



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:57 PM UTC

PDB ID : 8PMI / pdb_00008pmi
Title : Structure of Nall indica cultivar IR64, construct 36-458 in presence of peptide from FZP protein
Authors : Huang, L.Y.; Rety, S.; Xi, X.G.
Deposited on : 2023-06-28
Resolution : 2.83 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

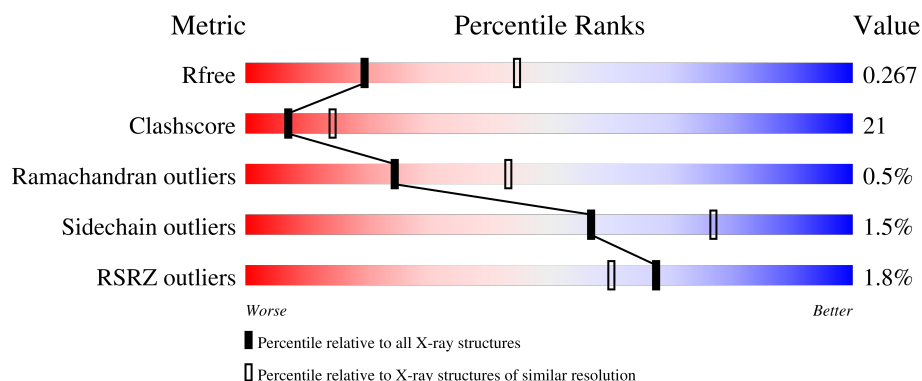
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	423	0% 58% 37% . .
1	B	423	0% 65% 31% .
1	C	423	2% 61% 35% . .
1	D	423	2% 58% 36% . .
1	E	423	3% 57% 38% . .

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Mol	Chain	Length	Quality of chain
1	F	423	2% 55% 40% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19163 atoms, of which 4 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 Protein NARROW LEAF 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3149	1996	552	589	12			
1	B	409	Total	C	N	O	S	0	0	0
			3160	2002	556	590	12			
1	C	408	Total	C	N	O	S	0	0	0
			3149	1996	552	589	12			
1	D	408	Total	C	N	O	S	0	0	0
			3149	1996	552	589	12			
1	E	408	Total	C	N	O	S	0	0	0
			3149	1996	552	589	12			
1	F	408	Total	C	N	O	S	0	0	0
			3149	1996	552	589	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ARG	HIS	variant	UNP B4XT64
B	233	ARG	HIS	variant	UNP B4XT64
C	233	ARG	HIS	variant	UNP B4XT64
D	233	ARG	HIS	variant	UNP B4XT64
E	233	ARG	HIS	variant	UNP B4XT64
F	233	ARG	HIS	variant	UNP B4XT64

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



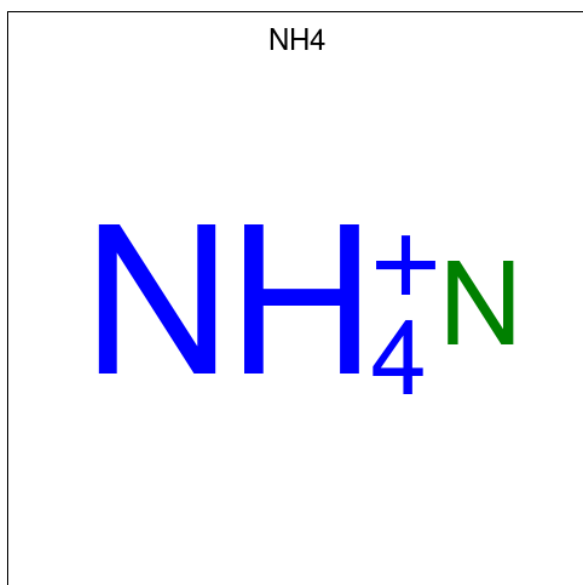
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	H	N	0	0
			5	4	1		

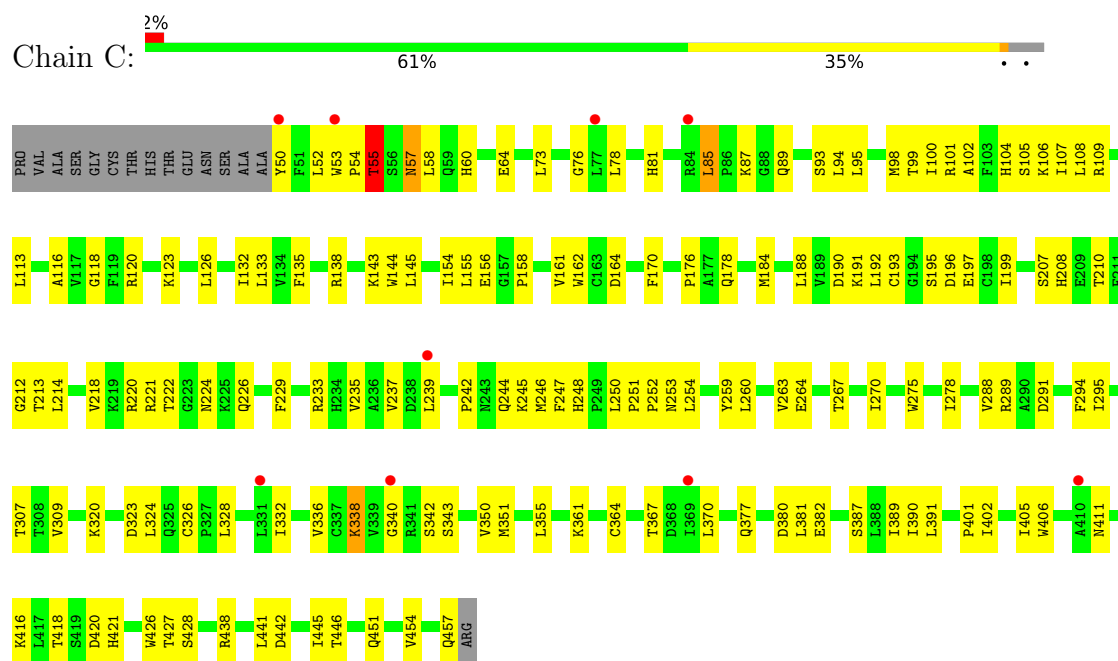
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain A:

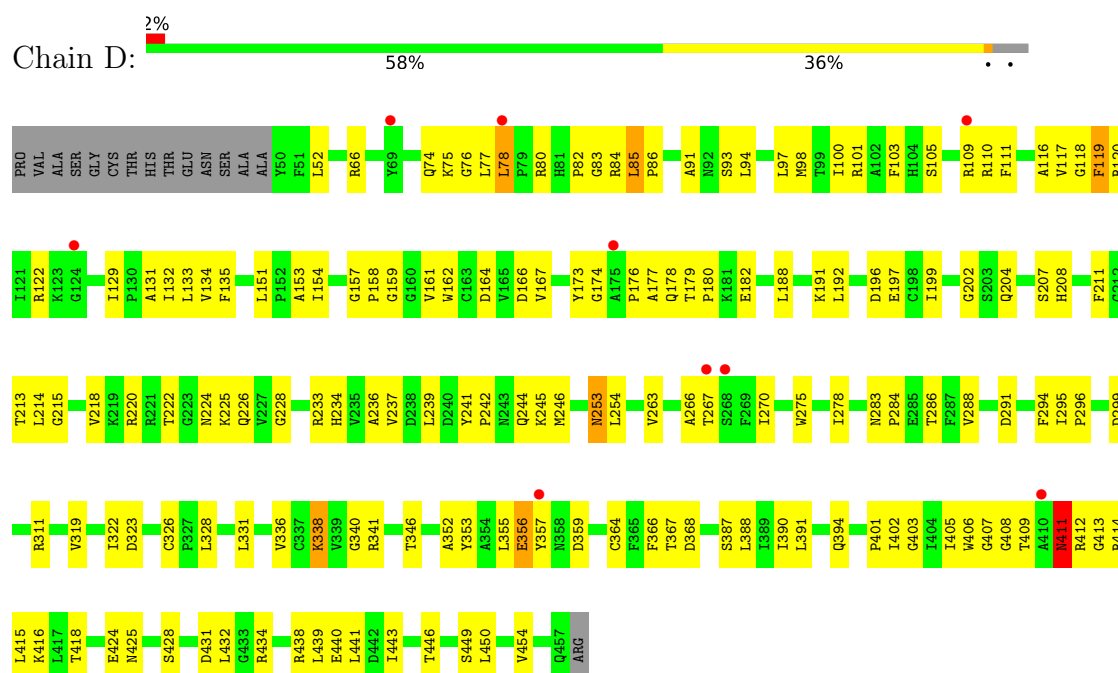
Amino Acid	Category
PRO	Green
VAL	Green
ALA	Green
SER	Green
GLY	Green
CYS	Green
THR	Green
HIS	Green
THR	Green
GLU	Green
ASN	Green
SER	Green
ALA	Green
ALA	Green
Y50	Green
F51	Yellow
T55	Green
S56	Green
A62	Green
A63	Green
E64	Green
G65	Green
R66	Yellow
A67	Green
N68	Green
Y69	Green
F70	Green
G71	Green
K75	Green
L78	Green
P79	Green
R80	Green
H81	Green
P82	Green
L85	Green
P86	Green
K87	Green
G88	Green
Q89	Green
L94	Green
L95	Green
D96	Green
L97	Green
R101	Green
S105	Green
K106	Green
I107	Green
L108	Green
R109	Green
S190	Green
F111	Green
F112	Green
L113	Yellow
G118	Green
F119	Green
R120	Green
L126	Green
A131	Green
I132	Green
L133	Green
V134	Green
F135	Green
V136	Green
A137	Green
R138	Green
H141	Green
K142	Green
K143	Green
W144	Yellow
L145	Green
Q149	Green
C150	Green
L151	Green
P152	Green
A153	Green
I154	Green
L155	Green
E156	Green
G160	Green
V161	Green
W162	Green
C163	Green
D164	Green
V165	Green
D166	Green
F170	Green
Y173	Green
A177	Green
Q178	Green
T179	Green
P180	Green
M184	Green
F185	Green
D190	Green
K191	Green
L192	Green
C193	Green
G194	Green
S195	Green
D196	Green
F197	Green
C198	Green
I199	Green
Q204	Green
V205	Green
G212	Green
T213	Green
L214	Green
I217	Green
V218	Green
K219	Green
R220	Green
R221	Green
K225	Green
F229	Green
L230	Green
R233	Green
H234	Green
V235	Green
A236	Green
L239	Green
Y240	Green
Q244	Green
K245	Green
M246	Green
P249	Green
L250	Green
L260	Green
G261	Green
A262	Green
V263	Green
E264	Green
R265	Green
S268	Green
F269	Green
I270	Green
W275	Green
I278	Yellow
Y279	Green
T282	Green
V288	Green
R289	Green
A290	Green
G403	Green
I404	Green
D291	Green
D292	Green
A293	Green
I295	Green
T307	Green
T308	Green
V309	Green
K320	Green
D323	Green
L324	Green
G325	Green
C326	Green
F327	Green
L328	Green
I332	Green
G333	Green
R334	Green
Q335	Green
V336	Green
C337	Green
K338	Green
R341	Green
S342	Green
S343	Green
G344	Green
H345	Green
T346	Green
L355	Green
D359	Green
E360	Green
T367	Green
D368	Green
I369	Green
L370	Green
R376	Green
E382	Green
G383	Green
I389	Green
I390	Green
L391	Green
Q394	Green
D395	Green
R400	Green
P401	Green
I402	Green
G403	Green
I404	Green
T405	Green
W406	Green
G407	Green
G408	Green
R414	Green
L415	Green
K416	Green
L417	Green
H421	Green
G422	Green
P423	Green
W426	Green
T427	Green
S428	Green
L432	Green
L441	Green
D442	Green
I443	Green
I444	Green
I445	Green
T446	Green
M447	Green
E448	Green
S449	Green
L450	Green
A453	Green
V454	Green
Q457	Green
ARG	Yellow

Chain B:

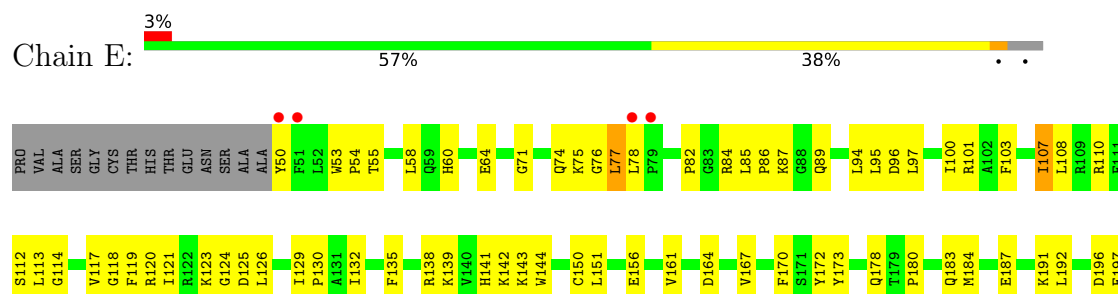
Token	Status
PRO	Unknown
VAL	Unknown
ALA	Unknown
SER	Unknown
GLY	Unknown
CYS	Unknown
THR	Unknown
HIS	Unknown
TRP	Unknown
GLU	Unknown
ASN	Unknown
SER	Unknown
ALA	Unknown
ALA	Unknown
Y50	Good
F51	Good
L52	Good
T55	Good
L58	Good
Q59	Good
A63	Good
R80	Good
H81	Good
L85	Good
P86	Good
K87	Good
G88	Good
Q89	Good
L94	Good
L95	Good
R101	Good
R109	Good
R110	Good
F111	Good
V117	Good
R120	Good
I132	Good
L133	Good
V134	Good
R138	Good
W144	Good
L145	Good
N146	Good
Q149	Good
C150	Good
L151	Good
E156	Good
V161	Good
D164	Good
V165	Good
H166	Good
V167	Good
V168	Good
A175	Good
P176	Good
A177	Good
Q178	Good
T179	Good
P180	Good
K181	Good
E182	Good
M184	Good
F185	Good
L188	Good
K191	Good
L192	Good
C193	Good
D196	Good
E197	Good
C198	Good
I199	Good
S207	Good
T210	Good
G212	Good
V218	Good
K219	Good
R220	Good
R221	Good
T222	Good
K225	Good
K226	Good
V227	Good
G228	Good
F229	Good
R233	Good
K234	Good
V235	Good
A236	Good
L239	Good
T240	Good
V241	Good
Q244	Good
K245	Good
M246	Good
V263	Good
T267	Good
D273	Good
V274	Good
W275	Good
I278	Good
N283	Good
T286	Good
V287	Good
P294	Good
I295	Good
P296	Good
T305	Good
T308	Good
V319	Good
K320	Good
D323	Good
C326	Good
P327	Good
L328	Good
V336	Good
C337	Good
K338	Good
V339	Good
G340	Good
S342	Good
S343	Good
G344	Good
Y353	Good
E360	Good
K361	Good
C364	Good
T367	Good
D368	Good
R376	Good
D380	Good
L381	Good
E382	Good
G383	Good
D384	Good
S385	Good
G386	Good
S387	Good
I390	Good
L391	Good
P401	Good
I402	Good
I405	Good
W406	Good
C407	Good
C408	Good
T409	Good
A410	Good
N411	Good
R412	Good
G413	Good
R414	Good
L415	Good
H421	Good
G422	Good
P423	Good
T427	Good
S428	Good
L441	Good
I444	Good
T446	Good
N447	Good
F448	Good
S449	Good
L450	Good
Q451	Good
Q455	Good
G456	Good
Q457	Good
R458	Good

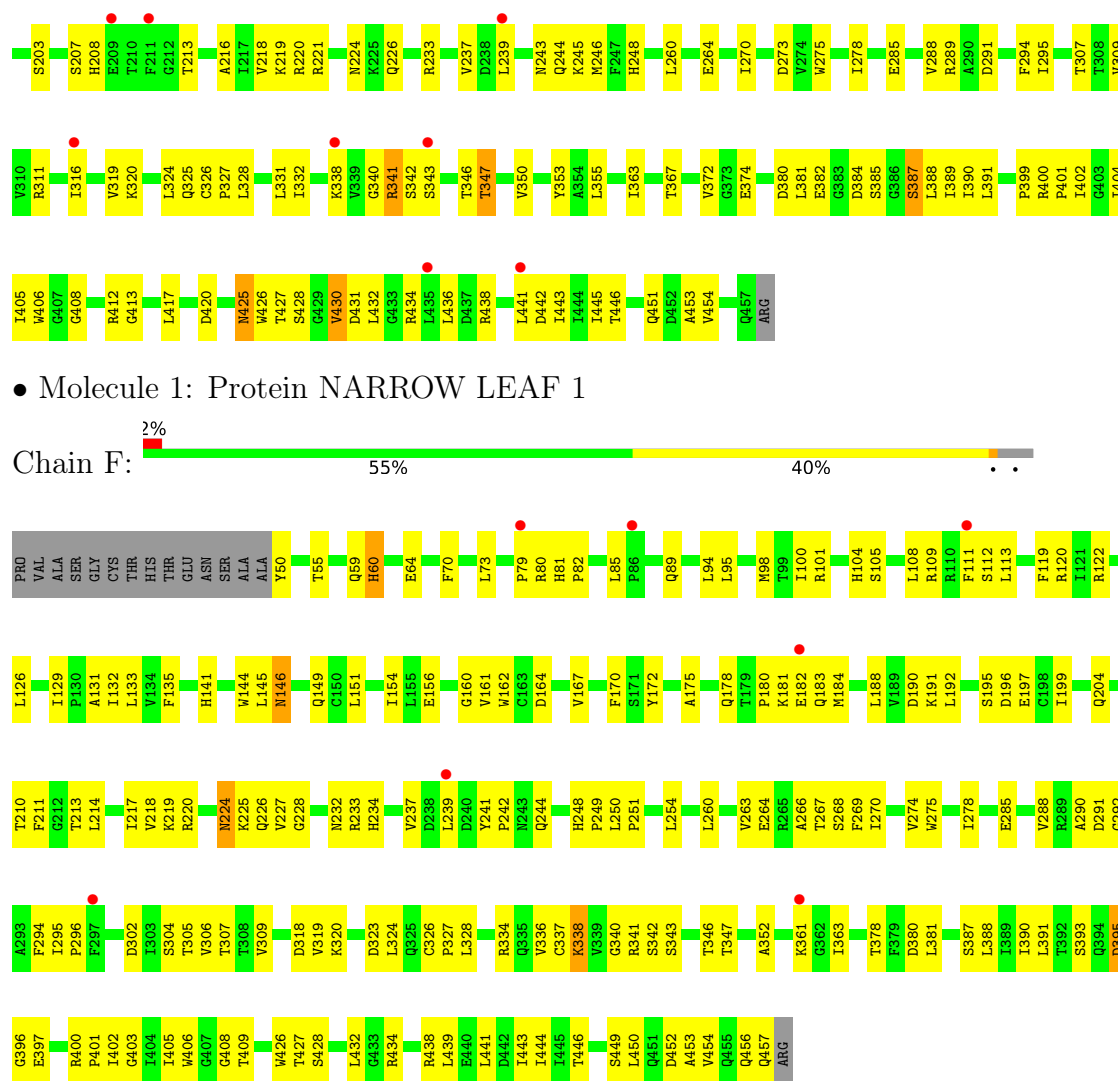


• Molecule 1: Protein NARROW LEAF 1



• Molecule 1: Protein NARROW LEAF 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.28Å 189.19Å 89.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.83 49.50 – 2.83	Depositor EDS
% Data completeness (in resolution range)	70.3 (49.50-2.83) 70.5 (49.50-2.83)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.268 0.206 , 0.267	Depositor DCC
R_{free} test set	2430 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19163	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NH4, SO4, ATP

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	0.16	0/3219	0.40	4/4371 (0.1%)
1	B	0.16	0/3230	0.32	0/4385
1	C	0.14	0/3219	0.34	2/4371 (0.0%)
1	D	0.13	0/3219	0.32	0/4371
1	E	0.12	0/3219	0.29	0/4371
1	F	0.13	0/3219	0.32	0/4371
All	All	0.14	0/19325	0.33	6/26240 (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	A	0	1
1	C	0	1
1	D	0	2
1	F	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLY	CA-C-N	8.15	136.21	122.20
1	A	65	GLY	C-N-CA	8.15	136.21	122.20
1	C	55	THR	CA-C-N	5.53	137.80	122.15
1	C	55	THR	C-N-CA	5.53	137.80	122.15
1	A	66	ARG	CA-C-N	5.27	128.08	120.38
1	A	66	ARG	C-N-CA	5.27	128.08	120.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	ARG	Peptide
1	C	55	THR	Peptide
1	D	174	GLY	Peptide
1	D	411	ASN	Peptide
1	F	60	HIS	Peptide

5.2 Too-close contacts

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	3149	0	3118	144	1
1	B	3160	0	3131	112	0
1	C	3149	0	3118	139	1
1	D	3149	0	3118	133	0
1	E	3149	0	3118	152	0
1	F	3149	0	3118	171	0
2	A	31	0	12	2	0
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	2	0
2	E	31	0	12	0	0
2	F	31	0	12	2	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	0	0	0
4	B	20	0	0	1	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	F	10	0	0	0	0
5	E	1	4	0	0	0
All	All	19159	4	18793	796	1

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 21.

All (796) 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:D:77:LEU:HD21	1:D:158:PRO:HA	1.10	1.09
1:F:184:MET:HG3	1:F:343:SER:HA	1.39	1.01
1:D:237:VAL:HA	1:D:244:GLN:HG2	1.41	1.01
1:E:82:PRO:HD2	1:E:85:LEU:HD23	1.42	1.01
1:C:178:GLN:HB3	1:C:210:THR:HG22	1.40	0.99
1:A:67:ALA:O	1:A:71:GLY:N	1.96	0.98
1:E:183:GLN:HB2	1:E:342:SER:HA	1.49	0.95
1:E:237:VAL:HA	1:E:244:GLN:HG2	1.47	0.94
1:F:336:VAL:HG12	1:F:391:LEU:HD23	1.50	0.94
1:E:95:LEU:HD12	1:E:325:GLN:HB3	1.49	0.94
1:C:118:GLY:HA2	1:C:332:ILE:HD13	1.48	0.93
1:B:239:LEU:HD23	1:E:239:LEU:HD22	1.48	0.93
1:E:341:ARG:HG3	1:E:342:SER:H	1.28	0.92
1:D:82:PRO:HD2	1:D:85:LEU:HD23	1.51	0.92
1:C:336:VAL:HG12	1:C:391:LEU:HD23	1.51	0.90
1:C:73:LEU:HD13	1:C:158:PRO:HB3	1.53	0.89
1:D:233:ARG:HB3	1:D:291:ASP:HB3	1.56	0.88
1:A:66:ARG:O	1:A:69:TYR:N	2.07	0.86
1:A:65:GLY:O	1:A:279:TYR:OH	1.94	0.84
1:A:106:LYS:HE3	1:A:282:THR:HG21	1.59	0.83
1:A:204:GLN:HB2	1:A:341:ARG:HG3	1.58	0.83
1:A:367:THR:HG21	1:A:428:SER:HB3	1.61	0.82
1:E:216:ALA:HB2	1:E:388:LEU:HD11	1.62	0.81
1:A:82:PRO:HD2	1:A:85:LEU:HD23	1.62	0.81
1:D:101:ARG:HB2	1:D:132:ILE:HD13	1.63	0.81
1:C:207:SER:HB3	1:C:246:MET:HE1	1.62	0.80
1:F:219:LYS:HG3	1:F:444:ILE:HD11	1.62	0.80
1:F:393:SER:OG	1:F:397:GLU:O	1.99	0.80
1:C:120:ARG:HH21	1:C:164:ASP:HB3	1.47	0.80
1:D:120:ARG:HH21	1:D:164:ASP:HB3	1.46	0.79
1:C:252:PRO:HG2	1:F:361:LYS:HE2	1.63	0.79
1:D:207:SER:HB3	1:D:246:MET:HE1	1.65	0.79
1:B:87:LYS:NZ	4:B:1006:SO4:O3	2.16	0.79
1:A:63:ALA:O	1:A:66:ARG:HB3	1.83	0.78
1:D:77:LEU:CD2	1:D:158:PRO:HA	2.04	0.78
1:A:95:LEU:HD11	1:A:278:ILE:HD11	1.65	0.78
1:D:413:GLY:O	1:D:425:ASN:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LYS:H	1:D:75:LYS:HD2	1.49	0.77
1:F:100:ILE:HD11	1:F:161:VAL:HG12	1.66	0.77
1:A:320:LYS:HG3	1:A:400:ARG:HH21	1.46	0.77
1:D:403:GLY:HA2	1:D:432:LEU:HB2	1.67	0.77
1:F:217:ILE:HG22	1:F:444:ILE:HD12	1.66	0.77
1:D:204:GLN:HB2	1:D:341:ARG:HG3	1.65	0.76
1:D:218:VAL:HG21	1:D:441:LEU:HD23	1.67	0.76
1:D:411:ASN:O	1:D:412:ARG:HG3	1.85	0.76
1:A:95:LEU:HD11	1:A:278:ILE:CD1	2.16	0.75
1:B:184:MET:HG3	1:B:343:SER:HA	1.67	0.75
1:F:219:LYS:HE3	1:F:444:ILE:CD1	2.17	0.75
1:F:251:PRO:HG2	1:F:254:LEU:HD13	1.66	0.75
1:E:207:SER:HB3	1:E:246:MET:HE1	1.68	0.75
1:C:118:GLY:HA2	1:C:332:ILE:CD1	2.17	0.75
1:B:80:ARG:HG2	1:B:81:HIS:H	1.50	0.75
1:C:239:LEU:HB2	1:F:239:LEU:HD22	1.69	0.74
1:F:220:ARG:HB3	1:F:225:LYS:HA	1.70	0.73
1:F:219:LYS:HE3	1:F:444:ILE:HD13	1.68	0.73
1:E:82:PRO:HG2	1:E:85:LEU:HA	1.69	0.73
1:C:237:VAL:HA	1:C:244:GLN:HG2	1.70	0.73
1:C:351:MET:HE2	1:C:351:MET:HA	1.71	0.72
1:E:60:HIS:O	1:E:64:GLU:HG2	1.88	0.72
1:E:107:ILE:HD12	1:E:110:ARG:HD2	1.69	0.72
1:A:67:ALA:O	1:A:70:PHE:N	2.23	0.72
1:B:193:CYS:SG	1:B:341:ARG:HG3	2.29	0.72
1:D:77:LEU:HD21	1:D:158:PRO:CA	2.05	0.71
1:F:213:THR:HG22	1:F:341:ARG:HG2	1.72	0.71
1:E:219:LYS:HD3	1:E:453:ALA:HB1	1.72	0.71
1:B:267:THR:HG22	1:E:50:TYR:HA	1.71	0.71
1:E:294:PHE:HB2	1:E:441:LEU:HD11	1.71	0.71
1:D:85:LEU:CD1	1:D:154:ILE:HG21	2.20	0.71
1:A:307:THR:OG1	1:A:309:VAL:HG12	1.91	0.70
1:D:83:GLY:O	1:D:85:LEU:HG	1.91	0.70
1:E:341:ARG:HG3	1:E:342:SER:N	2.04	0.70
1:F:108:LEU:O	1:F:112:SER:OG	2.08	0.70
1:D:134:VAL:HG11	1:D:151:LEU:HD11	1.74	0.70
1:F:95:LEU:CD1	1:F:278:ILE:HD13	2.21	0.70
1:A:239:LEU:HD12	1:D:239:LEU:HB3	1.73	0.70
1:A:51:PHE:HB2	1:D:266:ALA:O	1.91	0.69
1:E:338:LYS:HD2	1:E:387:SER:OG	1.92	0.69
1:B:212:GLY:HA3	1:B:235:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:HH21	1:D:239:LEU:HD21	1.56	0.69
1:E:82:PRO:HD2	1:E:85:LEU:CD2	2.22	0.69
1:E:123:LYS:O	1:E:123:LYS:HG2	1.92	0.69
1:F:95:LEU:HD12	1:F:278:ILE:HD13	1.75	0.69
1:B:305:THR:HG21	1:C:143:LYS:HD3	1.74	0.69
1:C:192:LEU:HD13	1:C:340:GLY:O	1.93	0.68
1:C:100:ILE:HD11	1:C:161:VAL:HG22	1.76	0.68
1:E:347:THR:HG23	1:E:374:GLU:HG2	1.74	0.68
1:D:446:THR:HG23	1:D:449:SER:H	1.58	0.68
1:C:264:GLU:HG3	1:F:55:THR:HG22	1.75	0.68
1:D:82:PRO:CD	1:D:85:LEU:HD23	2.23	0.68
1:C:367:THR:HG21	1:C:428:SER:HB3	1.76	0.68
1:D:357:TYR:CE2	1:D:359:ASP:HB3	2.30	0.67
1:F:192:LEU:HD13	1:F:340:GLY:O	1.94	0.67
1:E:320:LYS:HB2	1:E:400:ARG:HB3	1.75	0.67
1:A:336:VAL:HG12	1:A:391:LEU:HD23	1.75	0.67
1:E:101:ARG:HB2	1:E:132:ILE:HD13	1.75	0.67
1:A:55:THR:HG22	1:A:56:SER:H	1.60	0.67
1:A:156:GLU:OE2	1:A:160:GLY:HA2	1.95	0.67
1:F:319:VAL:HG23	1:F:443:ILE:HG21	1.76	0.67
1:F:291:ASP:OD2	1:F:406:TRP:NE1	2.24	0.66
1:B:184:MET:CG	1:B:343:SER:HA	2.25	0.66
1:D:270:ILE:HD13	1:D:438:ARG:HD3	1.77	0.66
1:D:390:ILE:HA	1:D:401:PRO:HA	1.76	0.66
1:B:246:MET:HE2	1:B:246:MET:HA	1.76	0.66
1:C:123:LYS:N	2:C:1001:ATP:O2G	2.26	0.66
1:C:212:GLY:HA3	1:C:235:VAL:HG11	1.77	0.66
1:D:267:THR:HG21	1:D:270:ILE:HD11	1.77	0.66
1:F:120:ARG:HH21	1:F:164:ASP:HB3	1.60	0.66
1:B:95:LEU:CD2	1:B:278:ILE:HD13	2.26	0.66
1:F:80:ARG:HH22	1:F:160:GLY:HA2	1.60	0.66
1:F:81:HIS:N	1:F:82:PRO:HD3	2.11	0.66
1:B:184:MET:HE2	1:B:381:LEU:HD11	1.77	0.66
1:C:390:ILE:HA	1:C:401:PRO:HA	1.78	0.66
1:D:177:ALA:O	1:D:179:THR:N	2.29	0.66
1:D:82:PRO:HD2	1:D:85:LEU:CD2	2.25	0.66
1:D:323:ASP:HB3	1:D:326:CYS:SG	2.36	0.66
1:E:213:THR:CG2	1:E:341:ARG:HG2	2.26	0.66
1:A:113:LEU:HD23	1:A:113:LEU:H	1.62	0.65
1:D:191:LYS:HB3	1:D:196:ASP:HB2	1.78	0.65
1:D:246:MET:HE2	1:D:246:MET:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ARG:HG2	1:E:442:ASP:OD2	1.96	0.65
1:B:305:THR:CG2	1:C:143:LYS:HD3	2.27	0.65
1:D:291:ASP:HB2	1:D:406:TRP:HE1	1.61	0.65
1:E:187:GLU:HG2	1:E:191:LYS:HE3	1.78	0.65
1:F:111:PHE:CD2	1:F:149:GLN:HG2	2.31	0.65
1:C:342:SER:HB3	1:C:381:LEU:HB2	1.78	0.65
1:E:94:LEU:HD21	1:E:353:TYR:CG	2.32	0.65
1:A:81:HIS:ND1	1:A:156:GLU:OE1	2.30	0.65
1:B:192:LEU:HD21	1:B:339:VAL:HG12	1.78	0.65
1:C:208:HIS:ND1	1:F:361:LYS:HD2	2.12	0.64
1:E:95:LEU:HG	1:E:324:LEU:CB	2.27	0.64
1:F:113:LEU:HD13	1:F:172:TYR:HE2	1.63	0.64
1:C:242:PRO:HG3	1:F:269:PHE:CG	2.32	0.64
1:E:389:ILE:HD11	1:E:405:ILE:HD13	1.79	0.64
1:C:245:LYS:O	1:C:246:MET:HE2	1.97	0.64
1:F:89:GLN:O	1:F:161:VAL:HA	1.97	0.64
1:D:204:GLN:CD	1:D:341:ARG:HD2	2.22	0.64
1:E:183:GLN:CB	1:E:342:SER:HA	2.27	0.64
1:A:135:PHE:HE2	1:A:355:LEU:HD13	1.61	0.64
1:A:134:VAL:HG11	1:A:151:LEU:HD21	1.79	0.64
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.62	0.63
1:C:178:GLN:CB	1:C:210:THR:HG22	2.25	0.63
1:B:168:VAL:HG11	1:B:415:LEU:HD11	1.79	0.63
1:E:203:SER:OG	1:E:311:ARG:NH2	2.29	0.63
1:C:213:THR:HG21	1:C:340:GLY:HA2	1.79	0.63
1:D:76:GLY:O	1:D:77:LEU:HD23	1.99	0.63
1:B:220:ARG:NH1	1:B:222:THR:O	2.32	0.63
1:E:113:LEU:HD12	1:E:114:GLY:N	2.14	0.63
1:E:289:ARG:HD3	1:E:406:TRP:CZ2	2.34	0.63
1:B:177:ALA:O	1:B:179:THR:N	2.31	0.63
1:D:236:ALA:O	1:D:244:GLN:HB3	1.99	0.63
1:B:446:THR:HG23	1:B:449:SER:H	1.64	0.62
1:C:253:ASN:OD1	1:F:361:LYS:HE3	1.99	0.62
1:E:71:GLY:O	1:E:75:LYS:HG2	1.99	0.62
1:C:391:LEU:HD21	1:C:402:ILE:HD13	1.82	0.62
1:D:131:ALA:HB2	1:D:164:ASP:HB2	1.80	0.62
1:A:101:ARG:HB2	1:A:132:ILE:HD13	1.82	0.62
1:A:120:ARG:HH21	1:A:164:ASP:HB3	1.64	0.62
1:B:193:CYS:HB3	1:C:138:ARG:NH2	2.15	0.62
1:F:182:GLU:HG2	1:F:183:GLN:H	1.65	0.62
1:A:359:ASP:OD1	1:A:360:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD13	1:A:162:TRP:CB	2.30	0.62
1:F:184:MET:CG	1:F:343:SER:HA	2.23	0.62
1:C:239:LEU:HB2	1:F:239:LEU:CD2	2.29	0.62
1:F:249:PRO:C	1:F:250:LEU:HD22	2.25	0.62
1:C:218:VAL:HG21	1:C:441:LEU:HD13	1.81	0.61
1:E:143:LYS:HE3	1:F:305:THR:HG21	1.82	0.61
1:F:275:TRP:CD1	1:F:288:VAL:HG11	2.35	0.61
1:A:82:PRO:HG2	1:A:85:LEU:H	1.63	0.61
1:C:135:PHE:HB3	1:C:170:PHE:HB3	1.82	0.61
1:F:204:GLN:HB2	1:F:341:ARG:HD2	1.83	0.61
1:B:239:LEU:HG	1:E:239:LEU:HB2	1.82	0.61
1:C:263:VAL:HG22	1:C:295:ILE:HG13	1.81	0.61
1:D:319:VAL:HG23	1:D:443:ILE:HG21	1.83	0.61
1:E:245:LYS:O	1:E:246:MET:HE2	2.00	0.61
1:B:191:LYS:HB3	1:B:196:ASP:HB2	1.81	0.61
1:A:151:LEU:HD13	2:A:1001:ATP:HN61	1.65	0.61
1:F:446:THR:HG23	1:F:449:SER:H	1.65	0.61
1:B:227:VAL:HG12	1:B:457:GLN:OE1	2.00	0.61
1:B:245:LYS:O	1:B:246:MET:HE2	2.01	0.61
1:C:104:HIS:O	1:C:108:LEU:HD13	2.00	0.61
1:B:101:ARG:HB2	1:B:132:ILE:HD13	1.83	0.61
1:A:204:GLN:CD	1:A:341:ARG:HD2	2.26	0.61
1:C:242:PRO:HG3	1:F:269:PHE:CD1	2.36	0.61
1:E:120:ARG:HH11	1:E:164:ASP:HB3	1.65	0.61
1:E:143:LYS:O	1:E:143:LYS:HD3	2.01	0.61
1:A:111:PHE:CZ	1:A:149:GLN:HG2	2.36	0.60
1:E:316:ILE:HA	1:E:399:PRO:HG2	1.82	0.60
1:A:177:ALA:HB2	1:A:382:GLU:OE1	2.01	0.60
1:C:445:ILE:HG13	1:C:446:THR:HG23	1.83	0.60
1:B:367:THR:HG21	1:B:428:SER:HB2	1.83	0.60
1:F:85:LEU:HD12	1:F:162:TRP:CG	2.37	0.60
1:F:387:SER:HB2	1:F:405:ILE:HD12	1.84	0.60
1:C:94:LEU:HB3	1:C:98:MET:HE3	1.83	0.60
1:F:80:ARG:HH22	1:F:160:GLY:CA	2.15	0.60
1:C:191:LYS:HB3	1:C:196:ASP:HB2	1.84	0.60
1:C:105:SER:O	1:C:109:ARG:HG2	2.02	0.60
1:C:233:ARG:HB3	1:C:291:ASP:HB3	1.84	0.60
1:A:193:CYS:HB3	1:B:138:ARG:NH2	2.17	0.60
1:C:76:GLY:O	1:C:78:LEU:HD13	2.01	0.60
1:E:95:LEU:HG	1:E:324:LEU:HB3	1.84	0.60
1:C:416:LYS:HE2	1:C:418:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:ILE:HG21	1:E:399:PRO:HB2	1.83	0.59
1:C:323:ASP:HB3	1:C:326:CYS:SG	2.42	0.59
1:A:105:SER:O	1:A:109:ARG:HG3	2.02	0.59
1:B:390:ILE:HA	1:B:401:PRO:HA	1.84	0.59
1:D:367:THR:HG21	1:D:428:SER:HB2	1.83	0.59
1:F:101:ARG:HB2	1:F:132:ILE:HD13	1.83	0.59
1:A:389:ILE:HG12	1:A:403:GLY:O	2.02	0.59
1:A:390:ILE:HA	1:A:401:PRO:HA	1.84	0.59
1:C:145:LEU:HD11	2:C:1001:ATP:C4	2.38	0.59
1:B:109:ARG:HH12	1:B:283:ASN:HB2	1.66	0.59
1:B:199:ILE:HG13	1:C:144:TRP:CH2	2.37	0.59
1:E:191:LYS:HB3	1:E:196:ASP:HB2	1.85	0.59
1:E:151:LEU:HD12	1:E:167:VAL:HG22	1.85	0.59
1:E:243:ASN:ND2	1:E:245:LYS:HE2	2.18	0.59
1:A:111:PHE:CE1	1:A:149:GLN:HG2	2.37	0.58
1:A:144:TRP:CH2	1:C:199:ILE:HG13	2.38	0.58
1:B:336:VAL:HG12	1:B:391:LEU:HD23	1.84	0.58
1:E:138:ARG:NH1	1:E:139:LYS:O	2.36	0.58
1:B:225:LYS:HE3	1:B:458:ARG:HH22	1.68	0.58
1:E:224:ASN:HB2	1:E:226:GLN:CD	2.28	0.58
1:D:353:TYR:HA	1:D:368:ASP:O	2.02	0.58
1:E:121:ILE:HG23	1:E:125:ASP:C	2.29	0.58
1:E:233:ARG:O	1:E:237:VAL:HG22	2.03	0.58
1:C:50:TYR:OH	1:F:438:ARG:HB3	2.03	0.58
1:D:207:SER:CB	1:D:246:MET:HE1	2.32	0.58
1:C:85:LEU:CG	1:C:154:ILE:HG21	2.34	0.58
1:F:219:LYS:NZ	1:F:449:SER:O	2.37	0.58
1:F:218:VAL:HG21	1:F:441:LEU:HD13	1.84	0.58
1:B:233:ARG:HH12	1:E:239:LEU:HD21	1.68	0.58
1:A:270:ILE:HG22	1:A:275:TRP:HB2	1.86	0.57
1:A:94:LEU:HD21	1:A:332:ILE:HD11	1.85	0.57
1:F:233:ARG:HH11	1:F:268:SER:CB	2.17	0.57
1:B:233:ARG:NH1	1:E:239:LEU:HD11	2.20	0.57
1:E:451:GLN:HA	1:E:454:VAL:HG12	1.84	0.57
1:A:323:ASP:HB3	1:A:326:CYS:SG	2.44	0.57
1:B:188:LEU:O	1:B:192:LEU:HD13	2.05	0.57
1:D:241:TYR:CD2	1:D:242:PRO:HD2	2.40	0.57
1:C:55:THR:OG1	1:C:57:ASN:OD1	2.21	0.57
1:A:191:LYS:HB3	1:A:196:ASP:HB2	1.86	0.57
1:E:94:LEU:HD11	1:E:117:VAL:HG23	1.87	0.57
1:E:192:LEU:HD13	1:E:340:GLY:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:LYS:HB3	1:F:196:ASP:HB2	1.86	0.57
1:D:336:VAL:HG12	1:D:391:LEU:HD23	1.86	0.57
1:E:406:TRP:CZ2	1:E:408:GLY:HA3	2.40	0.57
1:A:177:ALA:O	1:A:179:THR:N	2.38	0.57
1:B:361:LYS:HE3	1:E:208:HIS:NE2	2.19	0.57
1:F:307:THR:OG1	1:F:309:VAL:HG12	2.05	0.57
1:B:207:SER:HB3	1:B:246:MET:HE1	1.86	0.57
1:F:323:ASP:HB3	1:F:326:CYS:SG	2.45	0.57
1:A:196:ASP:OD1	1:A:197:GLU:N	2.37	0.56
1:E:270:ILE:CD1	1:E:438:ARG:HG3	2.35	0.56
1:E:347:THR:HG23	1:E:374:GLU:CG	2.35	0.56
1:A:294:PHE:HB2	1:A:441:LEU:HD11	1.85	0.56
1:B:239:LEU:CD2	1:E:239:LEU:HD22	2.29	0.56
1:D:411:ASN:O	1:D:411:ASN:ND2	2.39	0.56
1:E:319:VAL:HG23	1:E:443:ILE:HG21	1.87	0.56
1:F:146:ASN:HD21	1:F:149:GLN:HG3	1.71	0.56
1:B:275:TRP:CD1	1:B:288:VAL:HG11	2.40	0.56
1:D:94:LEU:HD12	1:D:94:LEU:H	1.70	0.56
1:D:275:TRP:CD1	1:D:288:VAL:HG11	2.41	0.56
1:E:113:LEU:HD13	1:E:172:TYR:CE2	2.41	0.56
1:F:341:ARG:HG3	1:F:342:SER:H	1.70	0.56
1:B:406:TRP:CE3	1:B:411:ASN:HB3	2.41	0.56
1:F:135:PHE:HB3	1:F:170:PHE:HB3	1.88	0.56
1:B:80:ARG:HG2	1:B:81:HIS:N	2.20	0.56
1:C:252:PRO:HD2	1:F:361:LYS:NZ	2.21	0.56
1:E:96:ASP:O	1:E:100:ILE:HG13	2.06	0.56
1:F:232:ASN:HA	1:F:292:GLY:HA2	1.86	0.56
1:D:109:ARG:HH12	1:D:283:ASN:HB2	1.71	0.56
1:A:338:LYS:HE3	1:A:346:THR:OG1	2.06	0.56
1:F:85:LEU:HD11	1:F:156:GLU:HG2	1.88	0.56
1:A:275:TRP:CD1	1:A:288:VAL:HG11	2.41	0.55
1:D:338:LYS:NZ	1:D:346:THR:OG1	2.31	0.55
1:E:380:ASP:OD1	1:E:427:THR:OG1	2.23	0.55
1:C:451:GLN:HA	1:C:454:VAL:HG12	1.88	0.55
1:E:55:THR:OG1	1:E:58:LEU:HG	2.05	0.55
1:A:406:TRP:CH2	1:A:408:GLY:HA3	2.41	0.55
1:B:411:ASN:ND2	1:B:412:ARG:HG3	2.21	0.55
1:E:89:GLN:O	1:E:161:VAL:HA	2.06	0.55
1:A:269:PHE:C	1:A:270:ILE:HD12	2.31	0.55
1:E:173:TYR:HB2	1:E:413:GLY:HA2	1.87	0.55
1:A:338:LYS:HD3	1:A:405:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:VAL:HA	1:F:244:GLN:HG2	1.89	0.55
1:D:135:PHE:HE2	1:D:355:LEU:HD13	1.70	0.55
1:D:322:ILE:HG23	1:D:331:LEU:HD22	1.88	0.55
1:E:248:HIS:HB2	1:E:260:LEU:HD11	1.87	0.55
1:E:404:ILE:CG2	1:E:430:VAL:HG22	2.37	0.55
1:E:113:LEU:HD13	1:E:172:TYR:HE2	1.72	0.55
1:F:274:VAL:HG12	1:F:438:ARG:HH12	1.72	0.55
1:D:86:PRO:O	1:D:162:TRP:NE1	2.36	0.55
1:E:233:ARG:HB3	1:E:291:ASP:HB3	1.88	0.55
1:B:120:ARG:HH21	1:B:164:ASP:HB3	1.72	0.54
1:F:178:GLN:HB3	1:F:210:THR:HB	1.89	0.54
1:B:207:SER:OG	1:B:210:THR:OG1	2.05	0.54
1:D:116:ALA:HB1	1:D:352:ALA:HB1	1.89	0.54
1:D:387:SER:HB2	1:D:405:ILE:HD11	1.90	0.54
1:E:246:MET:HE2	1:E:246:MET:HA	1.88	0.54
1:F:267:THR:HG23	1:F:439:LEU:HD21	1.88	0.54
1:B:239:LEU:HD21	1:E:239:LEU:HD13	1.90	0.54
1:C:307:THR:OG1	1:C:309:VAL:HG12	2.07	0.54
1:B:212:GLY:HA3	1:B:235:VAL:CG1	2.37	0.54
1:F:146:ASN:ND2	1:F:149:GLN:HG3	2.22	0.54
1:A:204:GLN:OE1	1:A:341:ARG:HD2	2.07	0.54
1:D:122:ARG:HA	2:D:1001:ATP:O2B	2.08	0.54
1:E:367:THR:HG21	1:E:428:SER:HB3	1.88	0.54
1:C:267:THR:HG22	1:F:50:TYR:HD1	1.72	0.54
1:E:207:SER:CB	1:E:246:MET:HE1	2.37	0.54
1:A:71:GLY:O	1:A:75:LYS:HG3	2.08	0.54
1:A:394:GLN:HG3	1:A:395:ASP:OD1	2.07	0.54
1:A:218:VAL:HG21	1:A:441:LEU:HD13	1.89	0.53
1:A:389:ILE:HG12	1:A:403:GLY:C	2.32	0.53
1:C:320:LYS:HB3	1:C:402:ILE:HG22	1.90	0.53
1:D:82:PRO:HG2	1:D:85:LEU:HA	1.90	0.53
1:D:233:ARG:HG2	1:D:234:HIS:H	1.72	0.53
1:A:221:ARG:HG2	1:A:442:ASP:OD2	2.08	0.53
1:A:270:ILE:HD13	1:A:290:ALA:HB3	1.90	0.53
1:B:176:PRO:HG3	1:B:408:GLY:HA2	1.90	0.53
1:C:120:ARG:NH2	1:C:164:ASP:HB3	2.19	0.53
1:B:85:LEU:HD11	1:B:156:GLU:OE2	2.09	0.53
1:C:226:GLN:HA	1:C:457:GLN:HG2	1.90	0.53
1:D:294:PHE:CD1	1:D:441:LEU:HD21	2.43	0.53
1:F:151:LEU:HD13	1:F:167:VAL:HG22	1.91	0.53
1:A:85:LEU:HD13	1:A:162:TRP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:OD1	1:C:197:GLU:N	2.41	0.53
1:A:107:ILE:HG22	1:A:110:ARG:HH12	1.73	0.53
1:F:154:ILE:HD13	1:F:164:ASP:HA	1.91	0.53
1:F:175:ALA:HB2	1:F:409:THR:HG23	1.89	0.53
1:A:62:ALA:O	1:A:66:ARG:HB2	2.08	0.53
1:A:118:GLY:HA2	1:A:332:ILE:HG12	1.90	0.53
1:C:320:LYS:HD2	1:C:391:LEU:CD1	2.38	0.53
1:D:196:ASP:OD1	1:D:197:GLU:N	2.42	0.53
1:A:82:PRO:HD2	1:A:85:LEU:CD2	2.37	0.53
1:F:131:ALA:HB2	1:F:164:ASP:HB2	1.89	0.53
1:F:406:TRP:CH2	1:F:408:GLY:HA3	2.44	0.53
1:E:213:THR:HG22	1:E:341:ARG:HG2	1.91	0.53
1:A:63:ALA:O	1:A:66:ARG:CB	2.54	0.53
1:B:55:THR:OG1	1:B:58:LEU:HD23	2.08	0.53
1:B:175:ALA:HA	1:B:409:THR:O	2.08	0.52
1:B:406:TRP:HE3	1:B:411:ASN:HB3	1.74	0.52
1:D:431:ASP:OD2	1:D:434:ARG:NH1	2.36	0.52
1:A:133:LEU:HD23	1:A:166:ASP:HB3	1.91	0.52
1:B:207:SER:CB	1:B:246:MET:HE1	2.40	0.52
1:D:224:ASN:OD1	1:D:226:GLN:HB3	2.10	0.52
1:F:334:ARG:HB3	1:F:391:LEU:HD22	1.91	0.52
1:F:336:VAL:HG12	1:F:391:LEU:CD2	2.31	0.52
1:F:388:LEU:HD23	1:F:390:ILE:HD11	1.89	0.52
1:A:265:ARG:HB3	1:D:52:LEU:HD23	1.91	0.52
1:C:253:ASN:ND2	1:C:254:LEU:HG	2.24	0.52
1:C:263:VAL:HG22	1:C:295:ILE:CG1	2.39	0.52
1:D:270:ILE:HD13	1:D:438:ARG:CD	2.39	0.52
1:B:342:SER:HB2	1:B:384:ASP:CG	2.35	0.52
1:C:220:ARG:NH2	1:C:222:THR:OG1	2.42	0.52
1:B:117:VAL:HG22	1:B:353:TYR:O	2.10	0.52
1:F:219:LYS:HD3	1:F:453:ALA:CB	2.40	0.52
1:A:56:SER:HB2	1:D:299:ASP:OD1	2.10	0.52
1:A:87:LYS:HD3	1:A:162:TRP:HZ2	1.75	0.52
1:E:119:PHE:HB2	1:E:126:LEU:HD11	1.90	0.52
1:E:332:ILE:N	1:E:332:ILE:HD12	2.25	0.52
1:A:233:ARG:HB3	1:A:291:ASP:HB3	1.91	0.52
1:D:263:VAL:HG22	1:D:295:ILE:HG13	1.91	0.52
1:E:141:HIS:HB3	1:E:144:TRP:CD1	2.45	0.52
1:A:67:ALA:HA	1:A:70:PHE:CD2	2.45	0.52
1:A:278:ILE:HG22	1:A:279:TYR:N	2.25	0.52
1:D:406:TRP:CH2	1:D:408:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HD12	1:A:295:ILE:N	2.24	0.51
1:C:85:LEU:HD21	1:C:154:ILE:HG21	1.93	0.51
1:D:208:HIS:ND1	1:D:253:ASN:OD1	2.39	0.51
1:C:126:LEU:HD22	1:C:351:MET:HE1	1.92	0.51
1:E:118:GLY:HA2	1:E:332:ILE:HG12	1.92	0.51
1:E:120:ARG:NH1	1:E:164:ASP:HB3	2.24	0.51
1:A:86:PRO:O	1:A:162:TRP:NE1	2.32	0.51
1:D:66:ARG:HD2	1:D:284:PRO:HA	1.93	0.51
1:B:218:VAL:HG21	1:B:441:LEU:HD13	1.92	0.51
1:C:237:VAL:HA	1:C:244:GLN:CG	2.40	0.51
1:B:110:ARG:HG2	1:B:111:PHE:CE2	2.45	0.51
1:B:80:ARG:HD2	1:B:156:GLU:OE2	2.10	0.51
1:F:98:MET:HE1	1:F:324:LEU:HD13	1.91	0.51
1:C:418:THR:OG1	1:C:421:HIS:HB2	2.10	0.51
1:F:145:LEU:HD11	2:F:1001:ATP:C4	2.45	0.51
1:F:426:TRP:HZ3	1:F:428:SER:HB3	1.75	0.51
1:A:270:ILE:CG2	1:A:275:TRP:HB2	2.41	0.51
1:B:239:LEU:CD2	1:E:239:LEU:HD13	2.41	0.51
1:A:185:PHE:CE1	1:B:423:PRO:HD3	2.46	0.51
1:B:59:GLN:O	1:B:63:ALA:N	2.33	0.51
1:E:431:ASP:OD2	1:E:434:ARG:NH1	2.38	0.51
1:F:80:ARG:NH2	1:F:160:GLY:HA2	2.26	0.51
1:C:176:PRO:HB3	1:C:382:GLU:HB3	1.93	0.51
1:A:85:LEU:HD21	1:A:156:GLU:OE1	2.11	0.50
1:A:153:ALA:O	1:A:154:ILE:HD13	2.10	0.50
1:A:212:GLY:HA3	1:A:235:VAL:HG11	1.92	0.50
1:A:370:LEU:HD11	1:A:426:TRP:HB2	1.93	0.50
1:C:184:MET:HG2	1:C:343:SER:HA	1.93	0.50
1:C:239:LEU:HD13	1:F:239:LEU:HB2	1.94	0.50
1:B:361:LYS:HG3	1:E:208:HIS:CE1	2.46	0.50
1:D:167:VAL:HG21	2:D:1001:ATP:C8	2.45	0.50
1:D:220:ARG:HG3	1:D:222:THR:H	1.76	0.50
1:E:184:MET:HE2	1:E:381:LEU:HD11	1.93	0.50
1:E:295:ILE:HD12	1:E:295:ILE:N	2.27	0.50
1:E:434:ARG:O	1:E:438:ARG:HG2	2.11	0.50
1:F:217:ILE:HD12	1:F:217:ILE:H	1.76	0.50
1:F:274:VAL:HG12	1:F:438:ARG:NH1	2.27	0.50
1:A:81:HIS:CE1	1:A:156:GLU:HB3	2.46	0.50
1:B:146:ASN:HD21	1:B:149:GLN:HG3	1.75	0.50
1:B:308:THR:HG21	1:B:444:ILE:HG22	1.92	0.50
1:E:218:VAL:HG21	1:E:441:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:HD12	1:A:332:ILE:N	2.26	0.50
1:C:50:TYR:HA	1:F:266:ALA:O	2.11	0.50
1:C:116:ALA:HB2	1:C:355:LEU:HD12	1.93	0.50
1:A:369:ILE:HD12	1:A:389:ILE:HD11	1.93	0.50
1:A:415:LEU:HD13	1:A:417:LEU:HG	1.93	0.50
1:B:387:SER:OG	1:B:405:ILE:HD12	2.11	0.50
1:C:93:SER:OG	1:C:324:LEU:O	2.19	0.50
1:F:133:LEU:HD12	1:F:352:ALA:HB2	1.93	0.50
1:E:220:ARG:HD3	1:E:226:GLN:OE1	2.12	0.50
1:E:404:ILE:HG22	1:E:430:VAL:HG22	1.94	0.50
1:F:233:ARG:HH11	1:F:268:SER:HB2	1.76	0.50
1:A:249:PRO:C	1:A:250:LEU:HD22	2.36	0.50
1:E:326:CYS:HB2	1:E:327:PRO:HD2	1.94	0.50
1:B:294:PHE:HB2	1:B:441:LEU:HD11	1.94	0.50
1:C:246:MET:HE2	1:C:246:MET:HA	1.94	0.50
1:F:452:ASP:O	1:F:456:GLN:HG3	2.12	0.50
1:D:118:GLY:HA2	1:D:328:LEU:HD23	1.93	0.49
1:C:85:LEU:HG	1:C:154:ILE:HG21	1.94	0.49
1:C:251:PRO:HD2	1:C:254:LEU:HB2	1.94	0.49
1:E:445:ILE:HG13	1:E:446:THR:HG23	1.93	0.49
1:A:113:LEU:HD21	1:A:136:VAL:C	2.37	0.49
1:B:263:VAL:HG22	1:B:295:ILE:HG13	1.95	0.49
1:E:320:LYS:HD3	1:E:400:ARG:HD3	1.94	0.49
1:E:343:SER:OG	1:E:346:THR:HG21	2.11	0.49
1:B:239:LEU:HG	1:E:239:LEU:HD13	1.94	0.49
1:B:323:ASP:HB3	1:B:326:CYS:SG	2.52	0.49
1:D:215:GLY:O	1:D:388:LEU:HG	2.12	0.49
1:A:65:GLY:O	1:A:279:TYR:CZ	2.65	0.49
1:B:196:ASP:OD1	1:B:197:GLU:N	2.45	0.49
1:C:54:PRO:HA	1:C:58:LEU:HD12	1.95	0.49
1:F:232:ASN:HD21	1:F:234:HIS:HB2	1.78	0.49
1:A:138:ARG:HH21	1:C:193:CYS:HB3	1.78	0.49
1:A:173:TYR:OH	1:A:414:ARG:HD3	2.13	0.49
1:A:184:MET:HG2	1:A:343:SER:HA	1.94	0.49
1:B:229:PHE:CE1	1:B:295:ILE:HB	2.48	0.49
1:E:390:ILE:CG2	1:E:399:PRO:HB2	2.43	0.49
1:F:341:ARG:HG3	1:F:342:SER:N	2.27	0.49
1:B:225:LYS:HG3	1:B:458:ARG:HH12	1.78	0.49
1:F:105:SER:O	1:F:109:ARG:HG2	2.12	0.49
1:E:84:ARG:O	1:E:85:LEU:HB2	2.12	0.49
1:E:285:GLU:OE1	1:E:363:ILE:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:HIS:HA	1:F:64:GLU:HG2	1.95	0.49
1:F:338:LYS:NZ	1:F:346:THR:OG1	2.38	0.49
1:F:363:ILE:HD12	1:F:363:ILE:N	2.27	0.49
1:C:251:PRO:HB3	1:F:361:LYS:HZ1	1.78	0.49
1:C:406:TRP:O	1:C:411:ASN:ND2	2.45	0.49
1:F:196:ASP:OD1	1:F:197:GLU:N	2.46	0.49
1:A:113:LEU:HD23	1:A:135:PHE:O	2.13	0.48
1:E:183:GLN:N	1:E:183:GLN:OE1	2.46	0.48
1:A:55:THR:HG22	1:A:56:SER:N	2.27	0.48
1:A:415:LEU:HD12	1:A:415:LEU:O	2.13	0.48
1:C:94:LEU:HD13	1:C:328:LEU:CD2	2.44	0.48
1:E:142:LYS:HE2	1:E:150:CYS:SG	2.54	0.48
1:A:205:VAL:HB	1:A:246:MET:HE3	1.95	0.48
1:D:357:TYR:CD2	1:D:359:ASP:HB3	2.48	0.48
1:E:95:LEU:HG	1:E:324:LEU:C	2.38	0.48
1:E:141:HIS:CE1	1:E:143:LYS:HB2	2.49	0.48
1:F:85:LEU:HG	1:F:154:ILE:HG21	1.94	0.48
1:A:221:ARG:HA	1:A:225:LYS:NZ	2.29	0.48
1:C:221:ARG:HD2	1:C:442:ASP:OD1	2.13	0.48
1:D:93:SER:O	1:D:97:LEU:HD23	2.13	0.48
1:D:180:PRO:HD2	1:D:211:PHE:CD2	2.48	0.48
1:D:414:ARG:HA	1:D:424:GLU:O	2.13	0.48
1:D:415:LEU:N	1:D:415:LEU:HD23	2.29	0.48
1:F:217:ILE:HD12	1:F:217:ILE:N	2.29	0.48
1:C:107:ILE:HG13	1:C:108:LEU:HD12	1.96	0.48
1:D:228:GLY:HA3	1:D:296:PRO:HA	1.96	0.48
1:F:380:ASP:O	1:F:381:LEU:HD23	2.14	0.48
1:A:233:ARG:O	1:A:233:ARG:HG2	2.13	0.48
1:C:85:LEU:HD22	1:C:85:LEU:N	2.29	0.48
1:A:66:ARG:O	1:A:68:ASN:N	2.47	0.48
1:C:207:SER:CB	1:C:246:MET:HE1	2.37	0.48
1:B:385:SER:OG	1:B:407:GLY:HA3	2.13	0.48
1:A:415:LEU:CD1	1:A:417:LEU:HG	2.44	0.47
1:C:295:ILE:HD12	1:C:295:ILE:N	2.29	0.47
1:E:391:LEU:HG	1:E:402:ILE:HD13	1.95	0.47
1:F:182:GLU:H	1:F:182:GLU:CD	2.22	0.47
1:B:239:LEU:CG	1:E:239:LEU:HD13	2.44	0.47
1:B:447:ASN:O	1:B:451:GLN:HG3	2.13	0.47
1:C:380:ASP:OD1	1:C:427:THR:OG1	2.27	0.47
1:F:406:TRP:CZ2	1:F:408:GLY:HA3	2.49	0.47
1:B:180:PRO:HB3	1:B:382:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLU:CG	1:F:55:THR:HG22	2.43	0.47
1:D:233:ARG:HG2	1:D:234:HIS:N	2.28	0.47
1:E:275:TRP:CD1	1:E:288:VAL:HG11	2.49	0.47
1:B:145:LEU:HD11	2:B:1001:ATP:C4	2.49	0.47
1:D:120:ARG:NH2	1:D:164:ASP:HB3	2.23	0.47
1:E:178:GLN:O	1:E:180:PRO:HD3	2.14	0.47
1:D:220:ARG:NH1	1:D:439:LEU:O	2.47	0.47
1:F:94:LEU:HD23	1:F:328:LEU:CD2	2.45	0.47
1:F:113:LEU:HD13	1:F:172:TYR:CE2	2.45	0.47
1:F:295:ILE:N	1:F:295:ILE:HD12	2.29	0.47
1:F:302:ASP:OD2	1:F:305:THR:HG23	2.13	0.47
1:A:212:GLY:HA3	1:A:235:VAL:CG1	2.45	0.47
1:A:219:LYS:HD3	1:A:453:ALA:HB1	1.95	0.47
1:A:450:LEU:O	1:A:454:VAL:HG23	2.15	0.47
1:B:184:MET:HG3	1:B:343:SER:CA	2.42	0.47
1:C:156:GLU:H	1:C:156:GLU:CD	2.22	0.47
1:D:192:LEU:HD23	1:D:311:ARG:NH2	2.30	0.47
1:D:295:ILE:N	1:D:295:ILE:HD12	2.29	0.47
1:B:286:THR:OG1	1:B:364:CYS:HB3	2.15	0.47
1:E:94:LEU:HD11	1:E:117:VAL:CG2	2.45	0.47
1:F:220:ARG:NH1	1:F:264:GLU:OE2	2.48	0.47
1:E:237:VAL:HA	1:E:244:GLN:CG	2.33	0.47
1:F:180:PRO:HD2	1:F:211:PHE:CE1	2.50	0.47
1:F:263:VAL:HA	1:F:295:ILE:HG13	1.97	0.47
1:F:450:LEU:O	1:F:454:VAL:HG23	2.14	0.47
1:E:97:LEU:HD21	1:E:328:LEU:HD11	1.96	0.47
1:F:104:HIS:O	1:F:108:LEU:HG	2.15	0.47
1:F:226:GLN:HG2	1:F:227:VAL:N	2.29	0.47
1:C:275:TRP:CD1	1:C:288:VAL:HG11	2.50	0.47
1:C:350:VAL:O	1:C:351:MET:HE2	2.15	0.47
1:F:85:LEU:HD11	1:F:156:GLU:CG	2.45	0.47
1:F:146:ASN:OD1	1:F:146:ASN:N	2.41	0.47
1:A:220:ARG:O	1:A:225:LYS:HD2	2.14	0.46
1:B:236:ALA:O	1:B:244:GLN:HB3	2.14	0.46
1:B:414:ARG:HB3	1:B:423:PRO:HB2	1.97	0.46
1:C:50:TYR:CD2	1:F:267:THR:HG22	2.50	0.46
1:C:118:GLY:CA	1:C:332:ILE:HD13	2.34	0.46
1:C:178:GLN:O	1:C:210:THR:HA	2.15	0.46
1:C:214:LEU:HD23	1:C:214:LEU:C	2.39	0.46
1:A:131:ALA:HB2	1:A:164:ASP:HB2	1.97	0.46
1:B:376:ARG:NE	1:B:421:HIS:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD23	1:D:166:ASP:HB3	1.97	0.46
1:E:94:LEU:HD21	1:E:353:TYR:CB	2.45	0.46
1:D:213:THR:HG21	1:D:340:GLY:HA2	1.97	0.46
1:D:267:THR:HG21	1:D:270:ILE:CD1	2.43	0.46
1:E:107:ILE:HD13	1:E:110:ARG:CZ	2.45	0.46
1:F:380:ASP:OD1	1:F:427:THR:OG1	2.26	0.46
1:A:244:GLN:HB2	1:A:263:VAL:HG23	1.96	0.46
1:C:94:LEU:N	1:C:94:LEU:HD22	2.30	0.46
1:C:246:MET:HG3	1:C:295:ILE:HG12	1.98	0.46
1:D:80:ARG:C	1:D:82:PRO:HD3	2.41	0.46
1:D:117:VAL:HG22	1:D:353:TYR:O	2.16	0.46
1:A:403:GLY:HA2	1:A:432:LEU:HB2	1.98	0.46
1:D:406:TRP:O	1:D:411:ASN:ND2	2.49	0.46
1:E:130:PRO:HB3	1:E:328:LEU:CD1	2.45	0.46
1:F:233:ARG:HH11	1:F:268:SER:HB3	1.81	0.46
1:B:376:ARG:HE	1:B:421:HIS:HB3	1.81	0.46
1:C:370:LEU:HD11	1:C:426:TRP:HB2	1.97	0.46
1:D:450:LEU:O	1:D:454:VAL:HG23	2.15	0.46
1:F:224:ASN:OD1	1:F:226:GLN:HB2	2.16	0.46
1:C:289:ARG:HD2	1:C:406:TRP:CZ2	2.51	0.46
1:D:438:ARG:HA	1:D:438:ARG:NE	2.30	0.46
1:F:120:ARG:NH2	1:F:164:ASP:HB3	2.28	0.46
1:B:380:ASP:OD1	1:B:427:THR:OG1	2.31	0.46
1:F:182:GLU:HG2	1:F:183:GLN:N	2.31	0.46
1:F:319:VAL:HG23	1:F:443:ILE:CG2	2.44	0.46
1:F:378:THR:HG21	1:F:381:LEU:HD21	1.98	0.46
1:A:111:PHE:CE2	1:A:149:GLN:HA	2.51	0.45
1:B:134:VAL:HG11	1:B:151:LEU:HD11	1.98	0.45
1:C:278:ILE:HD12	1:C:278:ILE:O	2.17	0.45
1:D:84:ARG:O	1:D:85:LEU:HB2	2.16	0.45
1:D:291:ASP:HB2	1:D:406:TRP:NE1	2.30	0.45
1:F:219:LYS:HD3	1:F:453:ALA:HB2	1.97	0.45
1:F:190:ASP:O	1:F:195:SER:HB2	2.16	0.45
1:A:250:LEU:HD21	1:B:138:ARG:CZ	2.46	0.45
1:B:360:GLU:OE1	1:B:360:GLU:N	2.44	0.45
1:C:106:LYS:HD2	1:C:109:ARG:HH21	1.82	0.45
1:C:389:ILE:HD11	1:C:405:ILE:HD13	1.98	0.45
1:D:199:ILE:HG13	1:F:144:TRP:CH2	2.52	0.45
1:E:183:GLN:HB2	1:E:342:SER:CA	2.34	0.45
1:C:184:MET:CG	1:C:343:SER:HA	2.46	0.45
1:F:395:ASP:OD1	1:F:396:GLY:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:ARG:O	1:F:438:ARG:HG2	2.17	0.45
1:A:81:HIS:HE1	1:A:156:GLU:HB3	1.81	0.45
1:A:217:ILE:HD12	1:A:217:ILE:N	2.32	0.45
1:B:241:TYR:CE2	1:E:363:ILE:HG13	2.51	0.45
1:B:353:TYR:HA	1:B:368:ASP:O	2.16	0.45
1:F:342:SER:HB3	1:F:381:LEU:HB2	1.98	0.45
1:A:369:ILE:CD1	1:A:389:ILE:HD11	2.46	0.45
1:B:89:GLN:O	1:B:161:VAL:HA	2.17	0.45
1:C:94:LEU:HD22	1:C:94:LEU:H	1.82	0.45
1:F:336:VAL:CG1	1:F:391:LEU:HD23	2.32	0.45
1:B:411:ASN:O	1:B:412:ARG:HB2	2.17	0.45
1:C:85:LEU:CD2	1:C:154:ILE:HG21	2.47	0.45
1:C:208:HIS:NE2	1:C:245:LYS:HB2	2.32	0.45
1:D:74:GLN:HA	1:D:103:PHE:HZ	1.81	0.45
1:A:214:LEU:HG	1:A:229:PHE:CD2	2.52	0.45
1:A:268:SER:HA	1:A:291:ASP:OD1	2.17	0.45
1:B:95:LEU:HD13	1:B:95:LEU:C	2.42	0.45
1:B:95:LEU:HD13	1:B:95:LEU:O	2.17	0.45
1:C:212:GLY:HA3	1:C:235:VAL:CG1	2.45	0.45
1:E:135:PHE:HB3	1:E:170:PHE:CB	2.47	0.45
1:E:388:LEU:HD22	1:E:432:LEU:HD22	1.98	0.45
1:A:193:CYS:HB3	1:B:138:ARG:HH21	1.81	0.45
1:C:270:ILE:CD1	1:C:438:ARG:HG3	2.46	0.45
1:B:267:THR:HG22	1:E:50:TYR:CA	2.43	0.44
1:C:126:LEU:HD22	1:C:351:MET:CE	2.47	0.44
1:C:361:LYS:HB2	1:F:241:TYR:OH	2.17	0.44
1:D:78:LEU:HD22	1:D:78:LEU:N	2.32	0.44
1:D:204:GLN:OE1	1:D:341:ARG:HD2	2.17	0.44
1:E:184:MET:HG2	1:E:343:SER:HA	1.99	0.44
1:E:324:LEU:HG	1:E:434:ARG:HH22	1.82	0.44
1:F:217:ILE:HG22	1:F:444:ILE:CD1	2.43	0.44
1:A:219:LYS:HD2	1:A:225:LYS:HE3	1.98	0.44
1:A:445:ILE:HG13	1:A:446:THR:HG23	1.99	0.44
1:B:150:CYS:SG	1:B:151:LEU:N	2.91	0.44
1:D:153:ALA:O	1:D:154:ILE:HD13	2.17	0.44
1:E:307:THR:HG22	1:E:309:VAL:H	1.80	0.44
1:F:95:LEU:HD11	1:F:278:ILE:HG21	1.98	0.44
1:F:251:PRO:HD2	1:F:254:LEU:HD22	2.00	0.44
1:A:95:LEU:HD11	1:A:278:ILE:HD12	1.98	0.44
1:A:143:LYS:NZ	1:C:197:GLU:HA	2.32	0.44
1:C:294:PHE:HB2	1:C:441:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ASP:OD1	1:C:421:HIS:ND1	2.50	0.44
1:E:289:ARG:HD3	1:E:406:TRP:CH2	2.52	0.44
1:F:141:HIS:HB3	1:F:144:TRP:CD1	2.52	0.44
1:D:253:ASN:ND2	1:D:254:LEU:HG	2.33	0.44
1:E:108:LEU:O	1:E:112:SER:OG	2.18	0.44
1:E:372:VAL:HG12	1:E:426:TRP:HB3	2.00	0.44
1:F:320:LYS:HA	1:F:400:ARG:HH21	1.83	0.44
1:C:102:ALA:HA	1:C:105:SER:OG	2.17	0.44
1:D:407:GLY:O	1:D:411:ASN:HB3	2.17	0.44
1:E:319:VAL:HG21	1:E:436:LEU:HD12	1.99	0.44
1:A:135:PHE:HB3	1:A:170:PHE:HB3	1.99	0.44
1:C:188:LEU:O	1:C:192:LEU:HG	2.18	0.44
1:D:245:LYS:O	1:D:246:MET:HE2	2.18	0.44
1:F:80:ARG:C	1:F:82:PRO:HD3	2.42	0.44
1:B:95:LEU:HD22	1:B:278:ILE:HD13	1.98	0.44
1:B:273:ASP:OD1	1:B:273:ASP:N	2.50	0.44
1:D:94:LEU:O	1:D:98:MET:HG3	2.18	0.44
1:D:214:LEU:C	1:D:214:LEU:HD23	2.43	0.44
1:D:356:GLU:HG3	1:D:366:PHE:CZ	2.53	0.44
1:F:129:ILE:HD12	1:F:129:ILE:N	2.33	0.44
1:B:120:ARG:HG3	1:B:166:ASP:HB2	2.00	0.43
1:C:239:LEU:CB	1:F:239:LEU:HD22	2.43	0.43
1:E:294:PHE:C	1:E:295:ILE:HD12	2.43	0.43
1:F:95:LEU:HD11	1:F:278:ILE:HD13	1.98	0.43
1:F:184:MET:HG3	1:F:343:SER:CA	2.28	0.43
1:A:221:ARG:HA	1:A:225:LYS:HZ3	1.82	0.43
1:D:411:ASN:HB2	1:D:428:SER:OG	2.18	0.43
1:E:74:GLN:HA	1:E:77:LEU:HG	2.01	0.43
1:F:228:GLY:HA3	1:F:296:PRO:HA	2.00	0.43
1:A:218:VAL:HG12	1:A:443:ILE:HA	2.00	0.43
1:A:414:ARG:HB3	1:A:423:PRO:HB2	2.01	0.43
1:C:263:VAL:HA	1:C:295:ILE:HG13	1.99	0.43
1:D:278:ILE:HD12	1:D:278:ILE:O	2.19	0.43
1:D:387:SER:HB2	1:D:405:ILE:CD1	2.48	0.43
1:F:122:ARG:NH1	2:F:1001:ATP:O1B	2.51	0.43
1:A:97:LEU:HD11	1:A:328:LEU:CD1	2.49	0.43
1:B:52:LEU:HD12	1:E:264:GLU:O	2.18	0.43
1:C:220:ARG:HD2	1:C:441:LEU:HD23	1.99	0.43
1:D:119:PHE:HA	1:D:129:ILE:O	2.19	0.43
1:E:144:TRP:CH2	1:F:199:ILE:HG13	2.53	0.43
1:E:216:ALA:HB2	1:E:388:LEU:CD1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:LYS:HD3	1:E:400:ARG:HH11	1.82	0.43
1:D:322:ILE:CG2	1:D:331:LEU:HD22	2.49	0.43
1:E:316:ILE:HG22	1:E:399:PRO:HG2	2.00	0.43
1:A:334:ARG:HB3	1:A:334:ARG:NH1	2.33	0.43
1:C:89:GLN:HB2	1:C:162:TRP:CD1	2.53	0.43
1:D:173:TYR:CZ	1:D:413:GLY:HA2	2.54	0.43
1:F:224:ASN:HD21	1:F:457:GLN:HB2	1.84	0.43
1:D:134:VAL:HG11	1:D:151:LEU:CD1	2.47	0.43
1:D:286:THR:HA	1:D:364:CYS:HB3	2.01	0.43
1:F:59:GLN:O	1:F:59:GLN:HG3	2.18	0.43
1:F:270:ILE:HD12	1:F:275:TRP:CZ3	2.53	0.43
1:A:190:ASP:C	1:A:195:SER:HB3	2.44	0.43
1:B:341:ARG:HG2	1:B:342:SER:N	2.31	0.43
1:C:95:LEU:HD11	1:C:278:ILE:HG12	2.01	0.43
1:E:273:ASP:OD1	1:E:273:ASP:N	2.51	0.43
1:D:311:ARG:H	1:D:311:ARG:HD3	1.84	0.43
1:E:87:LYS:HA	1:E:87:LYS:HD3	1.68	0.43
1:F:318:ASP:OD1	1:F:319:VAL:N	2.50	0.43
1:D:105:SER:O	1:D:109:ARG:HG3	2.19	0.43
1:F:248:HIS:HB2	1:F:260:LEU:HD11	2.00	0.43
1:B:320:LYS:HB3	1:B:402:ILE:HG22	2.00	0.42
1:C:101:ARG:HB2	1:C:132:ILE:HD13	2.01	0.42
1:D:226:GLN:H	1:D:226:GLN:CD	2.24	0.42
1:E:184:MET:HG2	1:E:342:SER:O	2.19	0.42
1:F:214:LEU:C	1:F:214:LEU:HD23	2.43	0.42
1:B:168:VAL:CG1	1:B:415:LEU:HD11	2.48	0.42
1:D:411:ASN:O	1:D:411:ASN:CG	2.60	0.42
1:E:124:GLY:HA2	1:E:417:LEU:O	2.18	0.42
1:E:412:ARG:NH1	1:E:425:ASN:OD1	2.51	0.42
1:A:236:ALA:O	1:A:244:GLN:HB3	2.19	0.42
1:D:91:ALA:HB1	1:D:97:LEU:HD22	1.99	0.42
1:E:420:ASP:OD1	1:E:420:ASP:N	2.52	0.42
1:F:390:ILE:HA	1:F:401:PRO:HA	2.01	0.42
1:B:182:GLU:O	1:B:184:MET:N	2.51	0.42
1:C:81:HIS:O	1:C:81:HIS:CG	2.72	0.42
1:E:82:PRO:CG	1:E:86:PRO:HD3	2.50	0.42
1:E:141:HIS:HB3	1:E:144:TRP:NE1	2.34	0.42
1:F:267:THR:OG1	1:F:290:ALA:O	2.37	0.42
1:A:67:ALA:C	1:A:69:TYR:N	2.78	0.42
1:A:199:ILE:HG13	1:B:144:TRP:CH2	2.55	0.42
1:A:338:LYS:O	1:A:345:HIS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLY:HA3	1:B:296:PRO:HA	2.01	0.42
1:C:93:SER:OG	1:C:326:CYS:O	2.38	0.42
1:D:220:ARG:O	1:D:225:LYS:HG2	2.19	0.42
1:D:220:ARG:NH2	1:D:440:GLU:OE1	2.53	0.42
1:C:60:HIS:O	1:C:64:GLU:HG2	2.20	0.42
1:C:161:VAL:O	1:C:161:VAL:HG13	2.18	0.42
1:C:248:HIS:HB3	1:C:260:LEU:HD11	2.01	0.42
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.72	0.42
1:F:199:ILE:O	1:F:306:VAL:HA	2.19	0.42
1:F:226:GLN:HG2	1:F:227:VAL:H	1.84	0.42
1:F:263:VAL:HG22	1:F:295:ILE:HG13	2.02	0.42
1:A:180:PRO:HG3	1:A:383:GLY:HA3	2.01	0.42
1:A:244:GLN:HB2	1:A:263:VAL:CG2	2.50	0.42
1:A:448:GLU:CD	1:A:448:GLU:H	2.26	0.42
1:B:151:LEU:HD12	1:B:167:VAL:HG22	2.01	0.42
1:E:129:ILE:N	1:E:129:ILE:HD12	2.35	0.42
1:E:347:THR:O	1:E:374:GLU:HG3	2.19	0.42
1:F:232:ASN:ND2	1:F:234:HIS:H	2.18	0.42
1:A:67:ALA:HA	1:A:70:PHE:HB2	2.02	0.42
1:A:391:LEU:HG	1:A:402:ILE:HD13	2.01	0.42
1:D:173:TYR:OH	1:D:414:ARG:HD2	2.19	0.42
1:D:188:LEU:O	1:D:192:LEU:HG	2.20	0.42
1:E:245:LYS:C	1:E:246:MET:HE2	2.45	0.42
1:A:376:ARG:CZ	1:A:421:HIS:HB3	2.50	0.42
1:C:133:LEU:N	1:C:133:LEU:HD12	2.35	0.42
1:D:77:LEU:CD2	1:D:159:GLY:H	2.33	0.42
1:E:85:LEU:HD21	1:E:156:GLU:OE1	2.20	0.42
1:F:241:TYR:CD1	1:F:242:PRO:HD2	2.54	0.42
1:A:89:GLN:O	1:A:161:VAL:HA	2.20	0.41
1:C:390:ILE:HG12	1:C:401:PRO:HB3	2.02	0.41
1:F:113:LEU:C	1:F:113:LEU:HD12	2.45	0.41
1:F:188:LEU:HG	1:F:192:LEU:CD1	2.50	0.41
1:F:219:LYS:HG2	1:F:227:VAL:HB	2.02	0.41
1:F:294:PHE:C	1:F:295:ILE:HD12	2.45	0.41
1:C:338:LYS:HD3	1:C:387:SER:HB2	2.01	0.41
1:E:135:PHE:HE2	1:E:355:LEU:HD13	1.85	0.41
1:F:119:PHE:HB2	1:F:126:LEU:HD11	2.01	0.41
1:E:390:ILE:HA	1:E:401:PRO:HA	2.02	0.41
1:F:70:PHE:HA	1:F:73:LEU:HD22	2.02	0.41
1:F:320:LYS:HA	1:F:400:ARG:NH2	2.35	0.41
1:A:151:LEU:CD1	2:A:1001:ATP:HN61	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLN:O	1:A:262:ALA:HA	2.21	0.41
1:C:53:TRP:HD1	1:F:264:GLU:C	2.28	0.41
1:D:100:ILE:HG12	1:D:157:GLY:HA3	2.02	0.41
1:D:391:LEU:HG	1:D:402:ILE:HG23	2.03	0.41
1:F:219:LYS:HG2	1:F:227:VAL:CB	2.50	0.41
1:F:248:HIS:HA	1:F:249:PRO:HA	1.92	0.41
1:F:326:CYS:HB3	1:F:327:PRO:HD2	2.01	0.41
1:F:338:LYS:HD2	1:F:338:LYS:C	2.45	0.41
1:A:199:ILE:HD13	1:A:260:LEU:HD21	2.01	0.41
1:B:340:GLY:O	1:B:344:GLY:N	2.51	0.41
1:B:376:ARG:HE	1:B:421:HIS:CG	2.38	0.41
1:D:394:GLN:N	1:D:394:GLN:OE1	2.53	0.41
1:B:409:THR:OG1	1:B:410:ALA:N	2.52	0.41
1:C:190:ASP:O	1:C:195:SER:HB3	2.21	0.41
1:A:230:LEU:HD12	1:A:293:ALA:O	2.20	0.41
1:A:250:LEU:HD21	1:B:138:ARG:NH1	2.35	0.41
1:B:94:LEU:HD23	1:B:328:LEU:CD2	2.51	0.41
1:C:108:LEU:HD11	1:C:155:LEU:HD11	2.01	0.41
1:C:214:LEU:HG	1:C:229:PHE:HB2	2.03	0.41
1:D:196:ASP:OD2	1:D:311:ARG:NH1	2.54	0.41
1:D:416:LYS:HE3	1:D:418:THR:O	2.21	0.41
1:E:384:ASP:O	1:E:387:SER:OG	2.38	0.41
1:F:337:CYS:HA	1:F:347:THR:HA	2.02	0.41
1:A:214:LEU:C	1:A:214:LEU:HD23	2.46	0.41
1:B:86:PRO:HG2	1:B:89:GLN:HB2	2.03	0.41
1:C:113:LEU:HD12	1:C:113:LEU:C	2.46	0.41
1:C:320:LYS:HD2	1:C:391:LEU:HD12	2.01	0.41
1:E:53:TRP:HB3	1:E:54:PRO:HD2	2.02	0.41
1:F:302:ASP:OD2	1:F:304:SER:OG	2.37	0.41
1:A:78:LEU:O	1:A:80:ARG:HG2	2.20	0.41
1:A:95:LEU:HB2	1:A:324:LEU:O	2.21	0.41
1:A:106:LYS:CE	1:A:282:THR:HG21	2.41	0.41
1:D:82:PRO:O	1:D:83:GLY:C	2.61	0.41
1:D:202:GLY:HA2	1:D:213:THR:CG2	2.50	0.41
1:E:347:THR:CG2	1:E:374:GLU:HG2	2.45	0.41
1:F:79:PRO:O	1:F:81:HIS:ND1	2.54	0.41
1:F:188:LEU:HG	1:F:192:LEU:HD11	2.03	0.41
1:A:138:ARG:HH11	1:C:250:LEU:HD11	1.85	0.41
1:B:197:GLU:O	1:B:197:GLU:HG2	2.21	0.41
1:C:391:LEU:CD2	1:C:402:ILE:HD13	2.50	0.41
1:D:182:GLU:O	1:D:182:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LYS:HG3	1:F:183:GLN:OE1	2.21	0.41
1:F:391:LEU:HG	1:F:402:ILE:HD13	2.02	0.41
1:E:107:ILE:HD13	1:E:110:ARG:NH1	2.36	0.40
1:E:224:ASN:HB2	1:E:226:GLN:NE2	2.35	0.40
1:F:85:LEU:HD12	1:F:162:TRP:CB	2.52	0.40
1:F:403:GLY:HA2	1:F:432:LEU:HB2	2.02	0.40
1:E:385:SER:HA	1:E:405:ILE:HG22	2.04	0.40
1:F:81:HIS:N	1:F:82:PRO:CD	2.82	0.40
1:C:247:PHE:CE1	1:C:259:TYR:HD1	2.39	0.40
1:D:176:PRO:HD3	1:D:409:THR:HA	2.04	0.40
1:E:76:GLY:O	1:E:78:LEU:N	2.55	0.40
1:E:180:PRO:HB2	1:E:382:GLU:O	2.21	0.40
1:F:285:GLU:OE1	1:F:363:ILE:HG13	2.21	0.40
1:A:141:HIS:CE1	1:A:143:LYS:HG3	2.56	0.40
1:C:224:ASN:HB2	1:C:226:GLN:OE1	2.20	0.40
1:C:94:LEU:O	1:C:98:MET:HG3	2.22	0.40
1:C:99:THR:HG22	1:C:158:PRO:HG2	2.03	0.40
1:D:100:ILE:HD11	1:D:161:VAL:HG22	2.03	0.40
1:D:110:ARG:HG2	1:D:111:PHE:CE2	2.57	0.40
1:E:77:LEU:HD21	1:E:103:PHE:HZ	1.87	0.40
1:E:331:LEU:HG	1:E:350:VAL:HG11	2.04	0.40

All (1) 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:A:279:TYR:OH	1:C:87:LYS:NZ[4_555]	2.13	0.07

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	406/423 (96%)	403 (99%)	2 (0%)	1 (0%)	43	62
1	B	407/423 (96%)	404 (99%)	0	3 (1%)	18	35
1	C	406/423 (96%)	406 (100%)	0	0	100	100
1	D	406/423 (96%)	402 (99%)	0	4 (1%)	12	24
1	E	406/423 (96%)	403 (99%)	1 (0%)	2 (0%)	24	43
1	F	406/423 (96%)	405 (100%)	0	1 (0%)	43	62
All	All	2437/2538 (96%)	2423 (99%)	3 (0%)	11 (0%)	24	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	409	THR
1	E	341	ARG
1	A	178	GLN
1	B	178	GLN
1	D	119	PHE
1	D	178	GLN
1	E	77	LEU
1	F	395	ASP
1	B	412	ARG
1	D	78	LEU
1	D	85	LEU

5.3.2 Protein sidechains ⓘ

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	339/350 (97%)	331 (98%)	8 (2%)	43	67
1	B	340/350 (97%)	337 (99%)	3 (1%)	70	84
1	C	339/350 (97%)	333 (98%)	6 (2%)	51	74
1	D	339/350 (97%)	335 (99%)	4 (1%)	63	80
1	E	339/350 (97%)	332 (98%)	7 (2%)	47	70
1	F	339/350 (97%)	336 (99%)	3 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2035/2100 (97%)	2004 (98%)	31 (2%)	57 77

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	68	ASN
1	A	113	LEU
1	A	126	LEU
1	A	144	TRP
1	A	145	LEU
1	A	278	ILE
1	A	448	GLU
1	B	319	VAL
1	B	338	LYS
1	B	455	GLN
1	C	52	LEU
1	C	57	ASN
1	C	85	LEU
1	C	338	LYS
1	C	364	CYS
1	C	377	GLN
1	D	253	ASN
1	D	338	LYS
1	D	356	GLU
1	D	411	ASN
1	E	107	ILE
1	E	197	GLU
1	E	278	ILE
1	E	347	THR
1	E	387	SER
1	E	425	ASN
1	E	430	VAL
1	F	146	ASN
1	F	224	ASN
1	F	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN

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Mol	Chain	Res	Type
1	A	358	ASN
1	B	60	HIS
1	B	89	GLN
1	B	456	GLN
1	C	345	HIS
1	C	375	ASN
1	D	335	GLN
1	E	57	ASN
1	E	421	HIS
1	F	90	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 7 are monoatomic and 1 is modelled with single atom - leaving 18 for Mogul analysis.

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	$\# Z > 2$
4	SO4	F	1004	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	B	1004	-	4,4,4	0.26	0	6,6,6	0.13	0
2	ATP	C	1001	3	32,33,33	0.53	1 (3%)	48,52,52	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	B	1001	3	32,33,33	0.77	2 (6%)	48,52,52	0.36	0
4	SO4	A	1004	-	4,4,4	0.23	0	6,6,6	0.19	0
4	SO4	A	1003	-	4,4,4	0.23	0	6,6,6	0.15	0
4	SO4	B	1006	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	F	1003	-	4,4,4	0.23	0	6,6,6	0.15	0
2	ATP	E	1001	3	32,33,33	0.26	0	48,52,52	0.31	0
2	ATP	D	1001	3	32,33,33	0.26	0	48,52,52	0.29	0
4	SO4	D	1003	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	B	1007	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	D	1004	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.09	0
2	ATP	A	1001	3	32,33,33	0.29	0	48,52,52	0.30	0
4	SO4	C	1003	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	C	1004	-	4,4,4	0.23	0	6,6,6	0.14	0
2	ATP	F	1001	3	32,33,33	0.39	0	48,52,52	0.35	0

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	ATP	C	1001	3	-	6/22/38/38	0/3/3/3
2	ATP	B	1001	3	-	12/22/38/38	0/3/3/3
2	ATP	E	1001	3	-	9/22/38/38	0/3/3/3
2	ATP	D	1001	3	-	6/22/38/38	0/3/3/3
2	ATP	A	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	F	1001	3	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ATP	PA-O3A	-3.07	1.56	1.59
2	B	1001	ATP	PB-O3B	-2.72	1.56	1.59
2	C	1001	ATP	PB-O3B	-2.11	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

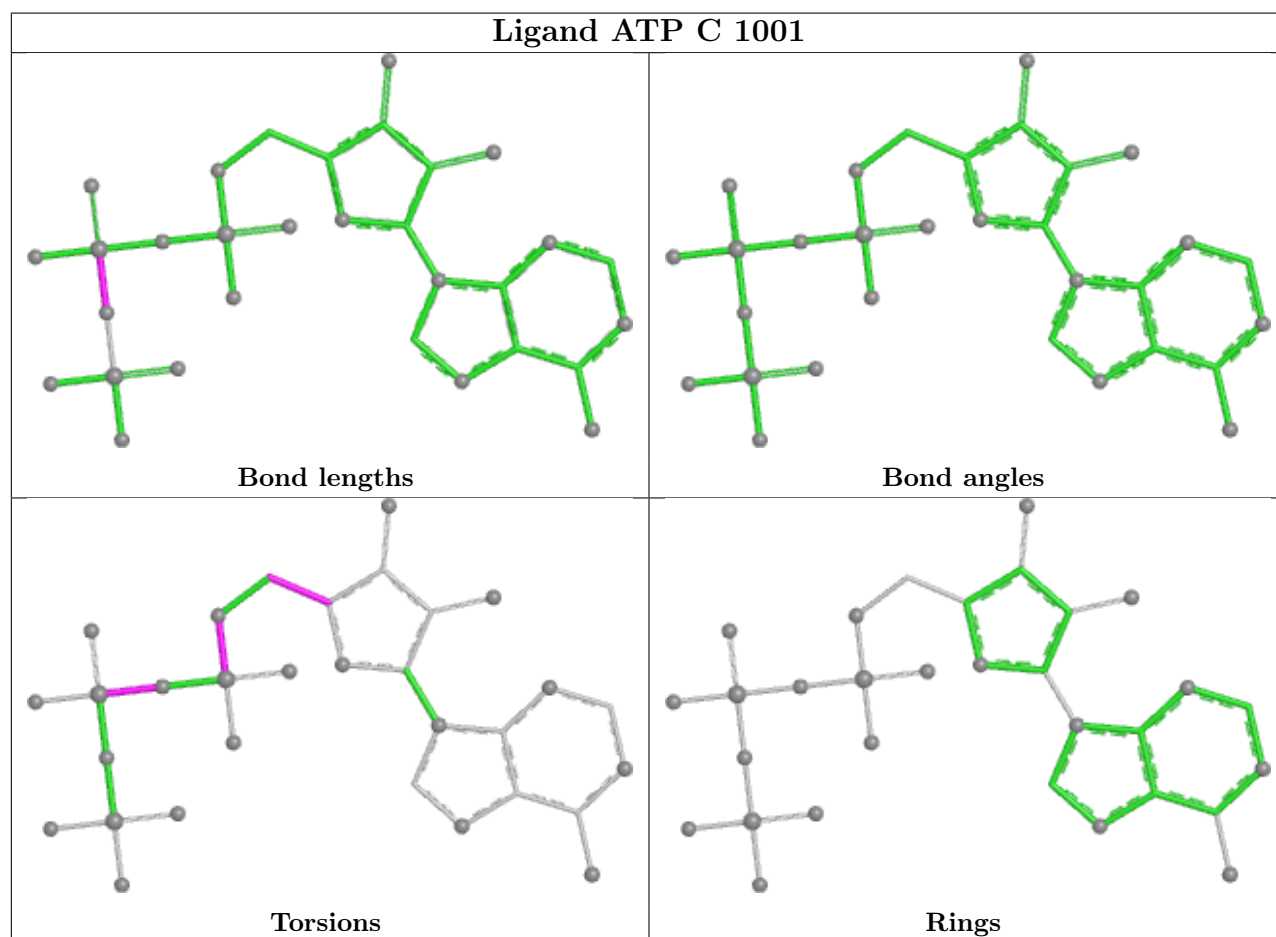
Mol	Chain	Res	Type	Atoms
2	B	1001	ATP	PB-O3B-PG-O2G
2	B	1001	ATP	C5'-O5'-PA-O1A
2	B	1001	ATP	C5'-O5'-PA-O3A
2	C	1001	ATP	C5'-O5'-PA-O1A
2	C	1001	ATP	C5'-O5'-PA-O3A
2	D	1001	ATP	C5'-O5'-PA-O1A
2	D	1001	ATP	C5'-O5'-PA-O3A
2	E	1001	ATP	PB-O3B-PG-O3G
2	E	1001	ATP	C5'-O5'-PA-O1A
2	E	1001	ATP	C5'-O5'-PA-O2A
2	E	1001	ATP	C5'-O5'-PA-O3A
2	B	1001	ATP	C3'-C4'-C5'-O5'
2	E	1001	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	O4'-C4'-C5'-O5'
2	C	1001	ATP	PA-O3A-PB-O1B
2	A	1001	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	PG-O3B-PB-O2B
2	B	1001	ATP	PB-O3A-PA-O2A
2	F	1001	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	C5'-O5'-PA-O2A
2	C	1001	ATP	C5'-O5'-PA-O2A
2	D	1001	ATP	C5'-O5'-PA-O2A
2	D	1001	ATP	C3'-C4'-C5'-O5'
2	C	1001	ATP	PA-O3A-PB-O2B
2	E	1001	ATP	C4'-C5'-O5'-PA
2	C	1001	ATP	C3'-C4'-C5'-O5'
2	D	1001	ATP	PG-O3B-PB-O2B
2	B	1001	ATP	PB-O3B-PG-O3G
2	A	1001	ATP	PG-O3B-PB-O3A
2	A	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PB-O3A-PA-O1A
2	D	1001	ATP	PG-O3B-PB-O1B
2	E	1001	ATP	PG-O3B-PB-O2B
2	F	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PB-O3B-PG-O1G
2	A	1001	ATP	PG-O3B-PB-O1B
2	B	1001	ATP	PG-O3B-PB-O1B
2	E	1001	ATP	PG-O3B-PB-O1B

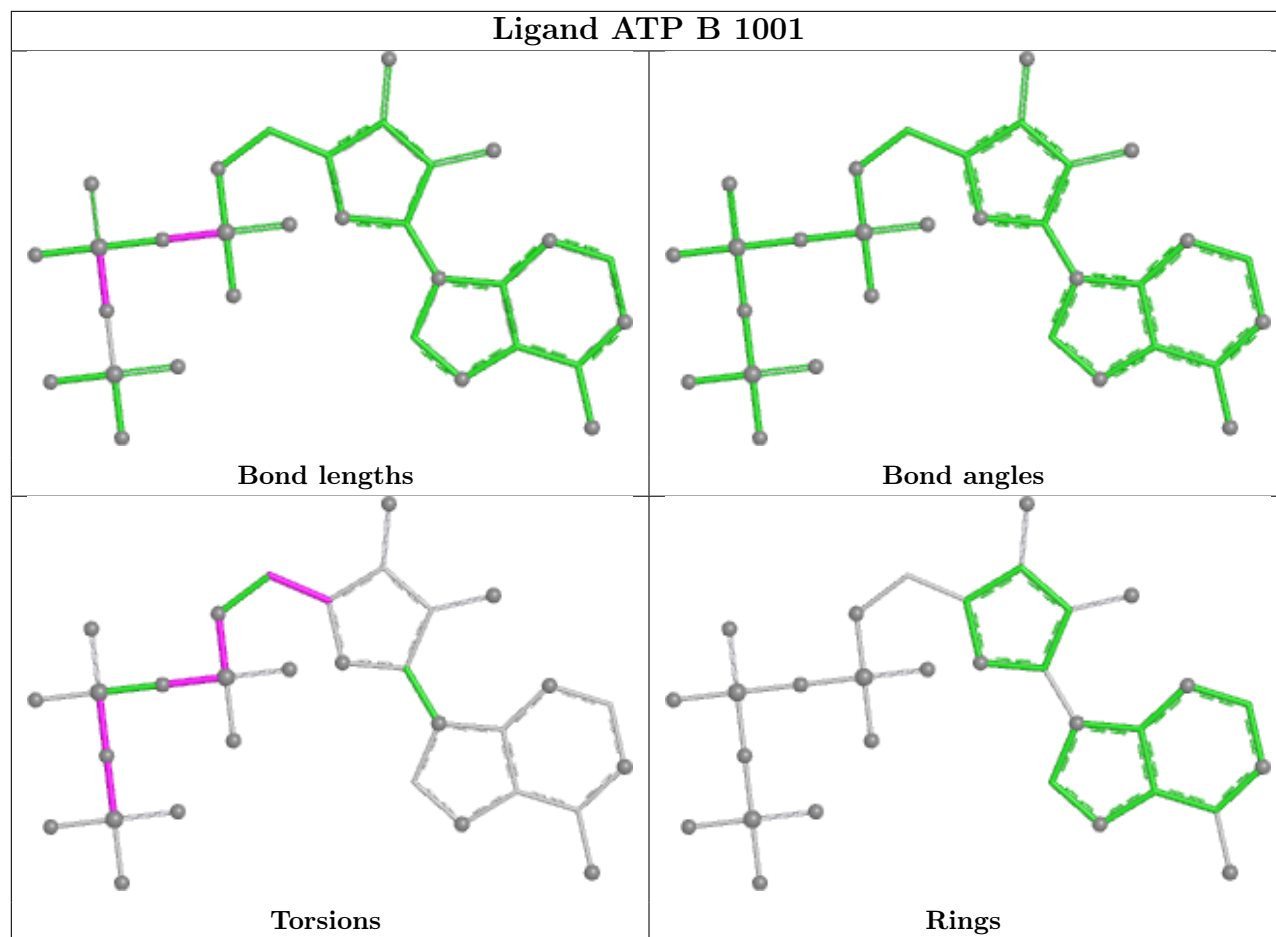
There are no ring outliers.

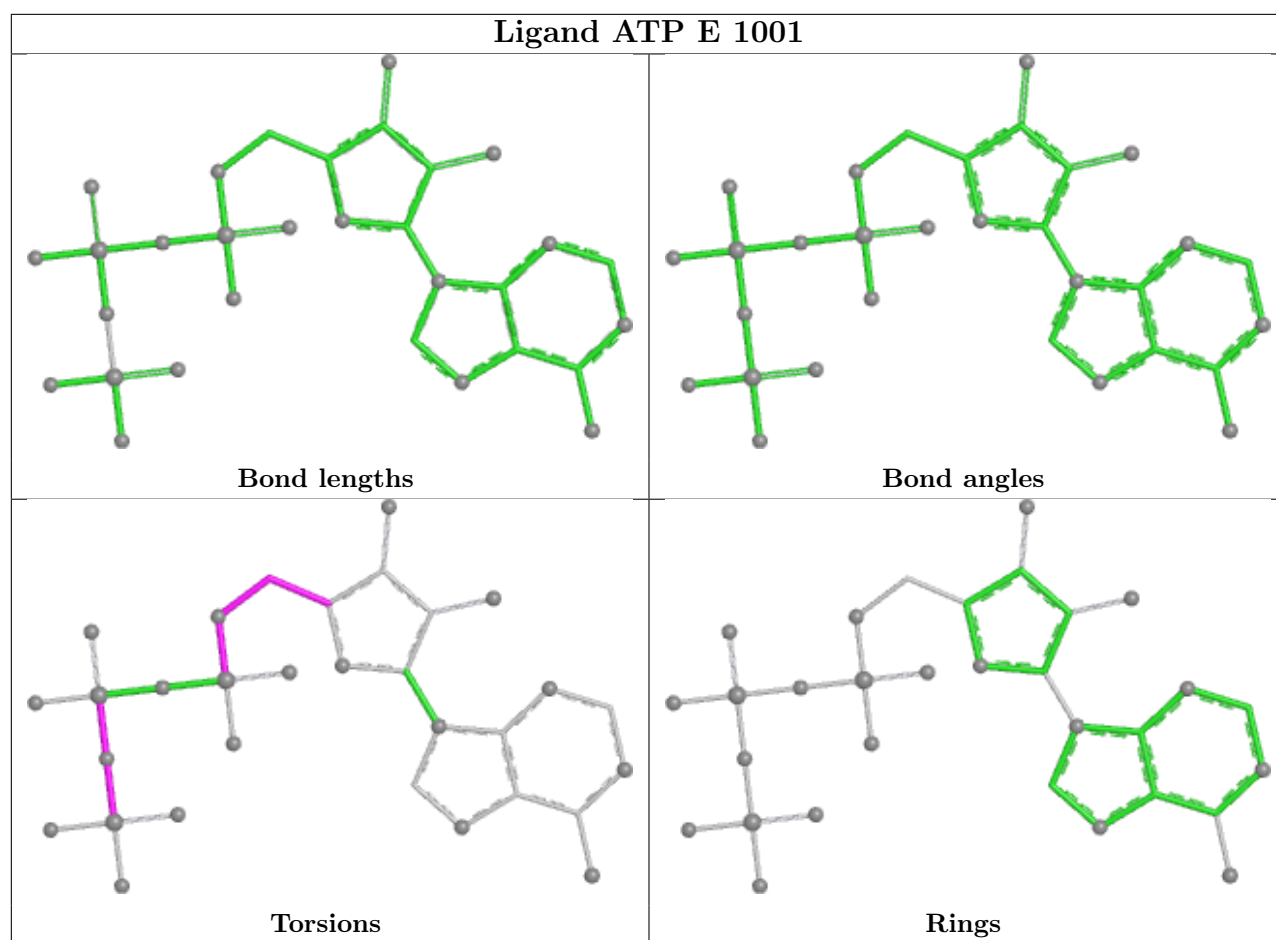
6 monomers are involved in 10 short contacts:

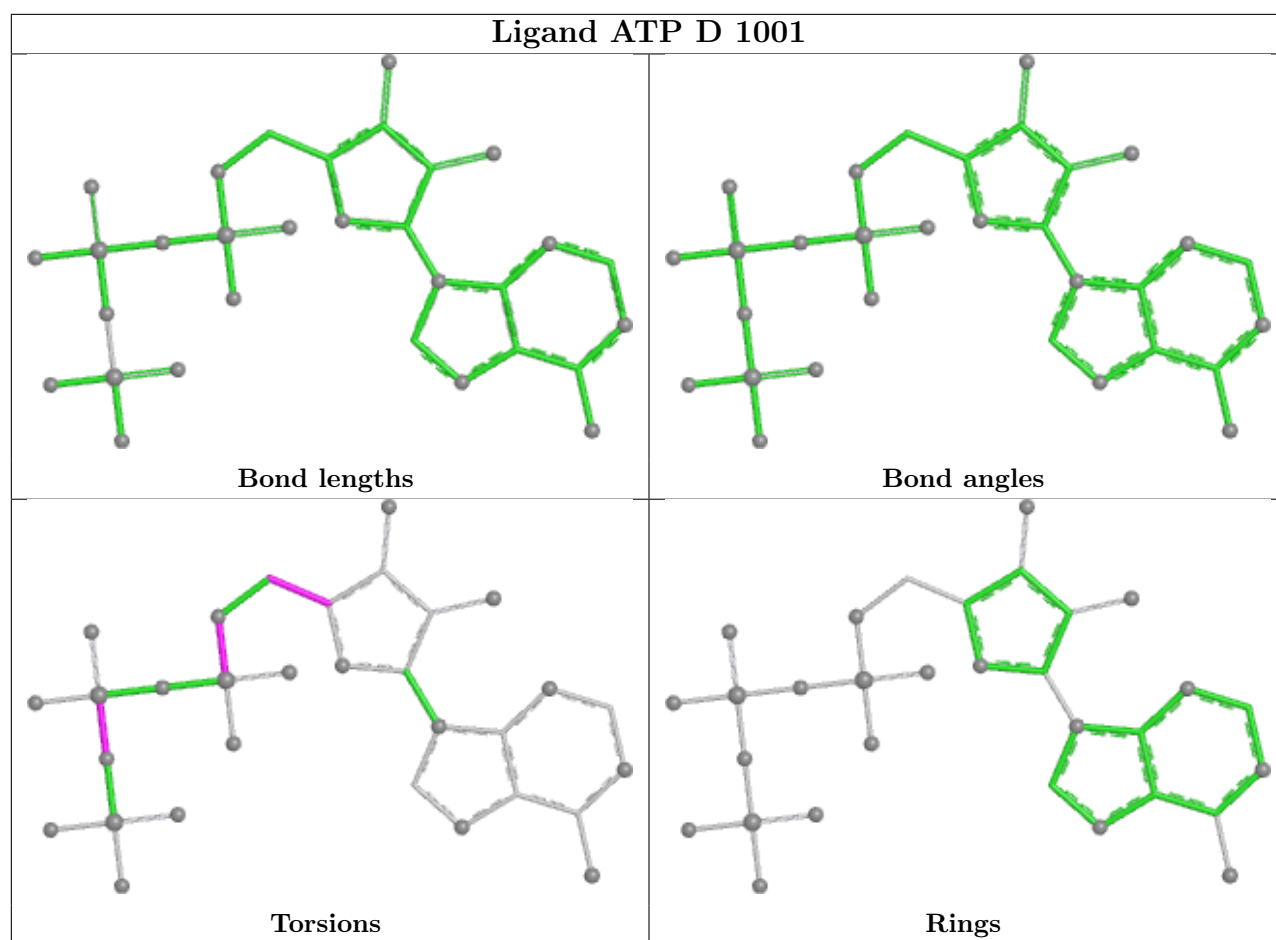
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	ATP	2	0
2	B	1001	ATP	1	0
4	B	1006	SO4	1	0
2	D	1001	ATP	2	0
2	A	1001	ATP	2	0
2	F	1001	ATP	2	0

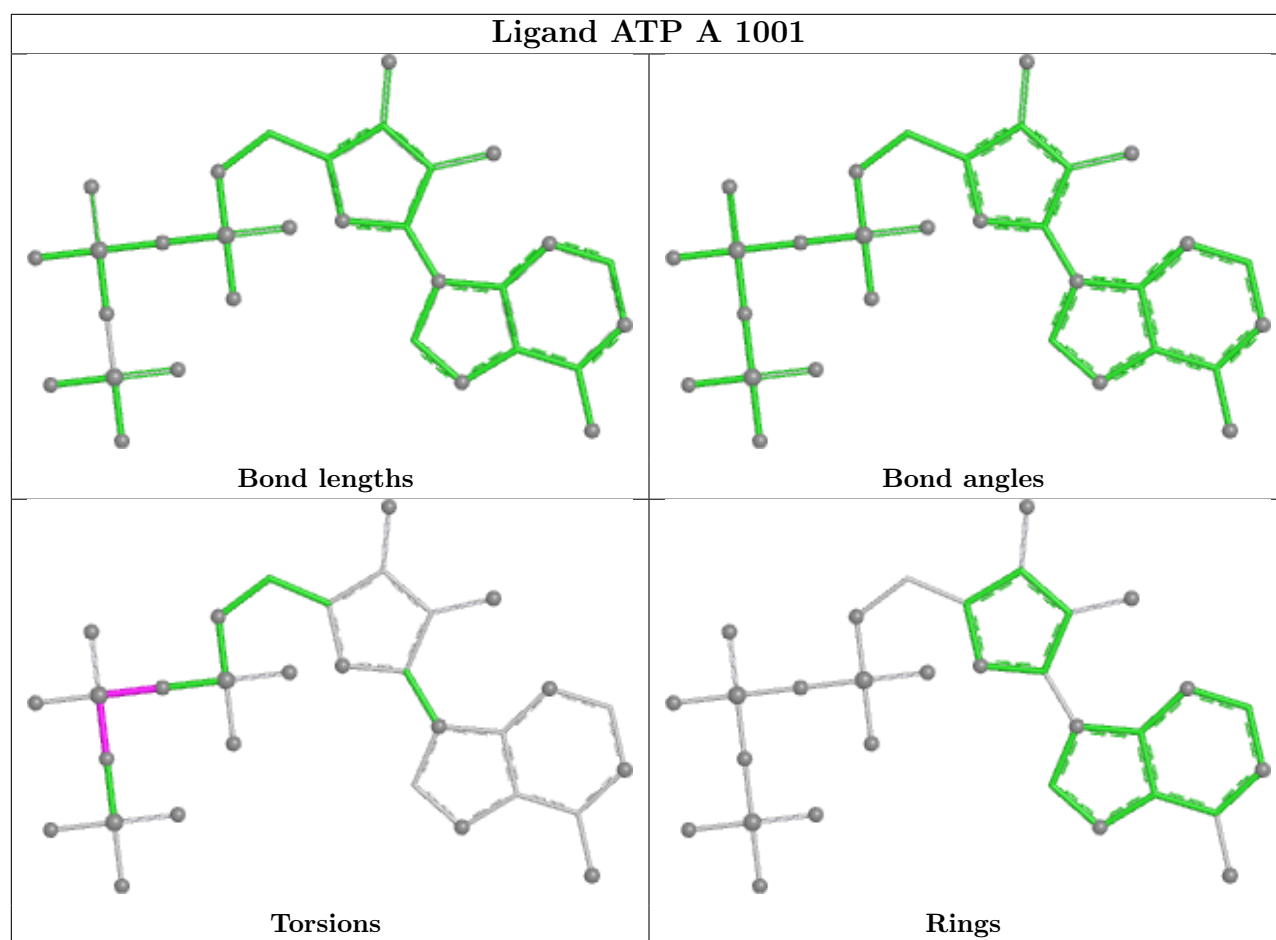
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

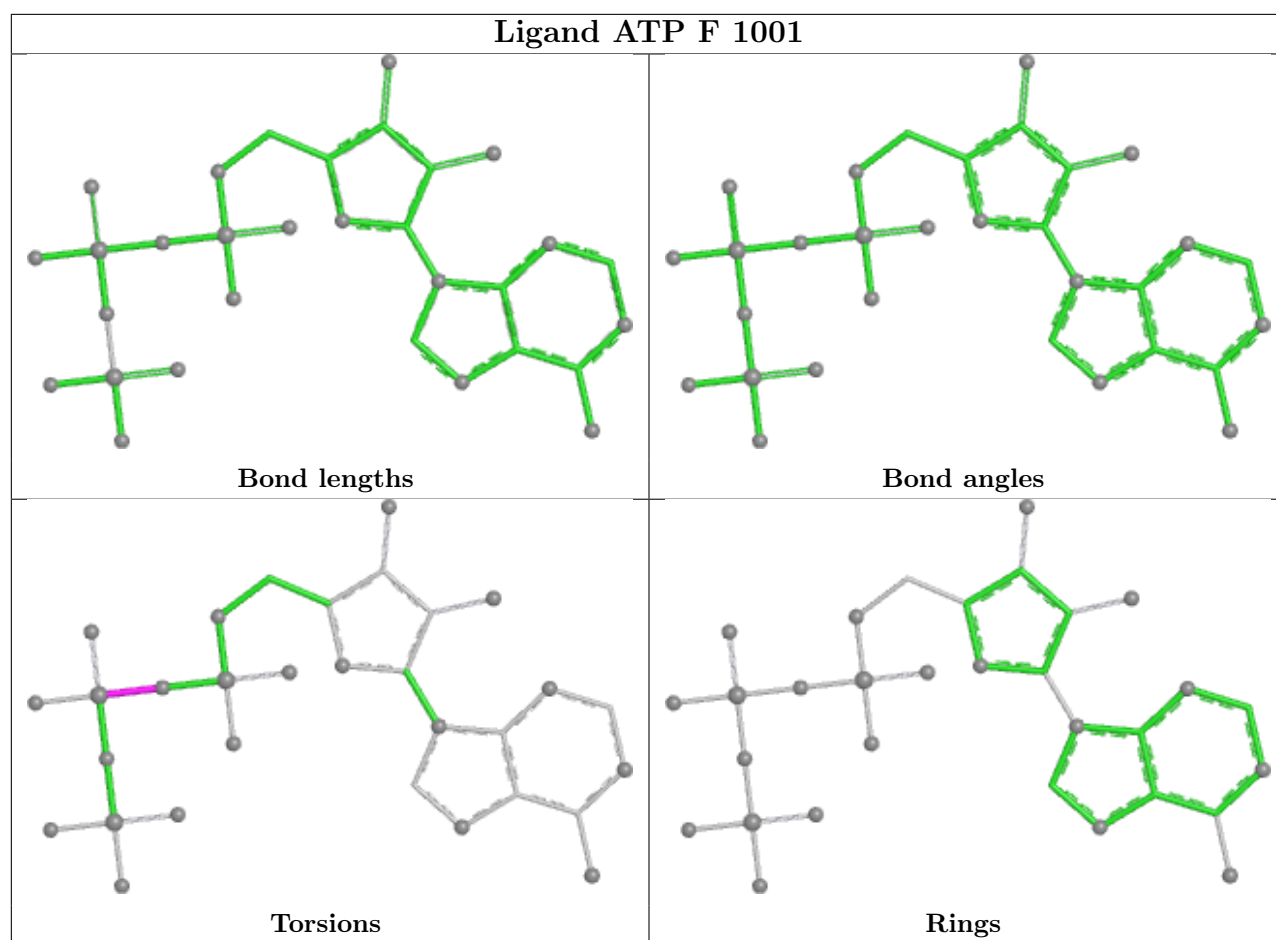












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	408/423 (96%)	-0.09	5 (1%) 76 71	37, 63, 112, 188	0
1	B	409/423 (96%)	-0.13	3 (0%) 84 80	32, 58, 122, 209	0
1	C	408/423 (96%)	0.16	9 (2%) 62 53	58, 83, 154, 221	0
1	D	408/423 (96%)	0.12	9 (2%) 62 53	53, 81, 140, 213	0
1	E	408/423 (96%)	0.22	12 (2%) 53 44	64, 90, 128, 214	0
1	F	408/423 (96%)	0.18	7 (1%) 69 62	55, 87, 153, 217	0
All	All	2449/2538 (96%)	0.08	45 (1%) 67 60	32, 80, 136, 221	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	79	PRO	3.5
1	C	410	ALA	3.3
1	B	409	THR	3.3
1	E	338	LYS	3.0
1	F	111	PHE	3.0
1	D	268	SER	2.9
1	F	86	PRO	2.9
1	B	109	ARG	2.8
1	C	331	LEU	2.8
1	D	267	THR	2.7
1	E	239	LEU	2.7
1	C	50	TYR	2.7
1	D	357	TYR	2.6
1	E	50	TYR	2.6
1	F	239	LEU	2.6
1	E	211	PHE	2.5
1	C	84	ARG	2.5
1	D	410	ALA	2.5
1	D	69	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	369	ILE	2.4
1	A	241	TYR	2.4
1	A	67	ALA	2.3
1	D	124	GLY	2.3
1	E	51	PHE	2.3
1	E	435	LEU	2.3
1	D	109	ARG	2.3
1	A	68	ASN	2.3
1	E	343	SER	2.3
1	A	65	GLY	2.3
1	D	175	ALA	2.2
1	F	79	PRO	2.2
1	D	78	LEU	2.2
1	E	78	LEU	2.2
1	A	278	ILE	2.2
1	E	316	ILE	2.2
1	E	209	GLU	2.2
1	F	361	LYS	2.1
1	F	297	PHE	2.1
1	F	182	GLU	2.1
1	C	340	GLY	2.1
1	C	77	LEU	2.0
1	C	239	LEU	2.0
1	C	53	TRP	2.0
1	E	441	LEU	2.0
1	B	185	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

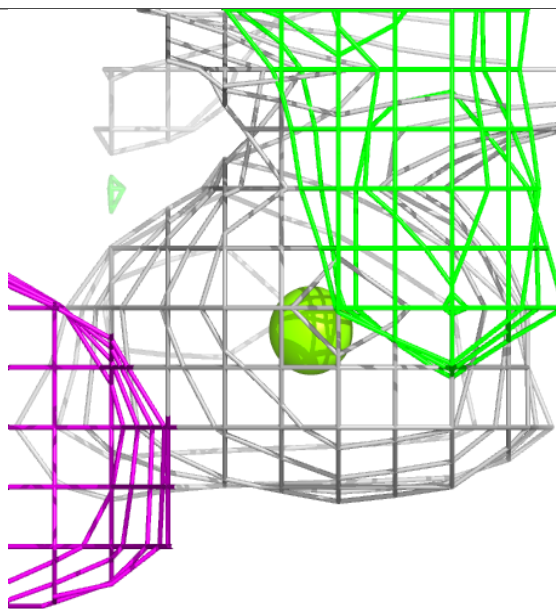
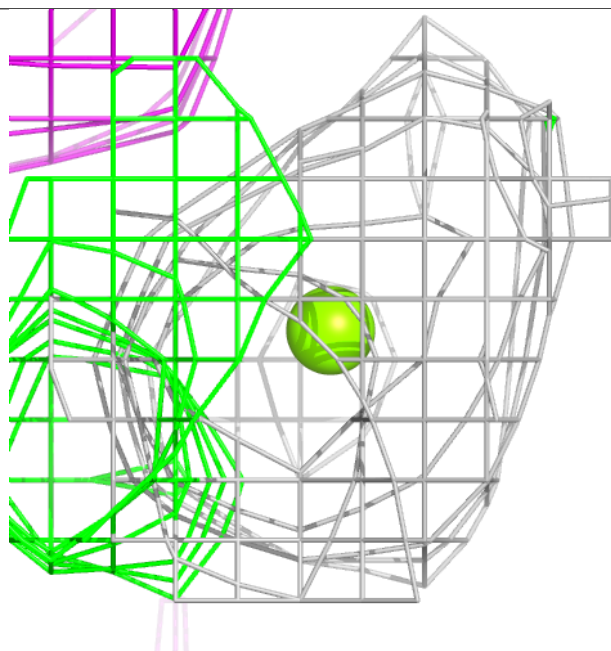
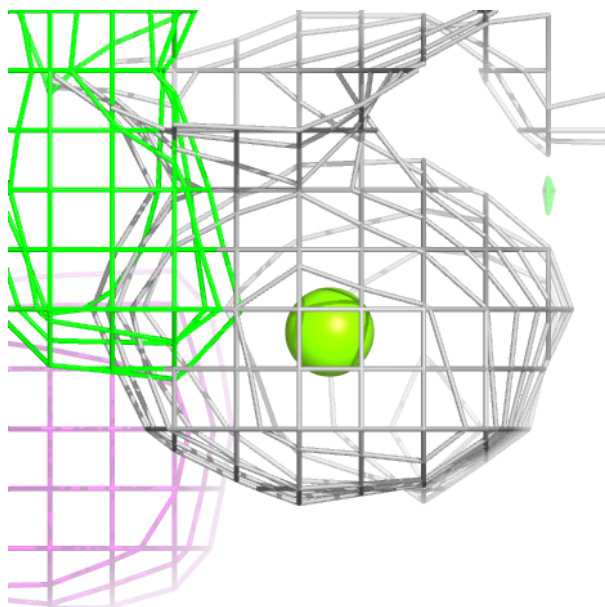
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	1003	5/5	0.79	0.16	102,104,115,119	0
4	SO4	F	1004	5/5	0.79	0.12	103,116,126,136	0
4	SO4	B	1005	5/5	0.82	0.17	86,96,125,128	0
4	SO4	B	1007	5/5	0.83	0.09	101,103,142,153	0
4	SO4	C	1004	5/5	0.83	0.20	97,106,112,127	0
4	SO4	B	1006	5/5	0.86	0.10	90,104,114,117	0
3	MG	B	1003	1/1	0.86	0.10	37,37,37,37	0
4	SO4	C	1003	5/5	0.86	0.17	106,106,113,125	0
4	SO4	A	1003	5/5	0.89	0.19	78,81,92,97	0
5	NH4	E	1003	1/1	0.89	0.07	70,84,84,84	0
4	SO4	D	1004	5/5	0.91	0.14	90,94,95,102	0
4	SO4	A	1004	5/5	0.92	0.13	62,80,97,104	0
4	SO4	D	1003	5/5	0.92	0.11	79,82,94,102	0
2	ATP	E	1001	31/31	0.93	0.10	76,102,120,121	0
2	ATP	C	1001	31/31	0.94	0.10	58,75,88,96	0
2	ATP	F	1001	31/31	0.94	0.09	54,62,74,77	0
2	ATP	D	1001	31/31	0.94	0.08	65,86,95,99	0
3	MG	B	1002	1/1	0.95	0.16	52,52,52,52	0
2	ATP	A	1001	31/31	0.96	0.07	53,68,83,96	0
4	SO4	B	1004	5/5	0.96	0.09	59,66,87,93	0
3	MG	D	1002	1/1	0.97	0.14	82,82,82,82	0
3	MG	F	1002	1/1	0.97	0.12	53,53,53,53	0
2	ATP	B	1001	31/31	0.97	0.07	34,44,57,59	0
3	MG	E	1002	1/1	0.98	0.09	94,94,94,94	0
3	MG	C	1002	1/1	0.98	0.13	63,63,63,63	0
3	MG	A	1002	1/1	0.98	0.13	64,64,64,64	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.

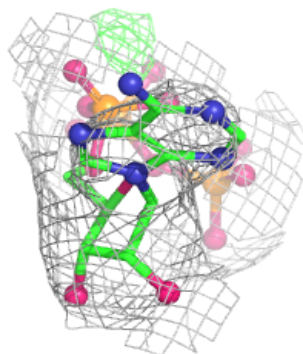
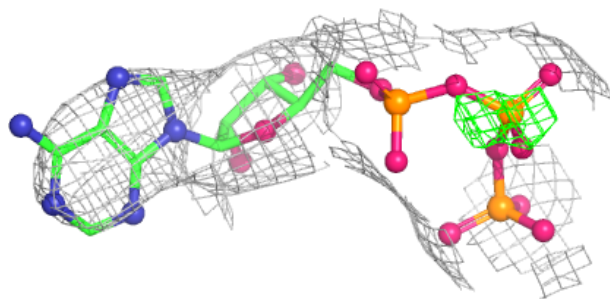
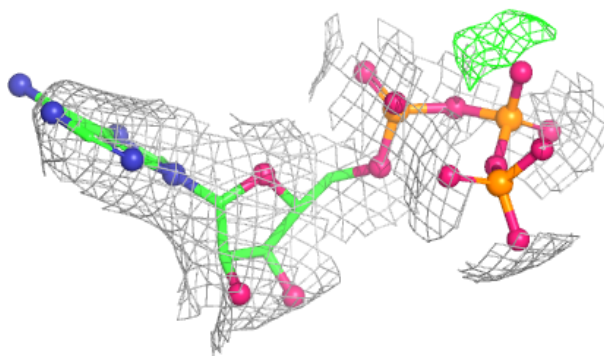
Electron density around MG B 1003:

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

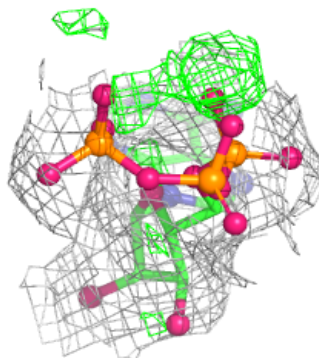
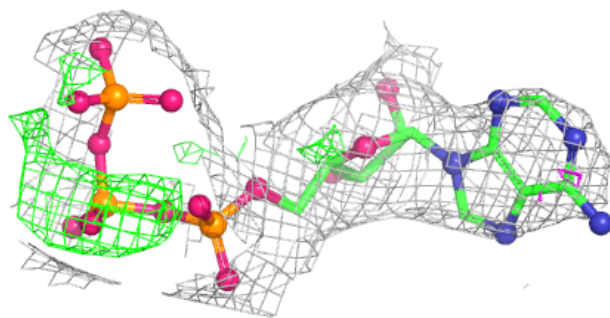
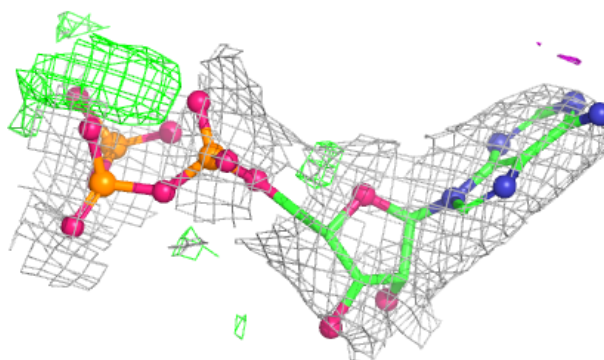


Electron density around ATP E 1001:

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

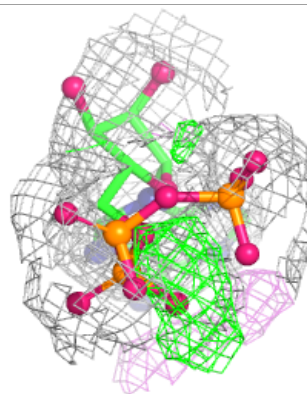
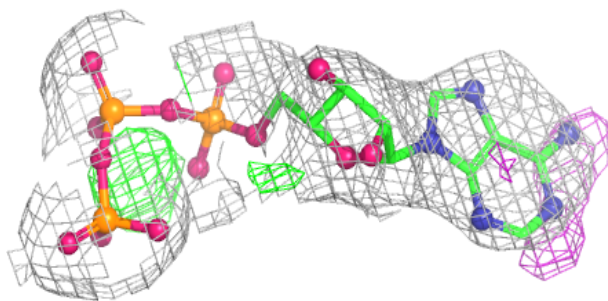
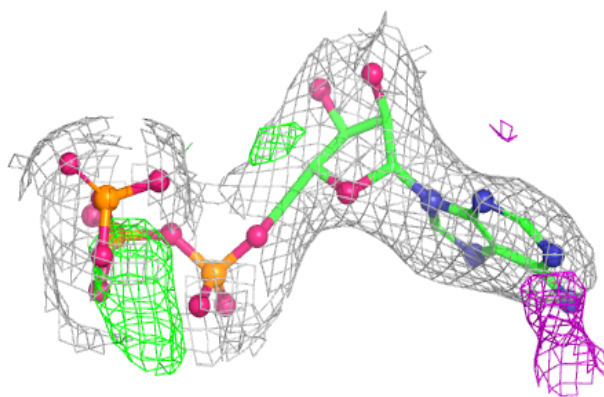
**Electron density around ATP C 1001:**

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

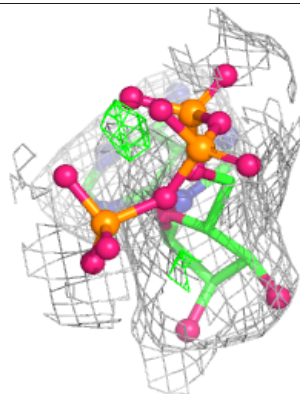
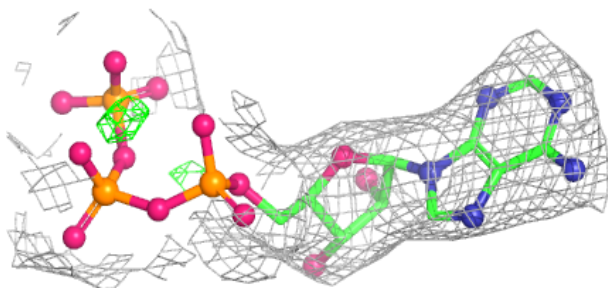
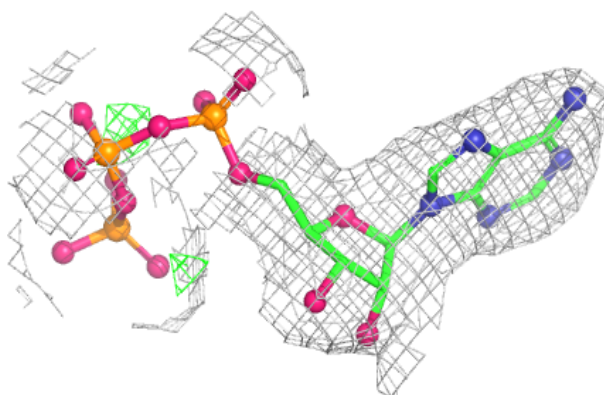


Electron density around ATP F 1001:

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

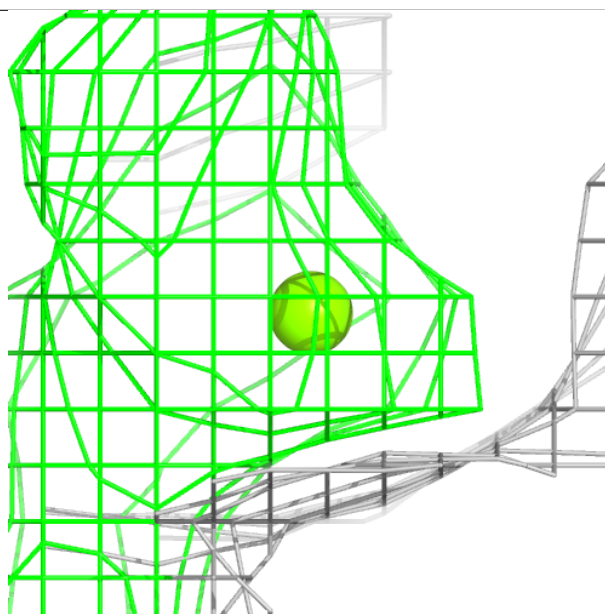
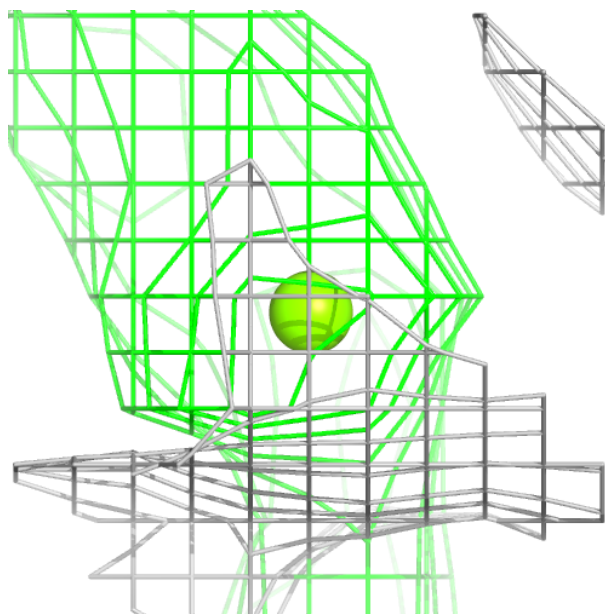
**Electron density around ATP D 1001:**

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



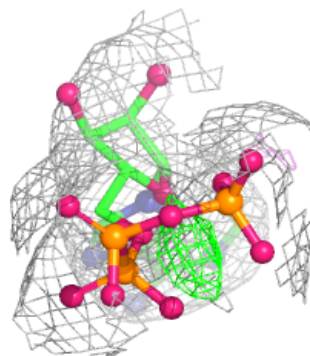
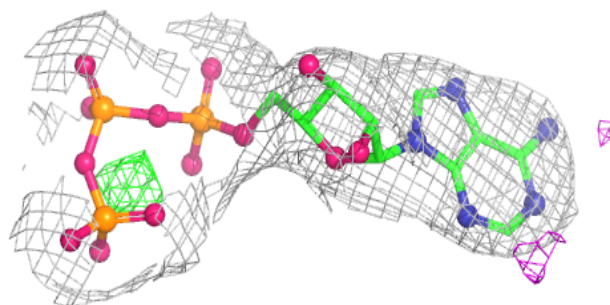
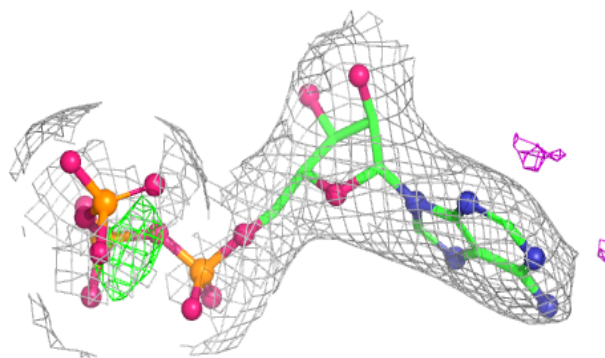
Electron density around MG B 1002:

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



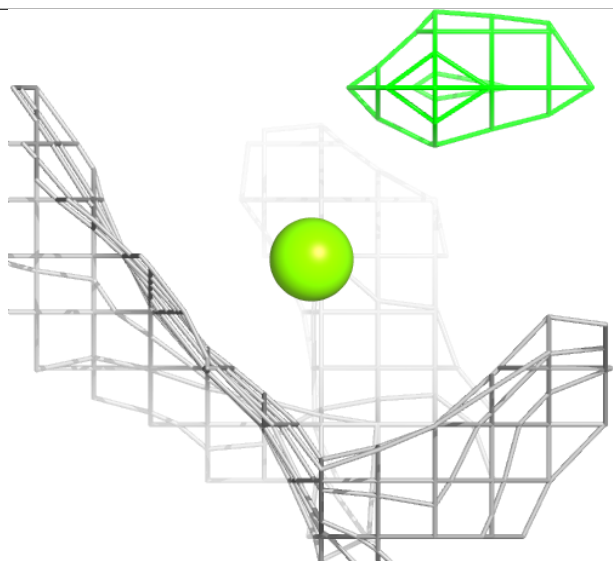
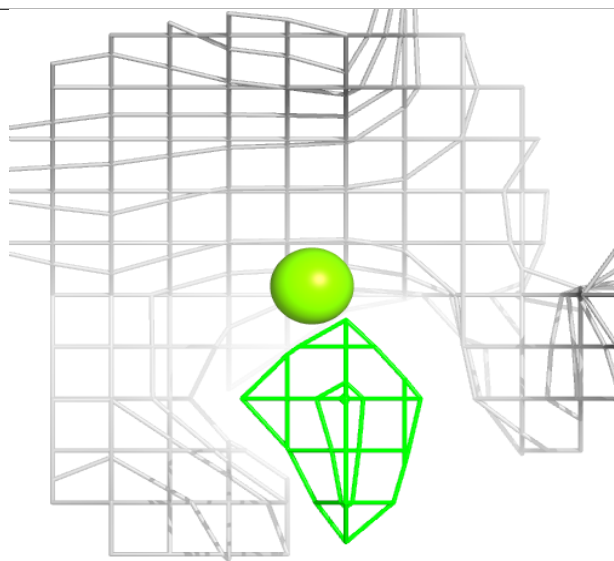
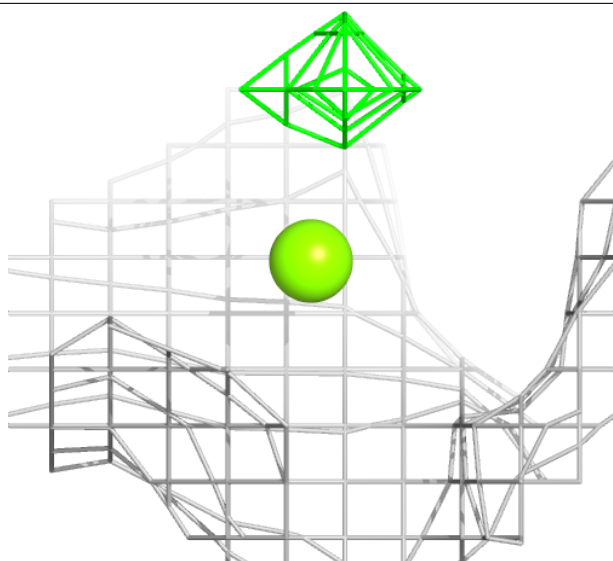
Electron density around ATP A 1001:

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



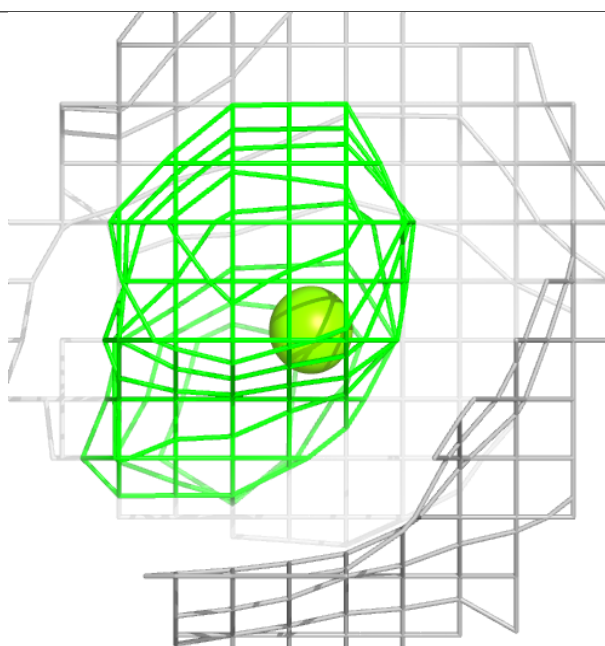
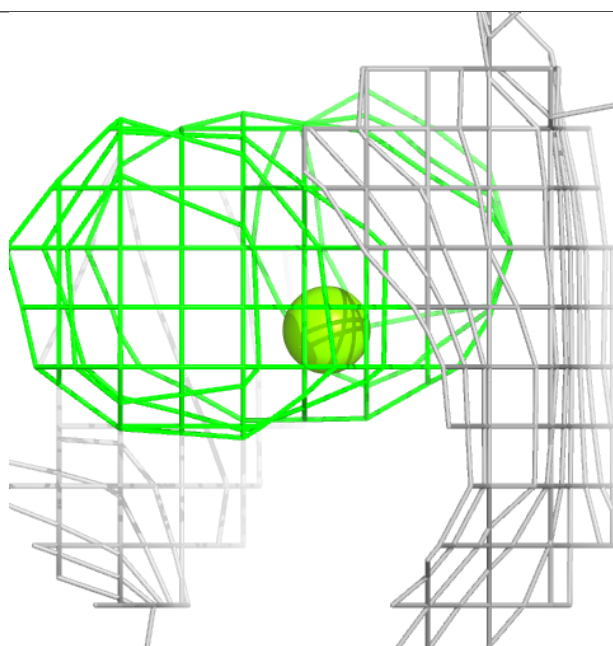
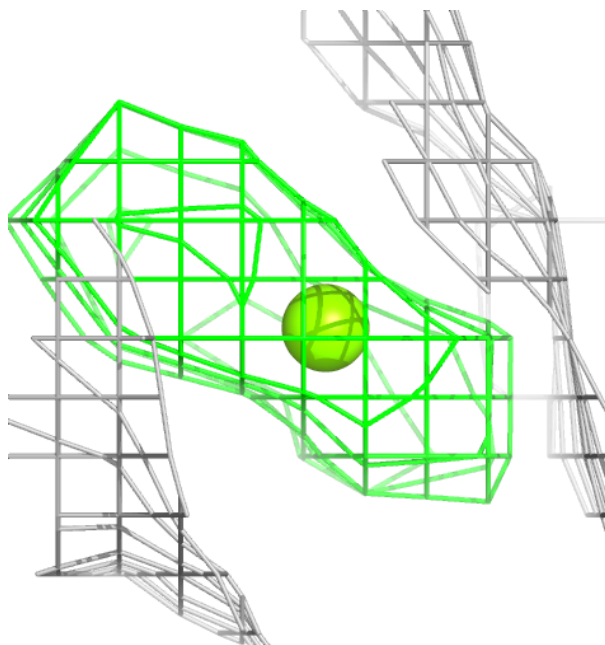
Electron density around MG D 1002:

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



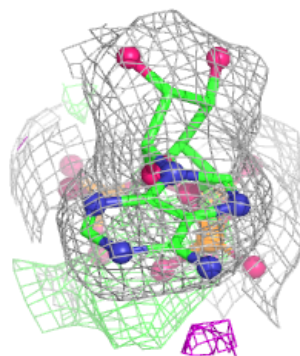
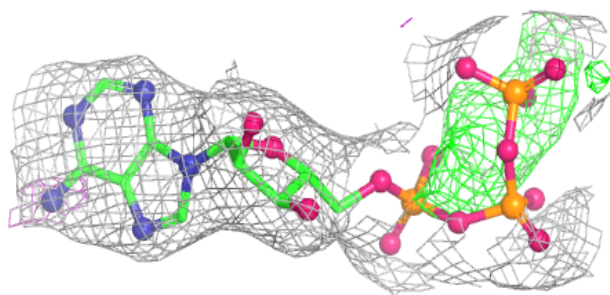
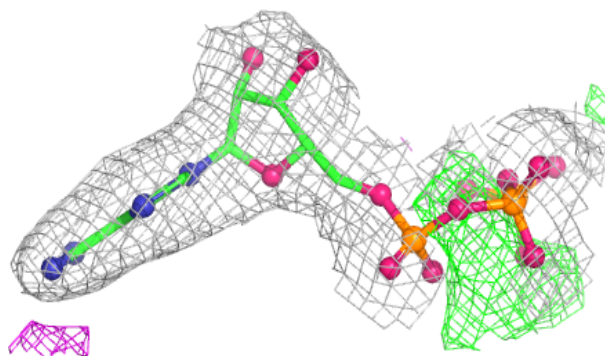
Electron density around MG F 1002:

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



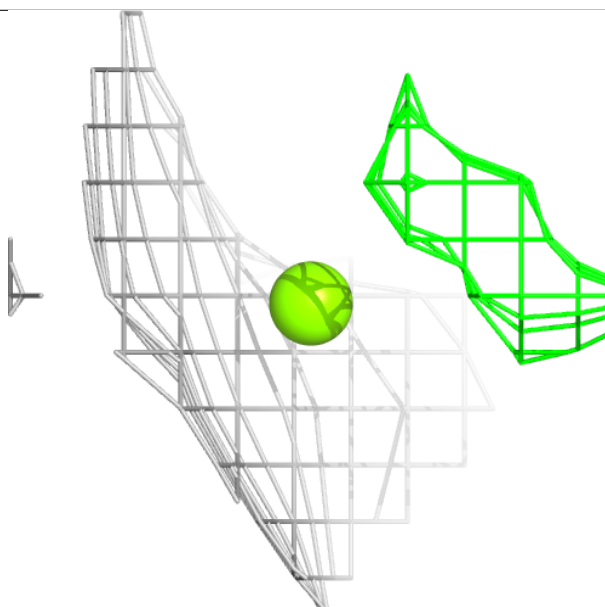
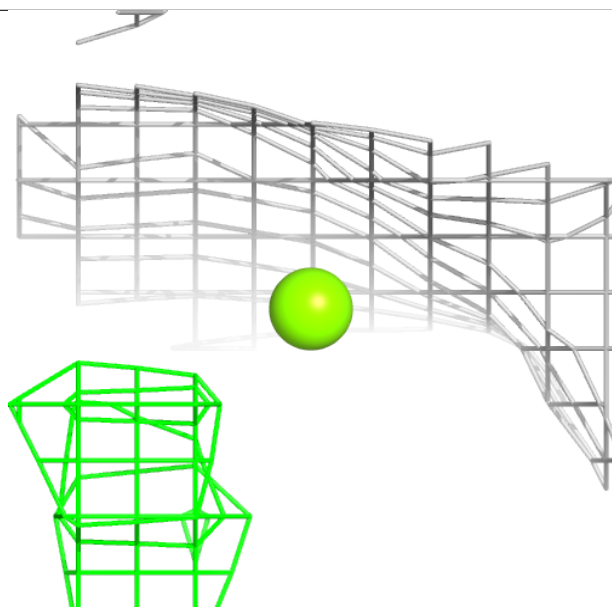
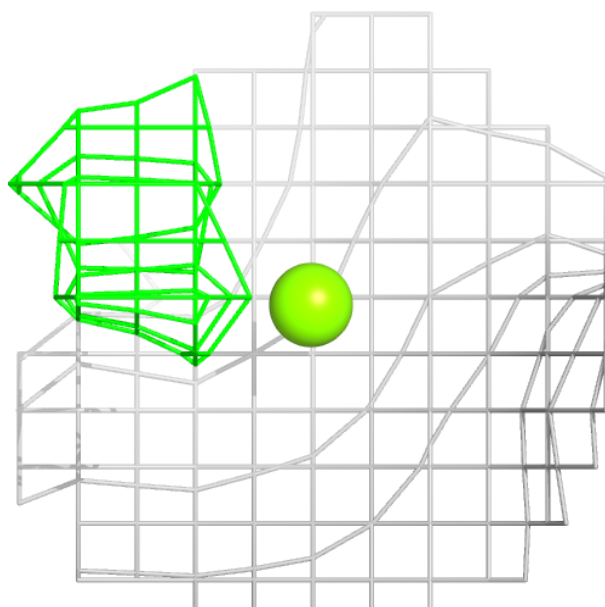
Electron density around ATP B 1001:

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



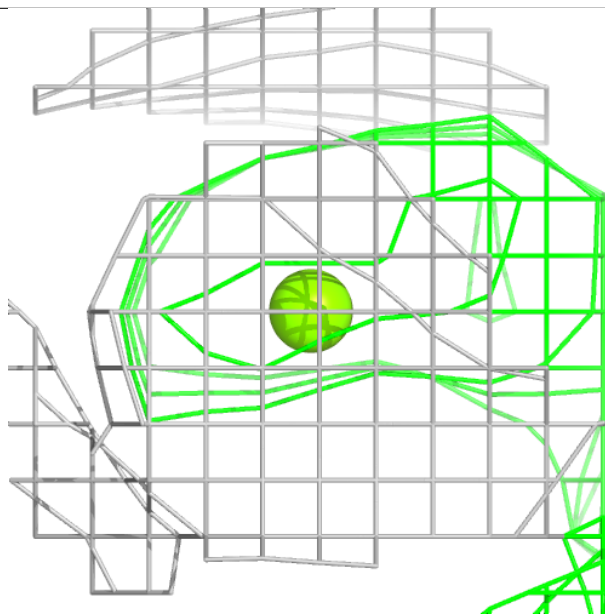
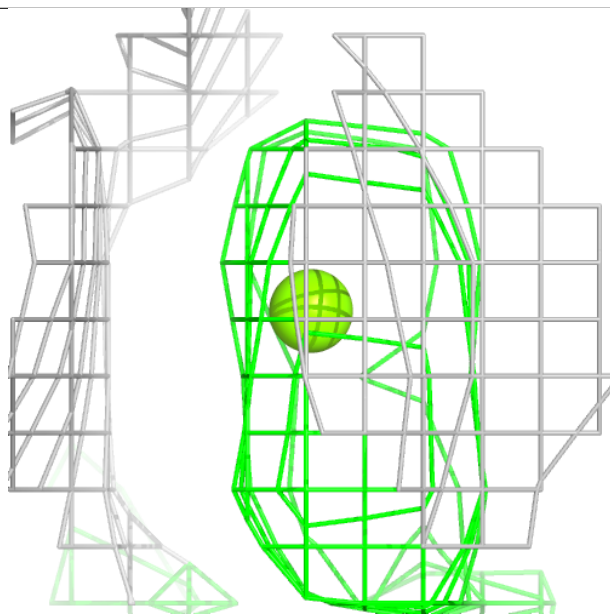
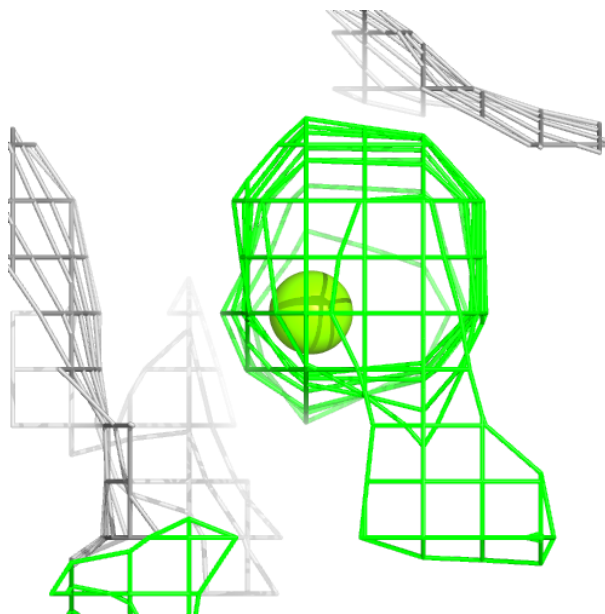
Electron density around MG E 1002:

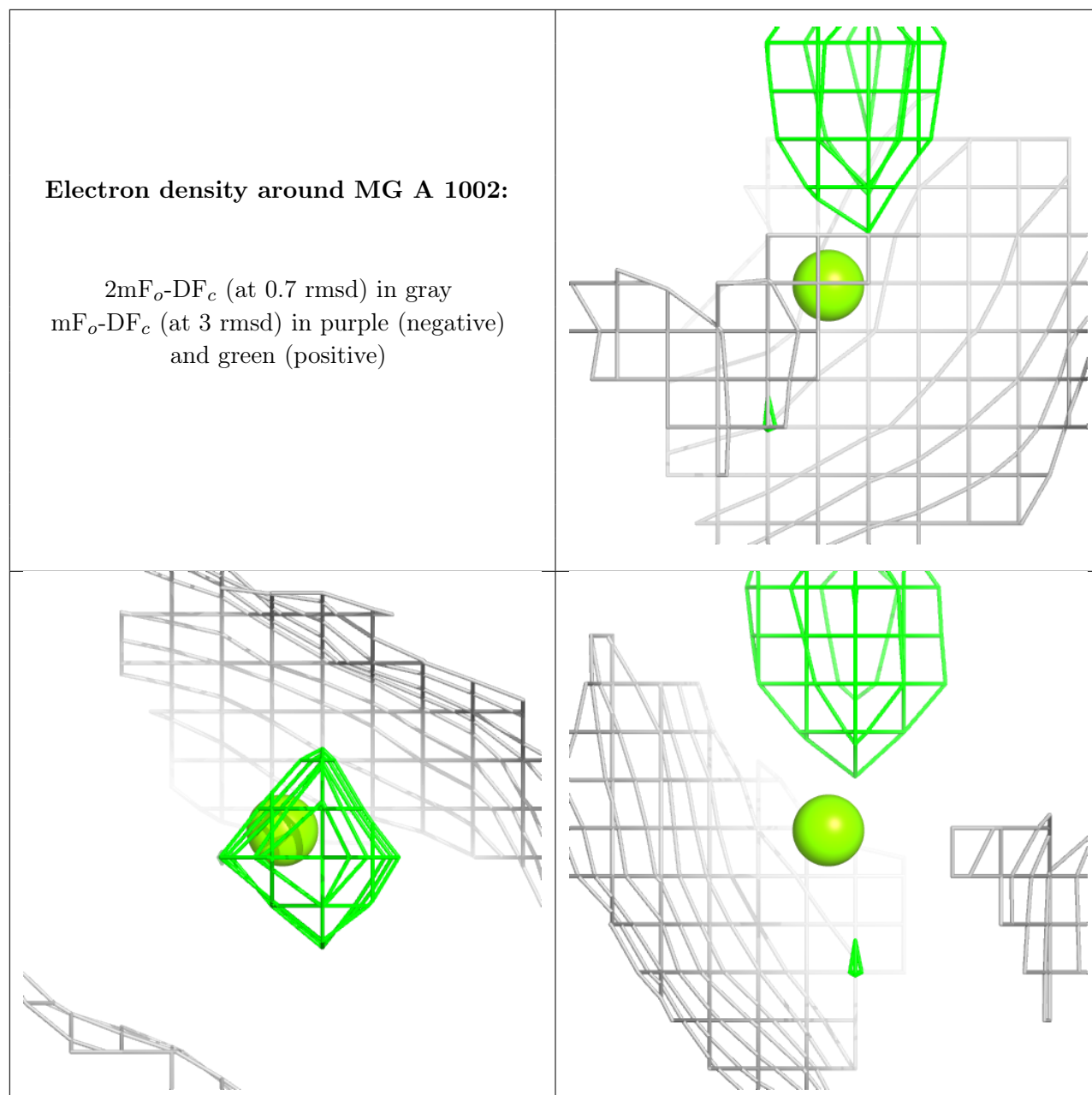
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG C 1002:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.