N	1:G:458:GLN:OE1	2.49	0.46
1:I:252:THR:HB	2:I:800:ADP:O1A	2.16	0.46
1:J:373:ASP:O	1:J:376:GLY:N	2.48	0.46
1:L:173:TYR:O	1:L:173:TYR:HD1	1.99	0.46
1:A:332:MET:HE2	1:A:362:ARG:HB3	1.96	0.46
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.51	0.46
1:H:355:PRO:O	1:H:358:ARG:HG2	2.15	0.46
1:A:173:TYR:HD1	1:A:173:TYR:O	1.98	0.46
1:B:453:ARG:HA	1:B:456:LEU:HD12	1.97	0.46
1:C:147:ARG:HG3	1:C:173:TYR:HB3	1.97	0.46
1:F:89:ARG:NH1	1:F:96:LEU:HD12	2.30	0.46
1:K:209:CYS:HB2	1:K:212:GLN:HG2	1.96	0.46
1:K:332:MET:HE2	1:K:362:ARG:HB3	1.96	0.46
1:K:26:LEU:HD21	1:K:45:LYS:HE2	1.96	0.46
2:J:800:ADP:O1B	1:K:359:ARG:NH1	2.49	0.46
1:B:407:VAL:O	1:B:410:ASP:HB2	2.16	0.46
1:D:355:PRO:O	1:D:358:ARG:HG2	2.15	0.46
1:F:146:ILE:HD11	1:F:168:THR:HG21	1.96	0.46
1:J:84:MET:HG3	1:J:89:ARG:HG3	1.97	0.46
1:L:209:CYS:HB2	1:L:212:GLN:NE2	2.31	0.46
1:D:107:ASP:N	1:D:107:ASP:OD1	2.46	0.46
1:D:453:ARG:HA	1:D:456:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:ARG:HG3	1:I:173:TYR:HB3	1.97	0.46
1:I:89:ARG:NH1	1:I:96:LEU:HD12	2.31	0.46
1:F:248:GLY:HA2	2:F:800:ADP:O3A	2.15	0.45
1:F:458:GLN:OE1	1:F:458:GLN:N	2.48	0.45
1:G:146:ILE:HD11	1:G:168:THR:HG21	1.96	0.45
1:H:55:ASP:O	1:H:71:VAL:HG12	2.16	0.45
1:I:158:MET:HB2	1:J:233:ILE:CG2	2.46	0.45
1:L:82:ILE:HG21	1:L:100:ILE:HD11	1.98	0.45
1:L:84:MET:HG3	1:L:89:ARG:HG3	1.98	0.45
1:A:208:GLY:HA2	1:A:376:GLY:CA	2.47	0.45
1:B:427:MET:CE	1:B:430:ILE:HB	2.41	0.45
1:E:332:MET:HE2	1:E:362:ARG:HB3	1.97	0.45
1:I:439:ALA:O	1:I:442:MET:HB2	2.16	0.45
1:L:270:ASN:HB3	1:L:273:GLU:HG2	1.98	0.45
1:B:316:THR:HG23	1:B:316:THR:O	2.15	0.45
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.98	0.45
1:E:453:ARG:HA	1:E:456:LEU:HD12	1.97	0.45
1:E:86:ARG:O	1:E:90:ASN:HB2	2.16	0.45
1:F:407:VAL:O	1:F:410:ASP:HB2	2.16	0.45
1:I:432:LEU:N	1:I:432:LEU:HD23	2.31	0.45
1:K:84:MET:HG3	1:K:89:ARG:HG3	1.97	0.45
1:L:355:PRO:O	1:L:358:ARG:HG2	2.16	0.45
1:A:133:VAL:HG13	1:A:443:ASN:HB2	1.98	0.45
1:C:332:MET:HE2	1:C:362:ARG:HB3	1.98	0.45
1:C:55:ASP:O	1:C:71:VAL:HG12	2.16	0.45
1:E:147:ARG:HG3	1:E:173:TYR:HB3	1.98	0.45
1:E:206:ILE:HG22	1:E:207:GLY:N	2.32	0.45
1:K:212:GLN:CD	1:K:212:GLN:H	2.19	0.45
1:B:270:ASN:HB3	1:B:273:GLU:HG2	1.98	0.45
1:E:86:ARG:HD3	1:E:204:ASP:OD2	2.17	0.45
1:E:328:LEU:HD23	1:E:357:LEU:HD21	1.98	0.45
1:E:407:VAL:O	1:E:410:ASP:HB2	2.16	0.45
1:F:328:LEU:HD23	1:F:357:LEU:HD21	1.99	0.45
1:K:133:VAL:HG13	1:K:443:ASN:CB	2.42	0.45
1:K:328:LEU:HD23	1:K:357:LEU:HD21	1.99	0.45
1:G:439:ALA:O	1:G:442:MET:HB2	2.17	0.45
1:J:146:ILE:HD11	1:J:168:THR:HG21	1.99	0.45
1:J:212:GLN:CD	1:J:212:GLN:H	2.20	0.45
1:G:232:ALA:HA	1:L:125:GLY:HA3	1.98	0.45
1:A:358:ARG:HB3	1:A:366:GLU:OE2	2.16	0.45
1:C:407:VAL:O	1:C:410:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:VAL:HG13	1:E:443:ASN:HB2	1.99	0.45
1:F:439:ALA:O	1:F:442:MET:HB2	2.17	0.45
1:G:82:ILE:HG21	1:G:100:ILE:HD11	1.97	0.45
1:A:407:VAL:O	1:A:410:ASP:HB2	2.16	0.45
1:G:373:ASP:O	1:G:377:ARG:HG3	2.17	0.45
1:I:453:ARG:HA	1:I:456:LEU:HD12	1.99	0.45
1:J:55:ASP:O	1:J:71:VAL:HG12	2.17	0.45
1:L:203:TYR:CE2	1:L:261:GLU:HG2	2.52	0.45
1:L:453:ARG:HA	1:L:456:LEU:HD12	1.99	0.45
1:C:373:ASP:O	1:C:377:ARG:HG3	2.16	0.45
1:E:458:GLN:N	1:E:458:GLN:OE1	2.50	0.45
1:H:146:ILE:HD11	1:H:168:THR:HG21	1.98	0.45
1:I:27:ILE:O	1:I:82:ILE:CG2	2.64	0.45
1:J:358:ARG:HB3	1:J:366:GLU:OE2	2.16	0.45
1:K:206:ILE:HG22	1:K:207:GLY:N	2.32	0.45
1:K:89:ARG:NH1	1:K:96:LEU:HD12	2.31	0.45
1:E:114:ILE:CD1	1:E:176:VAL:HG22	2.46	0.45
1:E:27:ILE:O	1:E:82:ILE:CG2	2.64	0.45
1:H:212:GLN:H	1:H:212:GLN:CD	2.20	0.45
1:H:27:ILE:O	1:H:82:ILE:CG2	2.64	0.45
1:H:89:ARG:NH1	1:H:96:LEU:HD12	2.32	0.45
1:J:439:ALA:O	1:J:442:MET:HB2	2.17	0.45
1:J:89:ARG:NH1	1:J:96:LEU:HD12	2.31	0.45
1:K:131:PHE:HB2	1:K:184:CYS:SG	2.56	0.45
1:K:453:ARG:HA	1:K:456:LEU:HD12	1.97	0.45
1:A:252:THR:OG1	2:A:800:ADP:O1B	2.35	0.44
1:B:86:ARG:O	1:B:87:VAL:C	2.56	0.44
1:E:206:ILE:CD1	1:E:253:LEU:HD22	2.46	0.44
1:K:55:ASP:O	1:K:71:VAL:HG12	2.17	0.44
1:L:105:CYS:O	1:L:108:VAL:HG23	2.16	0.44
1:L:131:PHE:HB2	1:L:184:CYS:SG	2.57	0.44
1:L:439:ALA:O	1:L:442:MET:HB2	2.17	0.44
1:A:335:LEU:HD22	1:A:336:LYS:O	2.17	0.44
1:C:27:ILE:O	1:C:82:ILE:CG2	2.64	0.44
1:G:212:GLN:H	1:G:212:GLN:CD	2.21	0.44
1:H:208:GLY:HA2	1:H:376:GLY:CA	2.47	0.44
1:H:453:ARG:HA	1:H:456:LEU:HD12	1.97	0.44
1:J:114:ILE:CD1	1:J:176:VAL:HG22	2.47	0.44
1:K:105:CYS:O	1:K:108:VAL:HG23	2.17	0.44
1:L:55:ASP:O	1:L:71:VAL:HG12	2.18	0.44
1:L:27:ILE:O	1:L:82:ILE:CG2	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:O	1:A:82:ILE:CG2	2.65	0.44
1:D:206:ILE:CD1	1:D:253:LEU:HD22	2.46	0.44
1:F:206:ILE:HG22	1:F:207:GLY:N	2.33	0.44
1:H:439:ALA:O	1:H:442:MET:HB2	2.18	0.44
1:I:270:ASN:HB3	1:I:273:GLU:HG2	1.98	0.44
1:L:328:LEU:HD23	1:L:357:LEU:HD21	2.00	0.44
1:B:105:CYS:O	1:B:108:VAL:HG23	2.17	0.44
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.47	0.44
1:L:358:ARG:HB3	1:L:366:GLU:OE2	2.18	0.44
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.53	0.44
1:G:209:CYS:HB2	1:G:212:GLN:HG2	1.95	0.44
1:I:146:ILE:HD11	1:I:168:THR:HG21	1.98	0.44
1:A:82:ILE:HG21	1:A:100:ILE:HD11	1.99	0.44
1:B:206:ILE:HG22	1:B:207:GLY:N	2.32	0.44
1:C:335:LEU:HD22	1:C:336:LYS:O	2.18	0.44
1:C:416:SER:OG	1:D:235:VAL:HG13	2.18	0.44
1:D:126:ILE:HG23	1:E:232:ALA:O	2.17	0.44
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.98	0.44
1:F:147:ARG:HG3	1:F:173:TYR:HB3	1.98	0.44
1:F:212:GLN:CD	1:F:212:GLN:H	2.21	0.44
1:J:270:ASN:HB3	1:J:273:GLU:HG2	2.00	0.44
1:A:206:ILE:CD1	1:A:253:LEU:HD22	2.46	0.44
1:G:355:PRO:O	1:G:358:ARG:HG2	2.17	0.44
1:I:252:THR:OG1	2:I:800:ADP:O3B	2.36	0.44
1:J:453:ARG:HA	1:J:456:LEU:HD12	1.99	0.44
1:B:136:LYS:HB3	1:B:137:PRO:HD3	2.00	0.44
1:C:432:LEU:N	1:C:432:LEU:HD23	2.33	0.44
1:L:407:VAL:O	1:L:410:ASP:HB2	2.17	0.44
1:L:89:ARG:NH1	1:L:96:LEU:HD12	2.33	0.44
1:A:441:VAL:O	1:A:444:SER:OG	2.34	0.44
1:D:89:ARG:NH1	1:D:96:LEU:HD12	2.33	0.44
1:E:439:ALA:O	1:E:442:MET:HB2	2.18	0.44
1:F:270:ASN:HB3	1:F:273:GLU:HG2	1.99	0.44
1:H:332:MET:HE2	1:H:362:ARG:HB3	2.00	0.44
1:I:208:GLY:HA2	1:I:376:GLY:CA	2.48	0.44
1:K:173:TYR:CD1	1:K:173:TYR:O	2.71	0.44
1:K:220:VAL:O	1:K:224:LEU:HB2	2.18	0.44
1:L:252:THR:HB	2:L:800:ADP:O1A	2.16	0.44
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.53	0.43
2:B:800:ADP:PB	1:C:359:ARG:HH12	2.41	0.43
1:E:89:ARG:NH1	1:E:96:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ASP:O	1:G:71:VAL:HG12	2.17	0.43
1:K:82:ILE:HG21	1:K:100:ILE:HD11	2.00	0.43
1:K:307:ASP:OD1	1:K:307:ASP:N	2.47	0.43
1:B:458:GLN:OE1	1:B:458:GLN:N	2.51	0.43
1:D:408:GLY:HA3	2:D:800:ADP:N7	2.33	0.43
1:E:427:MET:CE	1:E:430:ILE:HB	2.42	0.43
1:K:206:ILE:CD1	1:K:253:LEU:HD22	2.46	0.43
1:K:335:LEU:HD22	1:K:336:LYS:O	2.19	0.43
1:A:209:CYS:HB2	1:A:212:GLN:NE2	2.33	0.43
1:A:328:LEU:HD23	1:A:357:LEU:HD21	2.01	0.43
1:C:89:ARG:NH1	1:C:96:LEU:HD12	2.33	0.43
1:E:105:CYS:O	1:E:108:VAL:HG23	2.19	0.43
1:F:209:CYS:HB2	1:F:212:GLN:NE2	2.33	0.43
1:H:86:ARG:HD3	1:H:204:ASP:OD2	2.17	0.43
1:J:377:ARG:O	1:J:380:ILE:N	2.51	0.43
1:L:136:LYS:HB3	1:L:137:PRO:HD3	2.00	0.43
1:I:458:GLN:O	1:I:459:SER:HB3	2.19	0.43
1:J:423:ILE:O	1:J:427:MET:CB	2.66	0.43
1:C:84:MET:CG	1:C:89:ARG:HG3	2.48	0.43
1:G:105:CYS:O	1:G:108:VAL:HG23	2.18	0.43
1:G:206:ILE:HG22	1:G:207:GLY:N	2.33	0.43
1:G:89:ARG:NH1	1:G:96:LEU:HD12	2.32	0.43
1:K:136:LYS:HB3	1:K:137:PRO:HD3	2.00	0.43
1:L:335:LEU:HD22	1:L:336:LYS:O	2.19	0.43
1:A:136:LYS:HB3	1:A:137:PRO:HD3	2.01	0.43
1:D:55:ASP:O	1:D:71:VAL:HG12	2.18	0.43
1:E:427:MET:CA	1:E:427:MET:HE2	2.40	0.43
1:F:133:VAL:HG13	1:F:443:ASN:HB2	2.00	0.43
1:G:114:ILE:CD1	1:G:176:VAL:HG22	2.49	0.43
1:J:202:GLY:N	1:J:205:ASP:OD2	2.47	0.43
1:K:127:THR:HG23	1:K:438:ASP:CA	2.24	0.43
1:K:439:ALA:O	1:K:442:MET:HB2	2.18	0.43
1:J:335:LEU:HD22	1:J:336:LYS:O	2.18	0.43
1:C:252:THR:HB	2:C:800:ADP:O2A	2.18	0.43
1:D:27:ILE:O	1:D:82:ILE:CG2	2.65	0.43
1:D:316:THR:HG23	1:D:316:THR:O	2.18	0.43
1:D:423:ILE:O	1:D:427:MET:CB	2.67	0.43
1:G:28:VAL:HG22	1:G:98:ASP:N	2.34	0.43
1:J:432:LEU:N	1:J:432:LEU:HD23	2.34	0.43
1:L:206:ILE:CD1	1:L:253:LEU:HD22	2.48	0.43
1:B:212:GLN:H	1:B:212:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASN:HA	1:B:85:ASN:HD21	1.84	0.43
1:E:146:ILE:HD11	1:E:168:THR:HG21	2.00	0.43
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.54	0.43
1:G:332:MET:HE2	1:G:362:ARG:HB3	2.00	0.43
1:H:105:CYS:O	1:H:108:VAL:HG23	2.19	0.43
1:H:114:ILE:CD1	1:H:176:VAL:HG22	2.49	0.43
1:H:136:LYS:HB3	1:H:137:PRO:HD3	2.01	0.43
1:I:316:THR:O	1:I:316:THR:HG23	2.19	0.43
1:J:27:ILE:O	1:J:82:ILE:CG2	2.65	0.43
1:J:328:LEU:HD23	1:J:357:LEU:HD21	2.01	0.43
1:F:432:LEU:N	1:F:432:LEU:HD23	2.34	0.43
1:I:408:GLY:C	2:I:800:ADP:C8	2.92	0.43
1:I:248:GLY:HA2	2:I:800:ADP:O3A	2.19	0.43
1:J:117:LEU:HD21	1:J:185:GLU:O	2.18	0.43
1:A:105:CYS:O	1:A:108:VAL:HG23	2.19	0.42
1:A:212:GLN:NE2	1:A:212:GLN:H	2.16	0.42
1:B:55:ASP:O	1:B:71:VAL:HG12	2.18	0.42
1:D:82:ILE:HG21	1:D:100:ILE:HD11	2.00	0.42
1:D:252:THR:HB	2:D:800:ADP:O1A	2.19	0.42
1:F:55:ASP:O	1:F:71:VAL:HG12	2.19	0.42
1:G:173:TYR:CD1	1:G:173:TYR:O	2.72	0.42
1:I:55:ASP:O	1:I:71:VAL:HG12	2.19	0.42
1:J:105:CYS:O	1:J:108:VAL:HG23	2.19	0.42
1:K:358:ARG:HB3	1:K:366:GLU:OE2	2.19	0.42
1:E:270:ASN:HB3	1:E:273:GLU:HG2	2.01	0.42
1:G:316:THR:O	1:G:316:THR:HG23	2.19	0.42
1:K:407:VAL:O	1:K:410:ASP:HB2	2.19	0.42
1:L:220:VAL:O	1:L:224:LEU:HB2	2.19	0.42
1:L:86:ARG:O	1:L:87:VAL:C	2.57	0.42
1:D:328:LEU:HD23	1:D:357:LEU:HD21	2.00	0.42
1:G:136:LYS:HB3	1:G:137:PRO:HD3	2.02	0.42
1:G:158:MET:HA	1:G:387:ASN:O	2.19	0.42
1:H:408:GLY:C	2:H:800:ADP:C8	2.93	0.42
1:K:35:ASP:OD1	1:K:144:ARG:NH2	2.51	0.42
1:A:28:VAL:HG22	1:A:98:ASP:N	2.34	0.42
1:B:27:ILE:O	1:B:82:ILE:CG2	2.66	0.42
1:E:55:ASP:O	1:E:71:VAL:HG12	2.19	0.42
1:F:316:THR:HG23	1:F:316:THR:O	2.19	0.42
1:G:279:ALA:HB1	1:G:320:VAL:HG11	2.02	0.42
1:G:27:ILE:O	1:G:82:ILE:CG2	2.65	0.42
1:H:206:ILE:HG22	1:H:207:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:358:ARG:HB3	1:H:366:GLU:OE2	2.19	0.42
1:K:117:LEU:HD21	1:K:185:GLU:O	2.19	0.42
1:A:173:TYR:CD1	1:A:173:TYR:O	2.72	0.42
1:A:316:THR:HG23	1:A:316:THR:O	2.19	0.42
1:C:114:ILE:CD1	1:C:176:VAL:HG22	2.49	0.42
1:D:28:VAL:HG22	1:D:98:ASP:N	2.34	0.42
1:H:407:VAL:O	1:H:410:ASP:HB2	2.18	0.42
1:I:114:ILE:CD1	1:I:176:VAL:HG22	2.49	0.42
1:I:203:TYR:CE2	1:I:261:GLU:HG2	2.55	0.42
1:I:206:ILE:HG22	1:I:207:GLY:N	2.34	0.42
1:I:355:PRO:O	1:I:358:ARG:HG2	2.20	0.42
1:L:423:ILE:O	1:L:427:MET:CB	2.67	0.42
1:B:208:GLY:HA2	1:B:376:GLY:HA2	2.00	0.42
1:D:407:VAL:O	1:D:410:ASP:HB2	2.20	0.42
1:D:423:ILE:HG21	1:E:229:LEU:HD21	2.02	0.42
1:H:270:ASN:HB3	1:H:273:GLU:HG2	2.01	0.42
1:H:316:THR:HG23	1:H:316:THR:O	2.19	0.42
1:H:427:MET:CE	1:H:430:ILE:HB	2.42	0.42
1:J:28:VAL:HG22	1:J:98:ASP:N	2.34	0.42
1:L:35:ASP:OD1	1:L:36:ASN:N	2.52	0.42
1:L:408:GLY:C	2:L:800:ADP:C8	2.92	0.42
1:B:432:LEU:N	1:B:432:LEU:HD23	2.35	0.42
1:D:432:LEU:N	1:D:432:LEU:HD23	2.34	0.42
1:G:206:ILE:CD1	1:G:253:LEU:HD22	2.46	0.42
1:H:241:ILE:HA	1:H:365:ARG:O	2.19	0.42
1:C:206:ILE:HG22	1:C:207:GLY:N	2.34	0.42
1:E:335:LEU:HD22	1:E:336:LYS:O	2.20	0.42
1:G:432:LEU:HD23	1:G:432:LEU:N	2.34	0.42
1:H:206:ILE:CD1	1:H:253:LEU:HD22	2.46	0.42
1:H:408:GLY:HA3	2:H:800:ADP:N7	2.35	0.42
1:I:335:LEU:HD22	1:I:336:LYS:O	2.20	0.42
1:I:407:VAL:O	1:I:410:ASP:HB2	2.20	0.42
1:K:316:THR:HG23	1:K:316:THR:O	2.19	0.42
1:K:208:GLY:HA2	1:K:376:GLY:CA	2.49	0.42
1:B:250:GLY:CA	2:B:800:ADP:O1A	2.68	0.42
1:C:364:ASP:OD1	1:C:364:ASP:N	2.53	0.42
1:F:114:ILE:CD1	1:F:176:VAL:HG22	2.50	0.42
1:F:27:ILE:O	1:F:82:ILE:CG2	2.65	0.42
1:I:332:MET:HE2	1:I:362:ARG:HB3	2.02	0.42
1:K:423:ILE:O	1:K:427:MET:CB	2.67	0.42
1:A:30:GLU:HG2	1:A:96:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HG22	1:C:98:ASP:N	2.35	0.42
1:D:114:ILE:CD1	1:D:176:VAL:HG22	2.50	0.42
1:D:206:ILE:HG22	1:D:207:GLY:N	2.34	0.42
1:D:84:MET:CG	1:D:89:ARG:HG3	2.50	0.42
1:E:279:ALA:HB1	1:E:320:VAL:HG11	2.01	0.42
1:L:133:VAL:HG13	1:L:443:ASN:HB2	2.02	0.42
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.50	0.41
1:B:358:ARG:HB3	1:B:366:GLU:OE2	2.20	0.41
1:D:212:GLN:CD	1:D:212:GLN:H	2.23	0.41
1:D:27:ILE:HG22	1:D:28:VAL:N	2.35	0.41
1:G:203:TYR:CE2	1:G:261:GLU:HG2	2.54	0.41
1:H:84:MET:CG	1:H:89:ARG:HG3	2.50	0.41
1:B:120:ASP:CG	1:I:190:LYS:HZ3	2.23	0.41
1:I:26:LEU:O	1:I:99:VAL:HA	2.20	0.41
1:K:146:ILE:HD11	1:K:168:THR:HG21	2.01	0.41
1:L:202:GLY:N	1:L:205:ASP:OD2	2.45	0.41
1:L:432:LEU:N	1:L:432:LEU:HD23	2.35	0.41
1:F:105:CYS:O	1:F:108:VAL:HG23	2.19	0.41
1:K:212:GLN:NE2	1:K:212:GLN:H	2.17	0.41
1:K:427:MET:HE3	1:K:427:MET:HA	1.97	0.41
1:L:146:ILE:HD11	1:L:168:THR:HG21	2.02	0.41
1:B:332:MET:HE2	1:B:362:ARG:HB3	2.02	0.41
1:C:427:MET:CA	1:C:427:MET:HE2	2.40	0.41
1:D:437:ILE:HG21	1:D:442:MET:SD	2.59	0.41
1:E:432:LEU:HD23	1:E:432:LEU:N	2.35	0.41
1:H:432:LEU:HD23	1:H:432:LEU:N	2.34	0.41
1:J:313:ARG:HA	1:J:316:THR:HG22	2.02	0.41
1:L:208:GLY:HA2	1:L:376:GLY:HA2	2.03	0.41
1:C:105:CYS:O	1:C:108:VAL:HG23	2.20	0.41
1:C:423:ILE:O	1:C:427:MET:CB	2.68	0.41
1:E:358:ARG:HB3	1:E:366:GLU:OE2	2.21	0.41
1:E:454:TRP:HZ2	1:F:218:GLU:OE2	2.04	0.41
1:I:84:MET:CG	1:I:89:ARG:HG3	2.49	0.41
1:J:27:ILE:HG22	1:J:28:VAL:N	2.36	0.41
1:J:316:THR:HG23	1:J:316:THR:O	2.20	0.41
1:D:136:LYS:HB3	1:D:137:PRO:HD3	2.02	0.41
1:I:427:MET:CE	1:I:430:ILE:HB	2.42	0.41
1:L:316:THR:O	1:L:316:THR:HG23	2.19	0.41
1:A:26:LEU:O	1:A:99:VAL:HA	2.20	0.41
1:E:126:ILE:HB	1:E:439:ALA:HB2	2.02	0.41
1:G:202:GLY:N	1:G:205:ASP:OD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:GLN:H	1:I:212:GLN:NE2	2.18	0.41
1:J:407:VAL:O	1:J:410:ASP:HB2	2.21	0.41
1:C:212:GLN:H	1:C:212:GLN:NE2	2.18	0.41
1:F:437:ILE:HG21	1:F:442:MET:SD	2.61	0.41
1:G:212:GLN:NE2	1:G:212:GLN:H	2.18	0.41
1:K:432:LEU:N	1:K:432:LEU:HD23	2.35	0.41
1:D:197:SER:O	1:D:200:GLU:HB2	2.21	0.41
1:F:423:ILE:O	1:F:427:MET:CB	2.68	0.41
1:D:295:LYS:CG	1:H:193:ASP:OD1	2.68	0.41
1:I:328:LEU:HD23	1:I:357:LEU:HD21	2.02	0.41
1:I:423:ILE:O	1:I:427:MET:CB	2.69	0.41
1:L:313:ARG:HA	1:L:316:THR:HG22	2.03	0.41
1:A:220:VAL:O	1:A:224:LEU:HB2	2.21	0.41
1:B:209:CYS:HB2	1:B:212:GLN:NE2	2.35	0.41
1:B:27:ILE:HG22	1:B:28:VAL:N	2.36	0.41
1:B:423:ILE:O	1:B:427:MET:CB	2.69	0.41
1:C:136:LYS:HB3	1:C:137:PRO:HD3	2.03	0.41
1:E:423:ILE:O	1:E:427:MET:CB	2.69	0.41
1:E:39:VAL:HG13	1:E:69:CYS:SG	2.61	0.41
1:G:408:GLY:HA3	2:G:800:ADP:N7	2.36	0.41
1:K:313:ARG:HA	1:K:316:THR:HG22	2.02	0.41
1:A:208:GLY:HA2	1:A:376:GLY:HA2	2.02	0.41
2:B:800:ADP:PB	1:C:359:ARG:HH22	2.43	0.41
1:C:358:ARG:HB3	1:C:366:GLU:OE2	2.20	0.41
1:D:209:CYS:HB2	1:D:212:GLN:NE2	2.36	0.41
1:D:358:ARG:HB3	1:D:366:GLU:OE2	2.21	0.41
1:F:27:ILE:HG22	1:F:28:VAL:N	2.36	0.41
1:I:416:SER:OG	1:J:235:VAL:HG13	2.20	0.41
1:C:408:GLY:HA3	2:C:800:ADP:N7	2.35	0.41
1:E:424:ARG:NH1	1:F:218:GLU:O	2.54	0.41
1:H:212:GLN:H	1:H:212:GLN:NE2	2.19	0.41
1:I:27:ILE:HG22	1:I:28:VAL:N	2.36	0.41
1:K:373:ASP:O	1:K:377:ARG:HG3	2.20	0.41
1:A:379:GLU:O	1:A:382:GLN:HB2	2.21	0.40
1:C:328:LEU:HD23	1:C:357:LEU:HD21	2.02	0.40
1:D:332:MET:HE2	1:D:362:ARG:HB3	2.03	0.40
1:G:66:GLU:OE1	1:G:147:ARG:NH1	2.54	0.40
1:H:203:TYR:CE2	1:H:261:GLU:HG2	2.56	0.40
1:J:377:ARG:O	1:J:378:LEU:C	2.59	0.40
1:K:127:THR:CG2	1:K:438:ASP:HA	2.24	0.40
1:L:63:LYS:O	1:L:65:ARG:CG	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD22	1:B:336:LYS:O	2.21	0.40
1:B:373:ASP:O	1:B:377:ARG:HG3	2.21	0.40
1:B:408:GLY:HA3	2:B:800:ADP:N7	2.37	0.40
1:E:117:LEU:HD21	1:E:185:GLU:O	2.21	0.40
1:G:39:VAL:HG13	1:G:69:CYS:SG	2.62	0.40
1:I:136:LYS:HB3	1:I:137:PRO:HD3	2.03	0.40
1:K:203:TYR:CE2	1:K:261:GLU:HG2	2.56	0.40
1:K:279:ALA:HB1	1:K:320:VAL:HG11	2.03	0.40
1:A:427:MET:CE	1:A:430:ILE:HB	2.43	0.40
1:A:74:ASP:OD2	1:A:83:ARG:HD2	2.21	0.40
1:F:279:ALA:HB1	1:F:320:VAL:HG11	2.02	0.40
1:G:117:LEU:HD21	1:G:185:GLU:O	2.22	0.40
1:I:28:VAL:HG22	1:I:98:ASP:N	2.37	0.40
1:B:206:ILE:CD1	1:B:253:LEU:HD22	2.47	0.40
1:C:241:ILE:HA	1:C:365:ARG:O	2.21	0.40
1:D:270:ASN:HB3	1:D:273:GLU:HG2	2.02	0.40
1:F:28:VAL:HG22	1:F:98:ASP:N	2.37	0.40
1:I:439:ALA:O	1:I:442:MET:N	2.54	0.40
1:A:313:ARG:HA	1:A:316:THR:HG22	2.03	0.40
1:C:27:ILE:HG22	1:C:28:VAL:N	2.36	0.40
1:D:117:LEU:HD21	1:D:185:GLU:O	2.21	0.40
1:I:159:ARG:NH2	1:J:232:ALA:HA	2.37	0.40
1:L:408:GLY:HA3	2:L:800:ADP:N7	2.36	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:GLN:OE1	1:H:373:ASP:OD2[3_445]	1.72	0.48
1:K:115:HIS:ND1	1:L:185:GLU:OE1[4_545]	1.94	0.26
1:E:435:GLU:OE2	1:K:179:ASP:OD2[4_445]	2.02	0.18
1:A:402:GLU:OE2	1:J:373:ASP:OD2[3_545]	2.08	0.12

## 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	438/489 (90%)	407 (93%)	30 (7%)	1 (0%)	47	78
1	B	436/489 (89%)	405 (93%)	30 (7%)	1 (0%)	47	78
1	C	436/489 (89%)	404 (93%)	31 (7%)	1 (0%)	47	78
1	D	437/489 (89%)	404 (92%)	32 (7%)	1 (0%)	47	78
1	E	436/489 (89%)	404 (93%)	31 (7%)	1 (0%)	47	78
1	F	436/489 (89%)	405 (93%)	30 (7%)	1 (0%)	47	78
1	G	436/489 (89%)	405 (93%)	30 (7%)	1 (0%)	47	78
1	H	437/489 (89%)	407 (93%)	29 (7%)	1 (0%)	47	78
1	I	437/489 (89%)	406 (93%)	30 (7%)	1 (0%)	47	78
1	J	439/489 (90%)	404 (92%)	34 (8%)	1 (0%)	47	78
1	K	437/489 (89%)	406 (93%)	30 (7%)	1 (0%)	47	78
1	L	436/489 (89%)	405 (93%)	30 (7%)	1 (0%)	47	78
All	All	5241/5868 (89%)	4862 (93%)	367 (7%)	12 (0%)	47	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	271	GLY
1	F	271	GLY
1	A	271	GLY
1	D	271	GLY
1	E	271	GLY
1	H	271	GLY
1	J	271	GLY
1	B	271	GLY
1	C	271	GLY
1	I	271	GLY
1	G	271	GLY
1	L	271	GLY

### 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	377/418 (90%)	343 (91%)	34 (9%)	9	37
1	B	375/418 (90%)	343 (92%)	32 (8%)	10	40
1	C	375/418 (90%)	341 (91%)	34 (9%)	9	36
1	D	376/418 (90%)	343 (91%)	33 (9%)	10	38
1	E	375/418 (90%)	344 (92%)	31 (8%)	11	40
1	F	375/418 (90%)	344 (92%)	31 (8%)	11	40
1	G	375/418 (90%)	343 (92%)	32 (8%)	10	40
1	H	376/418 (90%)	347 (92%)	29 (8%)	13	43
1	I	376/418 (90%)	347 (92%)	29 (8%)	13	43
1	J	378/418 (90%)	345 (91%)	33 (9%)	10	38
1	K	376/418 (90%)	341 (91%)	35 (9%)	9	35
1	L	375/418 (90%)	341 (91%)	34 (9%)	9	36
All	All	4509/5016 (90%)	4122 (91%)	387 (9%)	10	39

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	45	LYS
1	A	52	PHE
1	A	59	LEU
1	A	69	CYS
1	A	76	THR
1	A	78	SER
1	A	81	LYS
1	A	95	ARG
1	A	96	LEU
1	A	103	GLN
1	A	108	VAL
1	A	173	TYR
1	A	184	CYS
1	A	193	ASP
1	A	199	ASN
1	A	210	ARG
1	A	212	GLN
1	A	213	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	253	LEU
1	A	273	GLU
1	A	307	ASP
1	A	316	THR
1	A	317	HIS
1	A	330	THR
1	A	335	LEU
1	A	337	GLN
1	A	358	ARG
1	A	359	ARG
1	A	362	ARG
1	A	416	SER
1	A	427	MET
1	A	434	ASP
1	A	438	ASP
1	B	22	ARG
1	B	45	LYS
1	B	52	PHE
1	B	59	LEU
1	B	64	ARG
1	B	69	CYS
1	B	76	THR
1	B	78	SER
1	B	81	LYS
1	B	96	LEU
1	B	101	SER
1	B	103	GLN
1	B	108	VAL
1	B	173	TYR
1	B	184	CYS
1	B	193	ASP
1	B	199	ASN
1	B	212	GLN
1	B	213	LEU
1	B	253	LEU
1	B	273	GLU
1	B	307	ASP
1	B	316	THR
1	B	317	HIS
1	B	335	LEU
1	B	337	GLN
1	B	358	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	359	ARG
1	B	362	ARG
1	B	427	MET
1	B	434	ASP
1	B	438	ASP
1	C	22	ARG
1	C	45	LYS
1	C	52	PHE
1	C	59	LEU
1	C	64	ARG
1	C	69	CYS
1	C	76	THR
1	C	78	SER
1	C	81	LYS
1	C	95	ARG
1	C	96	LEU
1	C	103	GLN
1	C	108	VAL
1	C	127	THR
1	C	173	TYR
1	C	184	CYS
1	C	193	ASP
1	C	199	ASN
1	C	212	GLN
1	C	213	LEU
1	C	253	LEU
1	C	273	GLU
1	C	307	ASP
1	C	316	THR
1	C	317	HIS
1	C	335	LEU
1	C	337	GLN
1	C	358	ARG
1	C	359	ARG
1	C	362	ARG
1	C	416	SER
1	C	427	MET
1	C	434	ASP
1	C	438	ASP
1	D	22	ARG
1	D	45	LYS
1	D	52	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	59	LEU
1	D	64	ARG
1	D	69	CYS
1	D	76	THR
1	D	78	SER
1	D	81	LYS
1	D	96	LEU
1	D	101	SER
1	D	103	GLN
1	D	108	VAL
1	D	173	TYR
1	D	184	CYS
1	D	193	ASP
1	D	199	ASN
1	D	210	ARG
1	D	212	GLN
1	D	213	LEU
1	D	253	LEU
1	D	273	GLU
1	D	307	ASP
1	D	316	THR
1	D	317	HIS
1	D	335	LEU
1	D	337	GLN
1	D	358	ARG
1	D	359	ARG
1	D	362	ARG
1	D	427	MET
1	D	434	ASP
1	D	438	ASP
1	E	22	ARG
1	E	45	LYS
1	E	52	PHE
1	E	59	LEU
1	E	64	ARG
1	E	69	CYS
1	E	76	THR
1	E	78	SER
1	E	81	LYS
1	E	103	GLN
1	E	108	VAL
1	E	173	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	184	CYS
1	E	193	ASP
1	E	199	ASN
1	E	212	GLN
1	E	213	LEU
1	E	253	LEU
1	E	273	GLU
1	E	307	ASP
1	E	316	THR
1	E	317	HIS
1	E	335	LEU
1	E	337	GLN
1	E	358	ARG
1	E	359	ARG
1	E	362	ARG
1	E	416	SER
1	E	427	MET
1	E	434	ASP
1	E	438	ASP
1	F	22	ARG
1	F	45	LYS
1	F	52	PHE
1	F	59	LEU
1	F	64	ARG
1	F	69	CYS
1	F	76	THR
1	F	78	SER
1	F	81	LYS
1	F	103	GLN
1	F	108	VAL
1	F	173	TYR
1	F	184	CYS
1	F	193	ASP
1	F	199	ASN
1	F	210	ARG
1	F	212	GLN
1	F	213	LEU
1	F	253	LEU
1	F	273	GLU
1	F	307	ASP
1	F	316	THR
1	F	317	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	335	LEU
1	F	337	GLN
1	F	358	ARG
1	F	359	ARG
1	F	362	ARG
1	F	427	MET
1	F	434	ASP
1	F	438	ASP
1	G	22	ARG
1	G	45	LYS
1	G	52	PHE
1	G	59	LEU
1	G	64	ARG
1	G	69	CYS
1	G	76	THR
1	G	78	SER
1	G	81	LYS
1	G	95	ARG
1	G	103	GLN
1	G	108	VAL
1	G	173	TYR
1	G	184	CYS
1	G	193	ASP
1	G	199	ASN
1	G	210	ARG
1	G	212	GLN
1	G	213	LEU
1	G	253	LEU
1	G	273	GLU
1	G	307	ASP
1	G	316	THR
1	G	317	HIS
1	G	335	LEU
1	G	337	GLN
1	G	358	ARG
1	G	359	ARG
1	G	362	ARG
1	G	427	MET
1	G	434	ASP
1	G	438	ASP
1	H	22	ARG
1	H	45	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	52	PHE
1	H	59	LEU
1	H	69	CYS
1	H	76	THR
1	H	78	SER
1	H	81	LYS
1	H	103	GLN
1	H	108	VAL
1	H	173	TYR
1	H	184	CYS
1	H	193	ASP
1	H	199	ASN
1	H	212	GLN
1	H	213	LEU
1	H	253	LEU
1	H	273	GLU
1	H	307	ASP
1	H	316	THR
1	H	317	HIS
1	H	335	LEU
1	H	337	GLN
1	H	358	ARG
1	H	359	ARG
1	H	362	ARG
1	H	427	MET
1	H	434	ASP
1	H	438	ASP
1	I	22	ARG
1	I	45	LYS
1	I	52	PHE
1	I	59	LEU
1	I	64	ARG
1	I	69	CYS
1	I	76	THR
1	I	78	SER
1	I	81	LYS
1	I	103	GLN
1	I	108	VAL
1	I	184	CYS
1	I	193	ASP
1	I	199	ASN
1	I	212	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	213	LEU
1	I	253	LEU
1	I	273	GLU
1	I	307	ASP
1	I	316	THR
1	I	317	HIS
1	I	335	LEU
1	I	337	GLN
1	I	358	ARG
1	I	359	ARG
1	I	362	ARG
1	I	427	MET
1	I	434	ASP
1	I	438	ASP
1	J	22	ARG
1	J	45	LYS
1	J	52	PHE
1	J	59	LEU
1	J	64	ARG
1	J	69	CYS
1	J	75	ASP
1	J	76	THR
1	J	78	SER
1	J	81	LYS
1	J	103	GLN
1	J	108	VAL
1	J	173	TYR
1	J	184	CYS
1	J	193	ASP
1	J	199	ASN
1	J	210	ARG
1	J	211	LYS
1	J	212	GLN
1	J	213	LEU
1	J	253	LEU
1	J	273	GLU
1	J	307	ASP
1	J	316	THR
1	J	317	HIS
1	J	335	LEU
1	J	337	GLN
1	J	358	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	359	ARG
1	J	362	ARG
1	J	427	MET
1	J	434	ASP
1	J	438	ASP
1	K	22	ARG
1	K	45	LYS
1	K	49	LEU
1	K	52	PHE
1	K	59	LEU
1	K	64	ARG
1	K	69	CYS
1	K	76	THR
1	K	78	SER
1	K	81	LYS
1	K	95	ARG
1	K	101	SER
1	K	103	GLN
1	K	108	VAL
1	K	127	THR
1	K	135	LEU
1	K	173	TYR
1	K	184	CYS
1	K	193	ASP
1	K	199	ASN
1	K	212	GLN
1	K	213	LEU
1	K	253	LEU
1	K	273	GLU
1	K	307	ASP
1	K	316	THR
1	K	317	HIS
1	K	335	LEU
1	K	337	GLN
1	K	358	ARG
1	K	359	ARG
1	K	362	ARG
1	K	427	MET
1	K	434	ASP
1	K	438	ASP
1	L	22	ARG
1	L	45	LYS

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Mol	Chain	Res	Type
1	L	52	PHE
1	L	59	LEU
1	L	64	ARG
1	L	69	CYS
1	L	76	THR
1	L	78	SER
1	L	81	LYS
1	L	95	ARG
1	L	103	GLN
1	L	108	VAL
1	L	140	LEU
1	L	173	TYR
1	L	184	CYS
1	L	193	ASP
1	L	199	ASN
1	L	210	ARG
1	L	211	LYS
1	L	212	GLN
1	L	213	LEU
1	L	253	LEU
1	L	273	GLU
1	L	307	ASP
1	L	316	THR
1	L	317	HIS
1	L	335	LEU
1	L	337	GLN
1	L	358	ARG
1	L	359	ARG
1	L	362	ARG
1	L	427	MET
1	L	434	ASP
1	L	438	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	199	ASN
1	A	212	GLN
1	B	91	ASN
1	B	199	ASN
1	B	212	GLN

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Mol	Chain	Res	Type
1	C	199	ASN
1	C	212	GLN
1	D	199	ASN
1	D	212	GLN
1	D	384	HIS
1	E	199	ASN
1	E	212	GLN
1	E	226	HIS
1	F	199	ASN
1	F	212	GLN
1	G	199	ASN
1	G	212	GLN
1	H	199	ASN
1	H	212	GLN
1	I	212	GLN
1	J	199	ASN
1	J	212	GLN
1	K	199	ASN
1	K	212	GLN
1	L	91	ASN
1	L	199	ASN
1	L	212	GLN

### 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 carbohydrates 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	ADP	A	800	-	24,29,29	1.43	4 (16%)	29,45,45	1.77	6 (20%)
2	ADP	C	800	-	24,29,29	1.21	2 (8%)	29,45,45	1.42	5 (17%)
2	ADP	L	800	-	24,29,29	1.12	3 (12%)	29,45,45	1.52	5 (17%)
2	ADP	H	800	-	24,29,29	1.15	1 (4%)	29,45,45	2.04	9 (31%)
2	ADP	E	800	-	24,29,29	1.08	1 (4%)	29,45,45	1.62	6 (20%)
2	ADP	J	800	-	24,29,29	1.45	3 (12%)	29,45,45	1.90	11 (37%)
2	ADP	D	800	-	24,29,29	1.37	4 (16%)	29,45,45	1.67	9 (31%)
2	ADP	F	800	-	24,29,29	1.24	3 (12%)	29,45,45	1.68	8 (27%)
2	ADP	B	800	-	24,29,29	1.14	2 (8%)	29,45,45	1.71	7 (24%)
2	ADP	I	800	-	24,29,29	1.35	3 (12%)	29,45,45	1.87	10 (34%)
2	ADP	K	800	-	24,29,29	1.20	3 (12%)	29,45,45	1.57	4 (13%)
2	ADP	G	800	-	24,29,29	1.21	3 (12%)	29,45,45	1.54	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	800	-	-	6/12/32/32	0/3/3/3
2	ADP	C	800	-	-	7/12/32/32	0/3/3/3
2	ADP	L	800	-	-	9/12/32/32	0/3/3/3
2	ADP	H	800	-	-	4/12/32/32	0/3/3/3
2	ADP	E	800	-	-	8/12/32/32	0/3/3/3
2	ADP	J	800	-	-	5/12/32/32	0/3/3/3
2	ADP	D	800	-	-	5/12/32/32	0/3/3/3
2	ADP	F	800	-	-	7/12/32/32	0/3/3/3
2	ADP	B	800	-	-	6/12/32/32	0/3/3/3
2	ADP	I	800	-	-	8/12/32/32	0/3/3/3
2	ADP	K	800	-	-	7/12/32/32	0/3/3/3
2	ADP	G	800	-	-	7/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	800	ADP	C5-C4	3.50	1.50	1.40
2	D	800	ADP	C5-C4	3.24	1.49	1.40
2	J	800	ADP	C2-N3	3.13	1.37	1.32
2	A	800	ADP	C5-C4	3.02	1.48	1.40
2	C	800	ADP	C5-C4	2.98	1.48	1.40
2	D	800	ADP	O4'-C1'	2.91	1.45	1.41
2	I	800	ADP	C2-N3	2.88	1.36	1.32
2	K	800	ADP	C5-C4	2.76	1.48	1.40
2	A	800	ADP	O4'-C1'	2.73	1.44	1.41
2	G	800	ADP	C5-C4	2.72	1.48	1.40
2	A	800	ADP	PA-O2A	-2.63	1.43	1.55
2	F	800	ADP	PA-O2A	-2.59	1.43	1.55
2	I	800	ADP	C5-C4	2.53	1.47	1.40
2	L	800	ADP	C5-C4	2.52	1.47	1.40
2	H	800	ADP	C5-C4	2.47	1.47	1.40
2	I	800	ADP	O4'-C1'	2.40	1.44	1.41
2	G	800	ADP	O4'-C1'	2.39	1.44	1.41
2	F	800	ADP	O4'-C1'	2.34	1.44	1.41
2	E	800	ADP	C5-C4	2.32	1.47	1.40
2	D	800	ADP	C2-N3	2.31	1.35	1.32
2	B	800	ADP	PA-O2A	-2.31	1.44	1.55
2	K	800	ADP	O4'-C1'	2.30	1.44	1.41
2	F	800	ADP	C5-C4	2.29	1.47	1.40
2	B	800	ADP	C5-N7	-2.28	1.31	1.39
2	C	800	ADP	C2-N3	2.27	1.35	1.32
2	A	800	ADP	C2-N3	2.20	1.35	1.32
2	G	800	ADP	C2-N3	2.14	1.35	1.32
2	K	800	ADP	C2-N3	2.11	1.35	1.32
2	J	800	ADP	PA-O1A	-2.11	1.43	1.50
2	D	800	ADP	PA-O2A	-2.10	1.45	1.55
2	L	800	ADP	PA-O2A	-2.08	1.45	1.55
2	L	800	ADP	C2-N3	2.02	1.35	1.32

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	800	ADP	O3B-PB-O3A	-4.66	89.02	104.64
2	A	800	ADP	O2B-PB-O3A	-4.63	89.10	104.64
2	H	800	ADP	O2B-PB-O3A	4.31	119.07	104.64
2	K	800	ADP	C3'-C2'-C1'	4.26	107.39	100.98
2	B	800	ADP	O2B-PB-O3A	-3.88	91.63	104.64
2	L	800	ADP	C3'-C2'-C1'	3.83	106.75	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	800	ADP	N3-C2-N1	-3.76	122.81	128.68
2	A	800	ADP	O3B-PB-O2B	3.68	121.72	107.64
2	H	800	ADP	O3B-PB-O1B	3.68	125.10	110.68
2	B	800	ADP	C3'-C2'-C1'	3.55	106.33	100.98
2	K	800	ADP	N3-C2-N1	-3.52	123.17	128.68
2	A	800	ADP	N3-C2-N1	-3.52	123.18	128.68
2	H	800	ADP	O2B-PB-O1B	-3.45	97.19	110.68
2	B	800	ADP	PA-O3A-PB	3.41	144.54	132.83
2	E	800	ADP	C4-C5-N7	-3.41	105.85	109.40
2	J	800	ADP	O5'-PA-O1A	-3.41	95.76	109.07
2	J	800	ADP	O2B-PB-O3A	-3.40	93.24	104.64
2	I	800	ADP	O3B-PB-O3A	3.39	116.01	104.64
2	A	800	ADP	C3'-C2'-C1'	3.37	106.05	100.98
2	E	800	ADP	N3-C2-N1	-3.36	123.42	128.68
2	E	800	ADP	C3'-C2'-C1'	3.32	105.97	100.98
2	C	800	ADP	N3-C2-N1	-3.29	123.53	128.68
2	G	800	ADP	O3B-PB-O3A	-3.22	93.84	104.64
2	B	800	ADP	N3-C2-N1	-3.22	123.65	128.68
2	H	800	ADP	C3'-C2'-C1'	3.20	105.80	100.98
2	F	800	ADP	N3-C2-N1	-3.19	123.69	128.68
2	D	800	ADP	O5'-PA-O1A	-3.18	96.63	109.07
2	D	800	ADP	O3A-PB-O1B	-3.13	93.85	111.19
2	F	800	ADP	O2B-PB-O3A	3.10	115.03	104.64
2	C	800	ADP	C3'-C2'-C1'	3.10	105.65	100.98
2	F	800	ADP	C4-C5-N7	-3.04	106.23	109.40
2	J	800	ADP	O3B-PB-O3A	3.00	114.71	104.64
2	J	800	ADP	O2A-PA-O5'	2.98	121.59	107.75
2	I	800	ADP	C3'-C2'-C1'	2.96	105.44	100.98
2	L	800	ADP	C4-C5-N7	-2.96	106.31	109.40
2	G	800	ADP	C3'-C2'-C1'	2.96	105.43	100.98
2	I	800	ADP	N3-C2-N1	-2.93	124.11	128.68
2	F	800	ADP	O3A-PB-O1B	-2.92	95.00	111.19
2	K	800	ADP	C4-C5-N7	-2.91	106.37	109.40
2	G	800	ADP	O2A-PA-O5'	-2.87	94.42	107.75
2	I	800	ADP	O2B-PB-O3A	-2.84	95.11	104.64
2	G	800	ADP	N3-C2-N1	-2.83	124.25	128.68
2	I	800	ADP	O2A-PA-O5'	2.82	120.82	107.75
2	K	800	ADP	O3A-PB-O1B	-2.81	95.58	111.19
2	I	800	ADP	C4-C5-N7	-2.80	106.48	109.40
2	C	800	ADP	O3A-PB-O1B	-2.79	95.69	111.19
2	H	800	ADP	N3-C2-N1	-2.78	124.33	128.68
2	F	800	ADP	C3'-C2'-C1'	2.78	105.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	ADP	C3'-C2'-C1'	2.78	105.16	100.98
2	I	800	ADP	PA-O3A-PB	2.74	142.22	132.83
2	F	800	ADP	O5'-PA-O1A	2.72	119.68	109.07
2	J	800	ADP	O2'-C2'-C3'	2.71	120.59	111.82
2	H	800	ADP	C4-C5-N7	-2.69	106.59	109.40
2	I	800	ADP	O5'-C5'-C4'	2.61	117.96	108.99
2	E	800	ADP	O3A-PB-O1B	-2.56	96.97	111.19
2	D	800	ADP	O2A-PA-O5'	2.54	119.53	107.75
2	F	800	ADP	PA-O3A-PB	2.47	141.30	132.83
2	I	800	ADP	O3A-PB-O1B	-2.46	97.57	111.19
2	F	800	ADP	O3B-PB-O2B	2.45	117.02	107.64
2	J	800	ADP	PA-O3A-PB	2.42	141.13	132.83
2	G	800	ADP	O3B-PB-O2B	2.42	116.88	107.64
2	H	800	ADP	O3B-PB-O2B	2.40	116.82	107.64
2	J	800	ADP	C2'-C3'-C4'	2.40	107.30	102.64
2	E	800	ADP	O2B-PB-O3A	2.39	112.67	104.64
2	H	800	ADP	O2A-PA-O1A	2.39	124.05	112.24
2	D	800	ADP	O5'-C5'-C4'	2.34	117.05	108.99
2	A	800	ADP	O3B-PB-O3A	-2.30	96.93	104.64
2	J	800	ADP	C3'-C2'-C1'	2.29	104.42	100.98
2	D	800	ADP	O2B-PB-O1B	2.23	119.41	110.68
2	B	800	ADP	O3B-PB-O2B	2.23	116.16	107.64
2	A	800	ADP	O4'-C4'-C3'	2.22	109.50	105.11
2	C	800	ADP	O2B-PB-O3A	2.21	112.06	104.64
2	E	800	ADP	C2-N1-C6	2.20	122.52	118.75
2	B	800	ADP	O5'-PA-O1A	2.19	117.62	109.07
2	D	800	ADP	N3-C2-N1	-2.18	125.26	128.68
2	J	800	ADP	C4-C5-N7	-2.18	107.13	109.40
2	J	800	ADP	O3A-PB-O1B	-2.18	99.11	111.19
2	G	800	ADP	C4-C5-N7	-2.13	107.18	109.40
2	C	800	ADP	C2'-C3'-C4'	2.12	106.77	102.64
2	B	800	ADP	C4-C5-N7	-2.12	107.19	109.40
2	J	800	ADP	N3-C2-N1	-2.08	125.43	128.68
2	L	800	ADP	O3B-PB-O3A	-2.08	97.67	104.64
2	L	800	ADP	O4'-C4'-C3'	2.07	109.22	105.11
2	D	800	ADP	C2'-C3'-C4'	2.05	106.63	102.64
2	I	800	ADP	O5'-PA-O1A	-2.04	101.10	109.07
2	D	800	ADP	O2'-C2'-C3'	2.03	118.37	111.82

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	ADP	PA-O3A-PB-O2B
2	A	800	ADP	C5'-O5'-PA-O1A
2	C	800	ADP	PA-O3A-PB-O2B
2	C	800	ADP	C5'-O5'-PA-O3A
2	C	800	ADP	O4'-C4'-C5'-O5'
2	L	800	ADP	C5'-O5'-PA-O1A
2	L	800	ADP	C5'-O5'-PA-O3A
2	L	800	ADP	O4'-C4'-C5'-O5'
2	H	800	ADP	C5'-O5'-PA-O2A
2	H	800	ADP	C5'-O5'-PA-O3A
2	H	800	ADP	O4'-C4'-C5'-O5'
2	E	800	ADP	PA-O3A-PB-O2B
2	E	800	ADP	C5'-O5'-PA-O3A
2	E	800	ADP	O4'-C4'-C5'-O5'
2	J	800	ADP	C5'-O5'-PA-O1A
2	J	800	ADP	C5'-O5'-PA-O2A
2	D	800	ADP	C5'-O5'-PA-O1A
2	D	800	ADP	C3'-C4'-C5'-O5'
2	F	800	ADP	PA-O3A-PB-O2B
2	F	800	ADP	C5'-O5'-PA-O1A
2	F	800	ADP	O4'-C4'-C5'-O5'
2	B	800	ADP	C5'-O5'-PA-O1A
2	B	800	ADP	C5'-O5'-PA-O2A
2	I	800	ADP	PA-O3A-PB-O3B
2	I	800	ADP	C5'-O5'-PA-O1A
2	I	800	ADP	C5'-O5'-PA-O3A
2	K	800	ADP	PA-O3A-PB-O2B
2	K	800	ADP	C5'-O5'-PA-O3A
2	K	800	ADP	O4'-C4'-C5'-O5'
2	G	800	ADP	PA-O3A-PB-O2B
2	G	800	ADP	PA-O3A-PB-O3B
2	G	800	ADP	C5'-O5'-PA-O2A
2	G	800	ADP	C5'-O5'-PA-O3A
2	A	800	ADP	O4'-C4'-C5'-O5'
2	J	800	ADP	O4'-C4'-C5'-O5'
2	J	800	ADP	C3'-C4'-C5'-O5'
2	D	800	ADP	O4'-C4'-C5'-O5'
2	F	800	ADP	C3'-C4'-C5'-O5'
2	B	800	ADP	O4'-C4'-C5'-O5'
2	B	800	ADP	C3'-C4'-C5'-O5'
2	I	800	ADP	O4'-C4'-C5'-O5'
2	I	800	ADP	C3'-C4'-C5'-O5'
2	G	800	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	G	800	ADP	C3'-C4'-C5'-O5'
2	A	800	ADP	C3'-C4'-C5'-O5'
2	C	800	ADP	C3'-C4'-C5'-O5'
2	L	800	ADP	C3'-C4'-C5'-O5'
2	H	800	ADP	C3'-C4'-C5'-O5'
2	E	800	ADP	C3'-C4'-C5'-O5'
2	K	800	ADP	C3'-C4'-C5'-O5'
2	L	800	ADP	PA-O3A-PB-O1B
2	D	800	ADP	PA-O3A-PB-O1B
2	I	800	ADP	PA-O3A-PB-O2B
2	A	800	ADP	C5'-O5'-PA-O3A
2	F	800	ADP	C5'-O5'-PA-O3A
2	L	800	ADP	PB-O3A-PA-O2A
2	E	800	ADP	PB-O3A-PA-O2A
2	B	800	ADP	PB-O3A-PA-O2A
2	A	800	ADP	C5'-O5'-PA-O2A
2	C	800	ADP	C5'-O5'-PA-O2A
2	E	800	ADP	C5'-O5'-PA-O1A
2	F	800	ADP	C5'-O5'-PA-O2A
2	K	800	ADP	C5'-O5'-PA-O1A
2	C	800	ADP	PA-O3A-PB-O1B
2	F	800	ADP	PA-O3A-PB-O1B
2	G	800	ADP	PA-O3A-PB-O1B
2	C	800	ADP	PA-O3A-PB-O3B
2	L	800	ADP	PA-O3A-PB-O2B
2	L	800	ADP	PA-O3A-PB-O3B
2	E	800	ADP	PA-O3A-PB-O3B
2	J	800	ADP	C5'-O5'-PA-O3A
2	B	800	ADP	C5'-O5'-PA-O3A
2	L	800	ADP	PB-O3A-PA-O1A
2	E	800	ADP	PB-O3A-PA-O1A
2	D	800	ADP	PB-O3A-PA-O2A
2	K	800	ADP	PB-O3A-PA-O2A
2	I	800	ADP	C5'-O5'-PA-O2A
2	I	800	ADP	PA-O3A-PB-O1B
2	K	800	ADP	PA-O3A-PB-O1B

There are no ring outliers.

12 monomers are involved in 47 short contacts:

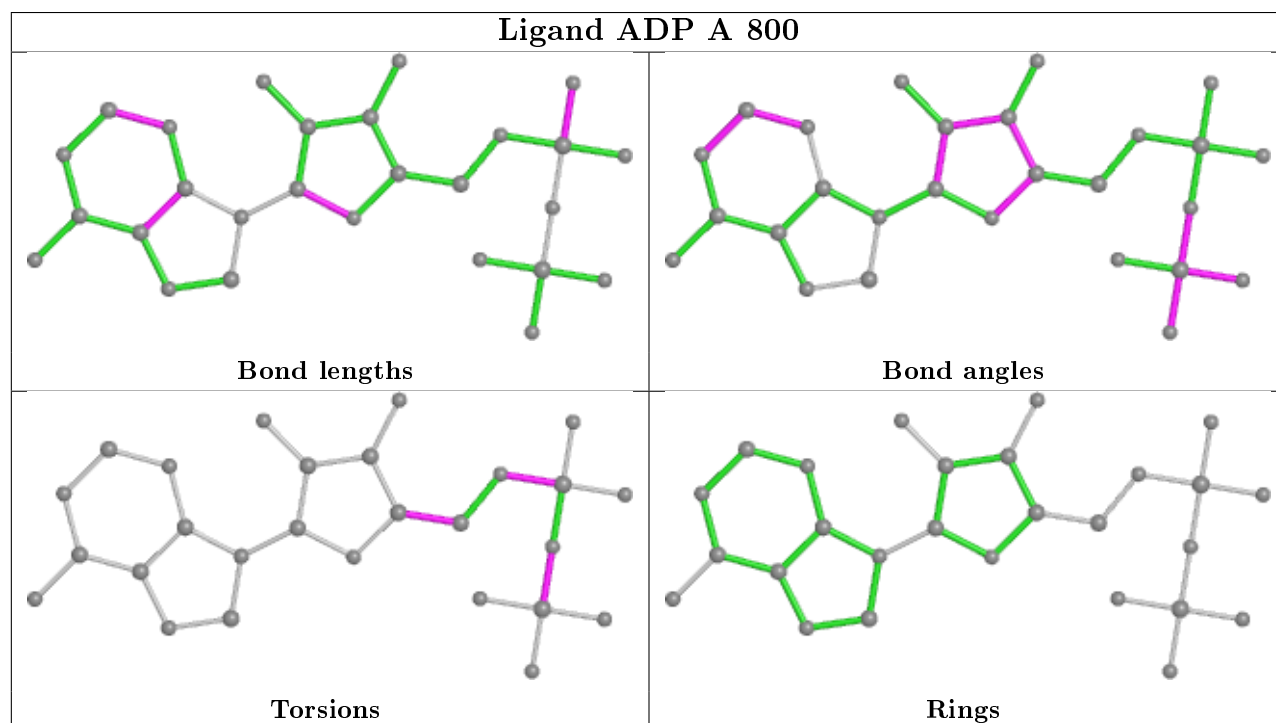
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	3	0

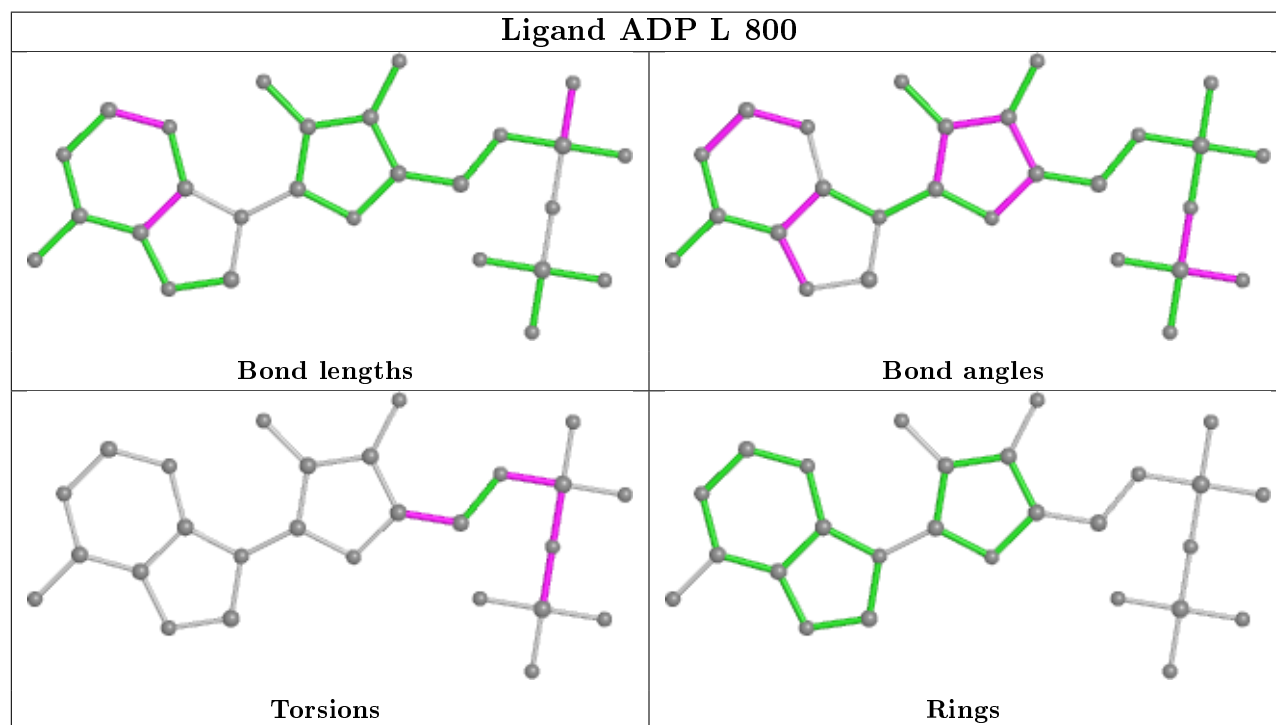
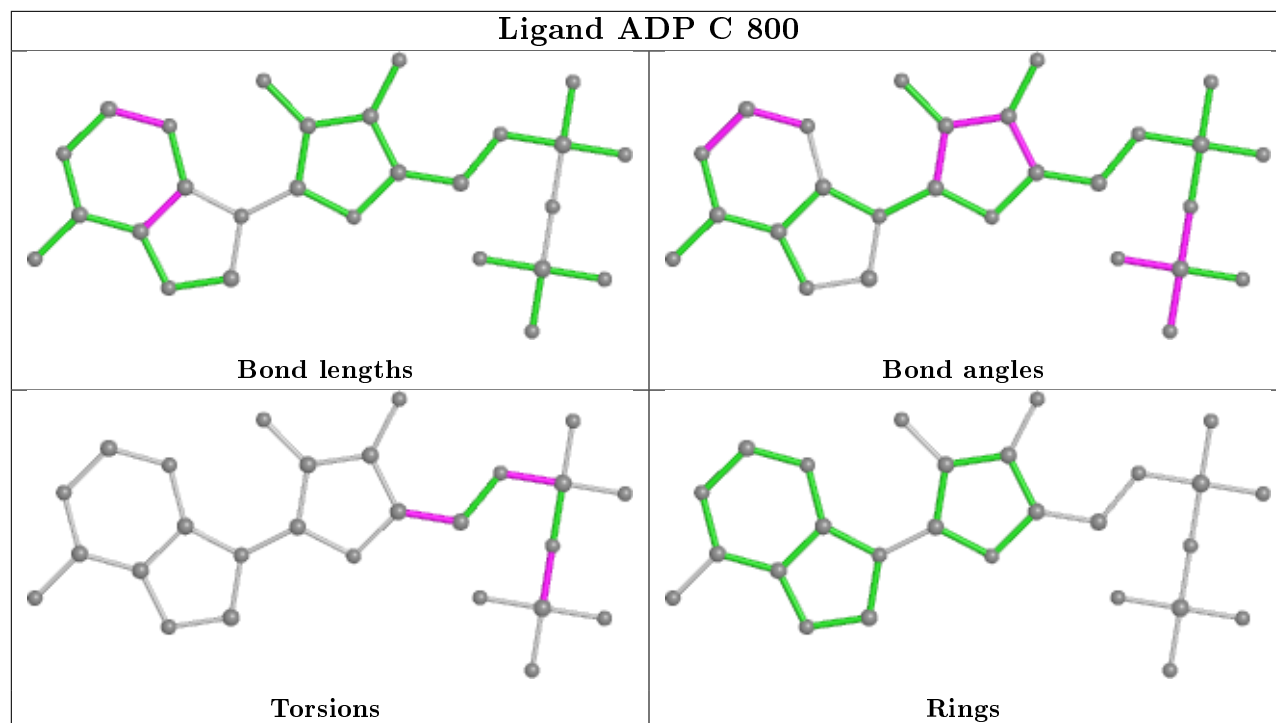
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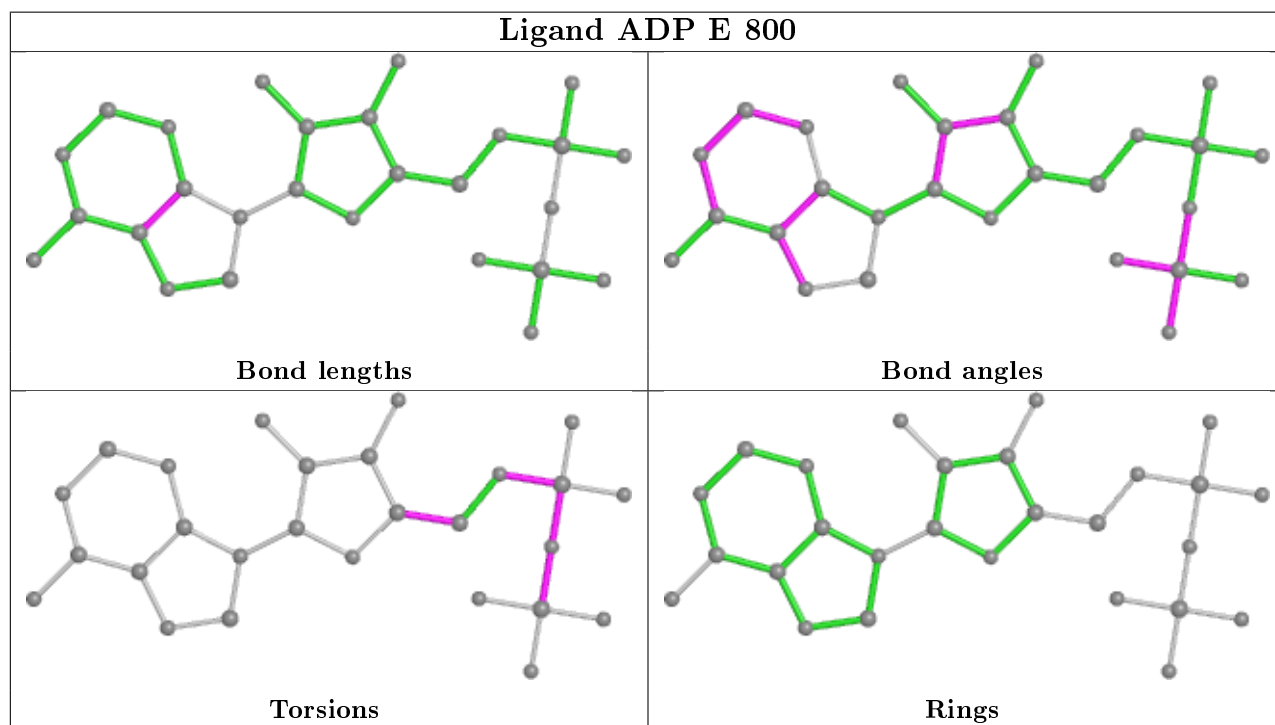
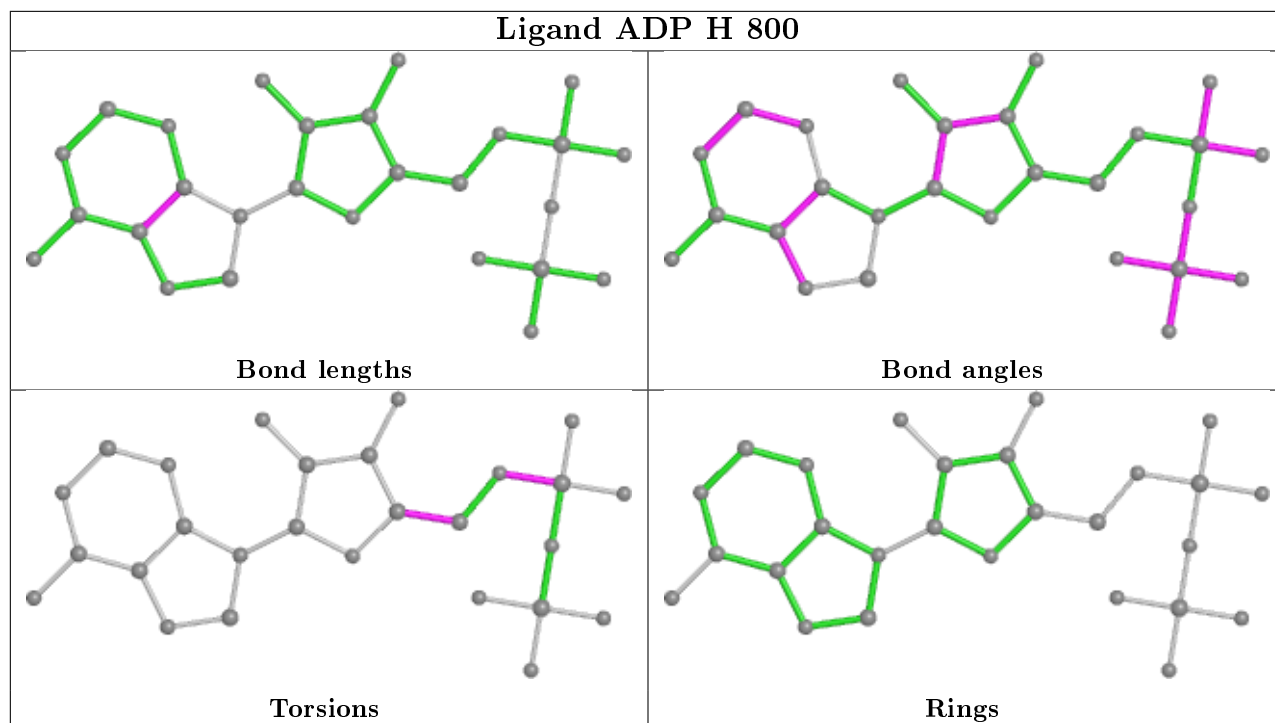
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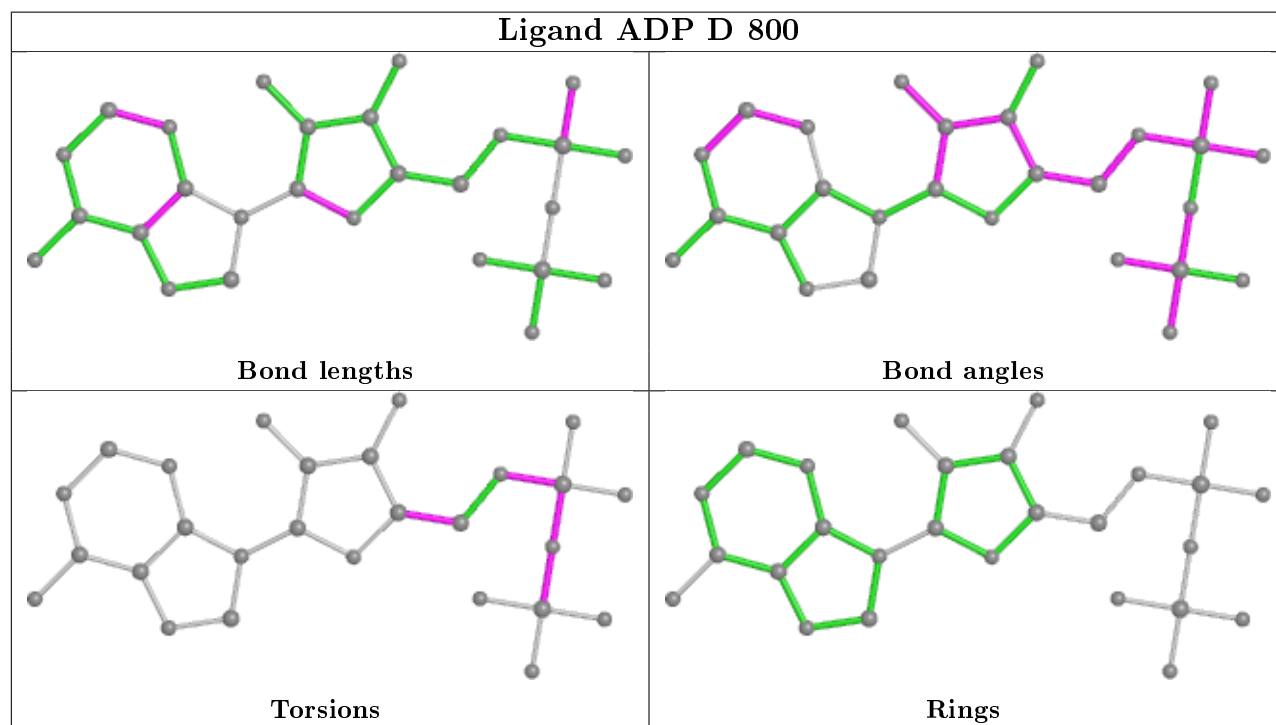
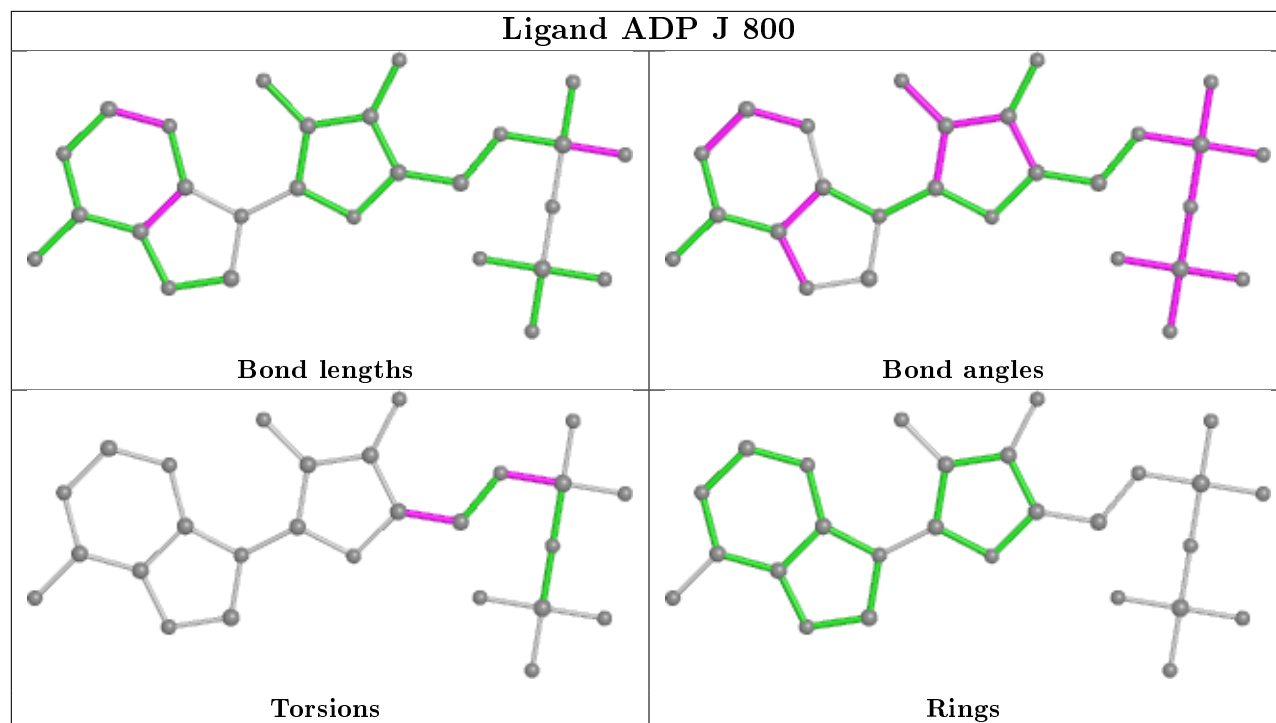
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	800	ADP	4	0
2	L	800	ADP	4	0
2	H	800	ADP	6	0
2	E	800	ADP	3	0
2	J	800	ADP	2	0
2	D	800	ADP	2	0
2	F	800	ADP	4	0
2	B	800	ADP	6	0
2	I	800	ADP	6	0
2	K	800	ADP	4	0
2	G	800	ADP	3	0

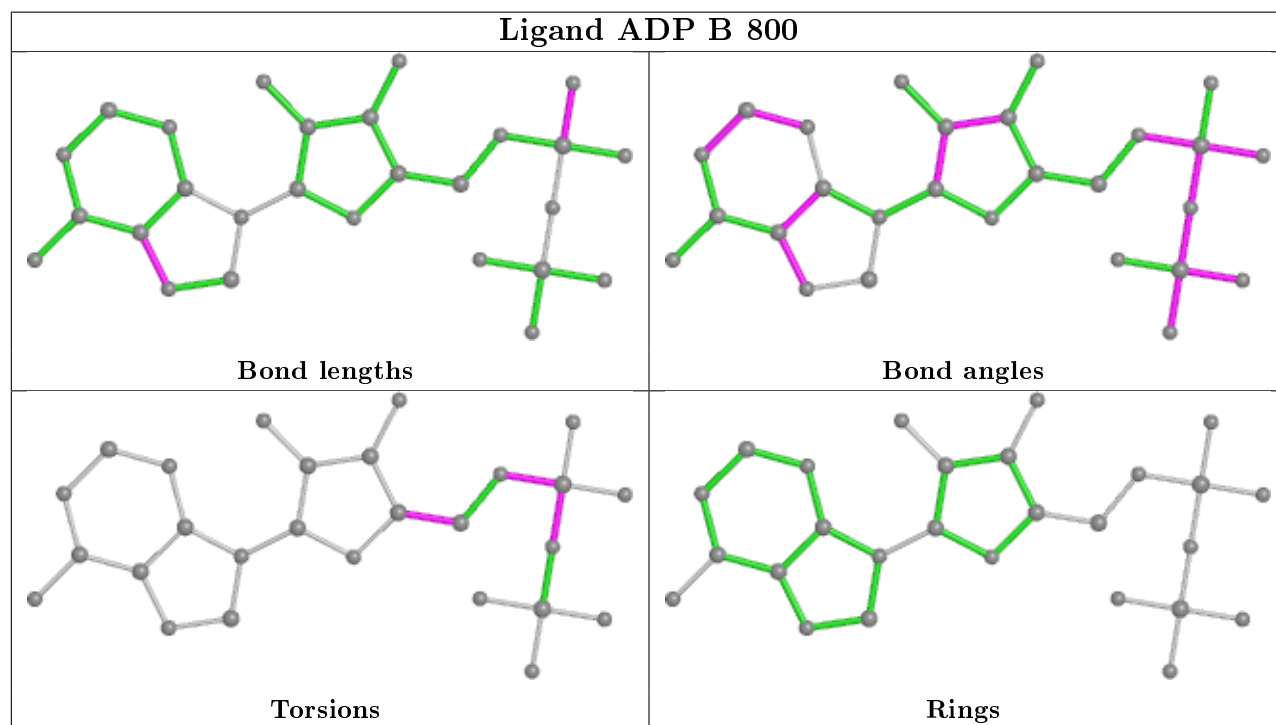
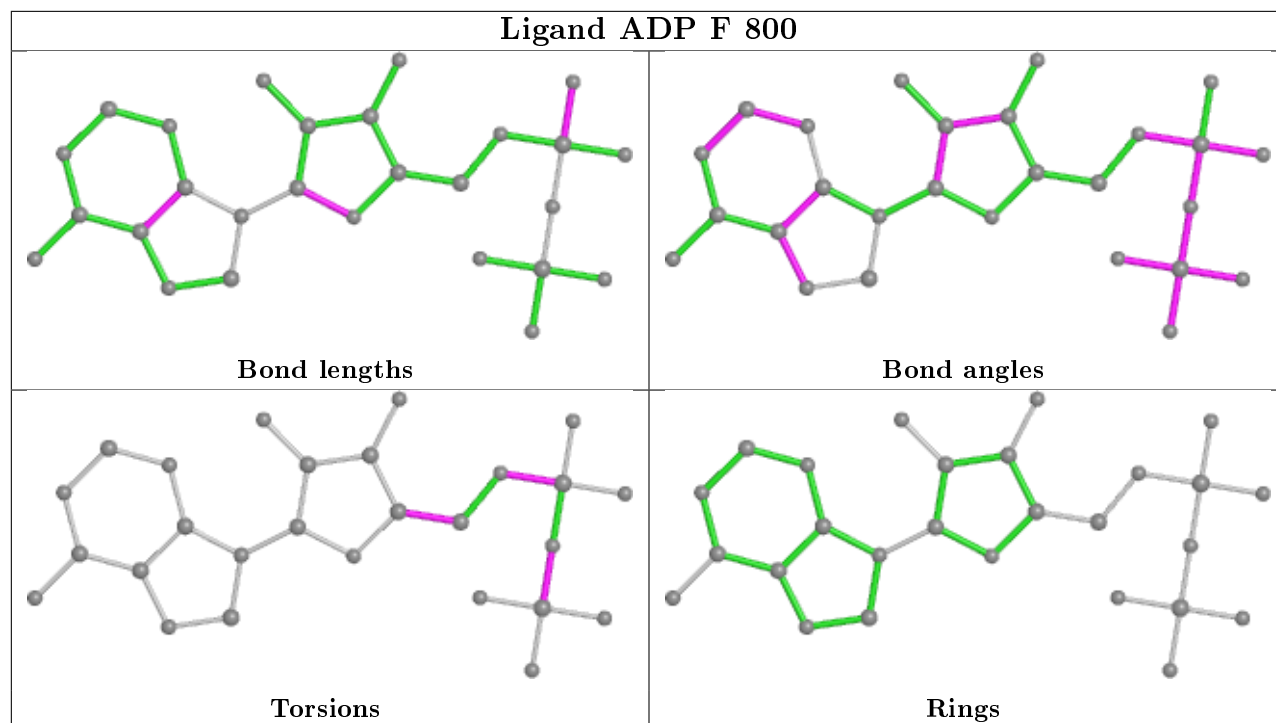
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

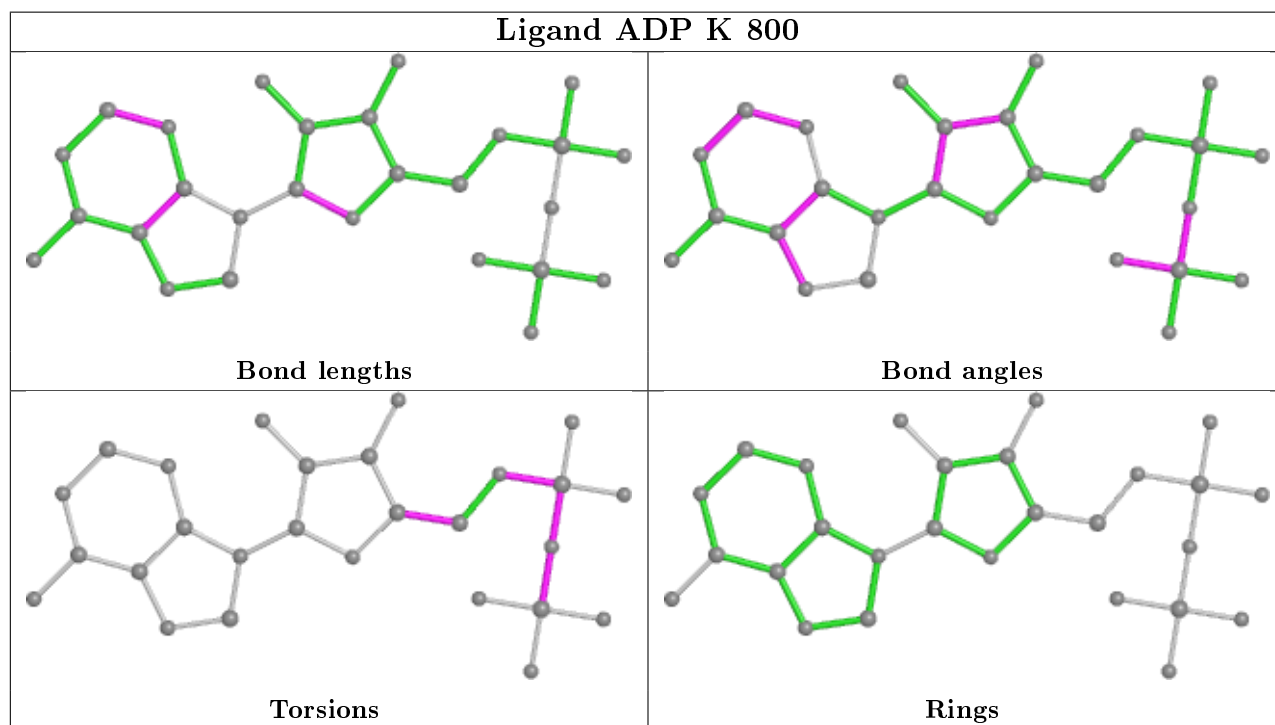
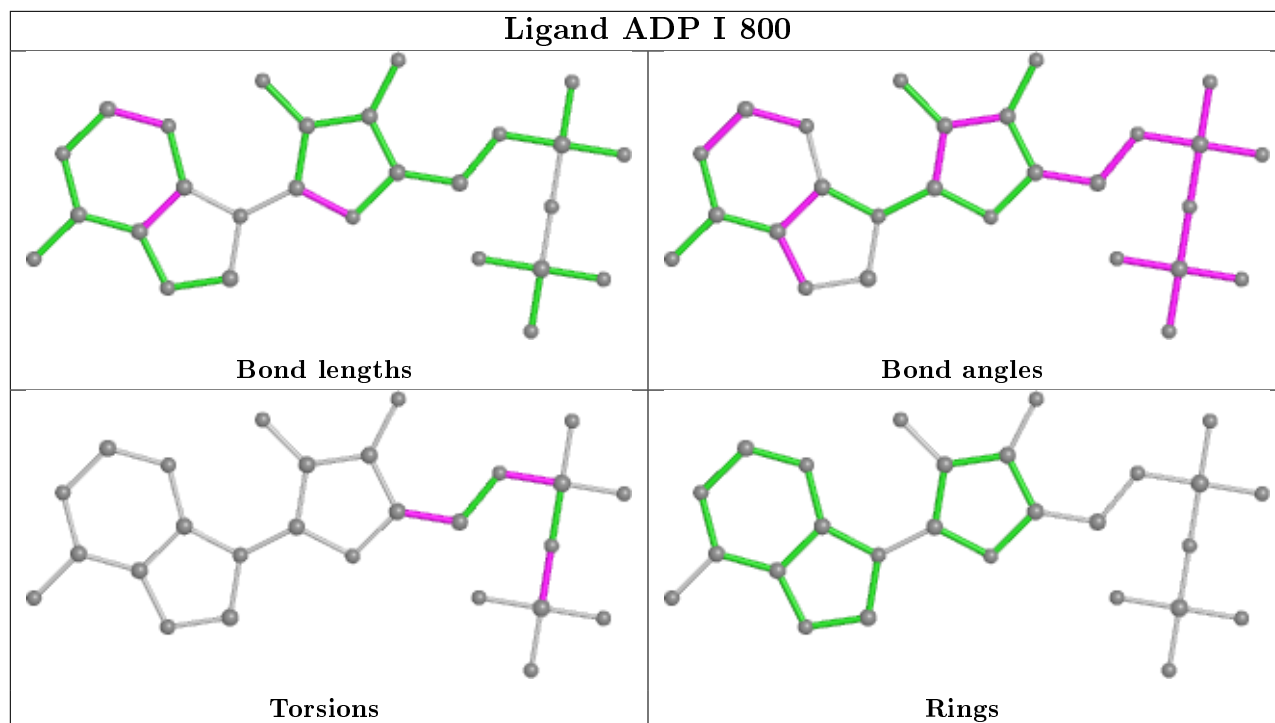


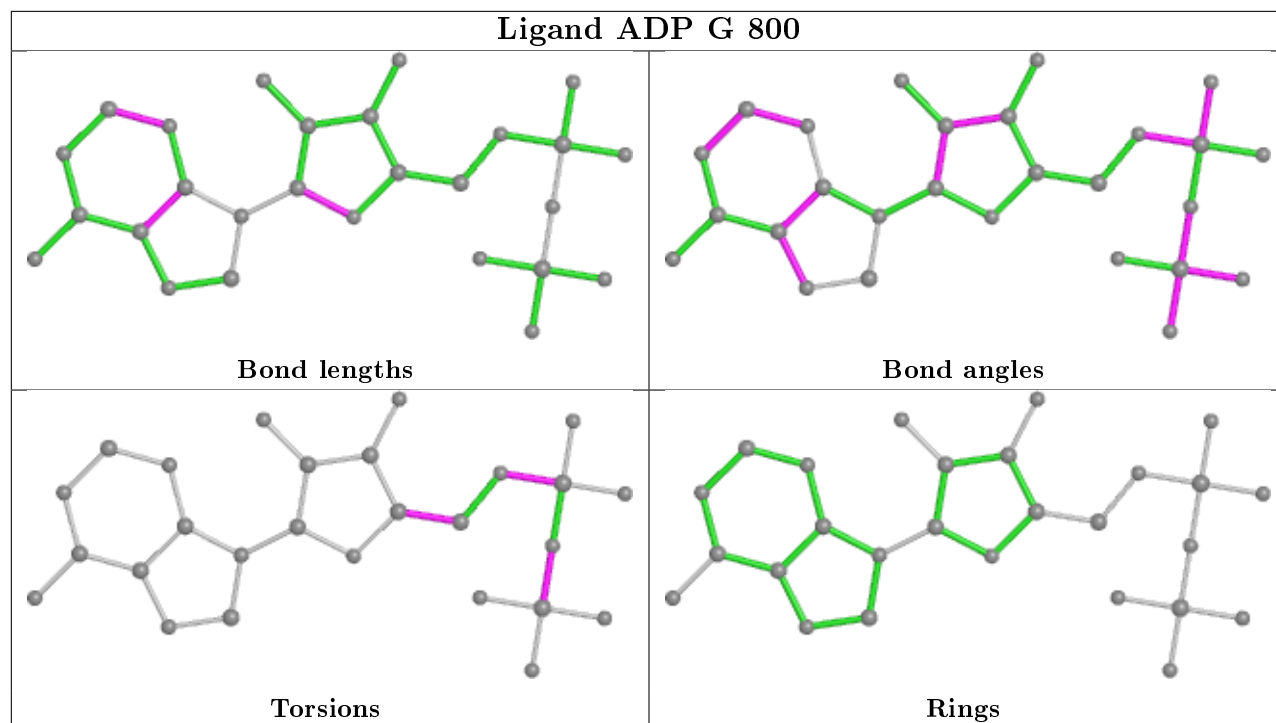












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	440/489 (89%)	0.04	3 (0%) 87 85	68, 120, 178, 241	0
1	B	438/489 (89%)	0.12	17 (3%) 39 32	69, 127, 192, 285	0
1	C	438/489 (89%)	0.54	47 (10%) 6 5	84, 157, 219, 330	0
1	D	439/489 (89%)	0.15	15 (3%) 45 37	79, 134, 192, 281	0
1	E	438/489 (89%)	0.57	43 (9%) 7 6	95, 161, 226, 269	0
1	F	438/489 (89%)	0.28	35 (7%) 12 10	82, 141, 198, 301	0
1	G	438/489 (89%)	0.17	22 (5%) 28 25	81, 139, 198, 298	0
1	H	439/489 (89%)	0.24	23 (5%) 27 24	78, 144, 217, 299	0
1	I	439/489 (89%)	0.14	17 (3%) 39 32	81, 138, 195, 302	0
1	J	441/489 (90%)	0.38	42 (9%) 8 7	87, 150, 202, 272	0
1	K	439/489 (89%)	-0.01	11 (2%) 57 49	71, 120, 180, 296	0
1	L	438/489 (89%)	-0.07	5 (1%) 80 76	70, 117, 176, 252	0
All	All	5265/5868 (89%)	0.21	280 (5%) 26 23	68, 136, 204, 330	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ASN	6.0
1	C	116	VAL	5.9
1	J	66	GLU	5.7
1	G	432	LEU	5.0
1	J	174	CYS	4.8
1	K	21	ASN	4.8
1	E	173	TYR	4.7
1	E	21	ASN	4.6
1	E	174	CYS	4.6
1	C	168	THR	4.6
1	J	175	ILE	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	282	SER	4.6
1	E	431	ASP	4.5
1	C	139	PHE	4.3
1	C	151	ILE	4.2
1	C	108	VAL	4.2
1	K	432	LEU	4.2
1	J	68	VAL	4.1
1	J	100	ILE	4.1
1	J	173	TYR	3.9
1	J	435	GLU	3.9
1	J	101	SER	3.9
1	E	172	PRO	3.9
1	H	459	SER	3.8
1	B	102	ILE	3.8
1	J	109	LYS	3.8
1	J	150	ASP	3.7
1	D	437	ILE	3.7
1	C	164	LYS	3.7
1	G	75	ASP	3.7
1	C	117	LEU	3.7
1	D	113	ARG	3.7
1	F	179	ASP	3.6
1	G	42	SER	3.6
1	G	43	GLN	3.6
1	F	175	ILE	3.5
1	J	434	ASP	3.5
1	C	83	ARG	3.4
1	E	198	LEU	3.4
1	C	432	LEU	3.4
1	I	179	ASP	3.4
1	E	108	VAL	3.4
1	K	434	ASP	3.4
1	F	435	GLU	3.4
1	E	146	ILE	3.3
1	G	433	GLU	3.3
1	C	41	LEU	3.3
1	G	99	VAL	3.3
1	F	116	VAL	3.3
1	I	134	TYR	3.3
1	C	115	HIS	3.3
1	E	126	ILE	3.3
1	E	58	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	230	PHE	3.3
1	B	100	ILE	3.3
1	C	405	GLY	3.2
1	J	102	ILE	3.2
1	E	102	ILE	3.2
1	H	102	ILE	3.2
1	B	23	PRO	3.2
1	J	433	GLU	3.2
1	C	94	VAL	3.2
1	F	113	ARG	3.2
1	L	437	ILE	3.1
1	F	176	VAL	3.1
1	C	73	SER	3.1
1	J	110	TYR	3.1
1	J	70	ILE	3.1
1	E	109	LYS	3.1
1	C	24	ASN	3.1
1	E	164	LYS	3.0
1	E	22	ARG	3.0
1	H	134	TYR	3.0
1	J	64	ARG	3.0
1	C	172	PRO	3.0
1	C	173	TYR	3.0
1	C	423	ILE	3.0
1	F	166	VAL	3.0
1	C	100	ILE	3.0
1	E	169	ASP	3.0
1	J	59	LEU	3.0
1	E	279	ALA	3.0
1	C	114	ILE	3.0
1	F	172	PRO	3.0
1	G	431	ASP	3.0
1	A	174	CYS	2.9
1	E	49	LEU	2.9
1	E	434	ASP	2.9
1	A	460	ASN	2.9
1	D	430	ILE	2.9
1	B	101	SER	2.9
1	I	437	ILE	2.9
1	L	428	ASP	2.9
1	J	21	ASN	2.8
1	J	92	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	109	LYS	2.8
1	G	437	ILE	2.8
1	J	176	VAL	2.8
1	F	182	ILE	2.7
1	J	67	ALA	2.7
1	J	58	LEU	2.7
1	H	103	GLN	2.7
1	J	62	LYS	2.7
1	C	40	SER	2.7
1	F	437	ILE	2.7
1	J	69	CYS	2.7
1	F	117	LEU	2.7
1	H	80	GLU	2.7
1	E	24	ASN	2.7
1	E	193	ASP	2.7
1	I	433	GLU	2.7
1	F	114	ILE	2.7
1	D	426	LYS	2.7
1	F	354	ASP	2.7
1	G	26	LEU	2.7
1	G	41	LEU	2.7
1	J	23	PRO	2.7
1	K	431	ASP	2.7
1	H	426	LYS	2.6
1	E	114	ILE	2.6
1	I	70	ILE	2.6
1	K	40	SER	2.6
1	H	434	ASP	2.6
1	F	108	VAL	2.6
1	B	173	TYR	2.6
1	G	78	SER	2.6
1	F	128	GLY	2.6
1	H	26	LEU	2.6
1	H	81	LYS	2.6
1	D	155	ARG	2.6
1	E	25	ARG	2.6
1	E	113	ARG	2.6
1	I	43	GLN	2.6
1	H	27	ILE	2.6
1	E	45	LYS	2.6
1	F	134	TYR	2.5
1	J	108	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	24	ASN	2.5
1	C	165	VAL	2.5
1	C	431	ASP	2.5
1	L	27	ILE	2.5
1	G	418	ALA	2.5
1	J	99	VAL	2.5
1	H	427	MET	2.5
1	C	109	LYS	2.5
1	K	435	GLU	2.5
1	K	41	LEU	2.5
1	B	22	ARG	2.5
1	C	63	LYS	2.5
1	G	73	SER	2.5
1	D	440	GLU	2.5
1	E	145	PRO	2.5
1	D	134	TYR	2.5
1	G	79	ASP	2.5
1	F	115	HIS	2.5
1	F	110	TYR	2.4
1	C	148	LYS	2.4
1	E	284	SER	2.4
1	C	107	ASP	2.4
1	C	111	GLY	2.4
1	F	434	ASP	2.4
1	J	146	ILE	2.4
1	D	158	MET	2.4
1	J	39	VAL	2.4
1	E	67	ALA	2.4
1	E	112	LYS	2.4
1	C	134	TYR	2.4
1	I	72	LEU	2.4
1	J	37	SER	2.4
1	B	82	ILE	2.4
1	F	70	ILE	2.4
1	F	165	VAL	2.4
1	I	71	VAL	2.4
1	J	168	THR	2.4
1	J	152	PHE	2.4
1	K	433	GLU	2.4
1	G	406	HIS	2.4
1	C	150	ASP	2.4
1	B	27	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	126	ILE	2.3
1	C	92	LEU	2.3
1	H	82	ILE	2.3
1	C	128	GLY	2.3
1	E	354	ASP	2.3
1	C	39	VAL	2.3
1	B	60	LYS	2.3
1	H	126	ILE	2.3
1	G	76	THR	2.3
1	E	281	GLU	2.3
1	F	174	CYS	2.3
1	B	169	ASP	2.3
1	G	102	ILE	2.3
1	J	436	THR	2.3
1	I	41	LEU	2.3
1	I	432	LEU	2.3
1	C	145	PRO	2.3
1	E	285	ASN	2.3
1	F	169	ASP	2.3
1	C	82	ILE	2.3
1	E	115	HIS	2.3
1	J	437	ILE	2.3
1	I	82	ILE	2.3
1	C	50	GLN	2.3
1	D	417	GLU	2.3
1	F	168	THR	2.3
1	J	235	VAL	2.3
1	C	102	ILE	2.2
1	C	110	TYR	2.2
1	D	157	GLY	2.2
1	J	172	PRO	2.2
1	H	433	GLU	2.2
1	B	427	MET	2.2
1	E	166	VAL	2.2
1	I	39	VAL	2.2
1	I	108	VAL	2.2
1	C	138	TYR	2.2
1	F	49	LEU	2.2
1	G	402	GLU	2.2
1	I	80	GLU	2.2
1	J	57	VAL	2.2
1	H	25	ARG	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	107	ASP	2.2
1	C	176	VAL	2.2
1	G	53	ARG	2.2
1	B	293	ALA	2.2
1	C	169	ASP	2.2
1	G	452	PHE	2.2
1	D	428	ASP	2.2
1	H	21	ASN	2.2
1	I	431	ASP	2.2
1	E	235	VAL	2.2
1	J	145	PRO	2.1
1	B	99	VAL	2.1
1	F	135	LEU	2.1
1	H	174	CYS	2.1
1	F	139	PHE	2.1
1	F	180	THR	2.1
1	G	405	GLY	2.1
1	J	143	TYR	2.1
1	K	72	LEU	2.1
1	J	151	ILE	2.1
1	E	165	VAL	2.1
1	H	41	LEU	2.1
1	D	109	LYS	2.1
1	H	40	SER	2.1
1	F	130	LEU	2.1
1	F	150	ASP	2.1
1	L	41	LEU	2.1
1	F	173	TYR	2.1
1	C	126	ILE	2.1
1	K	102	ILE	2.1
1	I	165	VAL	2.1
1	D	434	ASP	2.1
1	B	51	LEU	2.1
1	F	41	LEU	2.1
1	H	43	GLN	2.1
1	L	452	PHE	2.1
1	G	45	LYS	2.1
1	E	153	LEU	2.1
1	C	95	ARG	2.1
1	C	153	LEU	2.1
1	C	167	GLU	2.1
1	E	116	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	105	CYS	2.1
1	D	432	LEU	2.1
1	H	31	ALA	2.0
1	E	92	LEU	2.0
1	H	42	SER	2.0
1	K	459	SER	2.0
1	H	51	LEU	2.0
1	J	91	ASN	2.0
1	J	162	GLU	2.0
1	F	289	ALA	2.0
1	D	183	HIS	2.0
1	B	26	LEU	2.0
1	E	139	PHE	2.0
1	C	42	SER	2.0
1	I	102	ILE	2.0
1	A	145	PRO	2.0
1	E	229	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	C	800	27/27	0.91	0.25	73,89,104,105	0
2	ADP	L	800	27/27	0.91	0.26	63,67,71,72	0
2	ADP	A	800	27/27	0.93	0.24	67,70,80,82	0
2	ADP	E	800	27/27	0.93	0.23	98,100,111,114	0
2	ADP	F	800	27/27	0.93	0.25	81,89,92,95	0
2	ADP	I	800	27/27	0.93	0.25	85,91,94,96	0

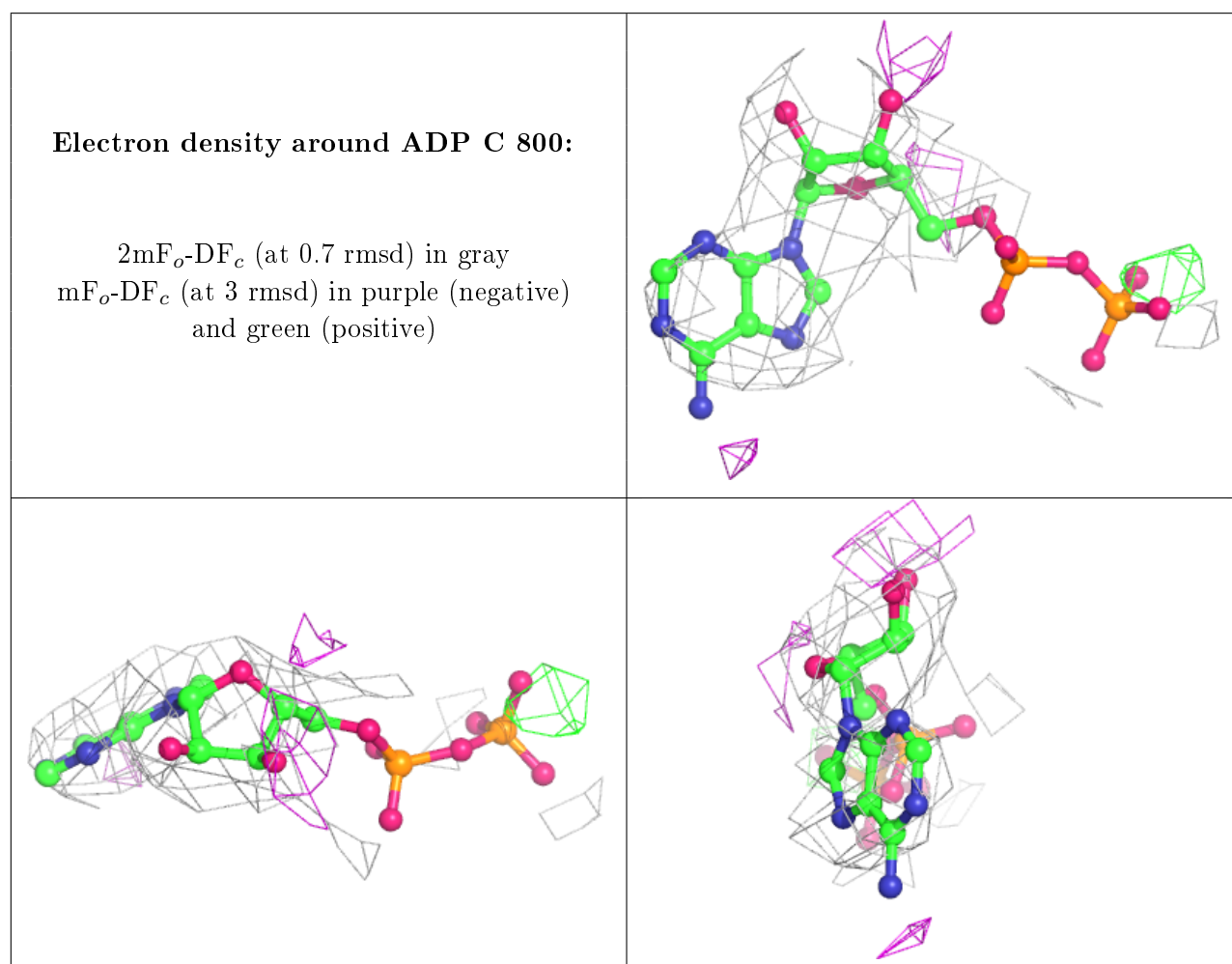
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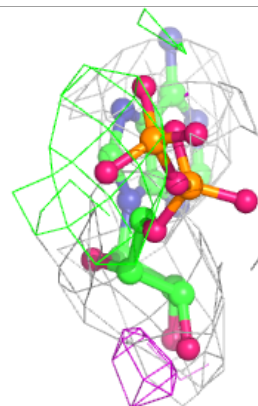
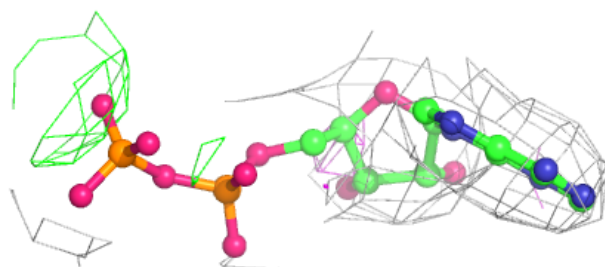
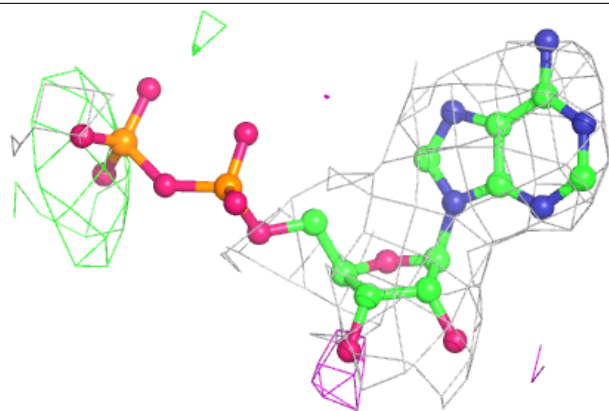
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	K	800	27/27	0.93	0.25	68,80,84,85	0
2	ADP	H	800	27/27	0.94	0.22	69,73,77,80	0
2	ADP	B	800	27/27	0.94	0.24	67,70,72,75	0
2	ADP	J	800	27/27	0.94	0.20	88,91,108,110	0
2	ADP	D	800	27/27	0.94	0.20	85,92,99,100	0
2	ADP	G	800	27/27	0.94	0.23	75,79,83,85	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.

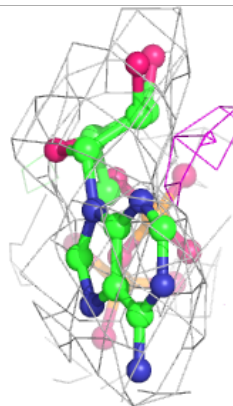
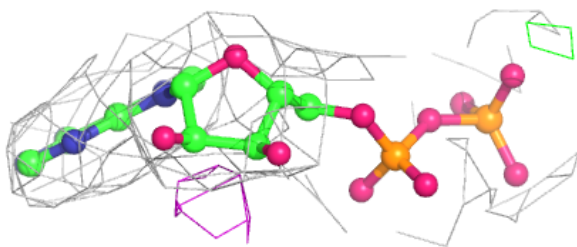
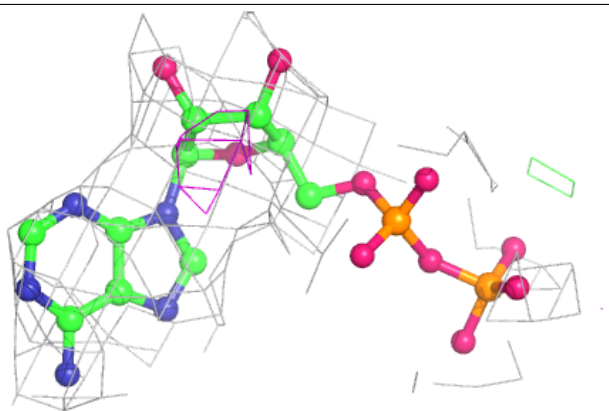


**Electron density around ADP L 800:**

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

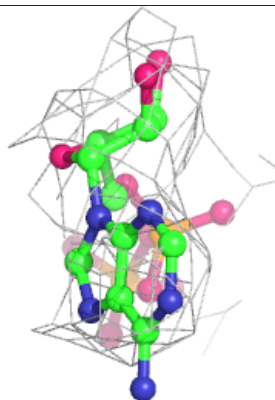
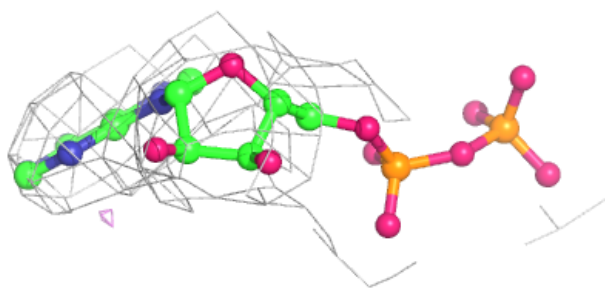
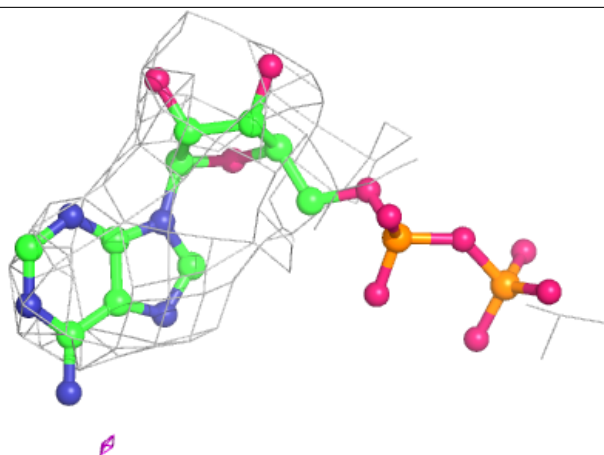
**Electron density around ADP A 800:**

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

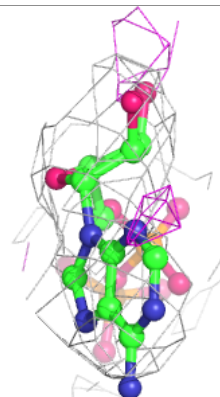
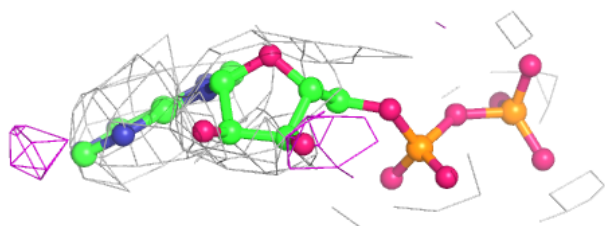
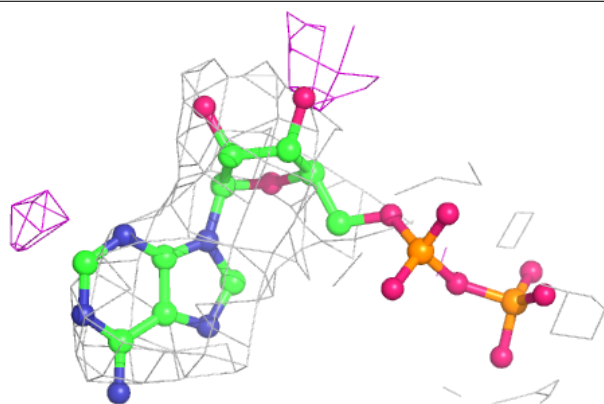


**Electron density around ADP E 800:**

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

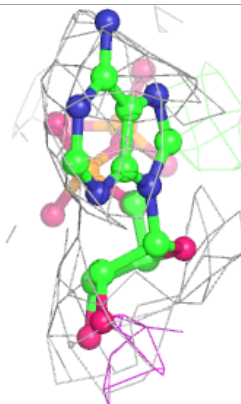
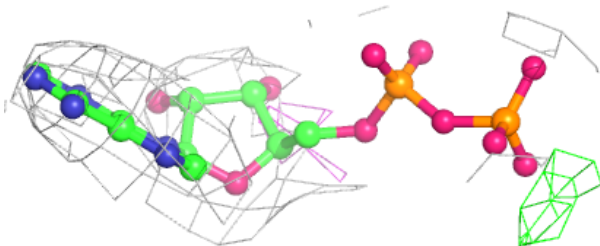
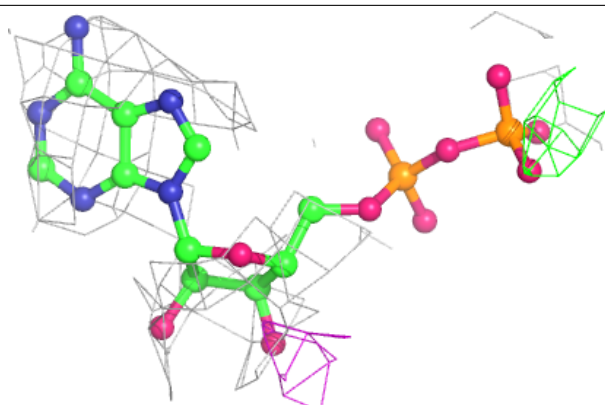
**Electron density around ADP F 800:**

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

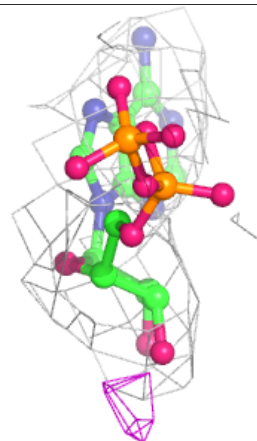
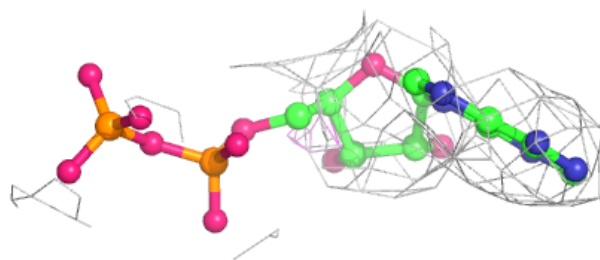
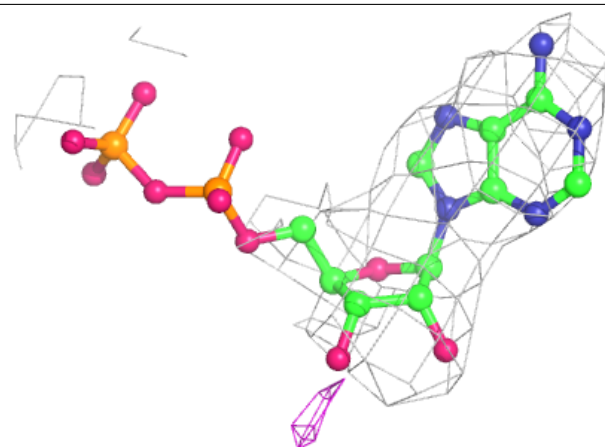


**Electron density around ADP I 800:**

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

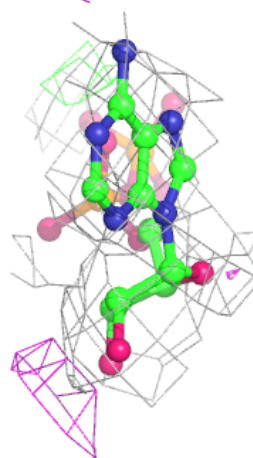
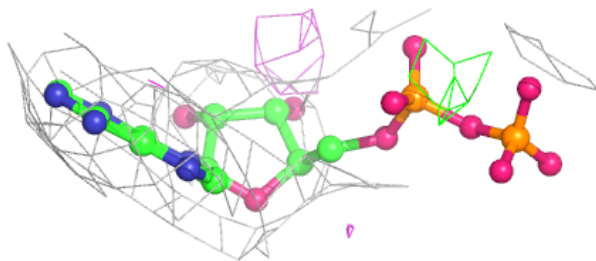
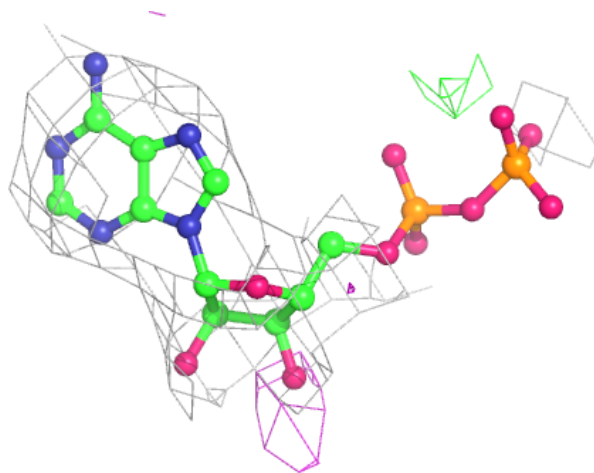
**Electron density around ADP K 800:**

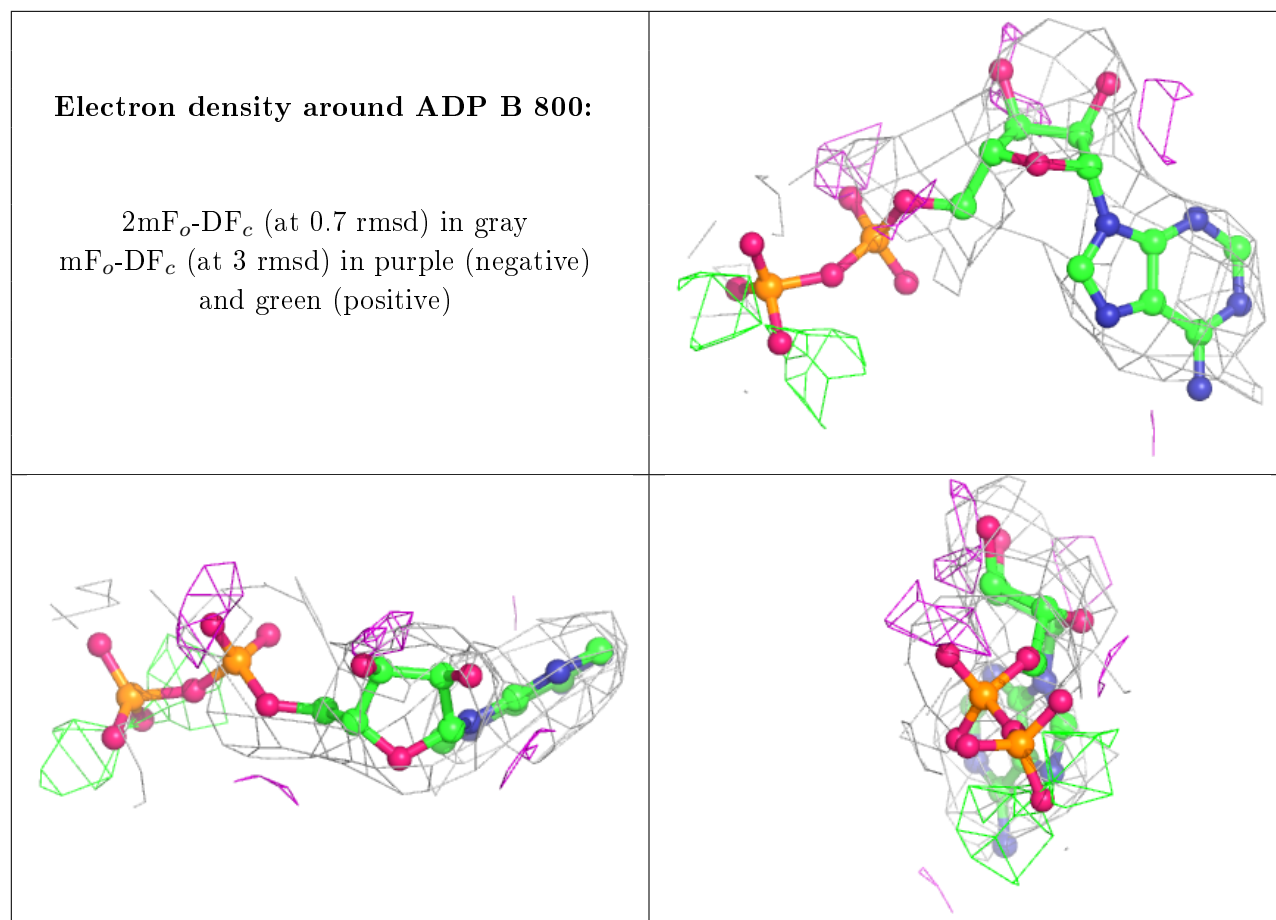
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADP H 800:**

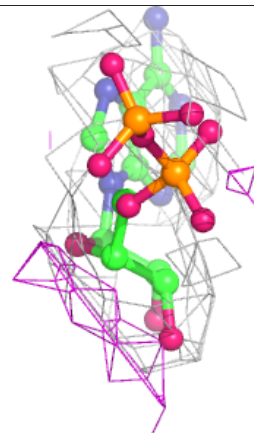
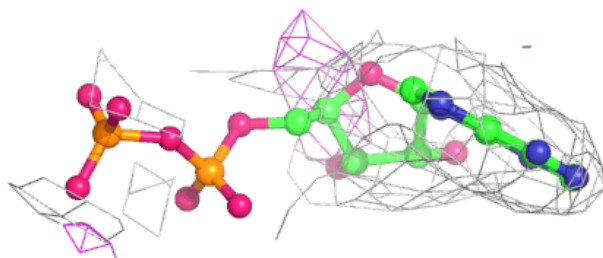
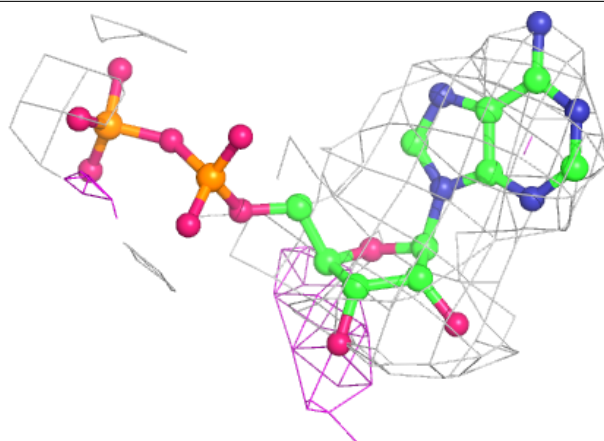
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

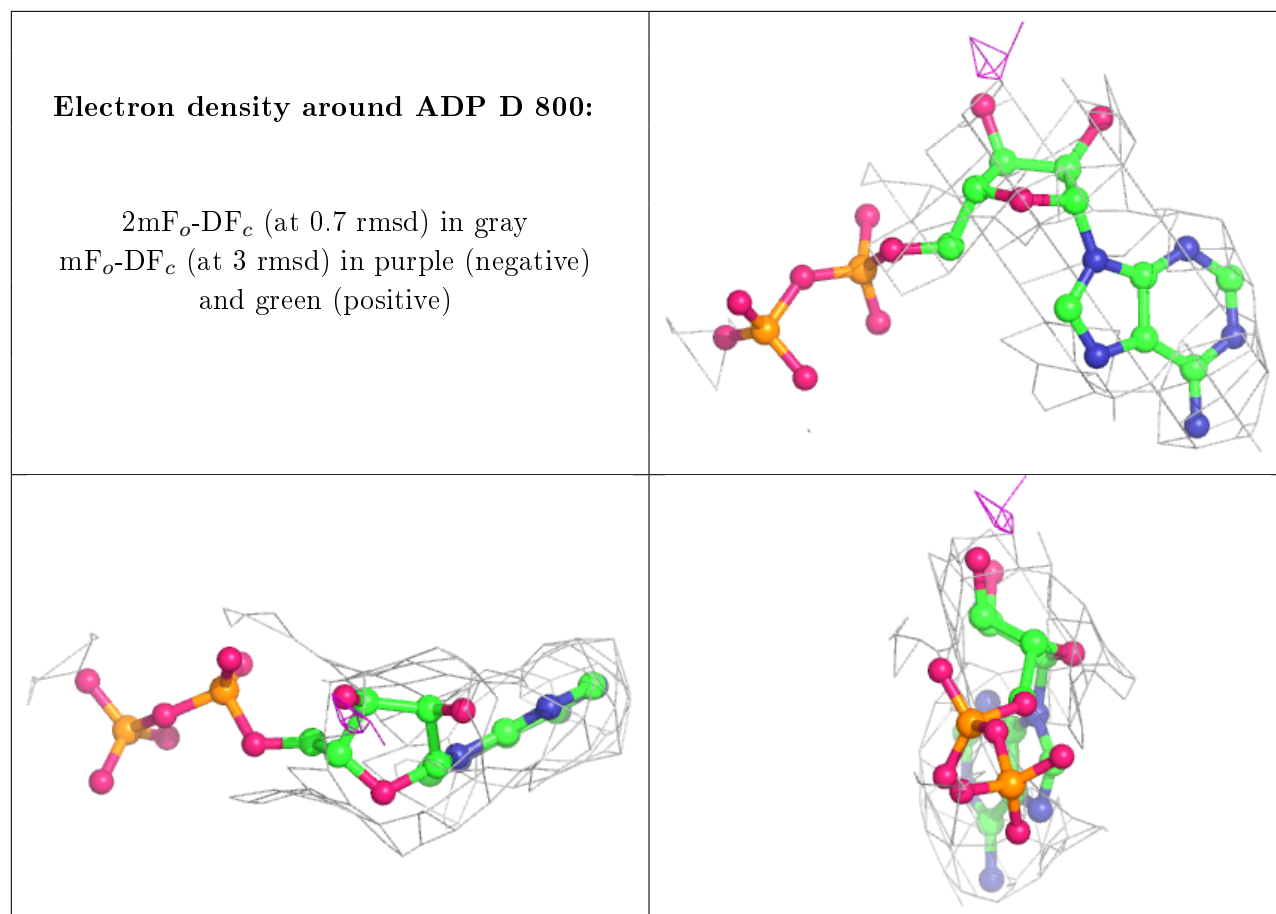




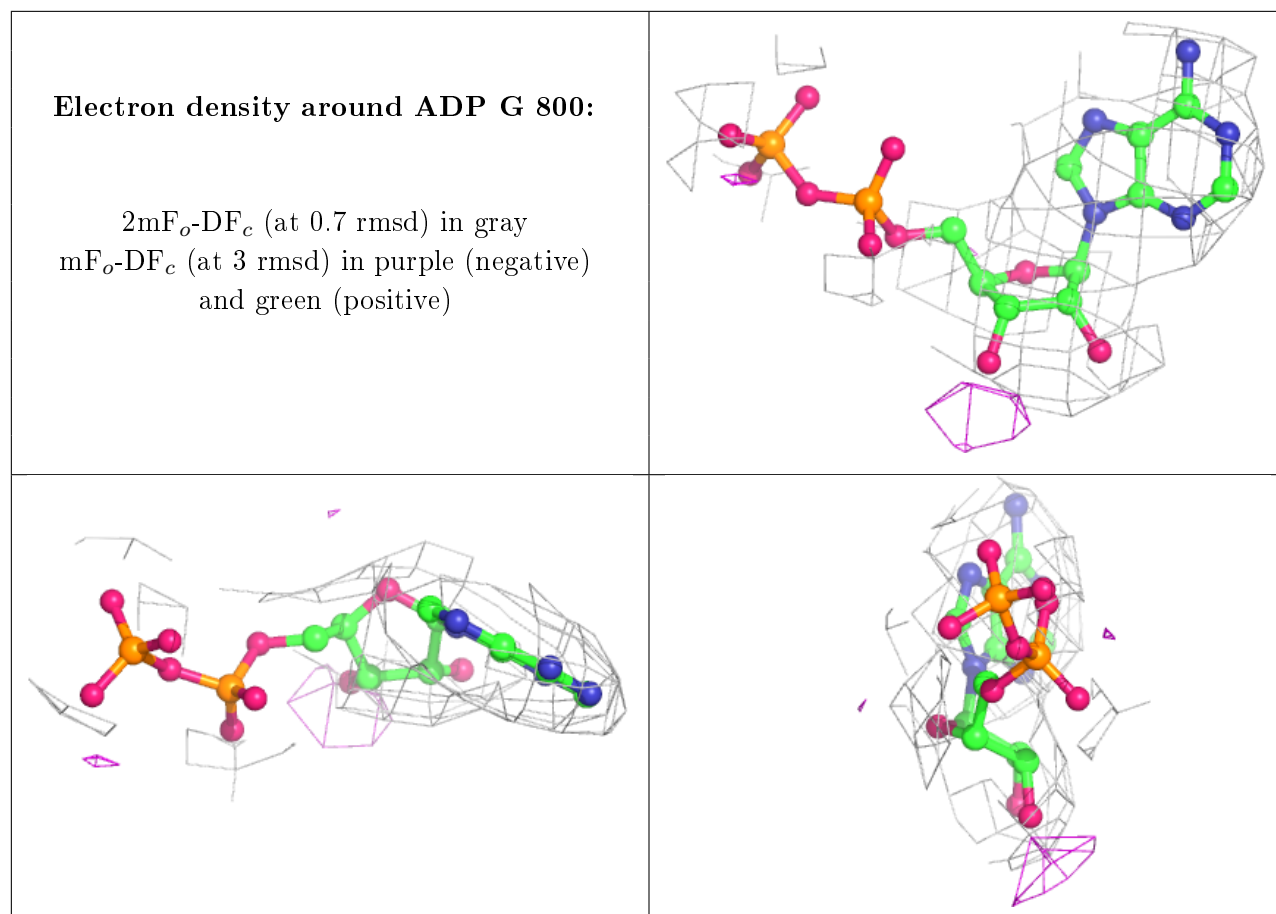
**Electron density around ADP J 800:**

$2mF_o-DF_c$  (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.