Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 09:20 PM EST

PDB ID	:	4KOD
Title	:	Structure of p97 N-D1 R155H mutant in complex with ADP
Authors	:	Xia, D.; Tang, W.K.
Deposited on	:	2013-05-11
Resolution	:	2.96 Å(reported)

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

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

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

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

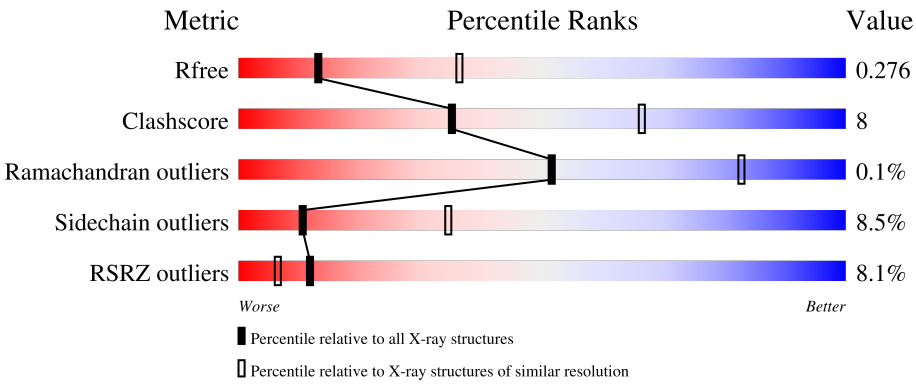
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	489	7% 72% 16% • 10%
1	B	489	4% 69% 20% • 10%
1	C	489	6% 68% 20% • 10%
1	D	489	7% 70% 19% • 10%
1	E	489	12% 70% 18% • 10%

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Mol	Chain	Length	Quality of chain
1	F	489	3% 68% 19% • 10%
1	G	489	6% 71% 17% • 11%
1	H	489	4% 71% 16% • 10%
1	I	489	7% 71% 17% • 10%
1	J	489	3% 73% 16% • 9%
1	K	489	18% 61% 23% 5% • 10%
1	L	489	9% 71% 18% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41760 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	438	3430	2154	607	651	18	0	0	0
1	B	439	3438	2158	609	653	18	0	0	0
1	C	438	3427	2152	605	652	18	0	0	0
1	D	439	3438	2158	609	653	18	0	0	0
1	E	439	3434	2157	606	653	18	0	0	0
1	F	438	3427	2152	605	652	18	0	0	0
1	G	437	3419	2148	603	650	18	0	0	0
1	H	438	3430	2154	607	651	18	0	0	0
1	I	440	3447	2164	611	654	18	0	0	0
1	J	445	3486	2187	619	662	18	0	0	0
1	K	438	3427	2152	605	652	18	0	0	0
1	L	442	3465	2175	615	657	18	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	HIS	ARG	engineered mutation	UNP P55072
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	HIS	-	expression tag	UNP P55072
A	487	HIS	-	expression tag	UNP P55072
A	488	HIS	-	expression tag	UNP P55072
A	489	HIS	-	expression tag	UNP P55072
B	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	UNP P55072
F	482	ARG	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
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
F	489	HIS	-	expression tag	UNP P55072
G	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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	155	HIS	ARG	engineered mutation	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

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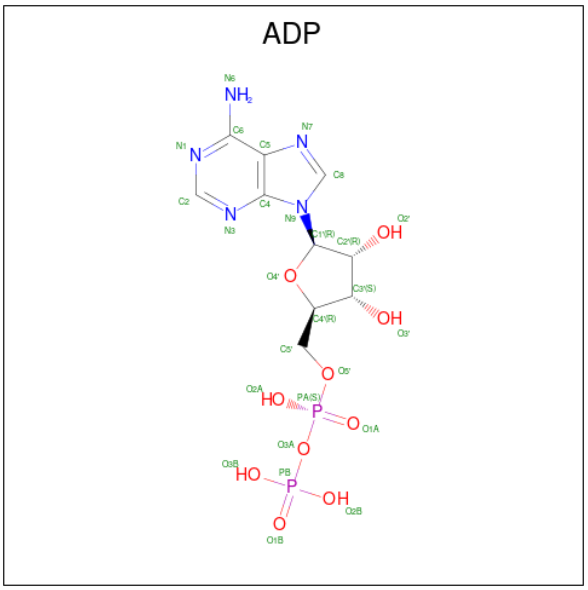
Chain	Residue	Modelled	Actual	Comment	Reference
J	489	HIS	-	expression tag	UNP P55072
K	155	HIS	ARG	engineered mutation	UNP P55072
K	482	ARG	-	expression tag	UNP P55072
K	483	SER	-	expression tag	UNP P55072
K	484	HIS	-	expression tag	UNP P55072
K	485	HIS	-	expression tag	UNP P55072
K	486	HIS	-	expression 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	155	HIS	ARG	engineered mutation	UNP P55072
L	482	ARG	-	expression tag	UNP P55072
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
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	14	14	14	0	0
3	B	9	9	9	0	0
3	C	14	14	14	0	0
3	D	17	17	17	0	0
3	E	17	17	17	0	0
3	F	15	15	15	0	0
3	G	11	11	11	0	0
3	H	16	16	16	0	0

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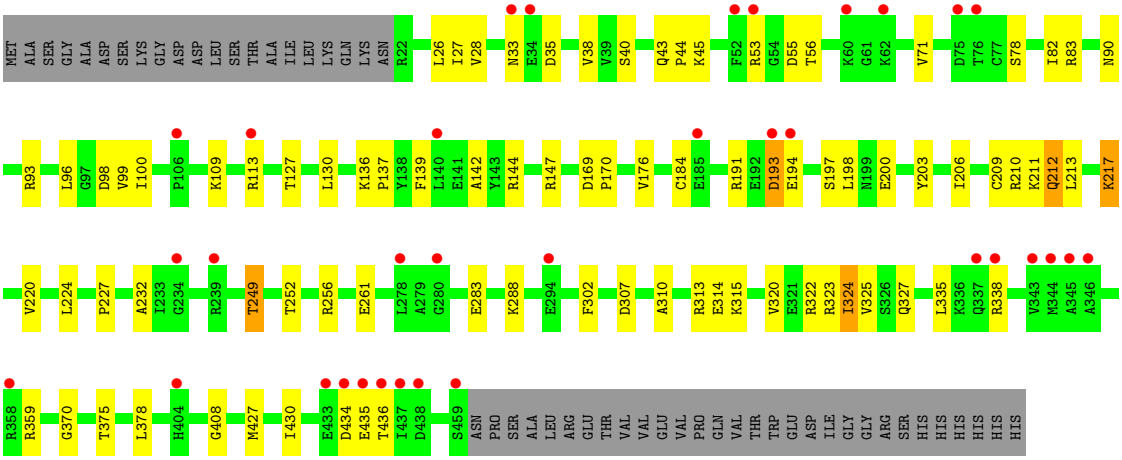
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	I	11	11	11	0	0
			Total	O		
3	J	17	17	17	0	0
			Total	O		
3	K	11	11	11	0	0
			Total	O		
3	L	16	16	16	0	0

3 Residue-property plots (i)

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

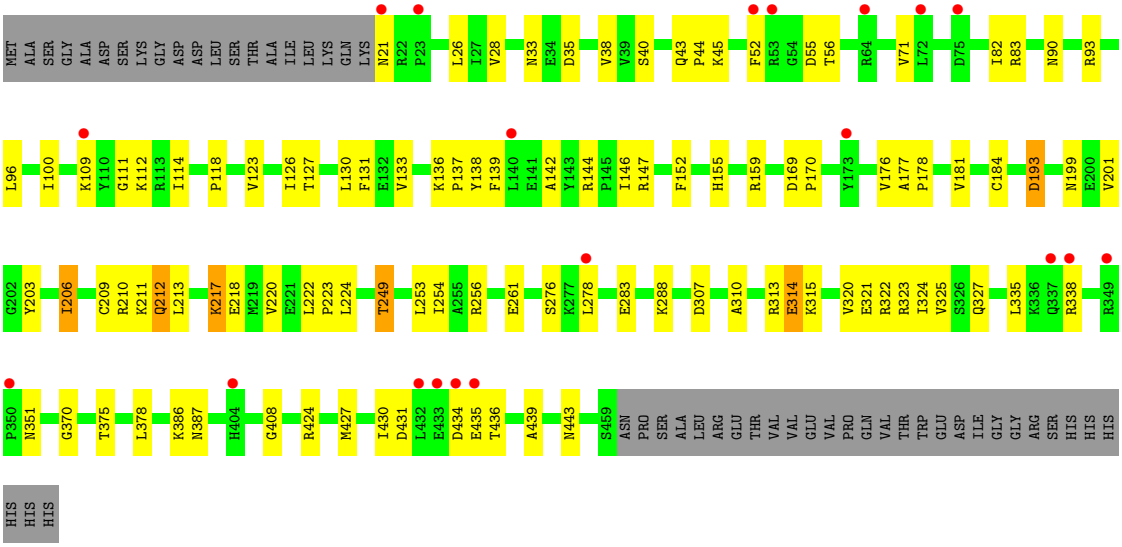
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



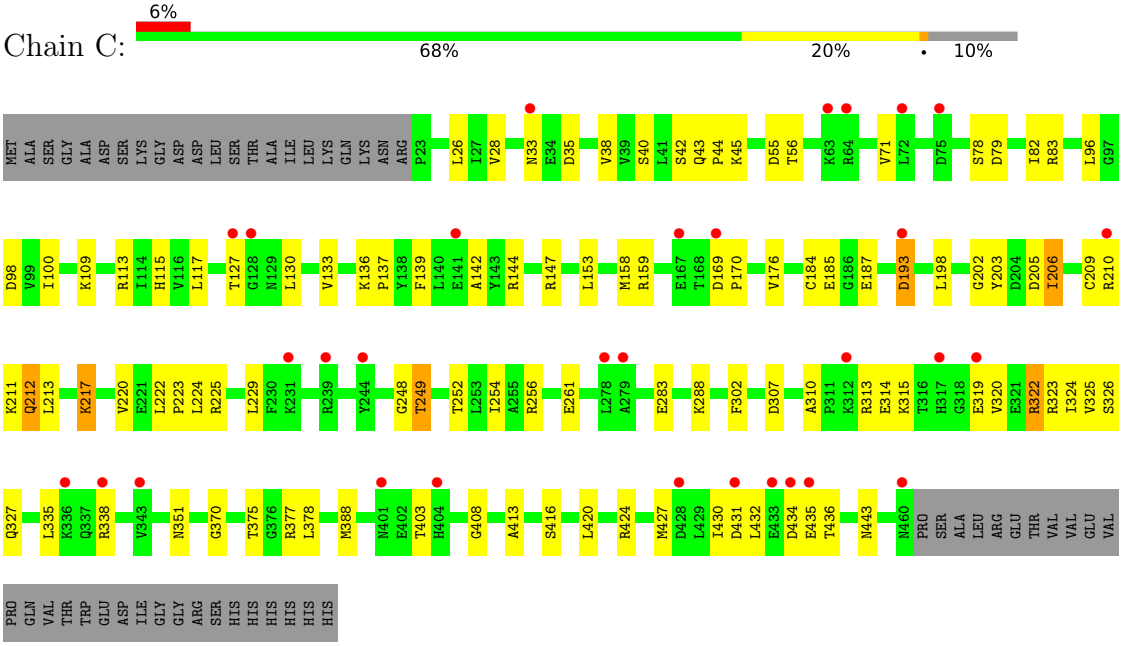
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:



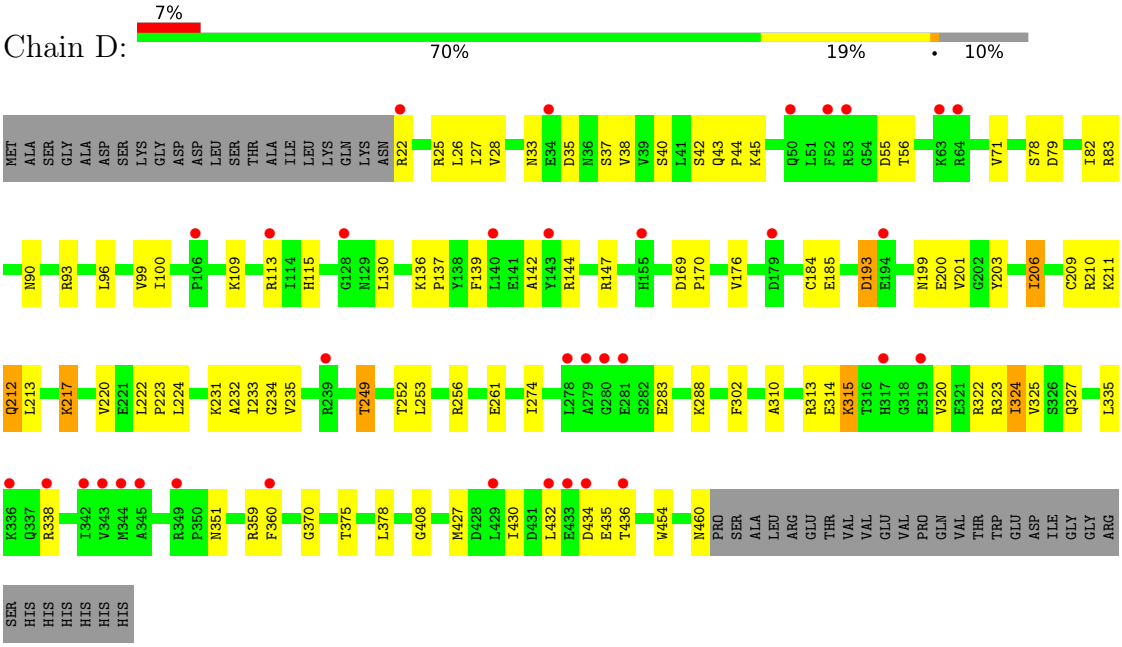
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



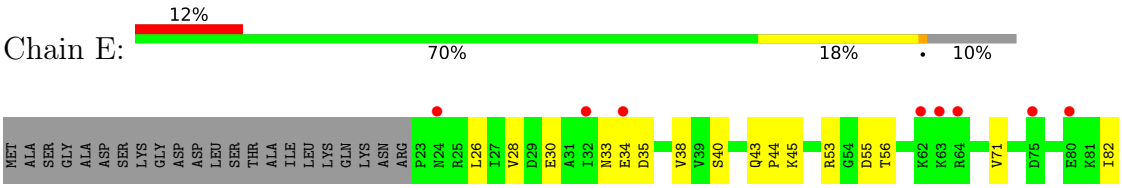
• Molecule 1: Transitional endoplasmic reticulum ATPase

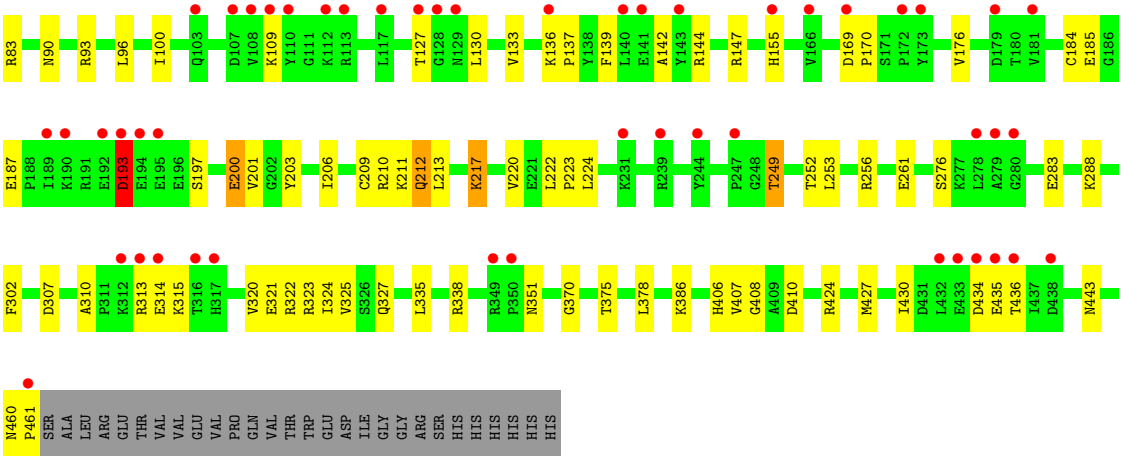
Chain D:



• Molecule 1: Transitional endoplasmic reticulum ATPase

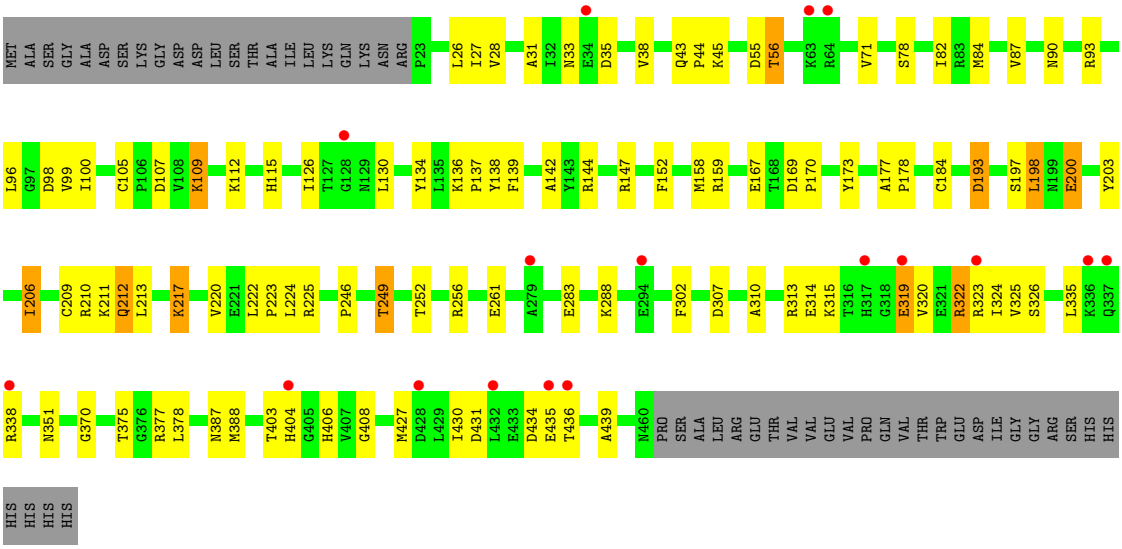
Chain E:





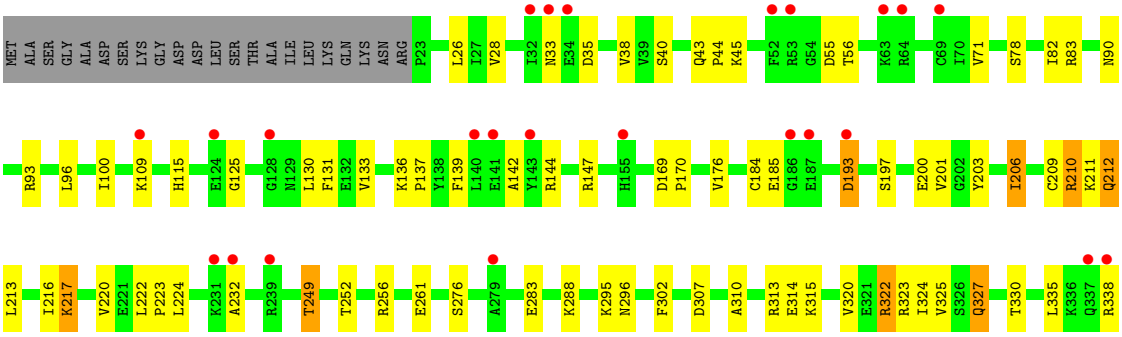
• Molecule 1: Transitional endoplasmic reticulum ATPase

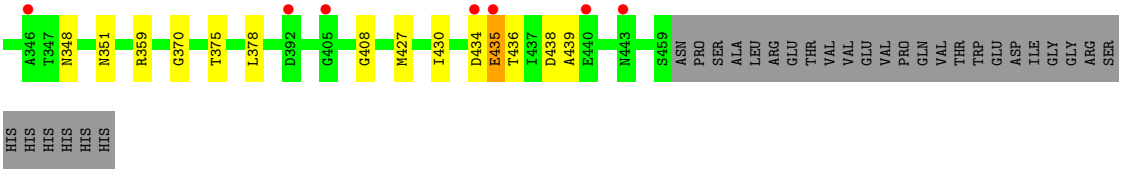
Chain F:



• Molecule 1: Transitional endoplasmic reticulum ATPase

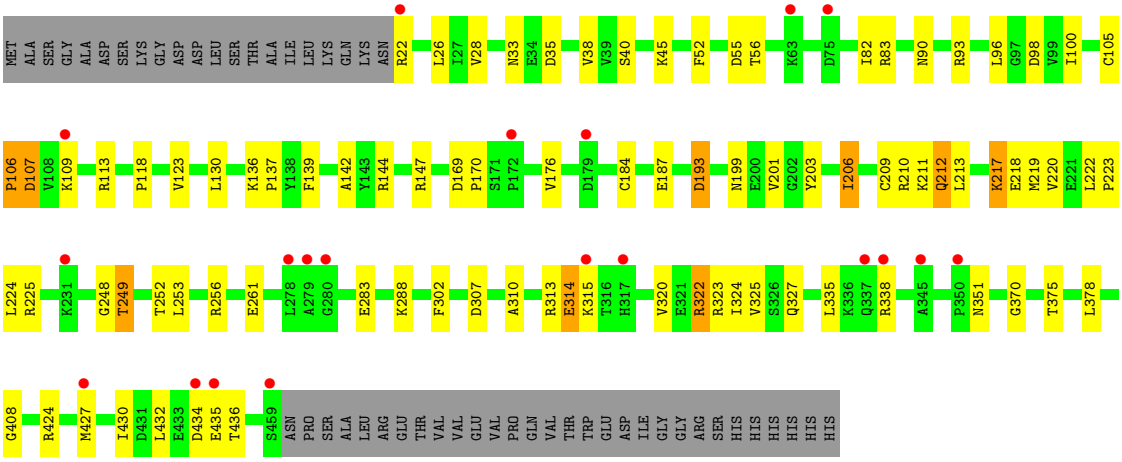
Chain G:





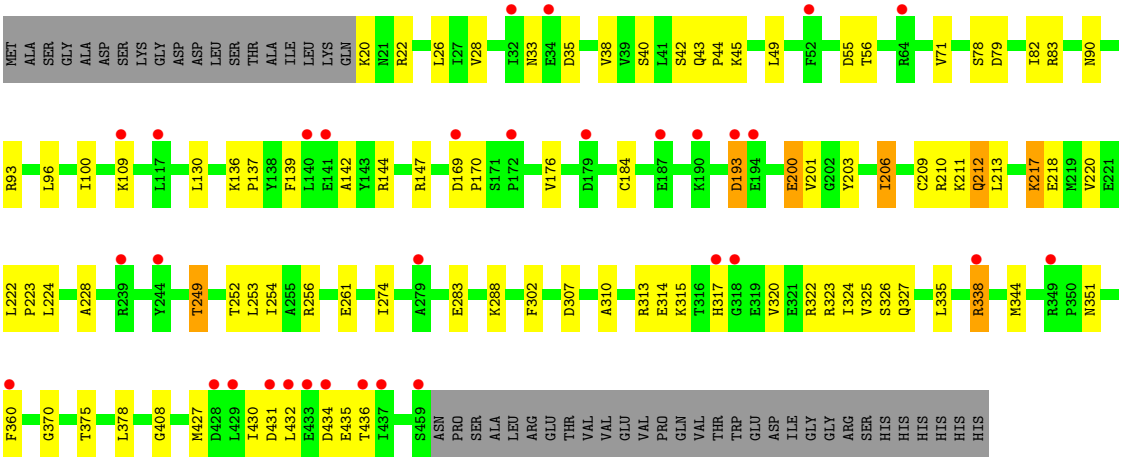
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain H:



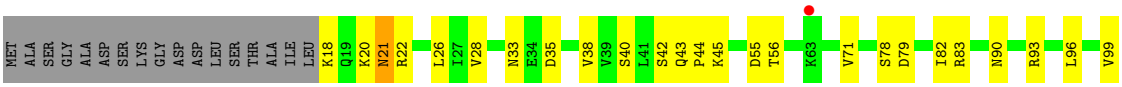
- Molecule 1: Transitional endoplasmic reticulum ATPase

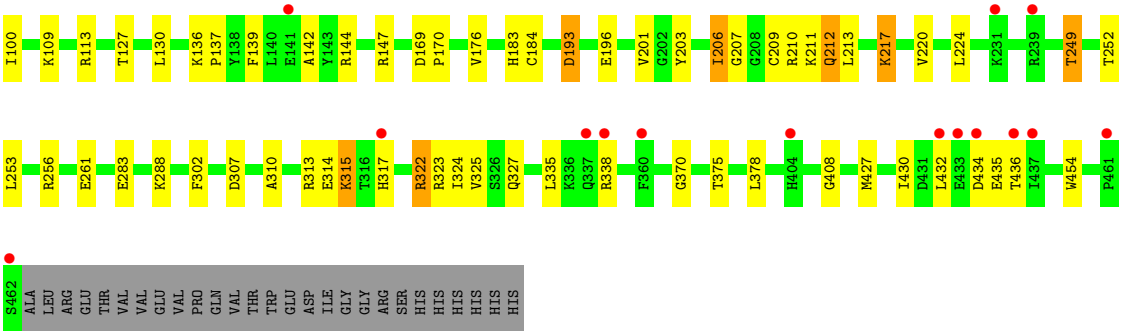
Chain I:



- Molecule 1: Transitional endoplasmic reticulum ATPase

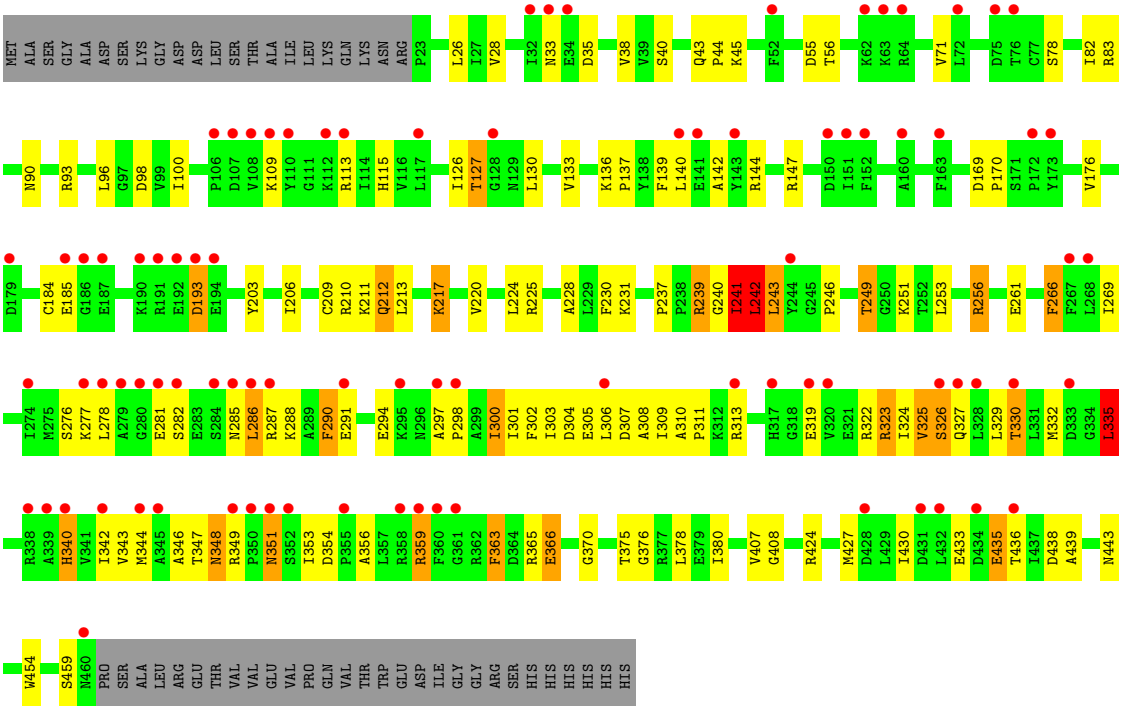
Chain J:





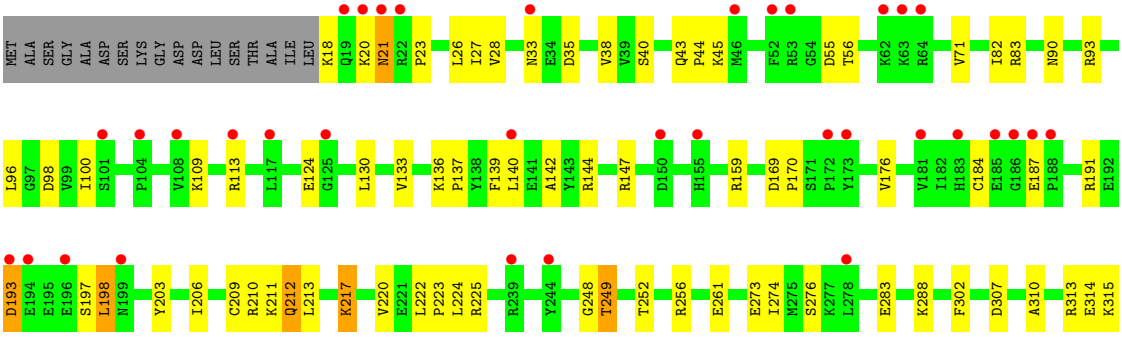
• Molecule 1: Transitional endoplasmic reticulum ATPase

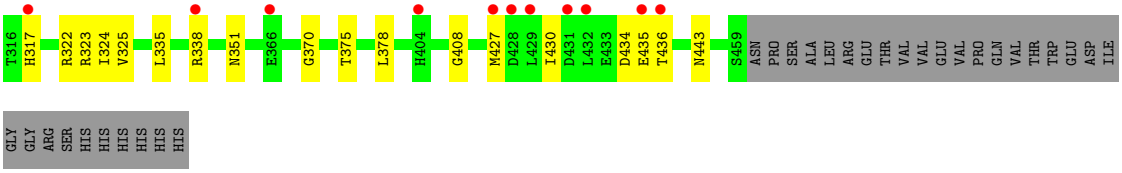
Chain K:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L:




T316
H317
R322
R323
I324
V325
L335
R338
N351
E366
G370
T375
L378
H404
G408
M427
D428
L429
I430
D431
L432
E433
D434
E435
T436
N443
S459
ASN
PRO
SER
ALA
LEU
ARG
GLU
THR
VAL
VAL
GLU
VAL
PRO
GLN
VAL
THR
TRP
GLU
ASP
ILE
GLY
GLY
ARG
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	146.52Å 170.74Å 256.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.99 – 2.96 21.99 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.0 (21.99-2.96) 88.3 (21.99-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.268 , 0.291 0.250 , 0.276	Depositor DCC
R_{free} test set	5937 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41760	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/3484	0.63	0/4708
1	B	0.47	0/3492	0.67	0/4719
1	C	0.38	0/3481	0.62	0/4704
1	D	0.39	0/3492	0.64	0/4719
1	E	0.40	1/3489 (0.0%)	0.68	3/4716 (0.1%)
1	F	0.48	0/3481	0.70	1/4704 (0.0%)
1	G	0.43	2/3473 (0.1%)	0.64	0/4693
1	H	0.42	0/3484	0.66	0/4708
1	I	0.40	0/3501	0.64	2/4730 (0.0%)
1	J	0.44	0/3541	0.66	0/4784
1	K	0.44	1/3481 (0.0%)	0.71	2/4704 (0.0%)
1	L	0.36	0/3519	0.62	0/4753
All	All	0.42	4/41918 (0.0%)	0.66	8/56642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	459	SER	C-N	8.47	1.53	1.34
1	E	193	ASP	CB-CG	-8.24	1.34	1.51
1	G	296	ASN	CG-ND2	-6.77	1.16	1.32
1	G	296	ASN	CG-OD1	-5.05	1.12	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	193	ASP	CB-CG-OD1	-16.01	103.89	118.30
1	E	193	ASP	CB-CG-OD2	7.36	124.93	118.30
1	I	360	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	K	242	LEU	CA-CB-CG	5.54	128.04	115.30
1	F	319	GLU	CB-CA-C	-5.48	99.43	110.40
1	E	193	ASP	CB-CA-C	-5.25	99.90	110.40
1	K	335	LEU	CA-CB-CG	5.23	127.34	115.30
1	I	360	PHE	CB-CG-CD2	5.11	124.38	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	239	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3480	44	0
1	B	3438	0	3486	66	1
1	C	3427	0	3474	74	0
1	D	3438	0	3486	61	0
1	E	3434	0	3481	60	0
1	F	3427	0	3474	71	1
1	G	3419	0	3468	55	1
1	H	3430	0	3480	54	0
1	I	3447	0	3499	49	1
1	J	3486	0	3538	46	0
1	K	3427	0	3474	132	0
1	L	3465	0	3520	56	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	4	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	27	0	12	3	0
2	I	27	0	12	2	0
2	J	27	0	12	2	0
2	K	27	0	12	3	0
2	L	27	0	12	4	0
3	A	14	0	0	2	0
3	B	9	0	0	0	0
3	C	14	0	0	0	0
3	D	17	0	0	1	0
3	E	17	0	0	2	0
3	F	15	0	0	0	0
3	G	11	0	0	4	0
3	H	16	0	0	0	0
3	I	11	0	0	1	0
3	J	17	0	0	2	0
3	K	11	0	0	1	0
3	L	16	0	0	0	0
All	All	41760	0	42004	681	2

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 8.

All (681) 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:433:GLU:HG3	1:K:436:THR:HG21	1.29	1.12
1:C:159:ARG:HD2	1:D:232:ALA:O	1.53	1.09
1:B:276:SER:HB3	1:F:326:SER:HB3	1.33	1.08
1:C:158:MET:HB2	1:D:233:ILE:HG22	1.36	1.07
1:I:209:CYS:HB2	1:I:212:GLN:HG2	1.36	1.03
1:K:240:GLY:HA3	1:K:363:PHE:CD1	1.95	1.02
1:J:209:CYS:HB2	1:J:212:GLN:HG2	1.41	1.00
1:D:209:CYS:HB2	1:D:212:GLN:HG2	1.52	0.91
1:B:209:CYS:HB2	1:B:212:GLN:HG2	1.53	0.90
1:C:413:ALA:HB2	1:D:360:PHE:HE1	1.36	0.90
1:K:256:ARG:HA	1:K:266:PHE:CE2	2.06	0.89
1:K:430:ILE:HG22	1:K:433:GLU:CB	2.03	0.88
1:L:209:CYS:HB2	1:L:212:GLN:HG2	1.56	0.88
1:I:209:CYS:HB2	1:I:212:GLN:CG	2.03	0.88
1:E:406:HIS:CD2	1:E:461:PRO:HB3	2.10	0.87
1:K:433:GLU:HG3	1:K:436:THR:CG2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:ARG:HH22	1:J:317:HIS:HB2	1.41	0.85
1:C:209:CYS:HB2	1:C:212:GLN:HG2	1.59	0.85
1:G:438:ASP:HA	3:G:910:HOH:O	1.77	0.84
1:B:276:SER:CB	1:F:326:SER:HB3	2.06	0.84
1:B:320:VAL:HG21	1:F:319:GLU:OE2	1.78	0.84
1:K:433:GLU:CG	1:K:436:THR:HG21	2.07	0.84
1:K:209:CYS:HB2	1:K:212:GLN:HG2	1.61	0.83
1:A:209:CYS:HB2	1:A:212:GLN:HG2	1.59	0.83
1:B:276:SER:HA	1:F:326:SER:HB2	1.59	0.83
1:K:430:ILE:HG22	1:K:433:GLU:HB2	1.59	0.82
1:E:209:CYS:HB2	1:E:212:GLN:HG2	1.60	0.82
1:K:298:PRO:HA	1:K:340:HIS:O	1.80	0.82
1:K:313:ARG:NH1	1:K:325:VAL:O	2.13	0.81
1:K:322:ARG:HA	1:K:325:VAL:HB	1.63	0.80
1:K:433:GLU:CG	1:K:436:THR:CG2	2.59	0.80
1:G:133:VAL:HG21	1:G:439:ALA:HB3	1.64	0.79
1:K:365:ARG:O	1:K:365:ARG:HG2	1.82	0.78
1:K:241:ILE:HD11	1:K:342:ILE:HG23	1.65	0.78
1:F:403:THR:HB	1:F:406:HIS:ND1	1.97	0.78
1:B:431:ASP:HB2	1:F:99:VAL:HG11	1.65	0.77
1:K:240:GLY:HA3	1:K:363:PHE:CE1	2.20	0.77
1:K:241:ILE:HG12	1:K:343:VAL:O	1.85	0.76
1:H:209:CYS:HB2	1:H:212:GLN:HG2	1.67	0.76
1:G:232:ALA:O	1:L:159:ARG:HD2	1.86	0.76
1:L:139:PHE:HA	1:L:142:ALA:HB2	1.68	0.75
1:K:256:ARG:HA	1:K:266:PHE:HE2	1.52	0.75
1:I:431:ASP:HB2	1:J:99:VAL:HG11	1.67	0.75
1:K:242:LEU:HD22	1:K:243:LEU:N	2.02	0.74
1:H:203:TYR:CE2	1:H:261:GLU:HG2	2.22	0.74
1:J:203:TYR:CE2	1:J:261:GLU:HG2	2.23	0.73
1:C:326:SER:HB3	1:E:276:SER:HB3	1.71	0.73
1:F:209:CYS:HB2	1:F:212:GLN:HG2	1.70	0.73
1:A:139:PHE:HA	1:A:142:ALA:HB2	1.70	0.73
1:C:431:ASP:HB2	1:D:99:VAL:CG1	2.19	0.73
1:K:139:PHE:HA	1:K:142:ALA:HB2	1.71	0.72
1:K:347:THR:HG22	1:K:348:ASN:H	1.54	0.72
1:G:276:SER:HB3	1:K:326:SER:HB2	1.69	0.72
1:F:139:PHE:HA	1:F:142:ALA:HB2	1.71	0.72
1:I:200:GLU:OE1	1:I:201:VAL:N	2.19	0.72
1:C:139:PHE:HA	1:C:142:ALA:HB2	1.71	0.72
1:B:201:VAL:HG11	1:B:253:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:VAL:CG2	1:F:319:GLU:OE2	2.38	0.72
1:E:193:ASP:N	1:E:193:ASP:OD1	2.18	0.72
1:I:139:PHE:HA	1:I:142:ALA:HB2	1.71	0.72
1:B:276:SER:HB3	1:F:326:SER:CB	2.18	0.72
1:D:139:PHE:HA	1:D:142:ALA:HB2	1.72	0.72
1:G:435:GLU:HG2	1:K:228:ALA:HB3	1.72	0.72
1:C:432:LEU:HA	1:D:25:ARG:HH21	1.55	0.71
1:G:139:PHE:HA	1:G:142:ALA:HB2	1.70	0.71
1:H:139:PHE:HA	1:H:142:ALA:HB2	1.72	0.71
1:E:139:PHE:HA	1:E:142:ALA:HB2	1.72	0.71
1:C:319:GLU:OE2	1:E:320:VAL:CG2	2.38	0.71
1:C:416:SER:HA	1:D:235:VAL:HG13	1.73	0.70
1:K:433:GLU:CB	1:K:436:THR:HG22	2.20	0.70
1:K:242:LEU:HD22	1:K:243:LEU:H	1.56	0.70
1:K:363:PHE:HE1	1:K:365:ARG:HB3	1.56	0.70
1:J:139:PHE:HA	1:J:142:ALA:HB2	1.71	0.70
1:J:201:VAL:HG11	1:J:253:LEU:HD12	1.72	0.70
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.26	0.70
1:F:98:ASP:OD1	1:F:225:ARG:NH2	2.24	0.70
1:B:276:SER:CB	1:F:326:SER:CB	2.70	0.69
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.27	0.69
1:B:139:PHE:HA	1:B:142:ALA:HB2	1.73	0.68
1:C:431:ASP:HB2	1:D:99:VAL:HG11	1.74	0.68
1:D:209:CYS:HB2	1:D:212:GLN:CG	2.22	0.68
1:F:158:MET:HA	1:F:387:ASN:O	1.93	0.68
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.28	0.68
1:B:276:SER:CA	1:F:326:SER:HB2	2.23	0.68
1:I:326:SER:HB2	1:K:276:SER:HB3	1.76	0.68
1:K:241:ILE:HA	1:K:365:ARG:NH1	2.09	0.68
1:F:115:HIS:CD2	1:F:167:GLU:OE2	2.47	0.68
1:C:158:MET:HB2	1:D:233:ILE:CG2	2.21	0.67
1:E:193:ASP:HB3	1:G:295:LYS:HE3	1.75	0.67
1:G:133:VAL:HG21	1:G:439:ALA:CB	2.24	0.67
1:G:209:CYS:HB2	1:G:212:GLN:HG2	1.76	0.67
1:K:127:THR:HB	1:K:438:ASP:OD1	1.94	0.67
1:H:106:PRO:HD2	1:H:107:ASP:OD1	1.93	0.67
1:A:53:ARG:NH2	3:A:909:HOH:O	2.26	0.67
1:I:249:THR:HG21	1:I:370:GLY:O	1.94	0.67
1:G:203:TYR:CE2	1:G:261:GLU:HG2	2.30	0.67
1:B:278:LEU:HA	1:F:323:ARG:NH1	2.10	0.66
1:F:126:ILE:HB	1:F:439:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:HIS:HB2	1:J:322:ARG:HH22	1.61	0.66
1:K:287:ARG:HA	1:K:290:PHE:HB2	1.76	0.66
1:J:249:THR:HG21	1:J:370:GLY:O	1.95	0.66
1:K:240:GLY:O	1:K:241:ILE:HD12	1.94	0.66
1:F:249:THR:HG21	1:F:370:GLY:O	1.97	0.65
1:I:203:TYR:CE2	1:I:261:GLU:HG2	2.32	0.65
1:B:276:SER:CA	1:F:326:SER:CB	2.74	0.65
1:L:203:TYR:CE2	1:L:261:GLU:HG2	2.30	0.65
1:C:249:THR:HG21	1:C:370:GLY:O	1.96	0.65
1:C:432:LEU:HA	1:D:25:ARG:NH2	2.12	0.64
1:H:432:LEU:HD21	1:L:21:ASN:HD22	1.61	0.64
1:K:203:TYR:CE2	1:K:261:GLU:HG2	2.32	0.64
1:L:98:ASP:OD1	1:L:225:ARG:NH2	2.31	0.64
1:K:136:LYS:HB3	1:K:137:PRO:HD3	1.80	0.64
1:E:249:THR:HG21	1:E:370:GLY:O	1.98	0.64
1:H:249:THR:HG21	1:H:370:GLY:O	1.97	0.64
1:A:249:THR:HG21	1:A:370:GLY:O	1.98	0.63
1:B:209:CYS:HB2	1:B:212:GLN:CG	2.24	0.63
1:C:413:ALA:HB2	1:D:360:PHE:CE1	2.26	0.63
1:E:187:GLU:HG3	1:L:124:GLU:HG2	1.80	0.63
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.81	0.63
1:J:209:CYS:HB2	1:J:212:GLN:CG	2.21	0.62
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.81	0.62
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.81	0.62
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.81	0.62
1:B:249:THR:HG21	1:B:370:GLY:O	1.99	0.62
1:C:158:MET:O	1:D:234:GLY:N	2.32	0.62
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.82	0.62
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.35	0.62
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.81	0.62
1:D:201:VAL:HG11	1:D:253:LEU:HD11	1.82	0.62
1:L:249:THR:HG21	1:L:370:GLY:O	1.99	0.62
1:G:283:GLU:OE2	1:G:323:ARG:HG2	2.00	0.61
1:E:133:VAL:HG13	1:E:443:ASN:HB2	1.82	0.61
1:G:249:THR:HG21	1:G:370:GLY:O	1.99	0.61
1:C:222:LEU:HD11	1:E:424:ARG:HG3	1.83	0.61
1:H:136:LYS:HB3	1:H:137:PRO:HD3	1.82	0.61
1:K:306:LEU:HA	1:K:346:ALA:O	2.01	0.61
1:A:434:ASP:HA	1:A:436:THR:H	1.66	0.61
1:E:406:HIS:CD2	1:E:461:PRO:CB	2.84	0.61
1:J:136:LYS:HB3	1:J:137:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ARG:CZ	1:E:321:GLU:OE1	2.49	0.61
1:G:136:LYS:HB3	1:G:137:PRO:HD3	1.82	0.61
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.37	0.60
1:K:249:THR:HG21	1:K:370:GLY:O	2.01	0.60
1:E:213:LEU:O	1:E:217:LYS:HG3	2.02	0.60
1:H:206:ILE:CD1	1:H:209:CYS:SG	2.89	0.60
1:J:283:GLU:OE2	1:J:323:ARG:HG2	2.02	0.60
1:F:158:MET:N	1:F:387:ASN:O	2.34	0.60
1:G:232:ALA:O	1:L:159:ARG:CD	2.50	0.60
1:J:201:VAL:HG11	1:J:253:LEU:CD1	2.31	0.60
1:L:209:CYS:HB2	1:L:212:GLN:CG	2.30	0.60
1:K:433:GLU:HB3	1:K:436:THR:HG22	1.83	0.59
1:I:136:LYS:HB3	1:I:137:PRO:HD3	1.84	0.59
1:G:327:GLN:HE21	1:L:276:SER:HB2	1.67	0.59
1:H:434:ASP:HA	1:H:436:THR:H	1.67	0.59
1:D:249:THR:HG21	1:D:370:GLY:O	2.01	0.59
1:K:302:PHE:HA	1:K:344:MET:O	2.02	0.59
1:I:222:LEU:HD11	1:K:424:ARG:HG3	1.84	0.59
1:G:359:ARG:NH2	2:L:800:ADP:O3B	2.36	0.59
1:E:434:ASP:HA	1:E:436:THR:H	1.68	0.58
1:I:434:ASP:HA	1:I:436:THR:H	1.68	0.58
1:B:434:ASP:HA	1:B:436:THR:H	1.69	0.58
1:L:136:LYS:HB3	1:L:137:PRO:HD3	1.85	0.58
1:B:276:SER:O	1:F:323:ARG:HG3	2.03	0.58
1:D:283:GLU:OE2	1:D:323:ARG:HG2	2.03	0.58
1:A:209:CYS:HB2	1:A:212:GLN:CG	2.32	0.58
1:C:283:GLU:OE2	1:C:323:ARG:HG2	2.04	0.58
1:F:434:ASP:HA	1:F:436:THR:H	1.69	0.58
1:D:434:ASP:HA	1:D:436:THR:H	1.69	0.57
1:E:283:GLU:OE2	1:E:323:ARG:HG2	2.04	0.57
1:J:206:ILE:HG13	1:J:207:GLY:N	2.18	0.57
1:J:434:ASP:HA	1:J:436:THR:H	1.68	0.57
1:A:283:GLU:OE2	1:A:323:ARG:HG2	2.04	0.57
1:C:213:LEU:O	1:C:217:LYS:HG3	2.05	0.57
1:K:301:ILE:HD12	1:K:343:VAL:HG22	1.87	0.57
1:A:213:LEU:O	1:A:217:LYS:HG3	2.04	0.57
1:D:35:ASP:HB3	1:D:38:VAL:HG12	1.87	0.57
1:K:285:ASN:HD21	1:K:288:LYS:HD2	1.69	0.57
1:F:213:LEU:O	1:F:217:LYS:HG3	2.05	0.57
1:L:35:ASP:HB3	1:L:38:VAL:HG12	1.88	0.56
1:G:434:ASP:HA	1:G:436:THR:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:213:LEU:O	1:K:217:LYS:HG3	2.05	0.56
1:K:241:ILE:CD1	1:K:342:ILE:HG23	2.32	0.56
1:E:201:VAL:HG11	1:E:253:LEU:HD12	1.88	0.56
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.87	0.56
1:C:434:ASP:HA	1:C:436:THR:H	1.70	0.56
1:F:158:MET:CA	1:F:387:ASN:O	2.54	0.56
1:L:434:ASP:HA	1:L:436:THR:H	1.69	0.56
1:J:35:ASP:HB3	1:J:38:VAL:HG12	1.86	0.56
1:I:220:VAL:HB	1:I:224:LEU:HD12	1.88	0.56
1:L:20:LYS:C	1:L:21:ASN:OD1	2.44	0.56
1:E:35:ASP:HB3	1:E:38:VAL:HG12	1.88	0.56
1:G:193:ASP:N	1:G:193:ASP:OD1	2.39	0.56
1:I:35:ASP:HB3	1:I:38:VAL:HG12	1.88	0.56
1:C:209:CYS:HB2	1:C:212:GLN:CG	2.34	0.56
1:K:347:THR:CG2	1:K:348:ASN:H	2.19	0.56
1:E:220:VAL:HB	1:E:224:LEU:HD12	1.88	0.56
1:D:201:VAL:HG11	1:D:253:LEU:CD1	2.36	0.55
1:E:53:ARG:N	3:E:905:HOH:O	2.38	0.55
1:K:35:ASP:HB3	1:K:38:VAL:HG12	1.88	0.55
1:L:213:LEU:O	1:L:217:LYS:HG3	2.05	0.55
1:L:220:VAL:HB	1:L:224:LEU:HD12	1.88	0.55
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.88	0.55
1:C:133:VAL:HG13	1:C:443:ASN:HB2	1.87	0.55
1:K:285:ASN:ND2	1:K:288:LYS:HB3	2.21	0.55
1:A:220:VAL:HB	1:A:224:LEU:HD12	1.88	0.55
1:D:220:VAL:HB	1:D:224:LEU:HD12	1.88	0.55
1:J:220:VAL:HB	1:J:224:LEU:HD12	1.88	0.55
1:B:201:VAL:HG11	1:B:253:LEU:CD1	2.35	0.55
1:K:297:ALA:HB1	1:K:340:HIS:O	2.07	0.55
1:F:158:MET:HG2	1:F:388:MET:HB3	1.88	0.55
1:H:220:VAL:HB	1:H:224:LEU:HD12	1.89	0.55
1:J:21:ASN:HA	1:J:22:ARG:HG2	1.88	0.55
1:K:304:ASP:HA	1:K:346:ALA:HB3	1.89	0.55
1:K:306:LEU:HA	1:K:347:THR:HA	1.88	0.55
1:B:220:VAL:HB	1:B:224:LEU:HD12	1.88	0.55
1:G:206:ILE:HD11	1:G:209:CYS:SG	2.47	0.55
1:I:218:GLU:OE1	1:K:454:TRP:HZ2	1.88	0.55
1:K:301:ILE:HB	1:K:343:VAL:HG13	1.88	0.55
1:B:213:LEU:O	1:B:217:LYS:HG3	2.07	0.55
1:C:319:GLU:OE2	1:E:320:VAL:HG21	2.07	0.55
1:F:283:GLU:OE2	1:F:323:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASP:OD1	1:C:225:ARG:NH2	2.39	0.54
1:D:193:ASP:OD1	1:D:193:ASP:N	2.40	0.54
1:B:133:VAL:HG13	1:B:443:ASN:HB2	1.89	0.54
1:G:125:GLY:HA2	1:K:231:LYS:HB3	1.89	0.54
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.88	0.54
1:F:142:ALA:HB1	1:F:144:ARG:HG3	1.90	0.54
1:K:193:ASP:OD1	1:K:193:ASP:N	2.39	0.54
1:A:35:ASP:HB3	1:A:38:VAL:HG12	1.88	0.54
1:B:35:ASP:HB3	1:B:38:VAL:HG12	1.90	0.54
1:C:35:ASP:HB3	1:C:38:VAL:HG12	1.89	0.54
1:F:206:ILE:O	1:F:206:ILE:CG1	2.54	0.54
1:G:35:ASP:HB3	1:G:38:VAL:HG12	1.87	0.54
1:H:35:ASP:HB3	1:H:38:VAL:HG12	1.89	0.54
1:H:218:GLU:OE1	1:J:454:TRP:HZ2	1.91	0.54
1:K:209:CYS:HB2	1:K:212:GLN:CG	2.35	0.54
1:C:222:LEU:HD11	1:E:424:ARG:CG	2.37	0.54
1:G:220:VAL:HB	1:G:224:LEU:HD12	1.88	0.54
1:I:432:LEU:HD23	1:J:21:ASN:HB2	1.90	0.54
1:K:300:ILE:HD11	1:K:344:MET:HG3	1.90	0.54
1:L:283:GLU:OE2	1:L:323:ARG:HG2	2.08	0.54
1:E:187:GLU:CG	1:L:124:GLU:HG2	2.38	0.54
1:G:322:ARG:HH22	1:L:317:HIS:HB2	1.73	0.54
1:F:220:VAL:HB	1:F:224:LEU:HD12	1.90	0.53
1:H:213:LEU:O	1:H:217:LYS:HG3	2.08	0.53
1:G:213:LEU:O	1:G:217:LYS:HG3	2.09	0.53
1:H:26:LEU:HD21	1:H:45:LYS:HE2	1.90	0.53
1:H:434:ASP:HA	1:H:436:THR:N	2.24	0.53
1:K:220:VAL:HB	1:K:224:LEU:HD12	1.91	0.53
1:K:322:ARG:CA	1:K:325:VAL:HB	2.36	0.53
1:J:249:THR:N	2:J:800:ADP:O2B	2.42	0.53
1:C:193:ASP:OD1	1:C:193:ASP:N	2.42	0.53
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.43	0.53
1:E:209:CYS:HB2	1:E:212:GLN:CG	2.33	0.53
1:F:197:SER:HB3	1:F:200:GLU:HG3	1.90	0.53
1:I:283:GLU:OE2	1:I:323:ARG:HG2	2.09	0.53
1:A:434:ASP:HA	1:A:436:THR:N	2.24	0.53
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.91	0.53
1:C:220:VAL:HB	1:C:224:LEU:HD12	1.89	0.53
1:F:35:ASP:HB3	1:F:38:VAL:HG12	1.90	0.53
1:K:300:ILE:HG13	1:K:342:ILE:O	2.08	0.53
1:C:82:ILE:HG21	1:C:100:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:GLY:HA3	1:K:231:LYS:O	2.09	0.53
1:B:55:ASP:O	1:B:71:VAL:HG12	2.09	0.52
1:F:26:LEU:HD21	1:F:45:LYS:HE2	1.91	0.52
1:H:82:ILE:HG21	1:H:100:ILE:HD11	1.91	0.52
1:H:424:ARG:HG3	1:L:222:LEU:HD11	1.91	0.52
1:J:193:ASP:OD1	1:J:193:ASP:N	2.42	0.52
1:K:282:SER:O	1:K:324:ILE:HG21	2.09	0.52
1:I:326:SER:CB	1:K:276:SER:HB3	2.38	0.52
1:D:434:ASP:HA	1:D:436:THR:N	2.24	0.52
1:E:434:ASP:HA	1:E:436:THR:N	2.24	0.52
1:J:434:ASP:HA	1:J:436:THR:N	2.24	0.52
1:K:436:THR:O	1:K:436:THR:HG23	2.07	0.52
1:B:434:ASP:HA	1:B:436:THR:N	2.25	0.52
1:I:193:ASP:OD1	1:I:193:ASP:N	2.41	0.52
1:K:82:ILE:HG21	1:K:100:ILE:HD11	1.92	0.52
1:F:90:ASN:O	1:F:93:ARG:NH1	2.43	0.52
1:I:434:ASP:HA	1:I:436:THR:N	2.24	0.52
1:A:227:PRO:HD2	3:A:906:HOH:O	2.10	0.52
1:I:432:LEU:CD2	1:J:21:ASN:HB2	2.39	0.52
1:J:82:ILE:HG21	1:J:100:ILE:HD11	1.91	0.52
1:H:219:MET:HE2	3:J:917:HOH:O	2.09	0.51
1:L:434:ASP:HA	1:L:436:THR:N	2.26	0.51
1:A:82:ILE:HG21	1:A:100:ILE:HD11	1.92	0.51
1:F:434:ASP:HA	1:F:436:THR:N	2.26	0.51
1:H:106:PRO:HD2	1:H:107:ASP:H	1.75	0.51
1:I:130:LEU:HD23	1:I:130:LEU:H	1.75	0.51
1:B:249:THR:N	2:B:800:ADP:O2B	2.44	0.51
1:I:213:LEU:O	1:I:217:LYS:HG3	2.10	0.51
1:C:139:PHE:CE1	1:C:176:VAL:HG11	2.46	0.51
1:D:139:PHE:CE1	1:D:176:VAL:HG11	2.46	0.51
1:G:310:ALA:HA	1:G:325:VAL:HG22	1.93	0.51
1:H:139:PHE:CE1	1:H:176:VAL:HG11	2.46	0.51
1:K:139:PHE:CE1	1:K:176:VAL:HG11	2.46	0.51
1:L:193:ASP:N	1:L:193:ASP:OD1	2.43	0.51
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.92	0.51
1:B:283:GLU:OE2	1:B:323:ARG:HG2	2.10	0.51
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.93	0.51
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.92	0.51
1:C:249:THR:N	2:C:800:ADP:O2B	2.44	0.51
1:E:155:HIS:HB3	1:E:386:LYS:O	2.10	0.51
1:I:338:ARG:HD2	3:I:901:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:GLU:HG2	1:K:308:ALA:CB	2.40	0.51
1:L:133:VAL:HG13	1:L:443:ASN:HB2	1.93	0.51
1:A:193:ASP:OD1	1:A:193:ASP:N	2.42	0.50
1:A:307:ASP:OD1	1:A:307:ASP:N	2.43	0.50
1:E:82:ILE:HG21	1:E:100:ILE:HD11	1.92	0.50
1:G:434:ASP:HA	1:G:436:THR:N	2.26	0.50
1:H:206:ILE:HD11	1:H:209:CYS:SG	2.51	0.50
1:K:241:ILE:HG12	1:K:343:VAL:C	2.31	0.50
1:B:139:PHE:CE1	1:B:176:VAL:HG11	2.46	0.50
1:B:193:ASP:N	1:B:193:ASP:OD1	2.44	0.50
1:C:222:LEU:HD11	1:E:424:ARG:HH11	1.76	0.50
1:C:322:ARG:NE	1:E:321:GLU:OE1	2.44	0.50
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.93	0.50
1:G:82:ILE:HG21	1:G:100:ILE:HD11	1.92	0.50
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.93	0.50
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.94	0.50
1:L:55:ASP:O	1:L:71:VAL:HG12	2.12	0.50
1:A:194:GLU:HB2	1:K:193:ASP:OD2	2.11	0.50
1:C:434:ASP:HA	1:C:436:THR:N	2.27	0.50
1:J:310:ALA:HA	1:J:325:VAL:HG22	1.94	0.50
1:H:52:PHE:O	1:H:55:ASP:HB2	2.12	0.50
1:H:106:PRO:CD	1:H:107:ASP:H	2.24	0.50
1:I:26:LEU:HD21	1:I:45:LYS:HE2	1.92	0.50
1:K:408:GLY:HA3	2:K:800:ADP:N7	2.27	0.50
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.94	0.50
1:J:213:LEU:O	1:J:217:LYS:HG3	2.12	0.50
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.94	0.50
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.94	0.50
1:F:377:ARG:NE	1:F:403:THR:O	2.45	0.50
1:H:206:ILE:O	1:H:206:ILE:HG13	2.12	0.50
1:K:430:ILE:HG22	1:K:433:GLU:HB3	1.92	0.49
1:B:424:ARG:HG3	1:F:222:LEU:HD11	1.95	0.49
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.94	0.49
1:F:130:LEU:HD23	1:F:130:LEU:H	1.78	0.49
1:H:314:GLU:HB2	1:J:315:LYS:NZ	2.27	0.49
1:K:26:LEU:HD21	1:K:45:LYS:HE2	1.93	0.49
1:K:305:GLU:CG	1:K:308:ALA:HA	2.42	0.49
1:C:326:SER:HB2	1:E:276:SER:HA	1.94	0.49
1:I:307:ASP:N	1:I:307:ASP:OD1	2.44	0.49
1:J:142:ALA:HB1	1:J:144:ARG:HG3	1.93	0.49
1:K:305:GLU:HG3	1:K:308:ALA:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:VAL:HG11	1:I:253:LEU:HD12	1.95	0.49
1:K:365:ARG:O	1:K:365:ARG:CG	2.56	0.49
1:D:213:LEU:O	1:D:217:LYS:HG3	2.11	0.49
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.94	0.49
1:J:26:LEU:HD21	1:J:45:LYS:HE2	1.94	0.49
1:L:40:SER:HB2	1:L:83:ARG:HB2	1.95	0.49
1:A:26:LEU:HD21	1:A:45:LYS:HE2	1.93	0.49
1:E:139:PHE:CE1	1:E:176:VAL:HG11	2.47	0.49
1:H:310:ALA:HA	1:H:325:VAL:HG22	1.94	0.49
1:B:278:LEU:HA	1:F:323:ARG:HH11	1.75	0.49
1:I:249:THR:N	2:I:800:ADP:O2B	2.46	0.49
2:C:800:ADP:O3B	1:D:359:ARG:NH2	2.46	0.49
1:E:142:ALA:HB1	1:E:144:ARG:HG3	1.95	0.49
1:F:408:GLY:HA3	2:F:800:ADP:N7	2.28	0.49
1:G:133:VAL:HG11	1:G:439:ALA:HB1	1.94	0.49
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.95	0.49
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.94	0.49
1:D:142:ALA:HB1	1:D:144:ARG:HG3	1.95	0.49
1:F:56:THR:OG1	1:F:105:CYS:O	2.30	0.49
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.95	0.49
1:K:40:SER:HB2	1:K:83:ARG:HB2	1.95	0.49
1:B:26:LEU:HD21	1:B:45:LYS:HE2	1.94	0.48
1:H:283:GLU:OE2	1:H:323:ARG:HG2	2.13	0.48
1:K:126:ILE:HB	1:K:439:ALA:HB2	1.94	0.48
1:H:408:GLY:HA3	2:H:800:ADP:N7	2.28	0.48
1:L:249:THR:N	2:L:800:ADP:O2B	2.47	0.48
1:B:130:LEU:H	1:B:130:LEU:HD23	1.78	0.48
1:B:427:MET:HA	1:B:430:ILE:HD12	1.95	0.48
1:C:252:THR:HA	1:C:302:PHE:CE2	2.48	0.48
1:I:82:ILE:HG21	1:I:100:ILE:HD11	1.94	0.48
1:I:90:ASN:O	1:I:93:ARG:NH1	2.46	0.48
1:K:306:LEU:HD23	1:K:346:ALA:HB1	1.95	0.48
1:A:249:THR:N	2:A:800:ADP:O2B	2.46	0.48
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.94	0.48
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.95	0.48
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.95	0.48
1:L:90:ASN:O	1:L:93:ARG:NH1	2.45	0.48
1:A:191:ARG:NH1	1:A:197:SER:HA	2.29	0.48
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.94	0.48
1:K:313:ARG:HD3	1:K:325:VAL:HG13	1.95	0.48
1:B:206:ILE:CD1	1:B:254:ILE:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:THR:N	2:F:800:ADP:O2B	2.46	0.48
1:G:55:ASP:O	1:G:71:VAL:HG12	2.14	0.48
1:G:130:LEU:H	1:G:130:LEU:HD23	1.78	0.48
1:H:98:ASP:OD1	1:H:225:ARG:NH2	2.45	0.48
1:I:142:ALA:HB1	1:I:144:ARG:HG3	1.95	0.48
1:J:130:LEU:HD23	1:J:130:LEU:H	1.78	0.48
1:K:130:LEU:HD23	1:K:130:LEU:H	1.79	0.48
1:L:82:ILE:HG21	1:L:100:ILE:HD11	1.96	0.48
1:C:153:LEU:HD13	1:C:198:LEU:HB2	1.94	0.48
1:G:26:LEU:HD21	1:G:45:LYS:HE2	1.96	0.48
1:I:408:GLY:HA3	2:I:800:ADP:N7	2.29	0.48
1:K:286:LEU:O	1:K:290:PHE:CD1	2.67	0.48
1:K:347:THR:HG22	1:K:348:ASN:N	2.23	0.48
1:G:249:THR:N	2:G:800:ADP:O2B	2.46	0.48
1:I:139:PHE:CE1	1:I:176:VAL:HG11	2.49	0.48
1:J:183:HIS:HB3	3:J:909:HOH:O	2.14	0.48
1:K:266:PHE:CD1	1:K:300:ILE:HG22	2.49	0.48
1:I:310:ALA:HA	1:I:325:VAL:HG22	1.95	0.48
1:C:26:LEU:HD21	1:C:45:LYS:HE2	1.95	0.48
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.95	0.48
1:K:142:ALA:HB1	1:K:144:ARG:HG3	1.96	0.48
1:K:230:PHE:CE1	1:K:237:PRO:HG3	2.49	0.48
1:L:26:LEU:HD21	1:L:45:LYS:HE2	1.95	0.48
1:D:130:LEU:HD23	1:D:130:LEU:H	1.78	0.47
1:F:138:TYR:CE2	1:F:152:PHE:CD2	3.02	0.47
1:A:408:GLY:HA3	2:A:800:ADP:N7	2.29	0.47
1:A:427:MET:HA	1:A:430:ILE:HD12	1.96	0.47
1:D:427:MET:HA	1:D:430:ILE:HD12	1.97	0.47
1:E:55:ASP:O	1:E:71:VAL:HG12	2.14	0.47
1:F:87:VAL:HA	1:F:198:LEU:HD11	1.95	0.47
1:K:241:ILE:HD11	1:K:342:ILE:HD12	1.95	0.47
1:G:408:GLY:HA3	2:G:800:ADP:N7	2.28	0.47
1:B:408:GLY:HA3	2:B:800:ADP:N7	2.30	0.47
1:E:26:LEU:HD21	1:E:45:LYS:HE2	1.95	0.47
1:E:34:GLU:N	3:E:909:HOH:O	2.27	0.47
1:F:109:LYS:NZ	1:F:173:TYR:O	2.47	0.47
1:F:203:TYR:CD2	1:F:261:GLU:HG2	2.50	0.47
1:H:130:LEU:HD23	1:H:130:LEU:H	1.79	0.47
1:C:427:MET:HA	1:C:430:ILE:HD12	1.97	0.47
1:E:249:THR:N	2:E:800:ADP:O2B	2.47	0.47
1:K:98:ASP:OD1	1:K:225:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:130:LEU:H	1.80	0.47
1:A:139:PHE:CE1	1:A:176:VAL:HG11	2.50	0.47
1:A:232:ALA:O	1:F:159:ARG:NE	2.48	0.47
1:C:408:GLY:HA3	2:C:800:ADP:N7	2.30	0.47
1:J:139:PHE:CE1	1:J:176:VAL:HG11	2.49	0.47
1:K:306:LEU:HB3	1:K:347:THR:HA	1.97	0.47
1:B:126:ILE:HB	1:B:439:ALA:HB2	1.95	0.47
1:D:252:THR:HA	1:D:302:PHE:CE2	2.50	0.47
1:D:408:GLY:HA3	2:D:800:ADP:N7	2.30	0.47
1:E:185:GLU:OE2	1:L:187:GLU:OE1	2.33	0.47
1:K:269:ILE:O	1:K:269:ILE:HG23	2.15	0.47
1:L:408:GLY:HA3	2:L:800:ADP:N7	2.29	0.47
1:I:222:LEU:HD11	1:K:424:ARG:CG	2.45	0.47
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.96	0.47
1:G:142:ALA:HB1	1:G:144:ARG:HG3	1.96	0.46
1:J:427:MET:HA	1:J:430:ILE:HD12	1.97	0.46
1:L:139:PHE:CE1	1:L:176:VAL:HG11	2.50	0.46
1:L:427:MET:HA	1:L:430:ILE:HD12	1.97	0.46
1:C:55:ASP:O	1:C:71:VAL:HG12	2.15	0.46
1:K:348:ASN:N	1:K:348:ASN:ND2	2.63	0.46
1:D:55:ASP:O	1:D:71:VAL:HG12	2.15	0.46
1:F:307:ASP:OD1	1:F:307:ASP:N	2.47	0.46
1:C:130:LEU:HD23	1:C:130:LEU:H	1.81	0.46
1:E:130:LEU:HD23	1:E:130:LEU:H	1.80	0.46
1:F:427:MET:HA	1:F:430:ILE:HD12	1.97	0.46
1:H:106:PRO:CD	1:H:107:ASP:N	2.76	0.46
1:I:427:MET:HA	1:I:430:ILE:HD12	1.97	0.46
1:K:430:ILE:CG2	1:K:433:GLU:CB	2.87	0.46
1:D:26:LEU:HD21	1:D:45:LYS:HE2	1.97	0.46
1:G:139:PHE:CE1	1:G:176:VAL:HG11	2.50	0.46
1:K:269:ILE:O	1:K:303:ILE:HA	2.16	0.46
1:C:142:ALA:HB1	1:C:144:ARG:HG3	1.97	0.46
1:E:408:GLY:HA3	2:E:800:ADP:N7	2.31	0.46
1:F:206:ILE:O	1:F:206:ILE:HG12	2.15	0.46
1:K:239:ARG:HD3	1:K:342:ILE:CD1	2.45	0.46
1:K:427:MET:HA	1:K:430:ILE:HD12	1.97	0.46
1:K:433:GLU:CB	1:K:436:THR:CG2	2.88	0.46
1:E:427:MET:HA	1:E:430:ILE:HD12	1.98	0.46
1:B:82:ILE:HG21	1:B:100:ILE:HD11	1.98	0.46
1:B:206:ILE:HD13	1:B:254:ILE:HG12	1.98	0.46
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:GLU:OE2	1:E:320:VAL:HG23	2.14	0.45
1:D:249:THR:N	2:D:800:ADP:O2B	2.48	0.45
1:L:137:PRO:HA	1:L:140:LEU:CD2	2.46	0.45
1:K:266:PHE:CD1	1:K:300:ILE:CG2	2.99	0.45
1:K:313:ARG:CZ	1:K:329:LEU:HD11	2.47	0.45
1:H:201:VAL:HG11	1:H:253:LEU:HD12	1.97	0.45
1:K:354:ASP:OD2	1:K:356:ALA:HB3	2.17	0.45
1:L:27:ILE:HA	1:L:98:ASP:O	2.16	0.45
1:L:140:LEU:O	1:L:140:LEU:HD12	2.15	0.45
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.98	0.45
1:C:202:GLY:O	1:C:205:ASP:HB2	2.16	0.45
1:E:252:THR:HA	1:E:302:PHE:CE2	2.52	0.45
1:A:55:ASP:O	1:A:71:VAL:HG12	2.16	0.45
1:C:322:ARG:NH2	1:E:321:GLU:OE1	2.50	0.45
1:F:320:VAL:HG22	1:F:323:ARG:NH2	2.32	0.45
1:G:320:VAL:N	1:K:319:GLU:OE2	2.50	0.45
1:H:427:MET:HA	1:H:430:ILE:HD12	1.99	0.45
1:J:408:GLY:HA3	2:J:800:ADP:N7	2.31	0.45
1:C:307:ASP:OD1	1:C:307:ASP:N	2.50	0.45
1:H:307:ASP:OD1	1:H:307:ASP:N	2.48	0.45
1:A:90:ASN:O	1:A:93:ARG:NH1	2.49	0.45
3:G:908:HOH:O	1:K:359:ARG:CG	2.65	0.45
1:J:307:ASP:OD1	1:J:307:ASP:N	2.49	0.45
1:L:248:GLY:N	2:L:800:ADP:O3B	2.43	0.45
1:D:90:ASN:O	1:D:93:ARG:NH1	2.50	0.45
1:F:43:GLN:N	1:F:44:PRO:HD2	2.32	0.45
1:F:193:ASP:OD1	1:F:193:ASP:N	2.48	0.45
1:B:218:GLU:OE1	1:D:454:TRP:HZ2	2.00	0.45
1:H:22:ARG:HG2	1:J:432:LEU:HG	1.98	0.45
1:K:322:ARG:HA	1:K:325:VAL:CB	2.41	0.45
1:C:431:ASP:HB3	1:D:27:ILE:HD11	1.99	0.44
1:F:55:ASP:O	1:F:71:VAL:HG12	2.17	0.44
1:K:242:LEU:O	1:K:366:GLU:HA	2.17	0.44
1:C:159:ARG:NH2	1:D:231:LYS:O	2.49	0.44
1:L:43:GLN:N	1:L:44:PRO:HD2	2.32	0.44
1:L:142:ALA:HB1	1:L:144:ARG:HG3	1.99	0.44
1:C:158:MET:HG2	1:C:388:MET:HB3	2.00	0.44
1:C:222:LEU:CD1	1:E:424:ARG:HH11	2.30	0.44
1:K:376:GLY:O	1:K:380:ILE:HG12	2.18	0.44
1:B:139:PHE:CD1	1:B:176:VAL:HG11	2.52	0.44
1:D:43:GLN:N	1:D:44:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:O	1:E:200:GLU:HB2	2.17	0.44
1:G:427:MET:HA	1:G:430:ILE:HD12	1.99	0.44
1:E:307:ASP:OD1	1:E:307:ASP:N	2.48	0.44
1:G:40:SER:HB2	1:G:83:ARG:HB2	1.99	0.44
3:G:908:HOH:O	1:K:359:ARG:HG3	2.16	0.44
1:J:40:SER:HB2	1:J:83:ARG:HB2	1.99	0.44
1:K:90:ASN:O	1:K:93:ARG:NH1	2.50	0.44
1:L:307:ASP:OD1	1:L:307:ASP:N	2.50	0.44
1:A:359:ARG:NH2	2:F:800:ADP:O3B	2.51	0.44
1:B:276:SER:HA	1:F:326:SER:CB	2.35	0.44
1:B:307:ASP:N	1:B:307:ASP:OD1	2.50	0.44
1:F:112:LYS:HD2	1:F:169:ASP:OD2	2.18	0.44
1:G:197:SER:O	1:G:200:GLU:HB2	2.18	0.44
1:H:118:PRO:HB2	1:H:123:VAL:HG11	1.99	0.44
1:H:222:LEU:N	1:H:223:PRO:HD2	2.32	0.44
1:L:130:LEU:H	1:L:130:LEU:HD23	1.82	0.44
1:C:420:LEU:HG	1:D:235:VAL:HG11	2.00	0.44
1:F:31:ALA:HB2	1:F:84:MET:C	2.38	0.44
1:F:252:THR:HA	1:F:302:PHE:CE2	2.53	0.44
1:K:133:VAL:HG13	1:K:443:ASN:HB2	2.00	0.44
1:K:347:THR:CG2	1:K:348:ASN:N	2.81	0.44
1:B:21:ASN:CA	1:D:432:LEU:HG	2.47	0.43
1:E:43:GLN:N	1:E:44:PRO:HD2	2.33	0.43
1:H:139:PHE:CD1	1:H:176:VAL:HG11	2.53	0.43
1:K:249:THR:N	2:K:800:ADP:O2B	2.51	0.43
1:G:43:GLN:N	1:G:44:PRO:HD2	2.33	0.43
1:H:142:ALA:HB1	1:H:144:ARG:HG3	2.00	0.43
1:K:286:LEU:HD21	1:K:287:ARG:HH21	1.81	0.43
1:B:114:ILE:HD11	1:B:146:ILE:HD11	2.00	0.43
1:B:155:HIS:HB3	1:B:386:LYS:O	2.18	0.43
1:F:27:ILE:HA	1:F:98:ASP:O	2.19	0.43
1:K:251:LYS:NZ	1:K:348:ASN:HB3	2.32	0.43
1:K:285:ASN:ND2	1:K:288:LYS:CB	2.81	0.43
1:C:222:LEU:N	1:C:223:PRO:HD2	2.33	0.43
1:D:206:ILE:O	1:D:206:ILE:CG1	2.61	0.43
1:K:140:LEU:HD12	3:K:905:HOH:O	2.18	0.43
1:E:90:ASN:O	1:E:93:ARG:NH1	2.51	0.43
1:G:276:SER:O	1:K:323:ARG:O	2.36	0.43
1:H:249:THR:N	2:H:800:ADP:O2B	2.52	0.43
1:E:40:SER:HB2	1:E:83:ARG:HB2	2.01	0.43
1:H:248:GLY:N	2:H:800:ADP:O3B	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:320:VAL:HG22	1:H:323:ARG:NH2	2.34	0.43
1:B:222:LEU:N	1:B:223:PRO:HD2	2.32	0.43
1:B:314:GLU:HB2	1:D:315:LYS:NZ	2.34	0.43
1:E:320:VAL:HG22	1:E:323:ARG:NH2	2.34	0.43
1:H:113:ARG:HB3	1:H:169:ASP:HB2	2.00	0.43
1:L:191:ARG:NH1	1:L:197:SER:HA	2.34	0.43
1:C:117:LEU:HD13	1:H:187:GLU:HG3	2.00	0.43
1:H:40:SER:HB2	1:H:83:ARG:HB2	2.01	0.43
1:K:55:ASP:O	1:K:71:VAL:HG12	2.18	0.43
1:K:239:ARG:HB3	1:K:335:LEU:HD12	2.01	0.43
1:C:229:LEU:CD1	1:E:427:MET:HE3	2.49	0.43
1:I:222:LEU:N	1:I:223:PRO:HD2	2.34	0.43
1:K:302:PHE:CZ	1:K:346:ALA:HB2	2.53	0.43
1:D:42:SER:OG	1:D:79:ASP:HA	2.19	0.42
1:J:43:GLN:N	1:J:44:PRO:HD2	2.34	0.42
1:J:55:ASP:O	1:J:71:VAL:HG12	2.19	0.42
1:K:43:GLN:N	1:K:44:PRO:HD2	2.34	0.42
1:A:43:GLN:N	1:A:44:PRO:HD2	2.34	0.42
1:C:206:ILE:HD13	1:C:254:ILE:HG12	2.01	0.42
1:C:424:ARG:HG3	1:D:222:LEU:HD11	2.02	0.42
1:I:176:VAL:HG13	1:I:176:VAL:O	2.20	0.42
1:K:242:LEU:CD1	1:K:363:PHE:HE2	2.32	0.42
1:K:433:GLU:CA	1:K:436:THR:HG22	2.48	0.42
1:B:159:ARG:C	1:B:387:ASN:OD1	2.58	0.42
1:B:177:ALA:HB1	1:B:178:PRO:HD2	2.01	0.42
1:D:199:ASN:O	1:D:200:GLU:C	2.57	0.42
1:D:222:LEU:N	1:D:223:PRO:HD2	2.34	0.42
1:E:30:GLU:OE2	1:E:217:LYS:HE2	2.19	0.42
1:G:222:LEU:N	1:G:223:PRO:HD2	2.34	0.42
1:I:55:ASP:O	1:I:71:VAL:HG12	2.20	0.42
1:I:252:THR:HA	1:I:302:PHE:CE2	2.54	0.42
1:K:115:HIS:HE1	1:K:185:GLU:HB2	1.85	0.42
1:B:111:GLY:HA2	1:B:170:PRO:CD	2.50	0.42
1:F:177:ALA:HB1	1:F:178:PRO:HD2	2.01	0.42
1:I:43:GLN:N	1:I:44:PRO:HD2	2.34	0.42
1:G:115:HIS:HE1	1:G:185:GLU:HB2	1.85	0.42
1:G:307:ASP:N	1:G:307:ASP:OD1	2.52	0.42
1:I:40:SER:HB2	1:I:83:ARG:HB2	2.01	0.42
1:J:252:THR:HA	1:J:302:PHE:CE2	2.55	0.42
1:A:27:ILE:HD11	1:F:431:ASP:HB3	2.01	0.42
1:C:187:GLU:HB2	1:H:187:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:THR:OG1	1:L:273:GLU:HA	2.19	0.42
1:H:252:THR:HA	1:H:302:PHE:CE2	2.55	0.42
1:K:246:PRO:O	1:K:249:THR:OG1	2.38	0.42
1:A:252:THR:HA	1:A:302:PHE:CE2	2.54	0.42
1:C:40:SER:HB2	1:C:83:ARG:HB2	2.01	0.42
1:C:229:LEU:HD12	1:E:427:MET:HE1	2.01	0.42
1:I:42:SER:OG	1:I:79:ASP:HA	2.20	0.42
1:F:126:ILE:CB	1:F:439:ALA:HB2	2.47	0.42
1:A:99:VAL:HG11	1:F:431:ASP:HB2	2.02	0.42
1:B:320:VAL:HG22	1:B:323:ARG:NH2	2.34	0.42
1:C:377:ARG:NE	1:C:403:THR:O	2.53	0.42
1:D:203:TYR:CE2	1:D:217:LYS:HD2	2.55	0.42
1:I:302:PHE:HA	1:I:344:MET:O	2.20	0.42
1:J:203:TYR:CD2	1:J:261:GLU:HG2	2.54	0.42
1:K:253:LEU:HD22	2:K:800:ADP:H2'	2.01	0.42
1:L:20:LYS:CB	1:L:21:ASN:OD1	2.68	0.42
1:A:324:ILE:HG22	1:A:325:VAL:N	2.35	0.41
1:C:42:SER:OG	1:C:79:ASP:HA	2.20	0.41
1:G:252:THR:HA	1:G:302:PHE:CE2	2.55	0.41
1:H:90:ASN:O	1:H:93:ARG:NH1	2.53	0.41
1:J:90:ASN:O	1:J:93:ARG:NH1	2.53	0.41
1:K:310:ALA:N	1:K:311:PRO:HD3	2.35	0.41
1:L:198:LEU:HD22	1:L:198:LEU:HA	1.81	0.41
1:F:222:LEU:N	1:F:223:PRO:HD2	2.35	0.41
1:G:320:VAL:HG22	1:G:323:ARG:NH2	2.35	0.41
1:K:212:GLN:CD	1:K:212:GLN:H	2.24	0.41
1:J:42:SER:OG	1:J:79:ASP:HA	2.19	0.41
1:B:112:LYS:O	1:B:181:VAL:N	2.52	0.41
1:D:113:ARG:HB3	1:D:169:ASP:HB2	2.03	0.41
1:B:90:ASN:O	1:B:93:ARG:NH1	2.54	0.41
1:B:118:PRO:HB2	1:B:123:VAL:HG11	2.02	0.41
1:B:321:GLU:OE1	1:F:322:ARG:CZ	2.68	0.41
1:C:320:VAL:HG22	1:C:323:ARG:NH2	2.36	0.41
1:D:324:ILE:HG22	1:D:325:VAL:N	2.36	0.41
1:F:35:ASP:HB3	1:F:38:VAL:CG1	2.49	0.41
1:G:176:VAL:O	1:G:176:VAL:HG13	2.20	0.41
1:G:232:ALA:O	1:L:159:ARG:NE	2.53	0.41
1:H:193:ASP:OD1	1:H:193:ASP:N	2.53	0.41
1:L:113:ARG:HB3	1:L:169:ASP:HB2	2.01	0.41
1:D:115:HIS:HE1	1:D:185:GLU:HB2	1.84	0.41
1:G:90:ASN:O	1:G:93:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:VAL:O	1:K:176:VAL:HG13	2.21	0.41
1:C:43:GLN:N	1:C:44:PRO:HD2	2.35	0.41
1:F:134:TYR:O	1:F:137:PRO:HD2	2.21	0.41
1:G:131:PHE:CD1	1:G:131:PHE:C	2.94	0.41
1:L:252:THR:HA	1:L:302:PHE:CE2	2.56	0.41
1:A:113:ARG:HB3	1:A:169:ASP:HB2	2.03	0.41
1:A:176:VAL:HG13	1:A:176:VAL:O	2.20	0.41
1:B:176:VAL:HG13	1:B:176:VAL:O	2.20	0.41
1:G:212:GLN:O	1:G:216:ILE:HG12	2.21	0.41
1:G:348:ASN:HB2	3:G:902:HOH:O	2.21	0.41
1:H:35:ASP:HB3	1:H:38:VAL:CG1	2.49	0.41
1:H:176:VAL:O	1:H:176:VAL:HG13	2.21	0.41
1:I:274:ILE:HD13	1:I:274:ILE:HA	1.95	0.41
1:K:348:ASN:N	1:K:348:ASN:HD22	2.19	0.41
1:L:35:ASP:HB3	1:L:38:VAL:CG1	2.50	0.41
1:A:320:VAL:HG22	1:A:323:ARG:NH2	2.35	0.41
1:D:37:SER:HA	3:D:914:HOH:O	2.21	0.41
1:I:206:ILE:HD13	1:I:254:ILE:HG12	2.03	0.41
1:L:20:LYS:C	1:L:21:ASN:CG	2.79	0.41
1:L:139:PHE:CD1	1:L:176:VAL:HG11	2.56	0.41
1:L:222:LEU:N	1:L:223:PRO:HD2	2.35	0.41
1:B:43:GLN:N	1:B:44:PRO:HD2	2.35	0.40
1:C:115:HIS:HE1	1:C:185:GLU:HB2	1.86	0.40
1:I:320:VAL:HG22	1:I:323:ARG:NH2	2.36	0.40
1:J:113:ARG:HB3	1:J:169:ASP:HB2	2.03	0.40
1:K:297:ALA:HB1	1:K:298:PRO:HA	2.02	0.40
1:A:27:ILE:HA	1:A:98:ASP:O	2.22	0.40
1:D:139:PHE:CD1	1:D:176:VAL:HG11	2.55	0.40
1:D:274:ILE:HD13	1:D:274:ILE:HA	1.95	0.40
1:I:228:ALA:CB	1:K:435:GLU:HG2	2.52	0.40
1:K:113:ARG:HB3	1:K:169:ASP:HB2	2.03	0.40
1:K:239:ARG:HD3	1:K:342:ILE:HG13	2.03	0.40
1:K:351:ASN:N	1:K:351:ASN:HD22	2.19	0.40
1:B:131:PHE:CD1	1:B:131:PHE:C	2.94	0.40
1:D:320:VAL:HG22	1:D:323:ARG:NH2	2.36	0.40
1:J:35:ASP:HB3	1:J:38:VAL:CG1	2.50	0.40
1:K:327:GLN:HA	1:K:330:THR:HG22	2.03	0.40
1:L:274:ILE:HD13	1:L:274:ILE:HA	1.96	0.40
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.57	0.40
1:A:197:SER:O	1:A:200:GLU:HB2	2.21	0.40
1:B:138:TYR:CE2	1:B:152:PHE:CD2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLY:N	2:C:800:ADP:O3B	2.44	0.40
1:C:326:SER:HB3	1:E:276:SER:CB	2.45	0.40
1:E:222:LEU:N	1:E:223:PRO:HD2	2.35	0.40
1:E:407:VAL:O	1:E:410:ASP:HB2	2.21	0.40
1:H:203:TYR:CD2	1:H:261:GLU:HG2	2.55	0.40
1:K:249:THR:HA	1:K:407:VAL:HG22	2.04	0.40
1:C:113:ARG:HB3	1:C:169:ASP:HB2	2.03	0.40
1:C:222:LEU:H	1:C:222:LEU:HD12	1.85	0.40
1:K:286:LEU:CD2	1:K:287:ARG:HH21	2.34	0.40

All (2) 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:F:404:HIS:CG	1:G:210:ARG:NH1[3_645]	1.92	0.28
1:B:52:PHE:CZ	1:I:49:LEU:O[4_455]	2.09	0.11

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	436/489 (89%)	419 (96%)	17 (4%)	0	100	100
1	B	437/489 (89%)	416 (95%)	21 (5%)	0	100	100
1	C	436/489 (89%)	418 (96%)	18 (4%)	0	100	100
1	D	437/489 (89%)	417 (95%)	20 (5%)	0	100	100
1	E	437/489 (89%)	418 (96%)	19 (4%)	0	100	100
1	F	436/489 (89%)	417 (96%)	19 (4%)	0	100	100
1	G	435/489 (89%)	418 (96%)	17 (4%)	0	100	100
1	H	436/489 (89%)	416 (95%)	19 (4%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	438/489 (90%)	418 (95%)	20 (5%)	0	100	100
1	J	443/489 (91%)	425 (96%)	18 (4%)	0	100	100
1	K	436/489 (89%)	398 (91%)	35 (8%)	3 (1%)	22	56
1	L	440/489 (90%)	419 (95%)	20 (4%)	1 (0%)	47	79
All	All	5247/5868 (89%)	4999 (95%)	243 (5%)	5 (0%)	51	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	23	PRO
1	K	241	ILE
1	K	277	LYS
1	K	359	ARG
1	H	106	PRO

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	375/418 (90%)	345 (92%)	30 (8%)	12	37
1	B	376/418 (90%)	346 (92%)	30 (8%)	12	37
1	C	375/418 (90%)	345 (92%)	30 (8%)	12	37
1	D	376/418 (90%)	345 (92%)	31 (8%)	11	36
1	E	376/418 (90%)	345 (92%)	31 (8%)	11	36
1	F	375/418 (90%)	343 (92%)	32 (8%)	10	34
1	G	374/418 (90%)	344 (92%)	30 (8%)	12	37
1	H	375/418 (90%)	344 (92%)	31 (8%)	11	35
1	I	377/418 (90%)	345 (92%)	32 (8%)	10	34
1	J	382/418 (91%)	349 (91%)	33 (9%)	10	34
1	K	375/418 (90%)	329 (88%)	46 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	379/418 (91%)	349 (92%)	30 (8%)	12	37
All	All	4515/5016 (90%)	4129 (92%)	386 (8%)	10	34

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	33	ASN
1	A	56	THR
1	A	78	SER
1	A	96	LEU
1	A	109	LYS
1	A	127	THR
1	A	147	ARG
1	A	184	CYS
1	A	193	ASP
1	A	198	LEU
1	A	206	ILE
1	A	210	ARG
1	A	211	LYS
1	A	212	GLN
1	A	217	LYS
1	A	249	THR
1	A	256	ARG
1	A	288	LYS
1	A	313	ARG
1	A	314	GLU
1	A	315	LYS
1	A	322	ARG
1	A	324	ILE
1	A	327	GLN
1	A	335	LEU
1	A	338	ARG
1	A	375	THR
1	A	378	LEU
1	A	435	GLU
1	B	28	VAL
1	B	33	ASN
1	B	56	THR
1	B	96	LEU
1	B	109	LYS
1	B	127	THR

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Mol	Chain	Res	Type
1	B	147	ARG
1	B	184	CYS
1	B	193	ASP
1	B	199	ASN
1	B	206	ILE
1	B	210	ARG
1	B	211	LYS
1	B	212	GLN
1	B	217	LYS
1	B	249	THR
1	B	256	ARG
1	B	288	LYS
1	B	313	ARG
1	B	314	GLU
1	B	315	LYS
1	B	322	ARG
1	B	324	ILE
1	B	327	GLN
1	B	335	LEU
1	B	338	ARG
1	B	351	ASN
1	B	375	THR
1	B	378	LEU
1	B	435	GLU
1	C	28	VAL
1	C	33	ASN
1	C	56	THR
1	C	78	SER
1	C	96	LEU
1	C	109	LYS
1	C	127	THR
1	C	147	ARG
1	C	184	CYS
1	C	193	ASP
1	C	206	ILE
1	C	210	ARG
1	C	211	LYS
1	C	212	GLN
1	C	217	LYS
1	C	249	THR
1	C	256	ARG
1	C	288	LYS

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Mol	Chain	Res	Type
1	C	313	ARG
1	C	314	GLU
1	C	315	LYS
1	C	322	ARG
1	C	324	ILE
1	C	327	GLN
1	C	335	LEU
1	C	338	ARG
1	C	351	ASN
1	C	375	THR
1	C	378	LEU
1	C	435	GLU
1	D	22	ARG
1	D	28	VAL
1	D	33	ASN
1	D	56	THR
1	D	78	SER
1	D	96	LEU
1	D	109	LYS
1	D	147	ARG
1	D	184	CYS
1	D	193	ASP
1	D	206	ILE
1	D	210	ARG
1	D	211	LYS
1	D	212	GLN
1	D	217	LYS
1	D	249	THR
1	D	256	ARG
1	D	288	LYS
1	D	313	ARG
1	D	314	GLU
1	D	315	LYS
1	D	322	ARG
1	D	324	ILE
1	D	327	GLN
1	D	335	LEU
1	D	338	ARG
1	D	351	ASN
1	D	375	THR
1	D	378	LEU
1	D	435	GLU

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Mol	Chain	Res	Type
1	D	460	ASN
1	E	28	VAL
1	E	33	ASN
1	E	56	THR
1	E	96	LEU
1	E	109	LYS
1	E	127	THR
1	E	147	ARG
1	E	184	CYS
1	E	193	ASP
1	E	200	GLU
1	E	206	ILE
1	E	210	ARG
1	E	211	LYS
1	E	212	GLN
1	E	217	LYS
1	E	249	THR
1	E	256	ARG
1	E	288	LYS
1	E	313	ARG
1	E	314	GLU
1	E	315	LYS
1	E	322	ARG
1	E	324	ILE
1	E	327	GLN
1	E	335	LEU
1	E	338	ARG
1	E	351	ASN
1	E	375	THR
1	E	378	LEU
1	E	435	GLU
1	E	460	ASN
1	F	28	VAL
1	F	33	ASN
1	F	56	THR
1	F	78	SER
1	F	96	LEU
1	F	107	ASP
1	F	109	LYS
1	F	147	ARG
1	F	184	CYS
1	F	193	ASP

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Mol	Chain	Res	Type
1	F	198	LEU
1	F	200	GLU
1	F	206	ILE
1	F	210	ARG
1	F	211	LYS
1	F	212	GLN
1	F	217	LYS
1	F	246	PRO
1	F	249	THR
1	F	256	ARG
1	F	288	LYS
1	F	313	ARG
1	F	314	GLU
1	F	315	LYS
1	F	322	ARG
1	F	324	ILE
1	F	335	LEU
1	F	338	ARG
1	F	351	ASN
1	F	375	THR
1	F	378	LEU
1	F	435	GLU
1	G	28	VAL
1	G	33	ASN
1	G	56	THR
1	G	78	SER
1	G	96	LEU
1	G	109	LYS
1	G	147	ARG
1	G	184	CYS
1	G	193	ASP
1	G	201	VAL
1	G	206	ILE
1	G	210	ARG
1	G	211	LYS
1	G	212	GLN
1	G	217	LYS
1	G	249	THR
1	G	256	ARG
1	G	288	LYS
1	G	313	ARG
1	G	314	GLU

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Mol	Chain	Res	Type
1	G	315	LYS
1	G	322	ARG
1	G	324	ILE
1	G	327	GLN
1	G	335	LEU
1	G	338	ARG
1	G	351	ASN
1	G	375	THR
1	G	378	LEU
1	G	435	GLU
1	H	28	VAL
1	H	33	ASN
1	H	56	THR
1	H	96	LEU
1	H	105	CYS
1	H	107	ASP
1	H	109	LYS
1	H	147	ARG
1	H	184	CYS
1	H	193	ASP
1	H	199	ASN
1	H	206	ILE
1	H	210	ARG
1	H	211	LYS
1	H	212	GLN
1	H	217	LYS
1	H	249	THR
1	H	256	ARG
1	H	288	LYS
1	H	313	ARG
1	H	314	GLU
1	H	315	LYS
1	H	322	ARG
1	H	324	ILE
1	H	327	GLN
1	H	335	LEU
1	H	338	ARG
1	H	351	ASN
1	H	375	THR
1	H	378	LEU
1	H	435	GLU
1	I	20	LYS

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Mol	Chain	Res	Type
1	I	22	ARG
1	I	28	VAL
1	I	33	ASN
1	I	56	THR
1	I	78	SER
1	I	96	LEU
1	I	109	LYS
1	I	147	ARG
1	I	184	CYS
1	I	193	ASP
1	I	200	GLU
1	I	206	ILE
1	I	210	ARG
1	I	211	LYS
1	I	212	GLN
1	I	217	LYS
1	I	249	THR
1	I	256	ARG
1	I	288	LYS
1	I	313	ARG
1	I	314	GLU
1	I	315	LYS
1	I	322	ARG
1	I	324	ILE
1	I	327	GLN
1	I	335	LEU
1	I	338	ARG
1	I	351	ASN
1	I	375	THR
1	I	378	LEU
1	I	435	GLU
1	J	18	LYS
1	J	20	LYS
1	J	21	ASN
1	J	28	VAL
1	J	33	ASN
1	J	56	THR
1	J	78	SER
1	J	96	LEU
1	J	109	LYS
1	J	127	THR
1	J	147	ARG

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Mol	Chain	Res	Type
1	J	184	CYS
1	J	193	ASP
1	J	196	GLU
1	J	206	ILE
1	J	210	ARG
1	J	211	LYS
1	J	212	GLN
1	J	217	LYS
1	J	249	THR
1	J	256	ARG
1	J	288	LYS
1	J	313	ARG
1	J	314	GLU
1	J	315	LYS
1	J	322	ARG
1	J	324	ILE
1	J	327	GLN
1	J	335	LEU
1	J	338	ARG
1	J	375	THR
1	J	378	LEU
1	J	435	GLU
1	K	28	VAL
1	K	33	ASN
1	K	56	THR
1	K	78	SER
1	K	96	LEU
1	K	109	LYS
1	K	127	THR
1	K	147	ARG
1	K	184	CYS
1	K	193	ASP
1	K	206	ILE
1	K	210	ARG
1	K	211	LYS
1	K	212	GLN
1	K	217	LYS
1	K	241	ILE
1	K	242	LEU
1	K	243	LEU
1	K	249	THR
1	K	256	ARG

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Mol	Chain	Res	Type
1	K	266	PHE
1	K	278	LEU
1	K	281	GLU
1	K	286	LEU
1	K	290	PHE
1	K	291	GLU
1	K	294	GLU
1	K	300	ILE
1	K	307	ASP
1	K	309	ILE
1	K	323	ARG
1	K	325	VAL
1	K	326	SER
1	K	330	THR
1	K	332	MET
1	K	335	LEU
1	K	340	HIS
1	K	348	ASN
1	K	349	ARG
1	K	351	ASN
1	K	353	ILE
1	K	363	PHE
1	K	366	GLU
1	K	375	THR
1	K	378	LEU
1	K	435	GLU
1	L	18	LYS
1	L	21	ASN
1	L	28	VAL
1	L	33	ASN
1	L	56	THR
1	L	96	LEU
1	L	109	LYS
1	L	147	ARG
1	L	184	CYS
1	L	193	ASP
1	L	198	LEU
1	L	206	ILE
1	L	210	ARG
1	L	211	LYS
1	L	212	GLN
1	L	217	LYS

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Mol	Chain	Res	Type
1	L	249	THR
1	L	256	ARG
1	L	288	LYS
1	L	313	ARG
1	L	314	GLU
1	L	315	LYS
1	L	322	ARG
1	L	324	ILE
1	L	335	LEU
1	L	338	ARG
1	L	351	ASN
1	L	375	THR
1	L	378	LEU
1	L	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	199	ASN
1	A	212	GLN
1	A	327	GLN
1	A	348	ASN
1	B	33	ASN
1	B	115	HIS
1	B	199	ASN
1	B	212	GLN
1	B	327	GLN
1	B	348	ASN
1	C	33	ASN
1	C	199	ASN
1	C	212	GLN
1	C	348	ASN
1	D	33	ASN
1	D	115	HIS
1	D	327	GLN
1	D	348	ASN
1	E	33	ASN
1	E	212	GLN
1	E	327	GLN
1	E	348	ASN
1	F	33	ASN

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Mol	Chain	Res	Type
1	F	115	HIS
1	F	183	HIS
1	F	212	GLN
1	F	348	ASN
1	G	212	GLN
1	G	327	GLN
1	G	348	ASN
1	H	33	ASN
1	H	212	GLN
1	H	327	GLN
1	H	348	ASN
1	I	33	ASN
1	I	327	GLN
1	I	348	ASN
1	J	33	ASN
1	J	212	GLN
1	J	317	HIS
1	J	327	GLN
1	J	348	ASN
1	K	33	ASN
1	K	348	ASN
1	K	351	ASN
1	L	33	ASN
1	L	50	GLN
1	L	212	GLN
1	L	327	GLN
1	L	348	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	B	800	-	24,29,29	0.99	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	A	800	-	24,29,29	0.89	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	L	800	-	24,29,29	0.91	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	G	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.41	4 (13%)
2	ADP	D	800	-	24,29,29	1.02	2 (8%)	29,45,45	1.53	5 (17%)
2	ADP	K	800	-	24,29,29	0.83	1 (4%)	29,45,45	1.55	4 (13%)
2	ADP	H	800	-	24,29,29	0.87	0	29,45,45	1.46	3 (10%)
2	ADP	C	800	-	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	I	800	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	J	800	-	24,29,29	1.15	2 (8%)	29,45,45	1.46	3 (10%)
2	ADP	E	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	3 (10%)
2	ADP	F	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	800	-	-	4/12/32/32	0/3/3/3
2	ADP	A	800	-	-	4/12/32/32	0/3/3/3
2	ADP	L	800	-	-	3/12/32/32	0/3/3/3
2	ADP	G	800	-	-	4/12/32/32	0/3/3/3
2	ADP	D	800	-	-	4/12/32/32	0/3/3/3
2	ADP	K	800	-	-	4/12/32/32	0/3/3/3
2	ADP	H	800	-	-	2/12/32/32	0/3/3/3
2	ADP	C	800	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	I	800	-	-	3/12/32/32	0/3/3/3
2	ADP	J	800	-	-	4/12/32/32	0/3/3/3
2	ADP	E	800	-	-	3/12/32/32	0/3/3/3
2	ADP	F	800	-	-	4/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	800	ADP	C2'-C1'	-2.61	1.49	1.53
2	D	800	ADP	C5-C4	2.52	1.47	1.40
2	L	800	ADP	C5-C4	2.49	1.47	1.40
2	G	800	ADP	C5-C4	2.40	1.47	1.40
2	J	800	ADP	C5-C4	2.36	1.47	1.40
2	C	800	ADP	C5-C4	2.30	1.47	1.40
2	F	800	ADP	C5-C4	2.28	1.47	1.40
2	E	800	ADP	C5-C4	2.26	1.46	1.40
2	B	800	ADP	C5-C4	2.13	1.46	1.40
2	D	800	ADP	C2'-C1'	-2.06	1.50	1.53
2	K	800	ADP	C5-C4	2.04	1.46	1.40
2	I	800	ADP	C5-C4	2.03	1.46	1.40
2	A	800	ADP	C5-C4	2.02	1.46	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	800	ADP	C3'-C2'-C1'	3.94	106.91	100.98
2	E	800	ADP	PA-O3A-PB	-3.84	119.66	132.83
2	D	800	ADP	PA-O3A-PB	-3.82	119.72	132.83
2	J	800	ADP	PA-O3A-PB	-3.80	119.80	132.83
2	H	800	ADP	N3-C2-N1	-3.79	122.76	128.68
2	F	800	ADP	PA-O3A-PB	-3.76	119.93	132.83
2	A	800	ADP	N3-C2-N1	-3.69	122.91	128.68
2	I	800	ADP	N3-C2-N1	-3.67	122.94	128.68
2	A	800	ADP	PA-O3A-PB	-3.62	120.42	132.83
2	B	800	ADP	PA-O3A-PB	-3.59	120.52	132.83
2	J	800	ADP	C3'-C2'-C1'	3.53	106.29	100.98
2	B	800	ADP	N3-C2-N1	-3.47	123.26	128.68
2	L	800	ADP	N3-C2-N1	-3.46	123.26	128.68
2	D	800	ADP	C3'-C2'-C1'	3.42	106.12	100.98
2	L	800	ADP	C3'-C2'-C1'	3.42	106.12	100.98
2	I	800	ADP	PA-O3A-PB	-3.37	121.27	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	800	ADP	PA-O3A-PB	-3.34	121.37	132.83
2	D	800	ADP	N3-C2-N1	-3.34	123.46	128.68
2	G	800	ADP	N3-C2-N1	-3.31	123.51	128.68
2	K	800	ADP	PA-O3A-PB	-3.30	121.50	132.83
2	H	800	ADP	C3'-C2'-C1'	3.27	105.90	100.98
2	I	800	ADP	C3'-C2'-C1'	3.27	105.90	100.98
2	E	800	ADP	C3'-C2'-C1'	3.23	105.84	100.98
2	E	800	ADP	N3-C2-N1	-3.21	123.66	128.68
2	C	800	ADP	C3'-C2'-C1'	3.19	105.79	100.98
2	C	800	ADP	N3-C2-N1	-3.19	123.70	128.68
2	J	800	ADP	N3-C2-N1	-3.19	123.70	128.68
2	G	800	ADP	PA-O3A-PB	-3.17	121.96	132.83
2	C	800	ADP	PA-O3A-PB	-3.14	122.06	132.83
2	L	800	ADP	PA-O3A-PB	-3.12	122.11	132.83
2	B	800	ADP	C3'-C2'-C1'	3.11	105.66	100.98
2	K	800	ADP	N3-C2-N1	-3.10	123.84	128.68
2	F	800	ADP	N3-C2-N1	-3.09	123.85	128.68
2	K	800	ADP	C4-C5-N7	-3.07	106.20	109.40
2	G	800	ADP	C3'-C2'-C1'	3.05	105.58	100.98
2	K	800	ADP	C3'-C2'-C1'	3.04	105.56	100.98
2	A	800	ADP	C3'-C2'-C1'	3.02	105.52	100.98
2	G	800	ADP	C4-C5-N7	-2.58	106.71	109.40
2	C	800	ADP	C4-C5-N7	-2.50	106.80	109.40
2	I	800	ADP	C4-C5-N7	-2.43	106.87	109.40
2	B	800	ADP	C4-C5-N7	-2.34	106.96	109.40
2	D	800	ADP	C2-N1-C6	2.34	122.75	118.75
2	D	800	ADP	C4-C5-N7	-2.32	106.98	109.40
2	F	800	ADP	C4-C5-N7	-2.29	107.01	109.40
2	L	800	ADP	C2-N1-C6	2.13	122.40	118.75
2	A	800	ADP	C4-C5-N7	-2.09	107.22	109.40

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	800	ADP	C5'-O5'-PA-O1A
2	J	800	ADP	C5'-O5'-PA-O1A
2	D	800	ADP	C5'-O5'-PA-O3A
2	F	800	ADP	C5'-O5'-PA-O3A
2	J	800	ADP	C5'-O5'-PA-O3A
2	L	800	ADP	C5'-O5'-PA-O1A
2	A	800	ADP	C5'-O5'-PA-O3A

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

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	ADP	2	0

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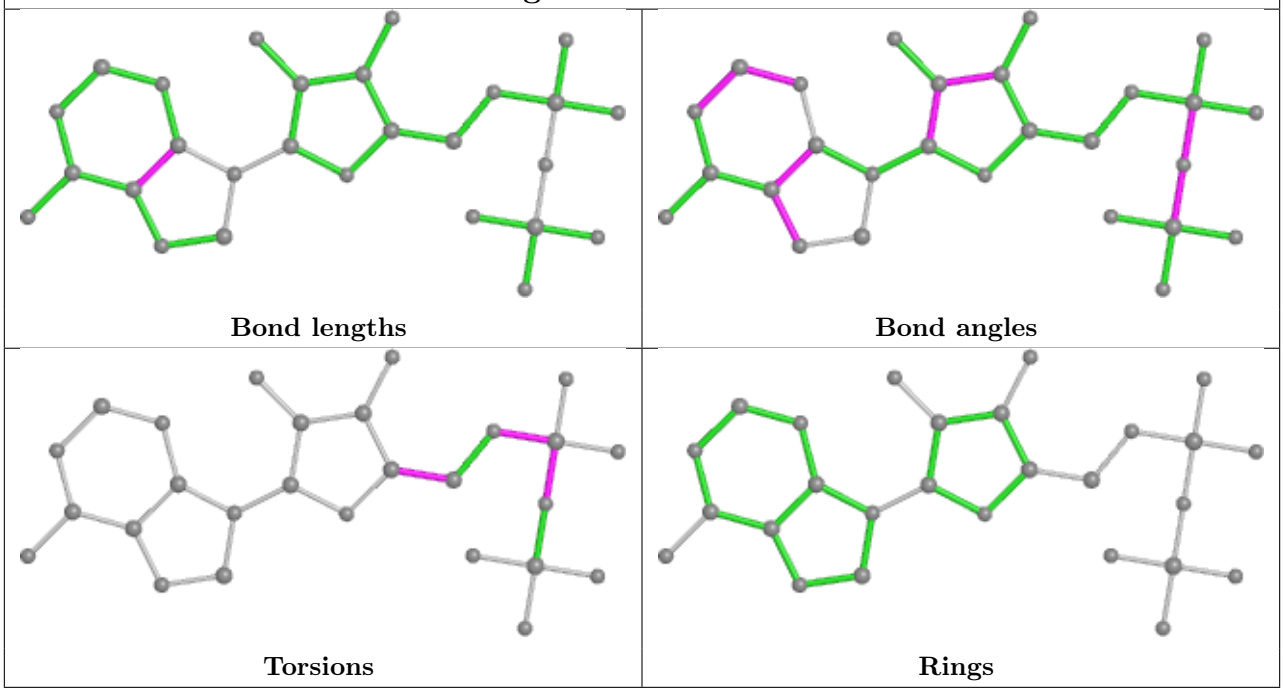
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	2	0
2	L	800	ADP	4	0
2	G	800	ADP	2	0
2	D	800	ADP	2	0
2	K	800	ADP	3	0
2	H	800	ADP	3	0
2	C	800	ADP	4	0
2	I	800	ADP	2	0
2	J	800	ADP	2	0
2	E	800	ADP	2	0
2	F	800	ADP	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 800



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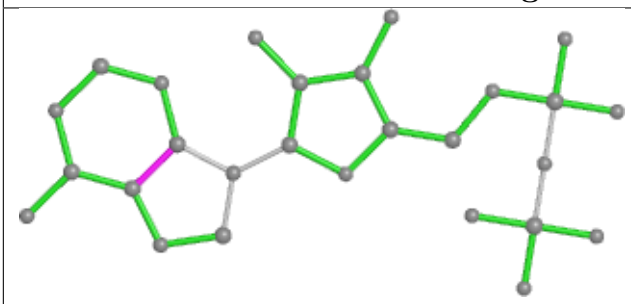
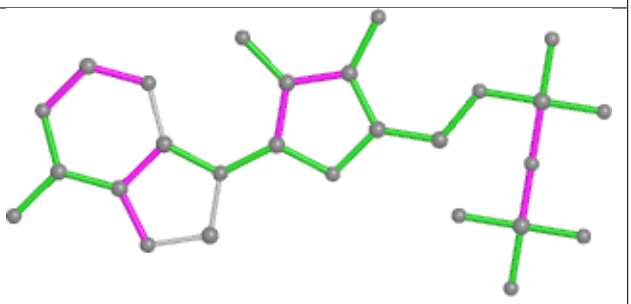
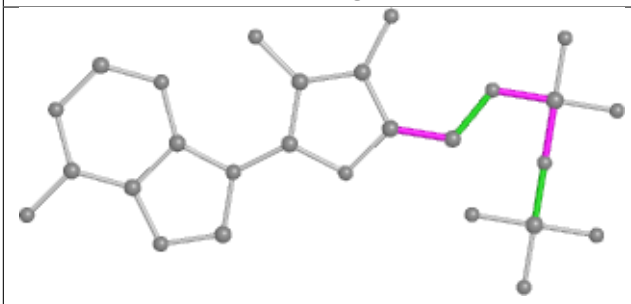
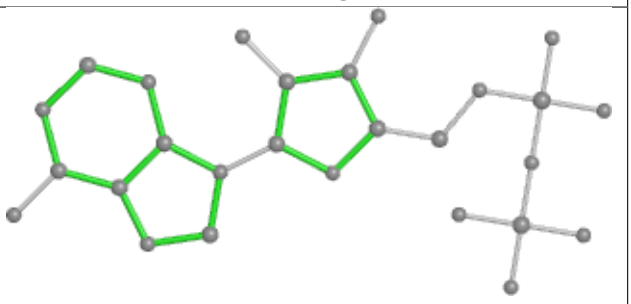
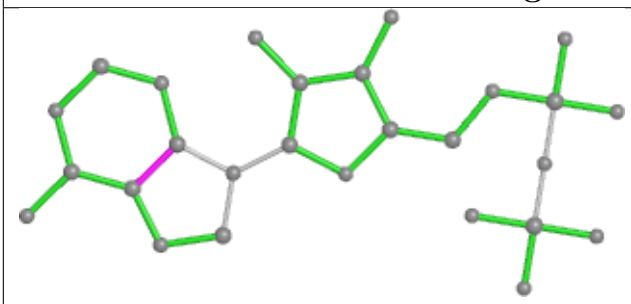
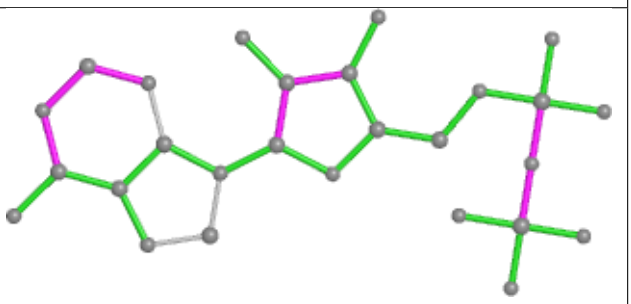
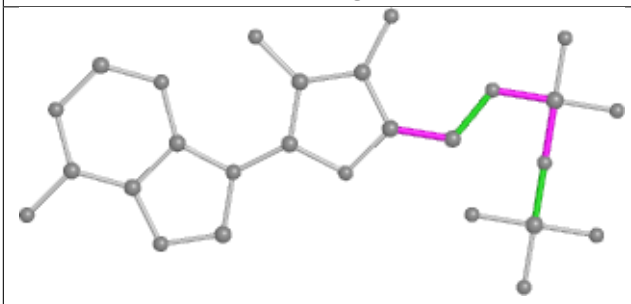
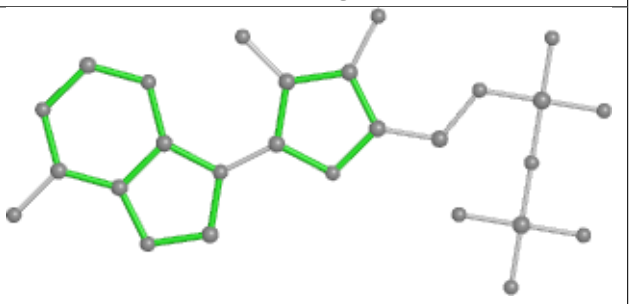
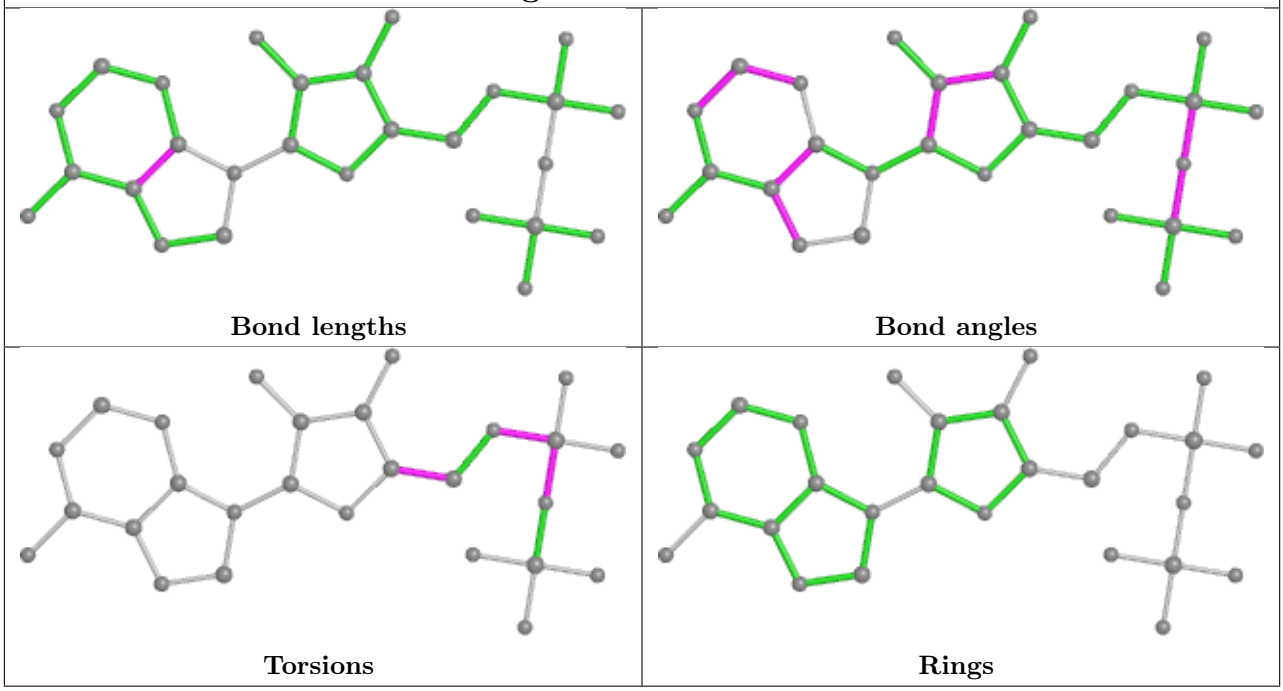
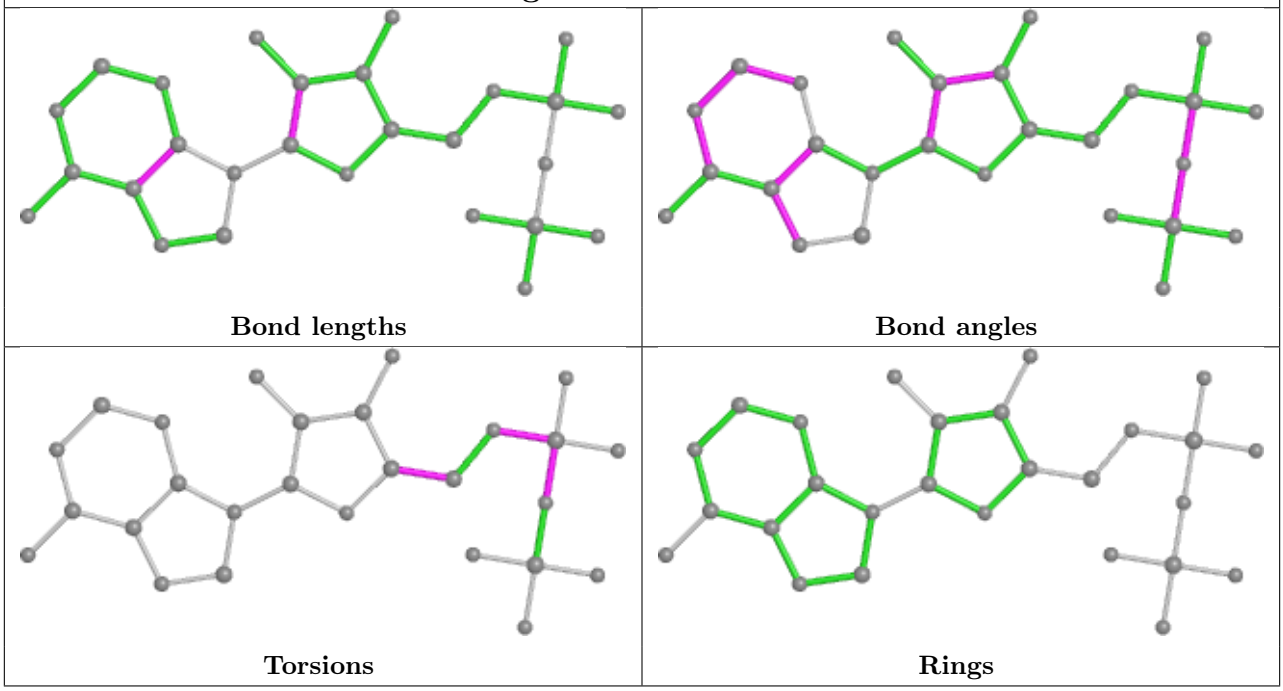
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP G 800



Ligand ADP D 800



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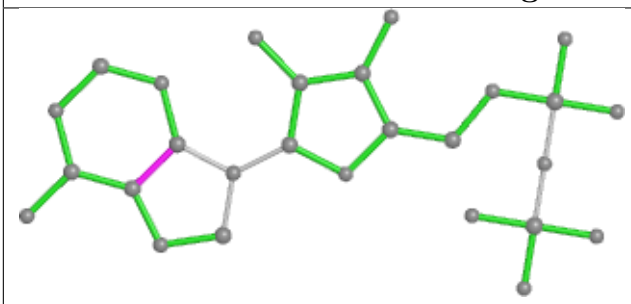
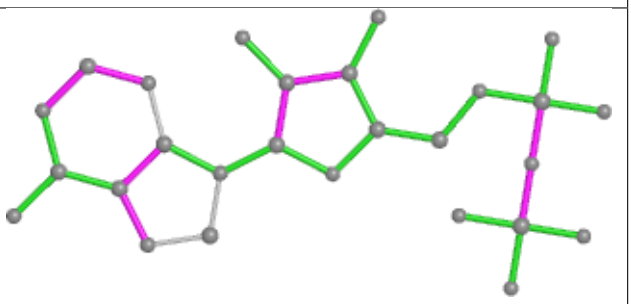
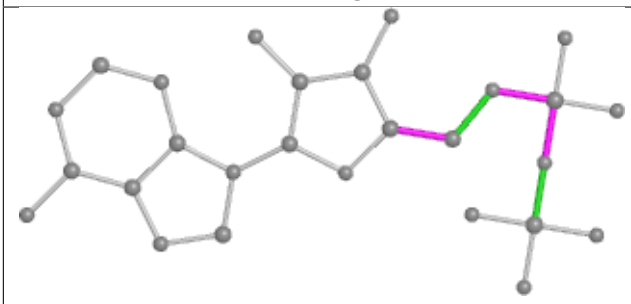
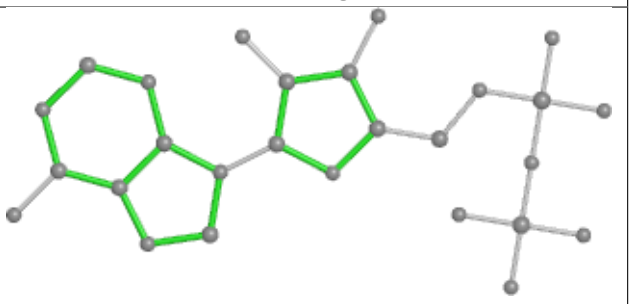
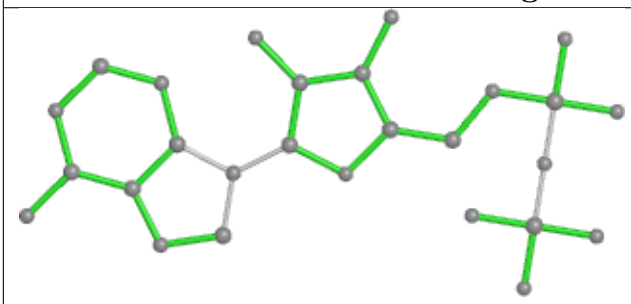
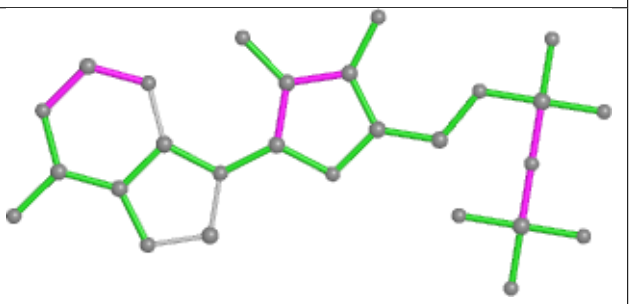
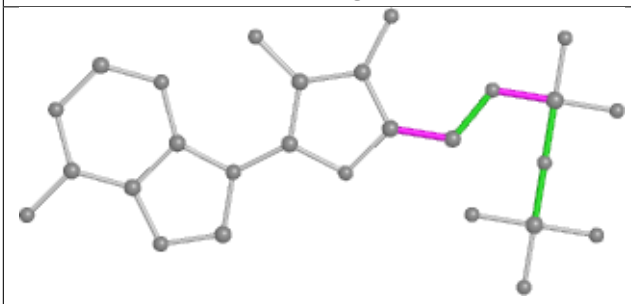
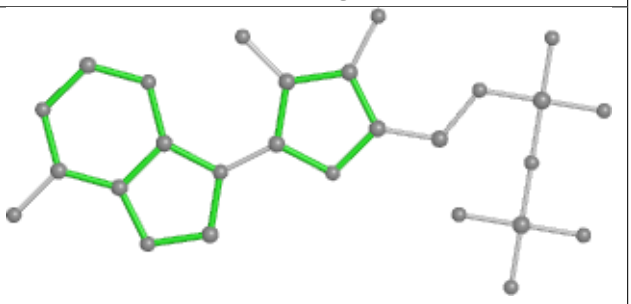
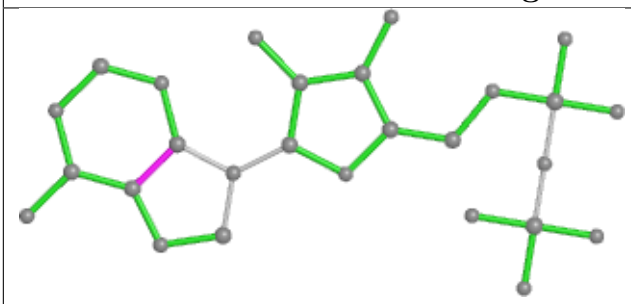
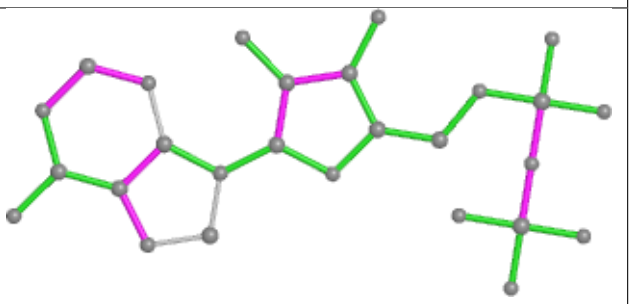
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP H 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

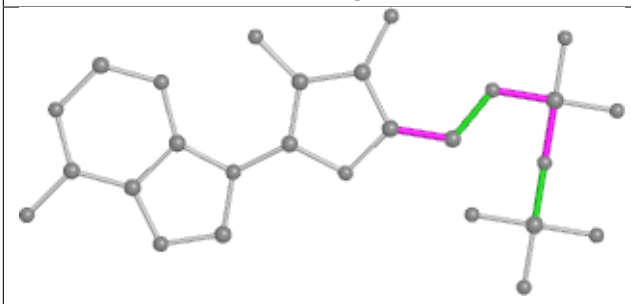
Ligand ADP C 800



Bond lengths



Bond angles



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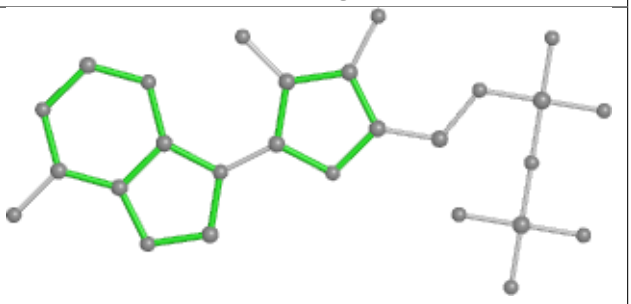
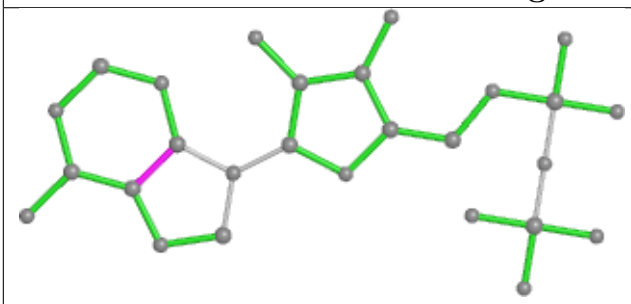


Rings

Ligand ADP I 800



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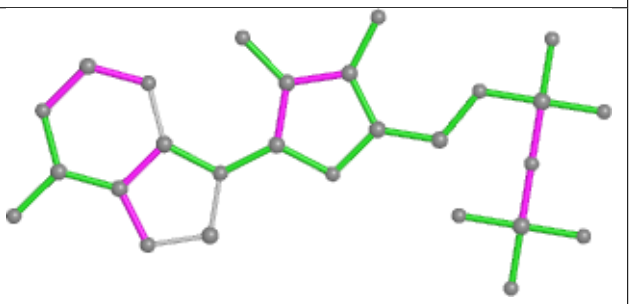

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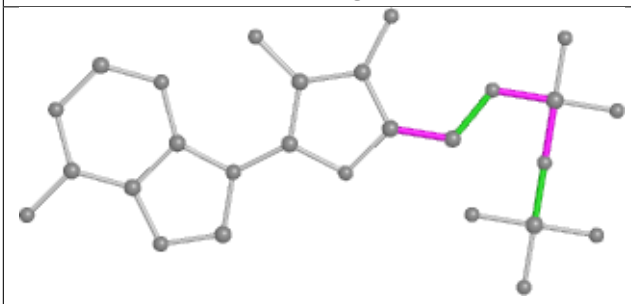

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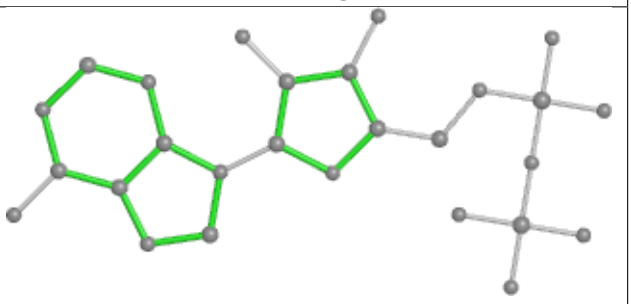
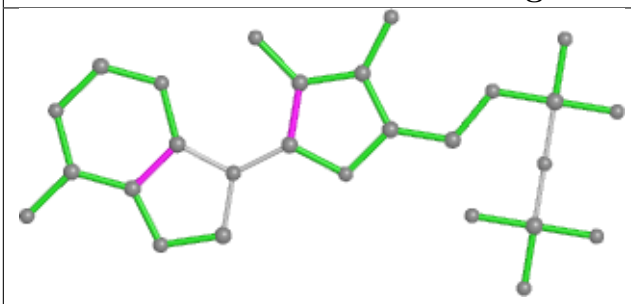
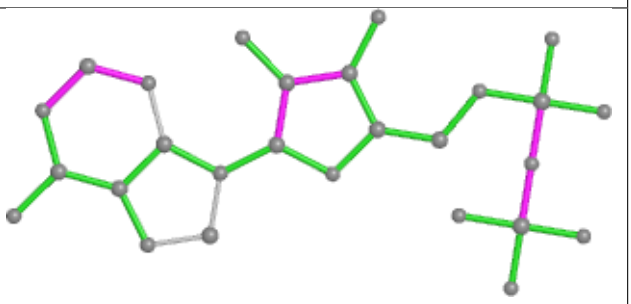
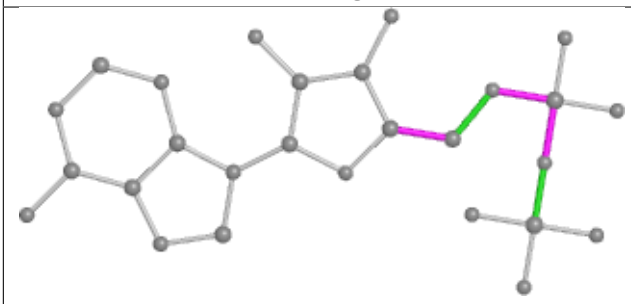
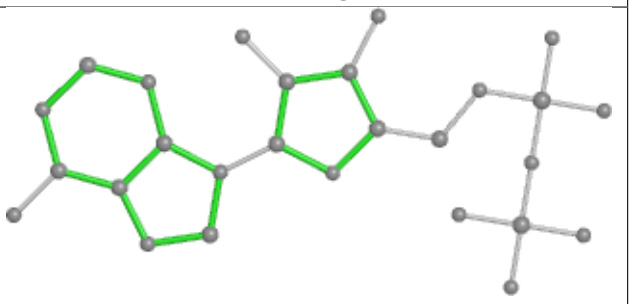
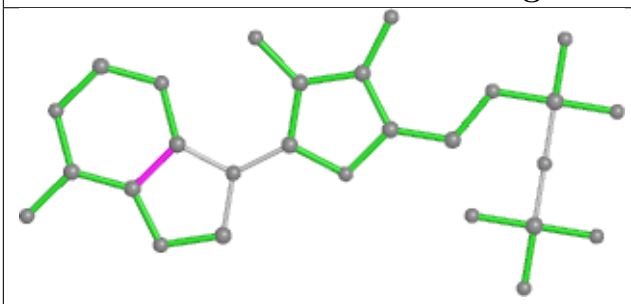
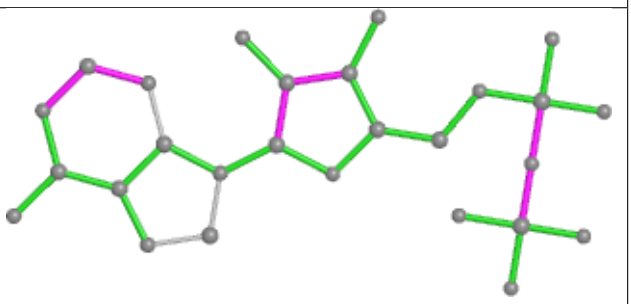
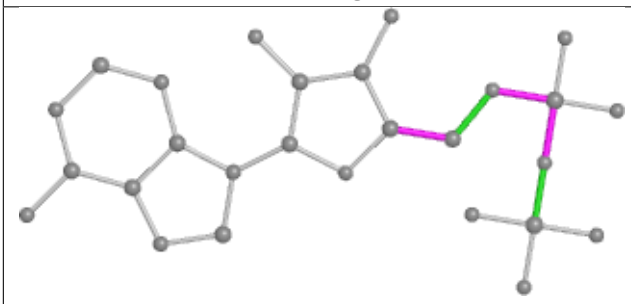
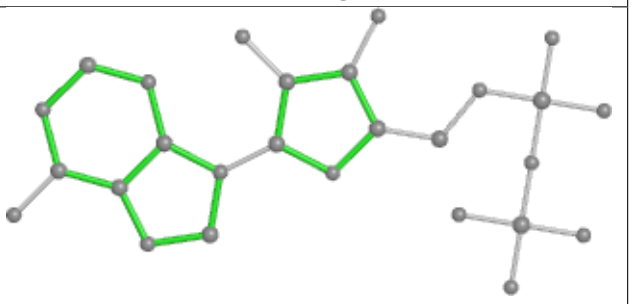
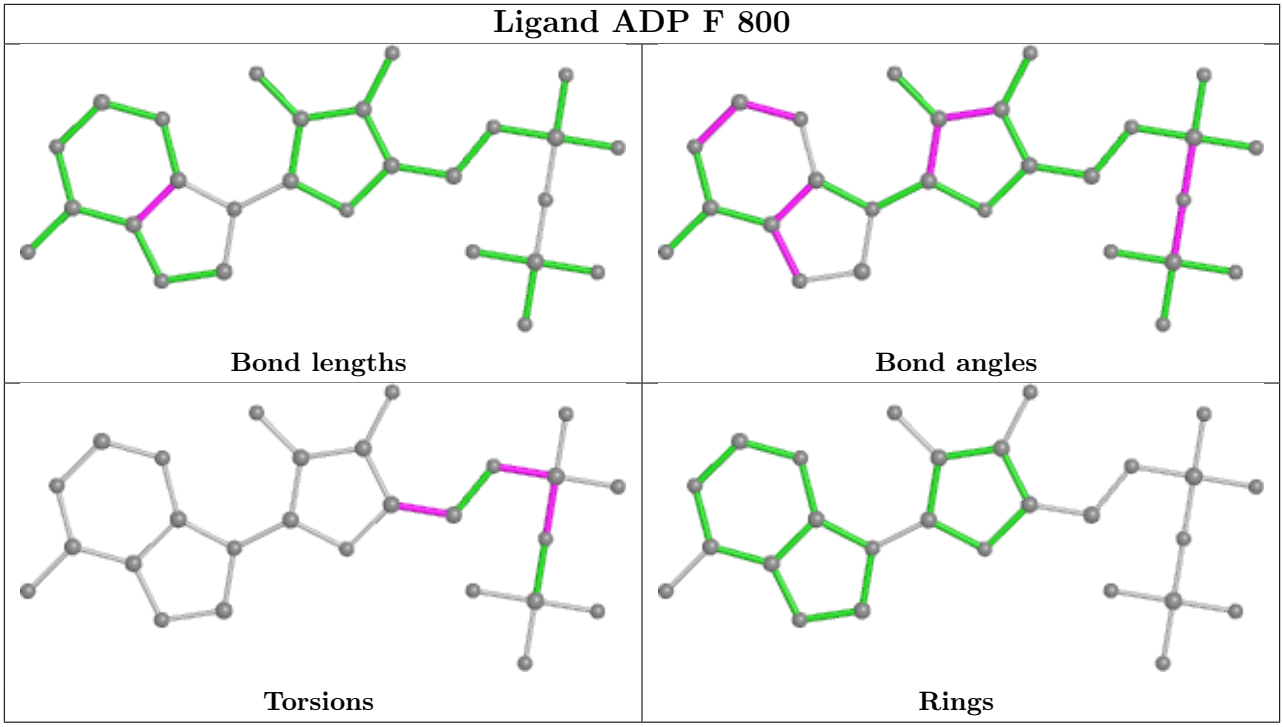


Rings

Ligand ADP J 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 800	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	438/489 (89%)	0.29	34 (7%)	13	7	71, 120, 172, 275	0
1	B	439/489 (89%)	-0.03	20 (4%)	32	20	57, 92, 153, 208	0
1	C	438/489 (89%)	0.19	31 (7%)	16	9	76, 120, 177, 233	0
1	D	439/489 (89%)	0.24	35 (7%)	12	7	60, 115, 176, 280	0
1	E	439/489 (89%)	0.52	57 (12%)	3	2	66, 132, 211, 261	0
1	F	438/489 (89%)	-0.01	17 (3%)	39	25	60, 95, 169, 215	0
1	G	437/489 (89%)	0.24	31 (7%)	16	9	60, 111, 169, 221	0
1	H	438/489 (89%)	0.06	20 (4%)	32	20	60, 105, 163, 233	0
1	I	440/489 (89%)	0.24	32 (7%)	15	8	61, 122, 182, 285	0
1	J	445/489 (91%)	-0.01	16 (3%)	42	28	50, 93, 153, 238	0
1	K	438/489 (89%)	0.82	87 (19%)	1	0	64, 142, 208, 239	0
1	L	442/489 (90%)	0.40	46 (10%)	6	4	76, 139, 204, 287	0
All	All	5271/5868 (89%)	0.25	426 (8%)	12	6	50, 115, 188, 287	0

All (426) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	279	ALA	9.2
1	I	432	LEU	8.3
1	D	433	GLU	7.7
1	E	279	ALA	7.7
1	E	432	LEU	7.3
1	K	432	LEU	7.2
1	I	436	THR	7.1
1	E	113	ARG	7.1
1	K	284	SER	6.8
1	K	460	ASN	6.3
1	E	435	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	K	109	LYS	5.9
1	K	279	ALA	5.8
1	G	434	ASP	5.7
1	I	437	ILE	5.6
1	H	435	GLU	5.6
1	K	194	GLU	5.6
1	F	317	HIS	5.5
1	E	166	VAL	5.5
1	L	187	GLU	5.4
1	L	432	LEU	5.4
1	A	435	GLU	5.2
1	K	278	LEU	5.2
1	J	436	THR	5.2
1	B	338	ARG	5.1
1	K	338	ARG	5.0
1	C	435	GLU	5.0
1	C	317	HIS	5.0
1	I	431	ASP	5.0
1	E	433	GLU	4.9
1	I	433	GLU	4.9
1	L	64	ARG	4.9
1	K	339	ALA	4.9
1	A	433	GLU	4.8
1	K	64	ARG	4.8
1	D	279	ALA	4.8
1	D	360	PHE	4.7
1	E	112	LYS	4.7
1	K	434	ASP	4.7
1	G	64	ARG	4.7
1	E	194	GLU	4.7
1	D	432	LEU	4.7
1	E	461	PRO	4.7
1	L	172	PRO	4.7
1	H	75	ASP	4.7
1	C	193	ASP	4.6
1	G	435	GLU	4.6
1	G	143	TYR	4.6
1	L	173	TYR	4.6
1	K	349	ARG	4.5
1	F	319	GLU	4.5
1	K	317	HIS	4.5
1	K	352	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	337	GLN	4.5
1	G	337	GLN	4.4
1	K	280	GLY	4.4
1	E	109	LYS	4.4
1	K	436	THR	4.4
1	K	340	HIS	4.4
1	I	279	ALA	4.3
1	K	277	LYS	4.3
1	L	53	ARG	4.3
1	B	53	ARG	4.3
1	G	338	ARG	4.3
1	K	173	TYR	4.3
1	I	428	ASP	4.2
1	J	434	ASP	4.2
1	L	63	LYS	4.2
1	D	434	ASP	4.2
1	J	433	GLU	4.2
1	B	337	GLN	4.2
1	K	350	PRO	4.2
1	F	337	GLN	4.2
1	L	21	ASN	4.1
1	J	239	ARG	4.1
1	K	112	LYS	4.1
1	L	244	TYR	4.1
1	J	461	PRO	4.0
1	A	345	ALA	4.0
1	A	338	ARG	4.0
1	E	108	VAL	4.0
1	K	286	LEU	4.0
1	L	101	SER	3.9
1	L	429	LEU	3.9
1	A	113	ARG	3.9
1	K	193	ASP	3.9
1	E	317	HIS	3.9
1	D	50	GLN	3.9
1	E	193	ASP	3.9
1	I	109	LYS	3.9
1	H	459	SER	3.8
1	G	63	LYS	3.8
1	K	63	LYS	3.8
1	E	280	GLY	3.8
1	A	76	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	108	VAL	3.8
1	K	140	LEU	3.8
1	L	181	VAL	3.8
1	K	128	GLY	3.8
1	A	75	ASP	3.8
1	I	349	ARG	3.8
1	E	75	ASP	3.7
1	C	141	GLU	3.7
1	K	141	GLU	3.7
1	K	163	PHE	3.7
1	I	34	GLU	3.7
1	J	317	HIS	3.7
1	A	344	MET	3.6
1	I	52	PHE	3.6
1	I	194	GLU	3.6
1	I	434	ASP	3.6
1	G	440	GLU	3.6
1	C	338	ARG	3.6
1	A	434	ASP	3.5
1	K	185	GLU	3.5
1	G	34	GLU	3.5
1	E	107	ASP	3.5
1	C	128	GLY	3.5
1	D	22	ARG	3.5
1	D	143	TYR	3.5
1	E	34	GLU	3.5
1	C	434	ASP	3.5
1	G	109	LYS	3.4
1	F	279	ALA	3.4
1	I	338	ARG	3.4
1	K	320	VAL	3.4
1	A	194	GLU	3.4
1	H	350	PRO	3.4
1	H	279	ALA	3.4
1	C	401	ASN	3.4
1	E	314	GLU	3.4
1	K	360	PHE	3.4
1	D	64	ARG	3.4
1	D	278	LEU	3.4
1	L	278	LEU	3.4
1	E	62	LYS	3.4
1	A	358	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	ARG	3.3
1	I	187	GLU	3.3
1	A	437	ILE	3.3
1	L	194	GLU	3.3
1	K	191	ARG	3.3
1	K	244	TYR	3.3
1	H	63	LYS	3.3
1	C	319	GLU	3.3
1	K	342	ILE	3.3
1	L	338	ARG	3.3
1	F	435	GLU	3.3
1	B	434	ASP	3.3
1	K	333	ASP	3.3
1	K	117	LEU	3.3
1	A	337	GLN	3.3
1	J	462	SER	3.3
1	L	404	HIS	3.3
1	E	136	LYS	3.3
1	I	459	SER	3.2
1	K	267	PHE	3.2
1	G	155	HIS	3.2
1	I	318	GLY	3.2
1	B	109	LYS	3.2
1	K	62	LYS	3.2
1	H	337	GLN	3.2
1	K	190	LYS	3.2
1	D	317	HIS	3.2
1	K	179	ASP	3.2
1	A	234	GLY	3.1
1	B	435	GLU	3.1
1	D	140	LEU	3.1
1	K	345	ALA	3.1
1	K	355	PRO	3.1
1	G	52	PHE	3.1
1	D	128	GLY	3.1
1	E	189	ILE	3.1
1	L	193	ASP	3.1
1	G	186	GLY	3.1
1	I	32	ILE	3.1
1	A	343	VAL	3.0
1	E	103	GLN	3.0
1	E	190	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	172	PRO	3.0
1	G	232	ALA	3.0
1	E	110	TYR	3.0
1	A	34	GLU	3.0
1	K	268	LEU	3.0
1	E	63	LYS	3.0
1	G	187	GLU	3.0
1	J	63	LYS	3.0
1	L	435	GLU	3.0
1	B	72	LEU	2.9
1	K	298	PRO	2.9
1	A	294	GLU	2.9
1	L	185	GLU	2.9
1	K	313	ARG	2.9
1	L	317	HIS	2.9
1	K	76	THR	2.9
1	K	107	ASP	2.9
1	K	143	TYR	2.9
1	C	231	LYS	2.9
1	D	280	GLY	2.9
1	D	436	THR	2.9
1	F	128	GLY	2.9
1	L	183	HIS	2.9
1	K	33	ASN	2.9
1	E	179	ASP	2.9
1	F	436	THR	2.9
1	D	343	VAL	2.8
1	A	62	LYS	2.8
1	I	141	GLU	2.8
1	K	113	ARG	2.8
1	F	336	LYS	2.8
1	L	62	LYS	2.8
1	F	404	HIS	2.8
1	H	280	GLY	2.8
1	C	63	LYS	2.8
1	L	113	ARG	2.8
1	D	63	LYS	2.8
1	B	350	PRO	2.8
1	K	295	LYS	2.8
1	L	20	LYS	2.8
1	C	433	GLU	2.8
1	K	358	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	143	TYR	2.8
1	B	21	ASN	2.7
1	K	428	ASP	2.7
1	C	404	HIS	2.7
1	A	239	ARG	2.7
1	I	64	ARG	2.7
1	K	187	GLU	2.7
1	K	287	ARG	2.7
1	K	75	ASP	2.7
1	D	281	GLU	2.7
1	K	186	GLY	2.7
1	K	151	ILE	2.7
1	F	63	LYS	2.7
1	A	106	PRO	2.7
1	L	188	PRO	2.7
1	B	404	HIS	2.7
1	L	125	GLY	2.7
1	C	169	ASP	2.7
1	K	106	PRO	2.7
1	D	34	GLU	2.7
1	K	32	ILE	2.7
1	A	60	LYS	2.6
1	E	129	ASN	2.6
1	E	244	TYR	2.6
1	J	432	LEU	2.6
1	G	392	ASP	2.6
1	H	434	ASP	2.6
1	B	433	GLU	2.6
1	G	33	ASN	2.6
1	E	127	THR	2.6
1	F	294	GLU	2.6
1	K	152	PHE	2.6
1	H	317	HIS	2.6
1	H	338	ARG	2.6
1	L	19	GLN	2.6
1	L	199	ASN	2.6
1	B	349	ARG	2.6
1	E	32	ILE	2.6
1	I	140	LEU	2.6
1	L	427	MET	2.6
1	H	427	MET	2.5
1	E	173	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	274	ILE	2.5
1	E	349	ARG	2.5
1	E	195	GLU	2.5
1	E	128	GLY	2.5
1	E	436	THR	2.5
1	K	328	LEU	2.5
1	K	319	GLU	2.5
1	A	404	HIS	2.5
1	E	140	LEU	2.5
1	G	32	ILE	2.5
1	D	338	ARG	2.5
1	E	80	GLU	2.5
1	K	110	TYR	2.5
1	D	52	PHE	2.4
1	I	193	ASP	2.4
1	C	127	THR	2.4
1	C	244	TYR	2.4
1	L	140	LEU	2.4
1	K	282	SER	2.4
1	E	181	VAL	2.4
1	E	312	LYS	2.4
1	L	186	GLY	2.4
1	A	278	LEU	2.4
1	C	278	LEU	2.4
1	D	106	PRO	2.4
1	E	350	PRO	2.4
1	I	360	PHE	2.4
1	H	109	LYS	2.4
1	H	172	PRO	2.4
1	D	336	LYS	2.4
1	A	459	SER	2.4
1	K	326	SER	2.4
1	K	150	ASP	2.4
1	G	140	LEU	2.4
1	C	239	ARG	2.4
1	F	338	ARG	2.4
1	K	330	THR	2.4
1	A	438	ASP	2.4
1	L	428	ASP	2.4
1	E	278	LEU	2.4
1	D	319	GLU	2.4
1	L	117	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	231	LYS	2.3
1	K	359	ARG	2.3
1	D	155	HIS	2.3
1	B	173	TYR	2.3
1	E	247	PRO	2.3
1	D	349	ARG	2.3
1	I	169	ASP	2.3
1	I	239	ARG	2.3
1	C	72	LEU	2.3
1	D	194	GLU	2.3
1	C	210	ARG	2.3
1	E	117	LEU	2.3
1	F	34	GLU	2.3
1	D	239	ARG	2.3
1	J	338	ARG	2.3
1	B	23	PRO	2.3
1	E	141	GLU	2.3
1	I	317	HIS	2.3
1	E	172	PRO	2.3
1	H	345	ALA	2.3
1	I	190	LYS	2.3
1	L	436	THR	2.3
1	L	155	HIS	2.3
1	E	169	ASP	2.3
1	G	193	ASP	2.3
1	L	150	ASP	2.3
1	C	279	ALA	2.3
1	G	128	GLY	2.3
1	K	361	GLY	2.3
1	E	192	GLU	2.3
1	K	192	GLU	2.3
1	L	196	GLU	2.3
1	H	179	ASP	2.3
1	F	323	ARG	2.3
1	L	46	MET	2.3
1	A	185	GLU	2.3
1	A	436	THR	2.3
1	K	285	ASN	2.3
1	K	351	ASN	2.3
1	B	140	LEU	2.3
1	L	431	ASP	2.2
1	G	53	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	231	LYS	2.2
1	K	306	LEU	2.2
1	L	108	VAL	2.2
1	L	52	PHE	2.2
1	E	438	ASP	2.2
1	J	437	ILE	2.2
1	E	64	ARG	2.2
1	K	34	GLU	2.2
1	H	22	ARG	2.2
1	K	52	PHE	2.2
1	C	33	ASN	2.2
1	C	336	LYS	2.2
1	E	316	THR	2.2
1	I	244	TYR	2.2
1	G	231	LYS	2.2
1	D	345	ALA	2.2
1	I	172	PRO	2.2
1	E	313	ARG	2.2
1	B	432	LEU	2.2
1	H	278	LEU	2.2
1	K	327	GLN	2.2
1	C	343	VAL	2.1
1	C	428	ASP	2.1
1	C	460	ASN	2.1
1	K	291	GLU	2.1
1	L	366	GLU	2.1
1	H	315	LYS	2.1
1	K	72	LEU	2.1
1	G	124	GLU	2.1
1	G	405	GLY	2.1
1	D	53	ARG	2.1
1	D	342	ILE	2.1
1	G	141	GLU	2.1
1	J	141	GLU	2.1
1	A	140	LEU	2.1
1	C	167	GLU	2.1
1	E	434	ASP	2.1
1	K	281	GLU	2.1
1	C	312	LYS	2.1
1	J	404	HIS	2.1
1	A	52	PHE	2.1
1	K	431	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	160	ALA	2.1
1	A	280	GLY	2.1
1	G	443	ASN	2.1
1	K	344	MET	2.1
1	D	113	ARG	2.1
1	G	239	ARG	2.1
1	I	429	LEU	2.1
1	C	75	ASP	2.1
1	J	231	LYS	2.1
1	A	33	ASN	2.1
1	L	33	ASN	2.1
1	J	360	PHE	2.1
1	A	193	ASP	2.1
1	F	428	ASP	2.1
1	I	179	ASP	2.1
1	D	344	MET	2.1
1	B	52	PHE	2.1
1	E	239	ARG	2.0
1	F	432	LEU	2.0
1	E	155	HIS	2.0
1	B	75	ASP	2.0
1	C	431	ASP	2.0
1	L	239	ARG	2.0
1	A	346	ALA	2.0
1	D	429	LEU	2.0
1	E	24	ASN	2.0
1	L	104	PRO	2.0
1	B	64	ARG	2.0
1	L	22	ARG	2.0
1	D	179	ASP	2.0
1	G	69	CYS	2.0
1	I	117	LEU	2.0
1	G	346	ALA	2.0
1	K	297	ALA	2.0
1	A	53	ARG	2.0
1	F	64	ARG	2.0
1	B	278	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 monosaccharides in this entry.

6.4 Ligands (i)

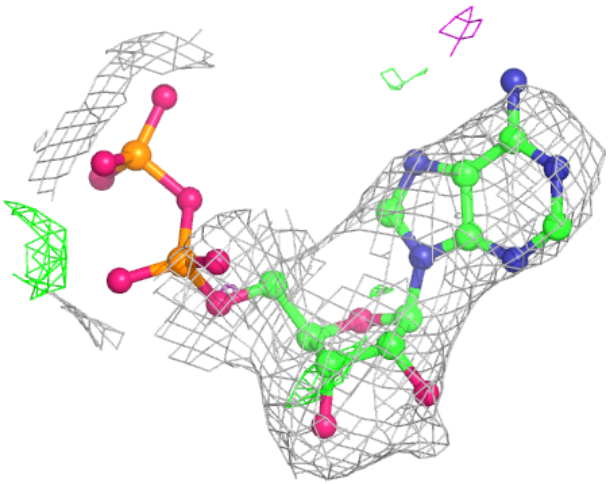
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

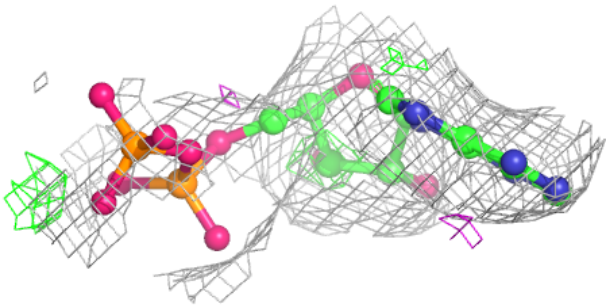
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	K	800	27/27	0.94	0.18	95,102,110,112	0
2	ADP	I	800	27/27	0.95	0.17	78,82,88,90	0
2	ADP	L	800	27/27	0.95	0.16	87,90,104,111	0
2	ADP	E	800	27/27	0.96	0.13	75,83,94,97	0
2	ADP	G	800	27/27	0.96	0.16	79,86,95,96	0
2	ADP	A	800	27/27	0.96	0.15	75,81,95,99	0
2	ADP	B	800	27/27	0.96	0.16	71,74,79,84	0
2	ADP	D	800	27/27	0.96	0.15	73,76,82,84	0
2	ADP	F	800	27/27	0.97	0.14	76,78,82,83	0
2	ADP	C	800	27/27	0.97	0.14	87,91,101,105	0
2	ADP	H	800	27/27	0.97	0.14	74,77,88,97	0
2	ADP	J	800	27/27	0.98	0.12	59,64,73,73	0

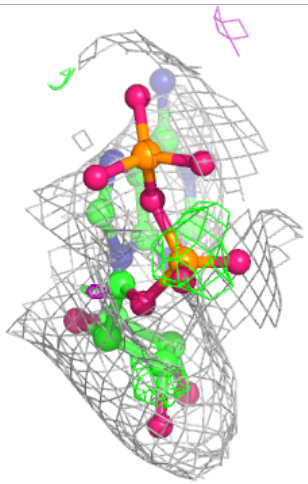
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

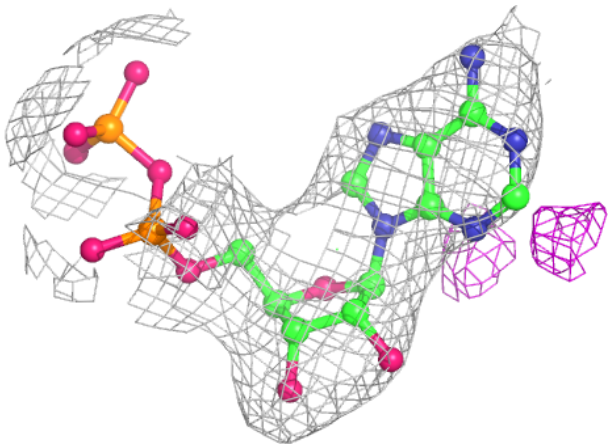


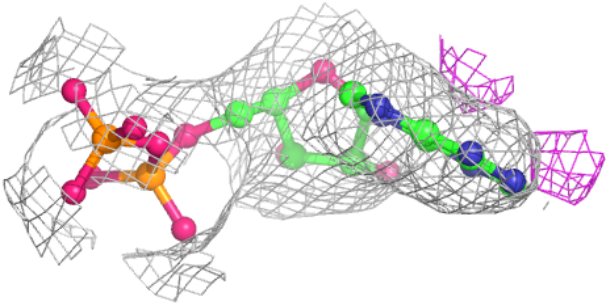


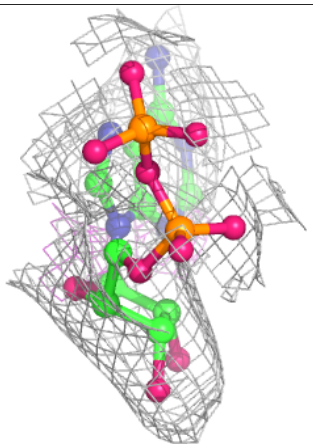


Electron density around ADP I 800:

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

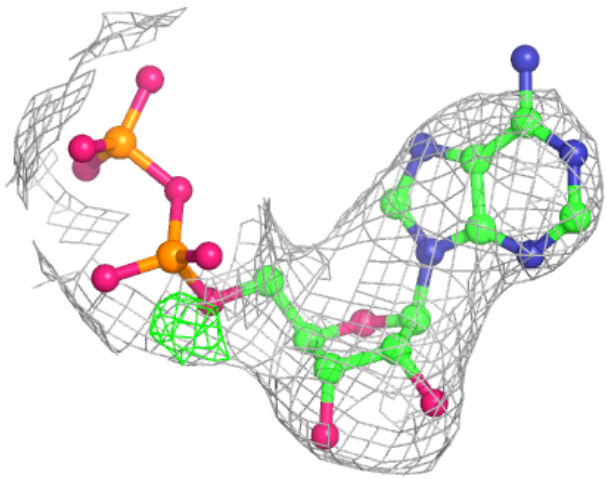


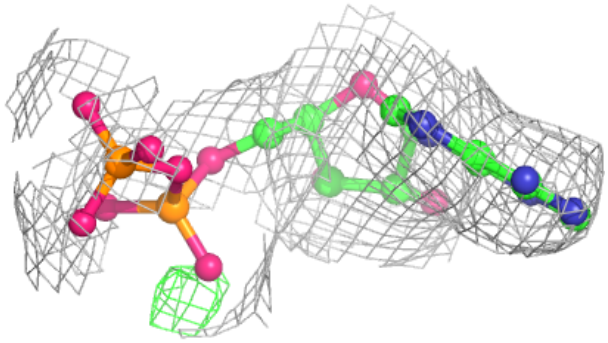


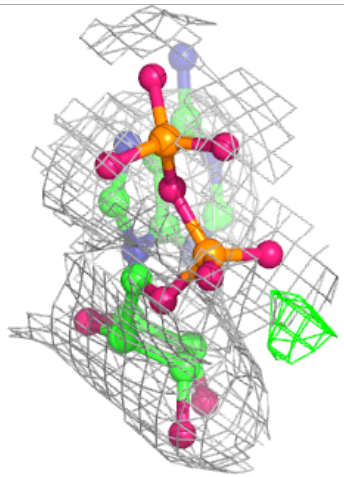


Electron density around ADP L 800:

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

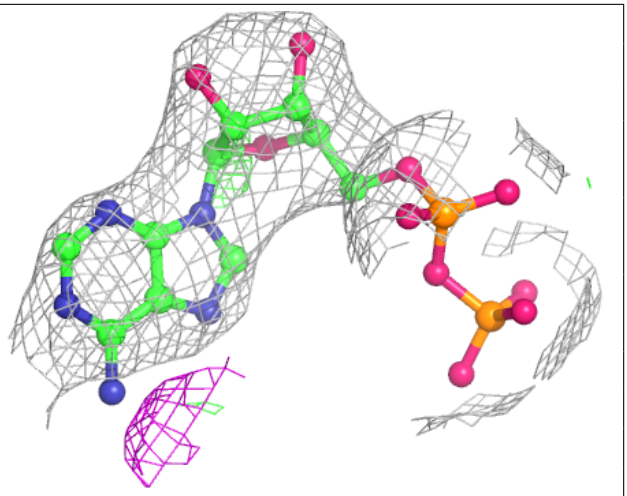


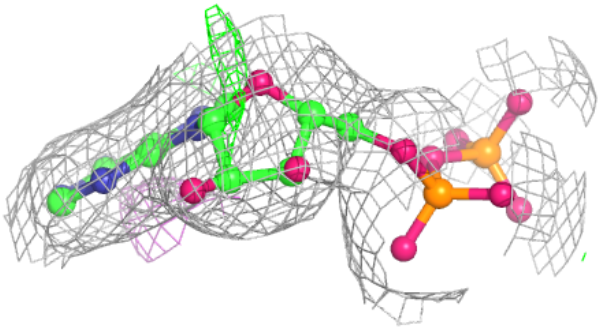


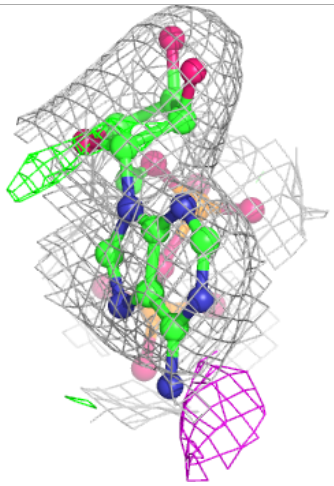


Electron density around ADP E 800:

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

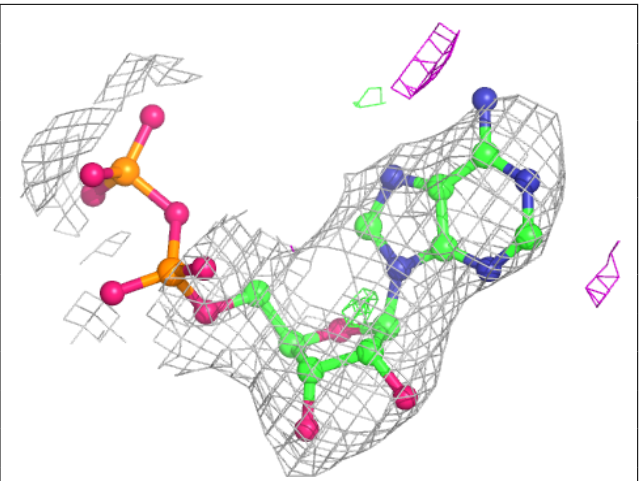


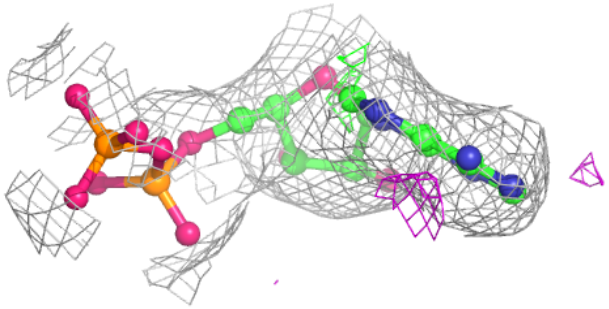


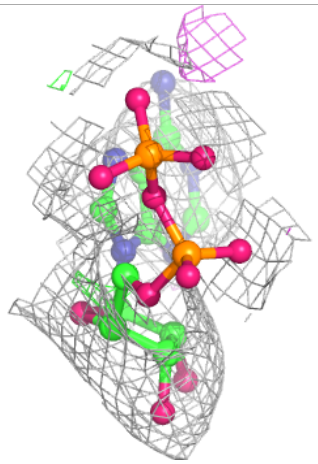


Electron density around ADP G 800:

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

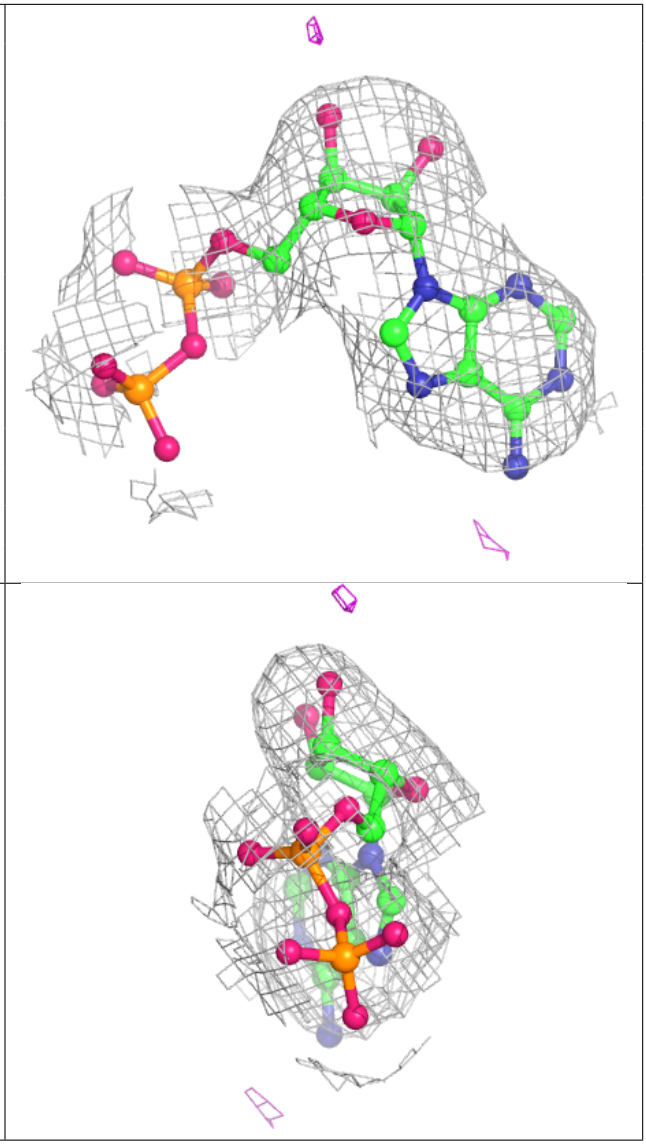






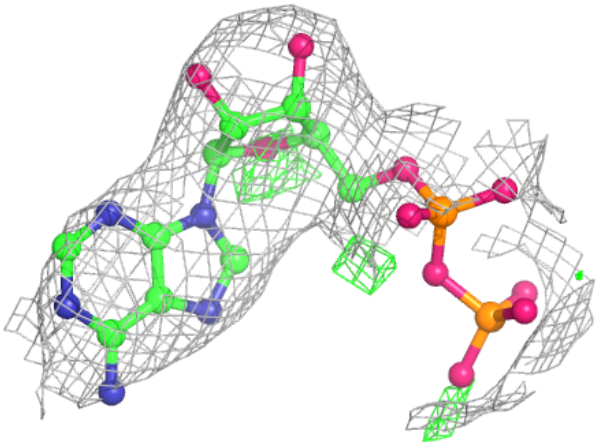
Electron density around ADP A 800:

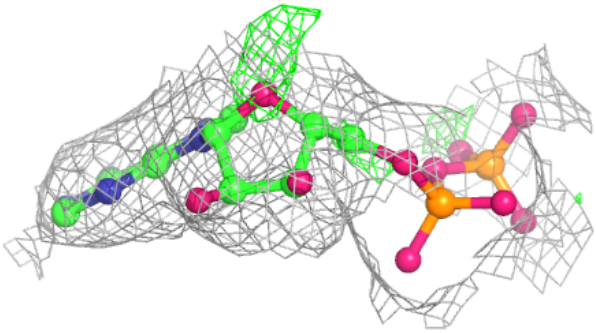
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

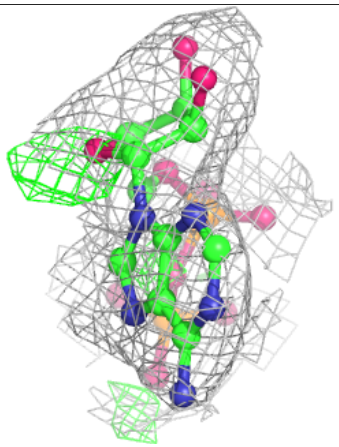


Electron density around ADP B 800:

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

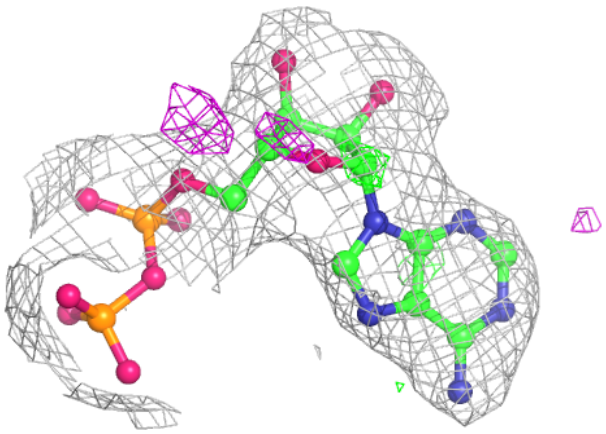


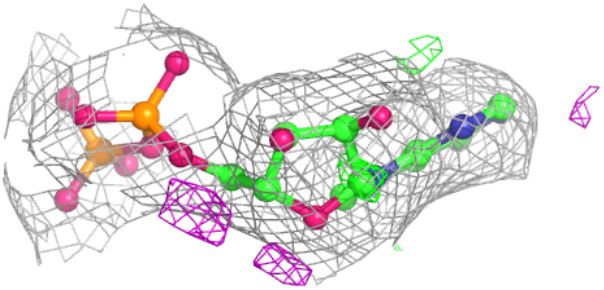


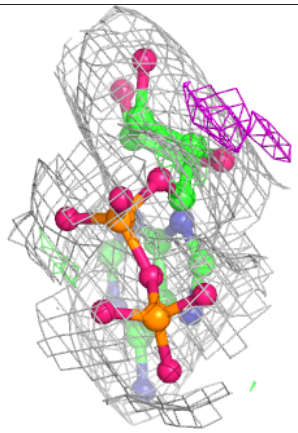


Electron density around ADP D 800:

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

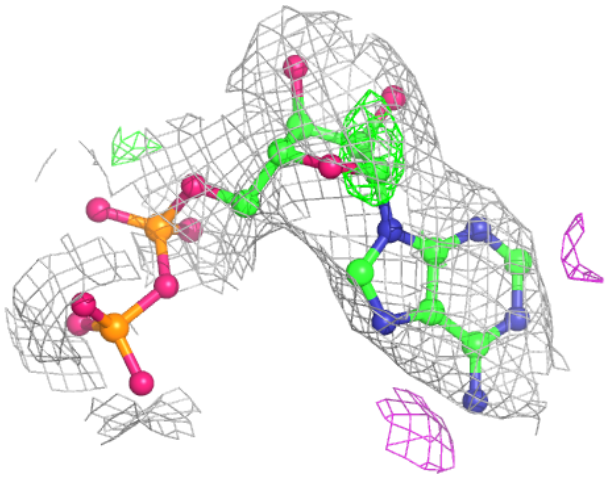


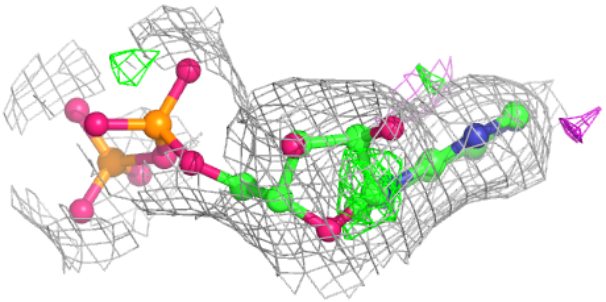


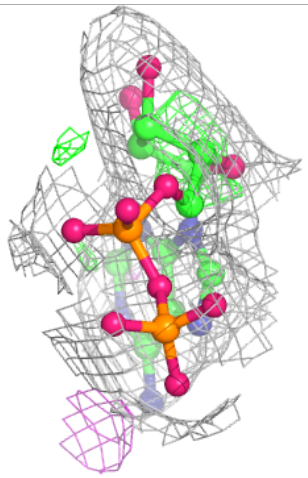


Electron density around ADP F 800:

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

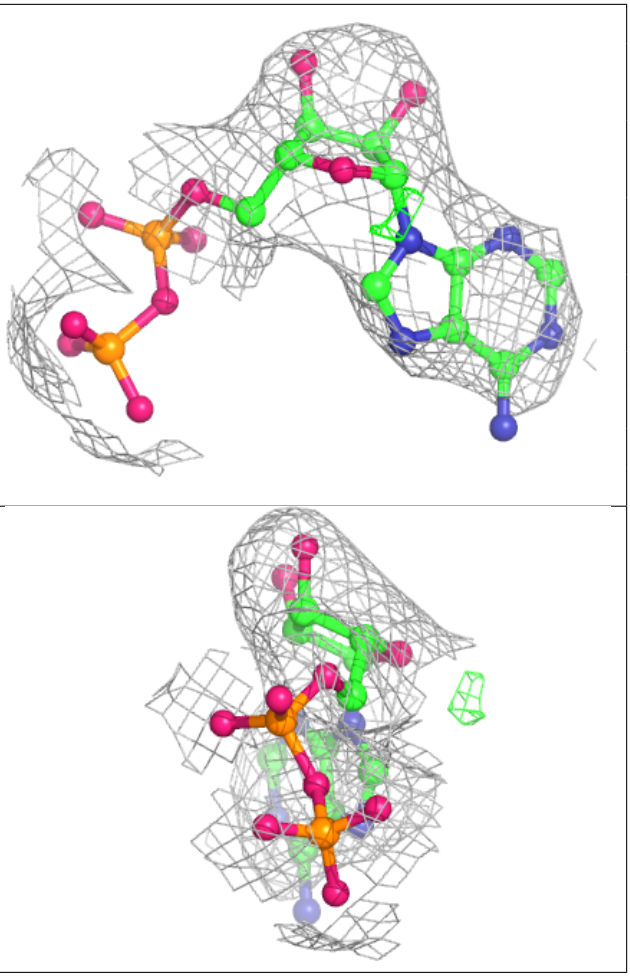






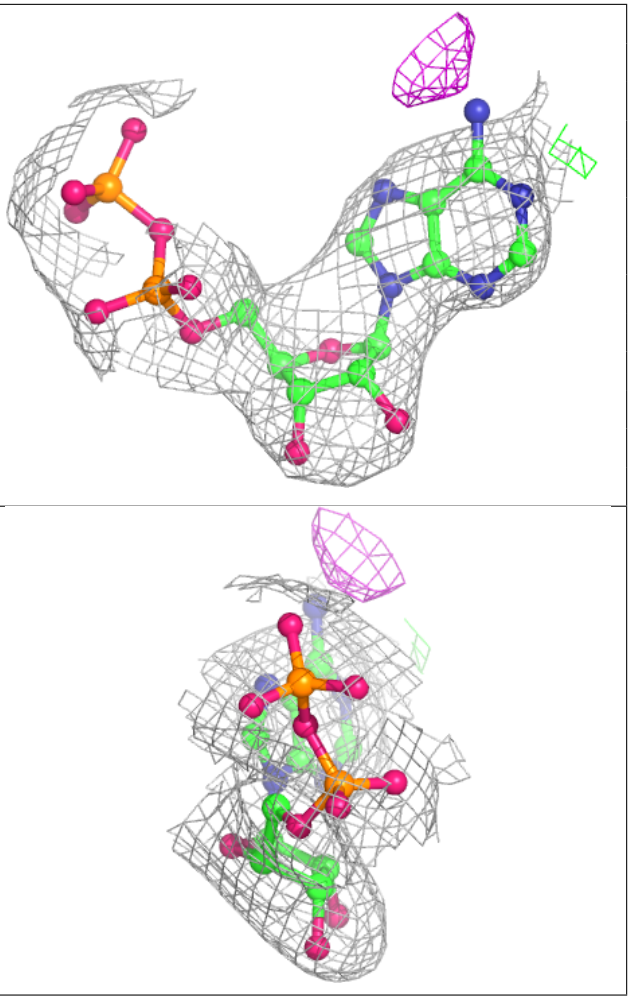
Electron density around ADP C 800:

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



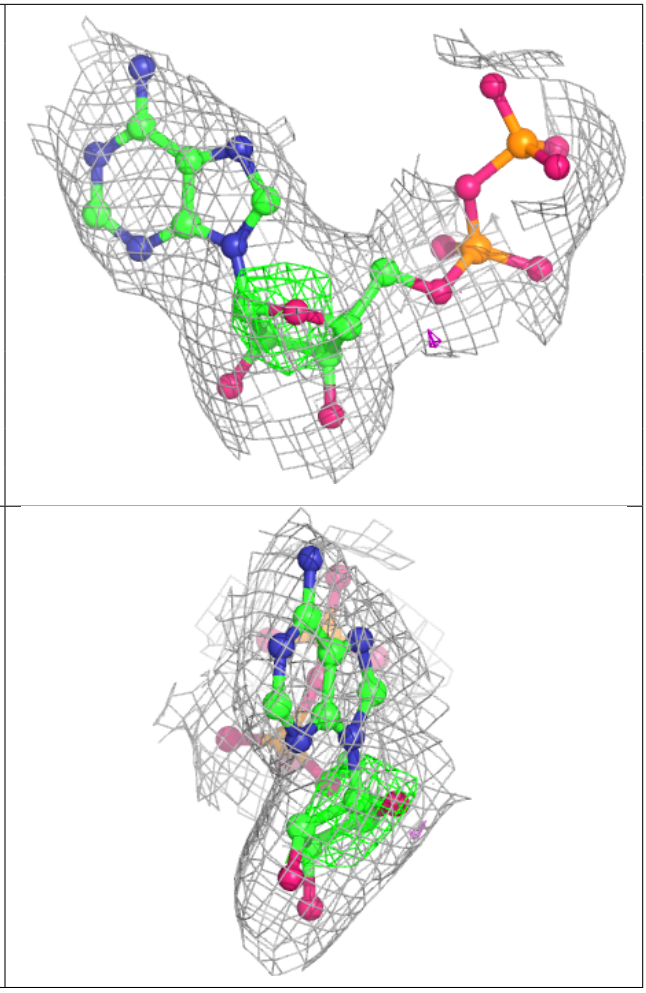
Electron density around ADP H 800:

$2mF_o$-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.