



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:45 pm BST

PDB ID : 3ZIA
Title : The structure of F1-ATPase from *Saccharomyces cerevisiae* inhibited by its regulatory protein IF1
Authors : Robinson, G.C.; Bason, J.V.; Montgomery, M.G.; Fearnley, I.M.; Mueller, D.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2013-01-07
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

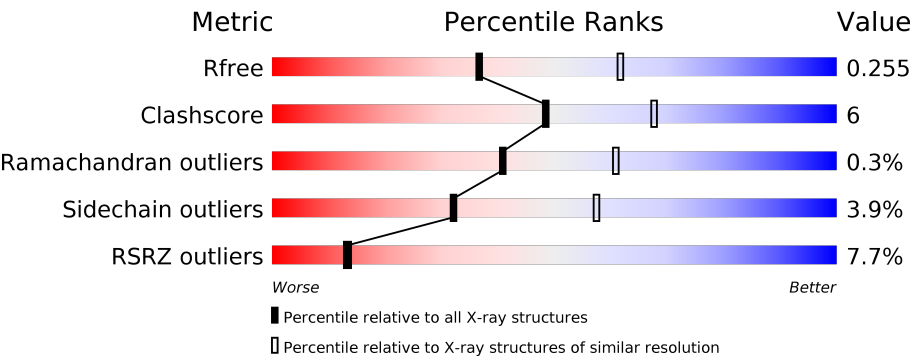
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	510	<div><div>5%</div><div><div></div><div>82%</div><div>12%</div><div>• 5%</div></div></div>
1	B	510	<div><div>5%</div><div><div></div><div>81%</div><div>12%</div><div>• 6%</div></div></div>
1	C	510	<div><div>7%</div><div><div></div><div>84%</div><div>11%</div><div>• 5%</div></div></div>
1	K	510	<div><div>7%</div><div><div></div><div>82%</div><div>12%</div><div>• 5%</div></div></div>
1	L	510	<div><div>%</div><div><div></div><div>81%</div><div>13%</div><div>• 6%</div></div></div>
1	M	510	<div><div>7%</div><div><div></div><div>84%</div><div>10%</div><div>• 5%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	478	
2	E	478	
2	F	478	
2	N	478	
2	O	478	
2	P	478	
3	G	278	
3	Q	278	
4	H	138	
4	R	138	
5	I	61	
5	S	61	
6	J	63	
6	T	63	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51906 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	B	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	K	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	L	480	Total	C	N	O	S	0	1	0
			3655	2310	648	694	3			
1	M	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	1	0
			3548	2251	603	687	7			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	O	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	P	469	Total	C	N	O	S	0	3	0
			3559	2260	603	689	7			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2057	1291	358	398	10			
3	Q	265	Total	C	N	O	S	0	1	0
			2063	1295	358	400	10			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			
4	R	124	Total	C	N	O	S	0	0	0
			937	594	156	185	2			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	58	Total	C	N	O	0	0	0
			450	283	79	88			
5	S	58	Total	C	N	O	0	0	0
			450	283	79	88			

- Molecule 6 is a protein called ATPASE INHIBITOR, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	36	Total	C	N	O	0	0	0
			283	168	55	60			
6	T	36	Total	C	N	O	0	0	0
			283	168	55	60			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	21	ALA	GLU	engineered mutation	UNP P01097
T	21	ALA	GLU	engineered mutation	UNP P01097

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	K	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	N	1	Total	Mg	0	0
			1	1		
8	L	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	M	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			4	2	2		
10	L	1	Total	C	O	0	0
			4	2	2		
10	L	1	Total	C	O	0	0
			4	2	2		
10	M	1	Total	C	O	0	0
			4	2	2		
10	O	1	Total	C	O	0	0
			4	2	2		
10	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	18	Total	O	0	0
			18	18		
11	B	90	Total	O	0	0
			90	90		
11	C	94	Total	O	0	0
			94	94		
11	D	37	Total	O	0	0
			37	37		
11	E	20	Total	O	0	0
			20	20		
11	F	81	Total	O	0	0
			81	81		

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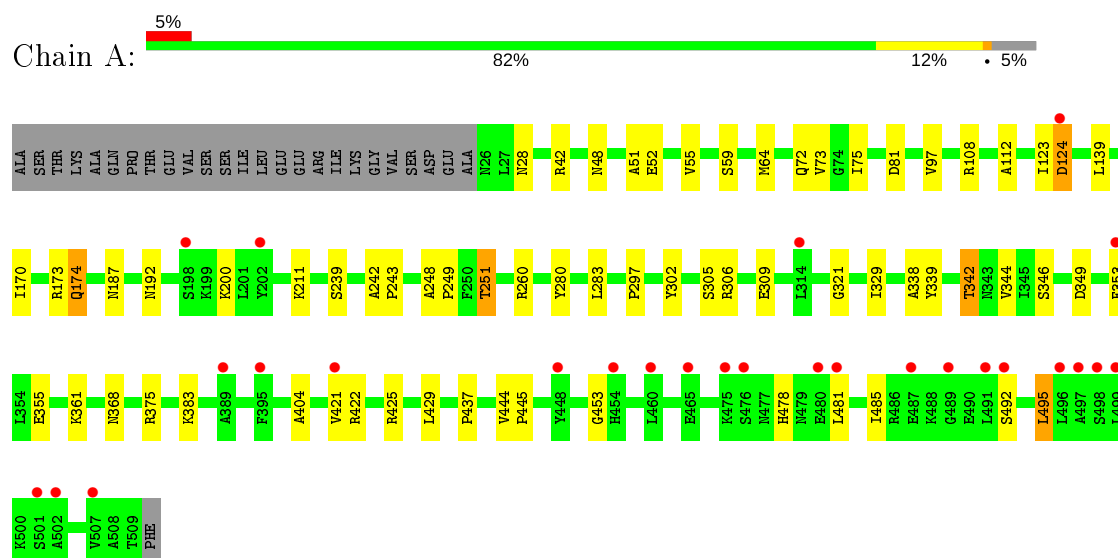
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	11	Total 11	O 11	0	0
11	H	1	Total 1	O 1	0	0
11	I	1	Total 1	O 1	0	0
11	K	27	Total 27	O 27	0	0
11	L	156	Total 156	O 156	0	0
11	M	76	Total 76	O 76	0	0
11	N	32	Total 32	O 32	0	0
11	O	52	Total 52	O 52	0	0
11	P	68	Total 68	O 68	0	0
11	Q	8	Total 8	O 8	0	0
11	R	1	Total 1	O 1	0	0

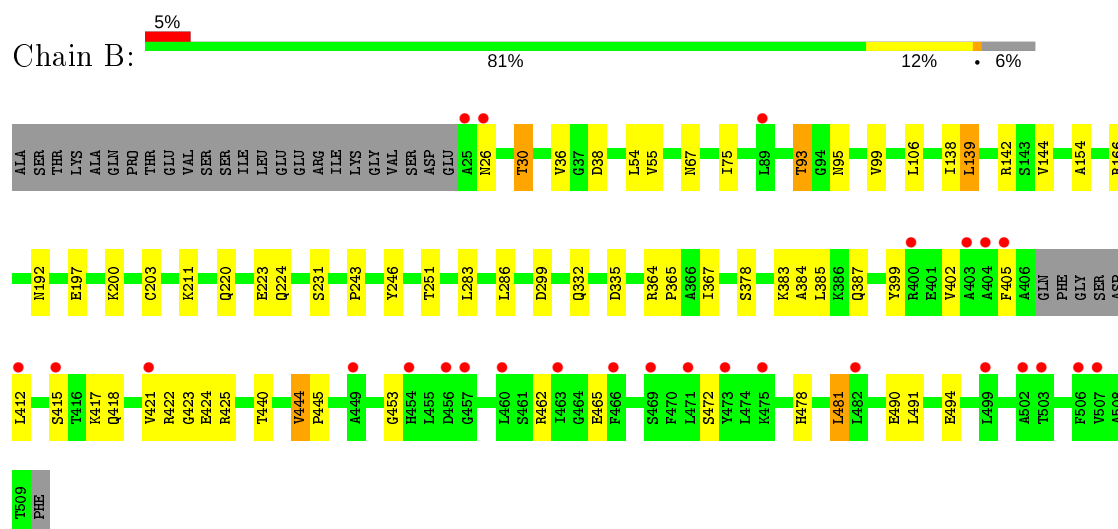
3 Residue-property plots [i](#)

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

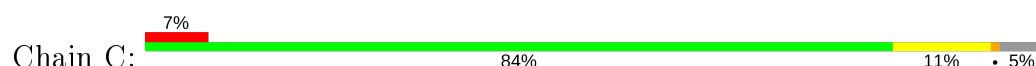
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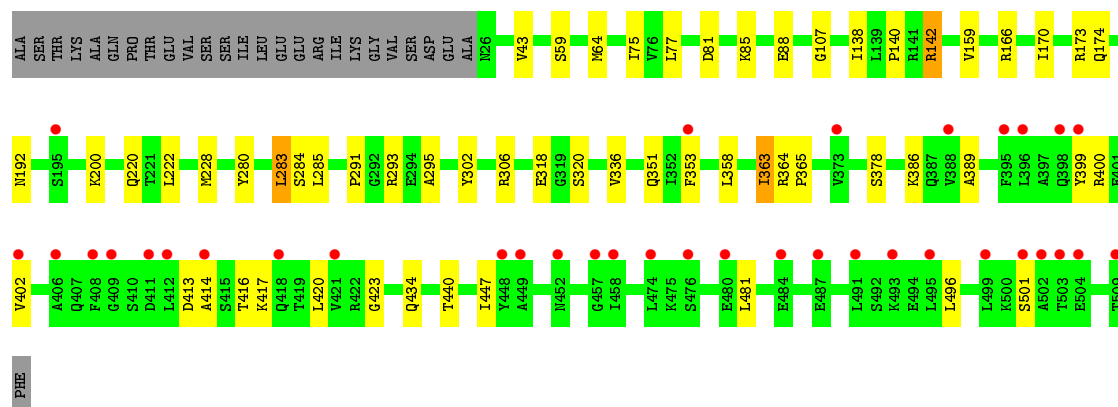


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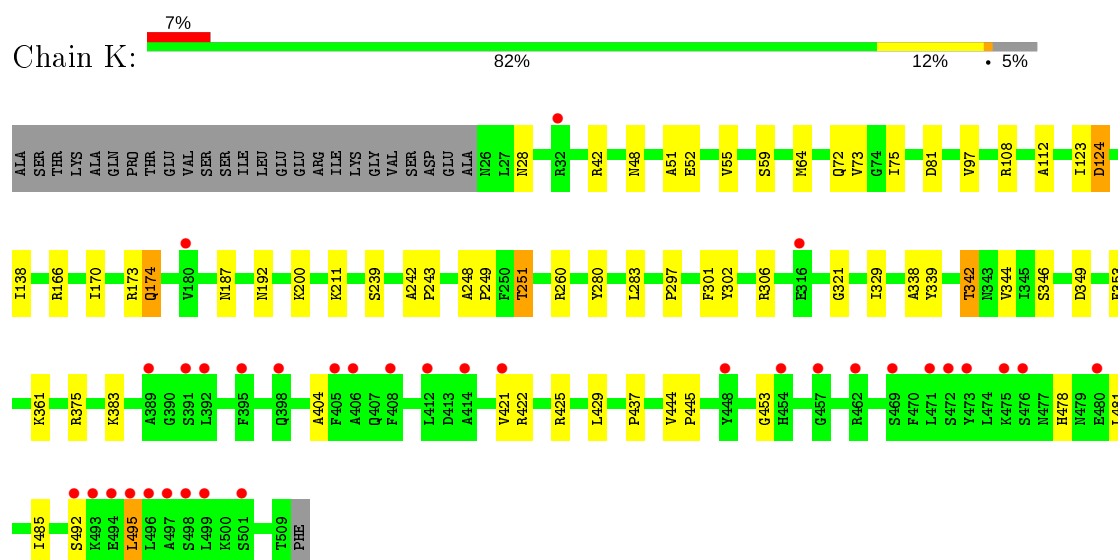


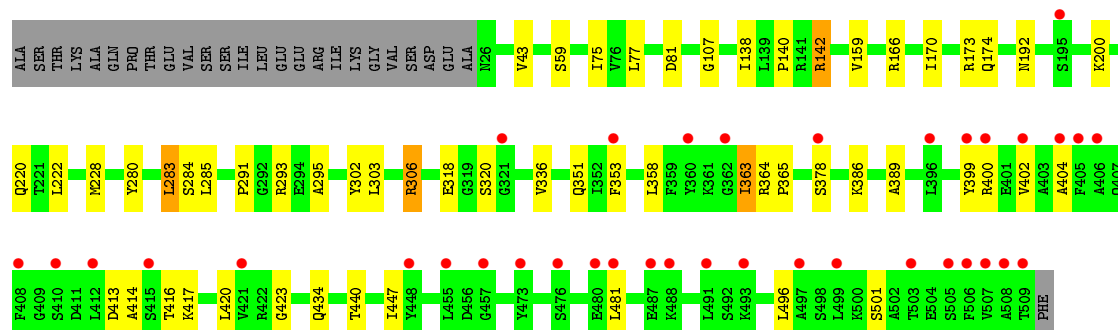
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



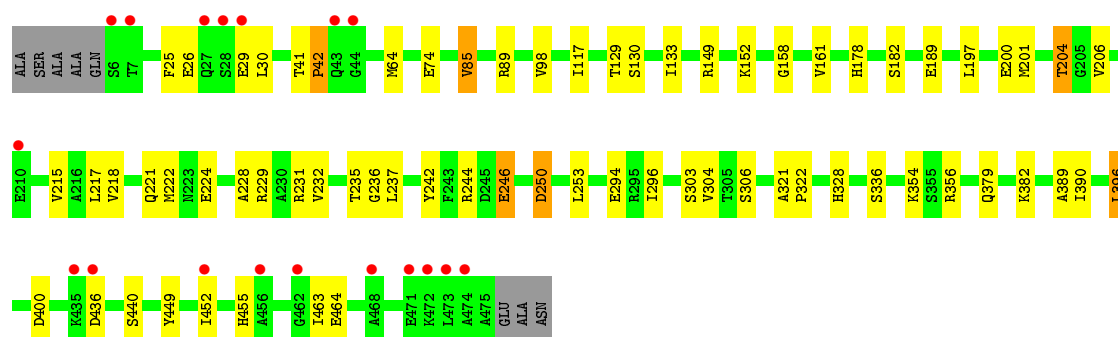
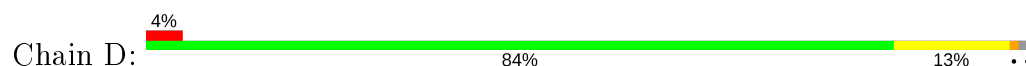


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

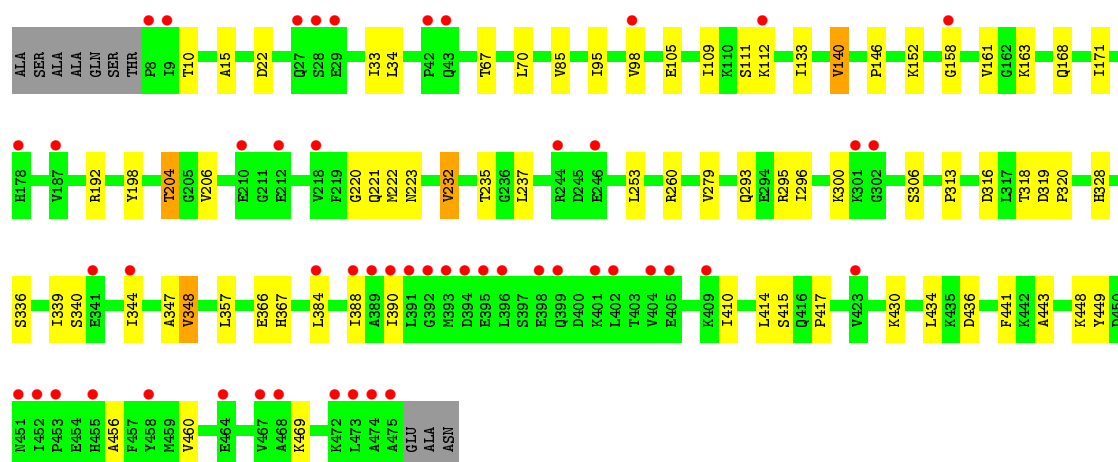
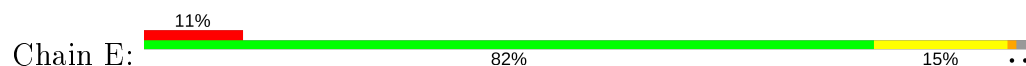




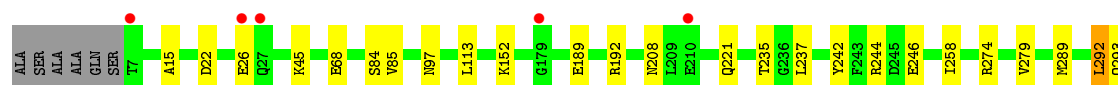
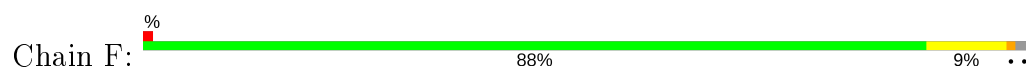
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

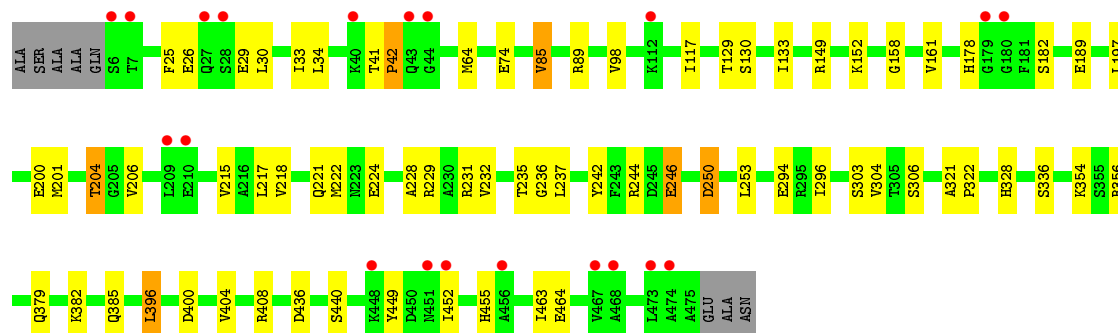
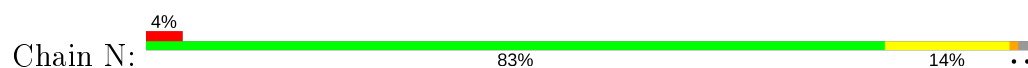


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

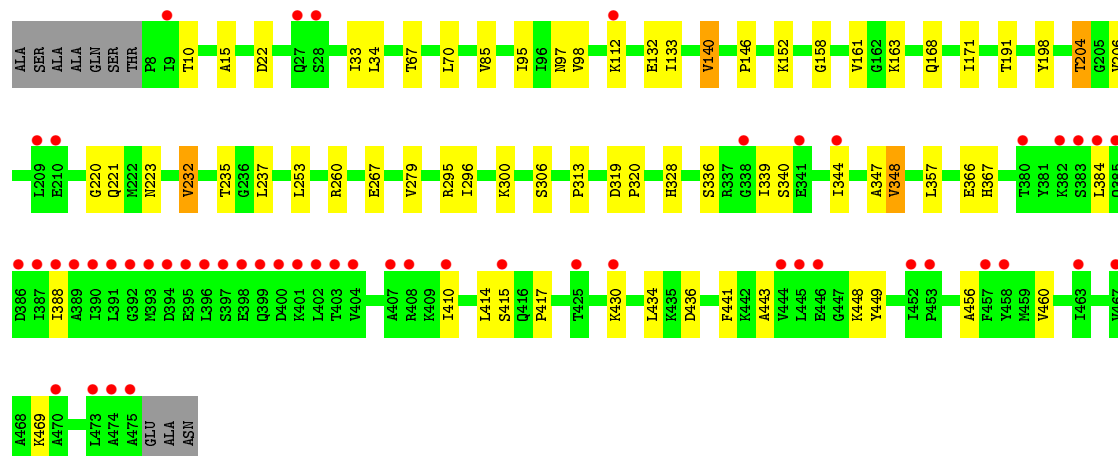
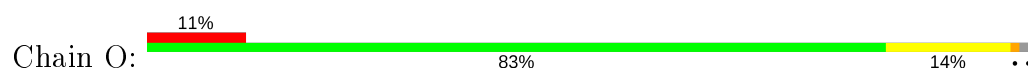




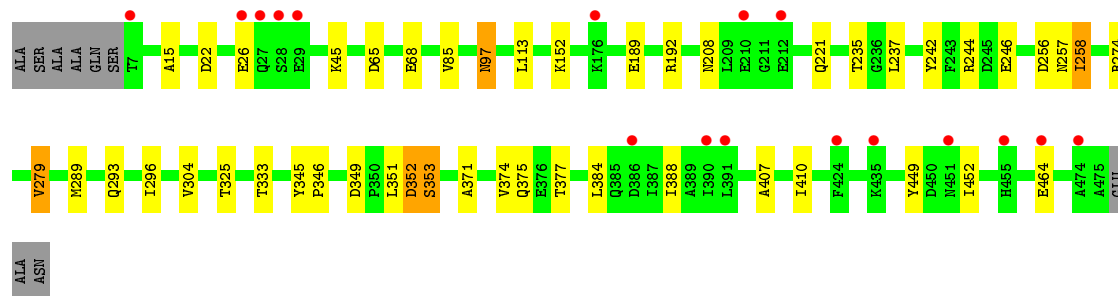
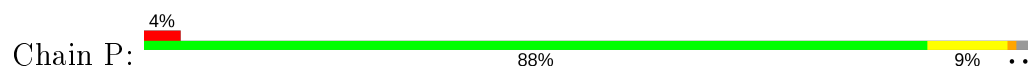
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



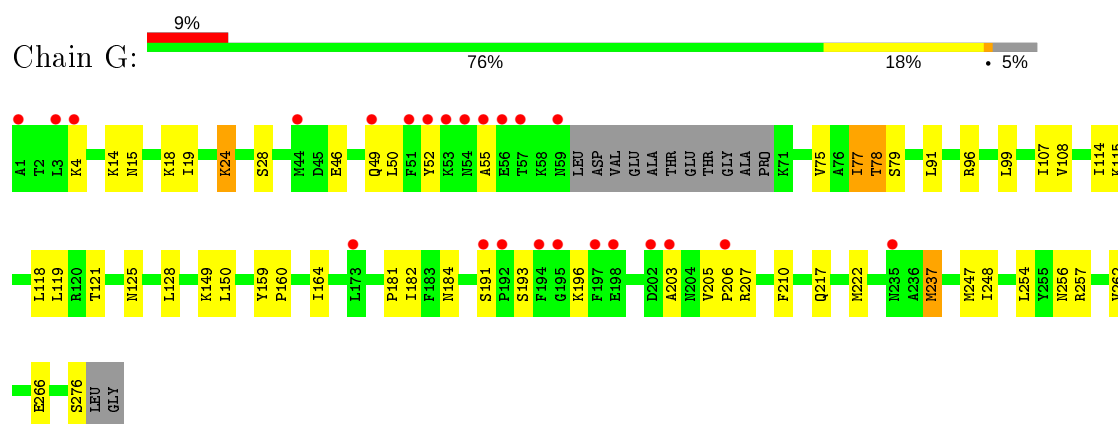
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



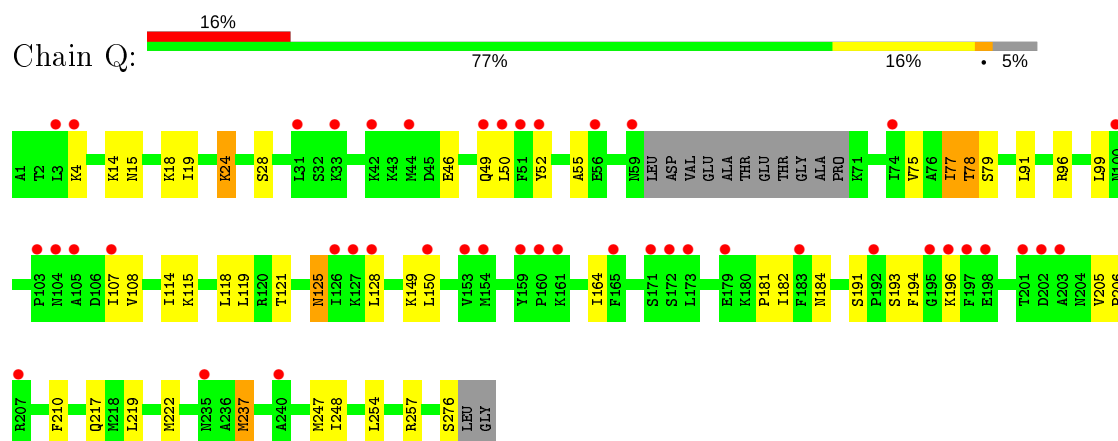
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



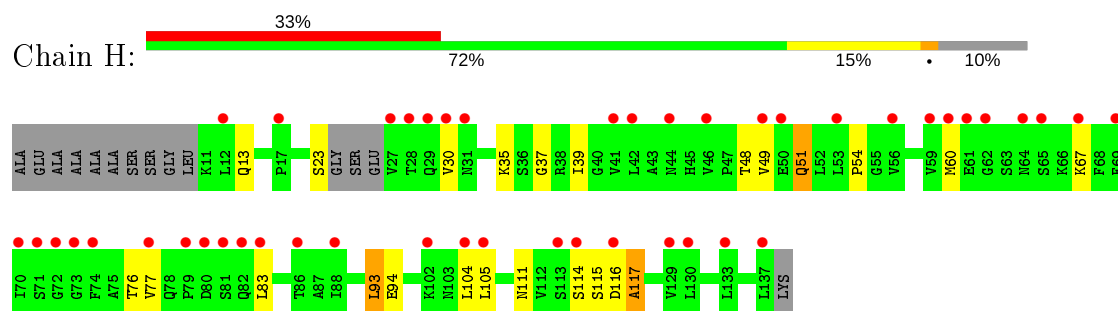
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



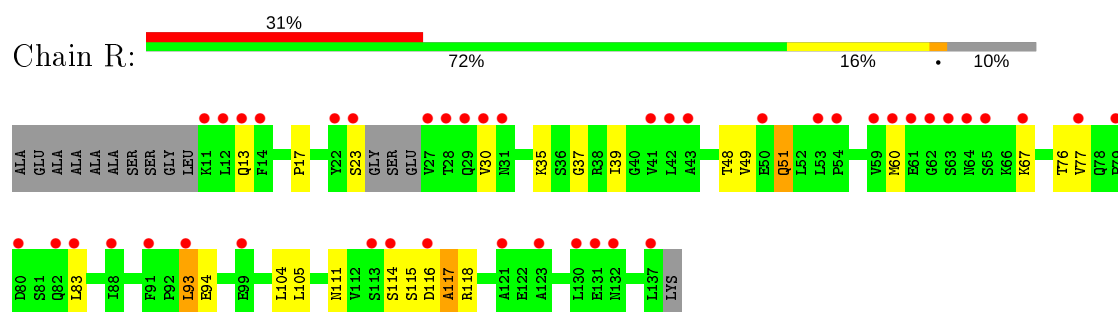
- Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



- Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



- Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



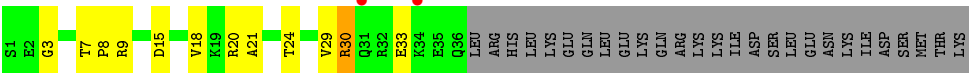
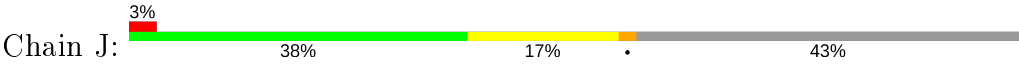
- Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



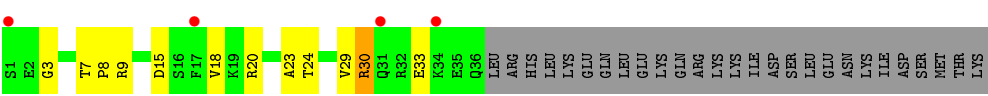
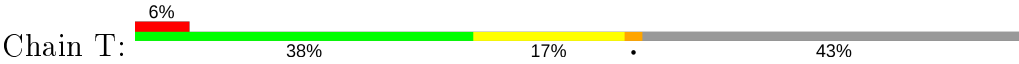
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



• Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL



• Molecule 6: ATPASE INHIBITOR, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.22Å 187.85Å 181.81Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	181.81 – 2.50 40.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (181.81-2.50) 98.3 (40.91-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.224 , 0.262 0.218 , 0.255	Depositor DCC
R_{free} test set	13570 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k 0.004 for -h,l,k 0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51906	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, ATP, ADP, EDO

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	0.39	0/3736	0.55	0/5057
1	B	0.50	0/3712	0.62	0/5023
1	C	0.47	0/3736	0.58	0/5057
1	K	0.39	0/3736	0.55	0/5057
1	L	0.53	0/3712	0.63	0/5023
1	M	0.46	0/3736	0.58	0/5057
2	D	0.42	0/3605	0.55	0/4889
2	E	0.42	0/3592	0.58	0/4870
2	F	0.50	0/3607	0.63	0/4891
2	N	0.41	0/3605	0.55	0/4889
2	O	0.45	0/3592	0.59	0/4870
2	P	0.49	0/3624	0.62	0/4914
3	G	0.38	0/2082	0.52	0/2800
3	Q	0.38	0/2091	0.52	0/2812
4	H	0.37	0/950	0.55	0/1288
4	R	0.38	0/950	0.55	0/1288
5	I	0.43	0/457	0.55	0/619
5	S	0.44	0/457	0.55	0/619
6	J	0.42	0/286	0.62	0/379
6	T	0.41	0/286	0.61	0/379
All	All	0.45	0/51552	0.58	0/69781

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3680	0	3763	45	0
1	B	3655	0	3751	36	0
1	C	3680	0	3763	47	0
1	K	3680	0	3763	42	0
1	L	3655	0	3751	34	0
1	M	3680	0	3763	48	0
2	D	3549	0	3620	45	0
2	E	3536	0	3610	48	0
2	F	3548	0	3624	30	0
2	N	3549	0	3620	46	0
2	O	3536	0	3610	42	0
2	P	3559	0	3641	30	0
3	G	2057	0	2127	38	0
3	Q	2063	0	2133	32	0
4	H	937	0	947	18	0
4	R	937	0	947	22	0
5	I	450	0	452	20	0
5	S	450	0	452	20	0
6	J	283	0	267	11	0
6	T	283	0	267	12	0
7	A	31	0	12	0	0
7	K	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	P	1	0	0	0	0
9	B	27	0	12	0	0
9	C	27	0	12	1	0
9	D	27	0	12	0	0
9	E	27	0	12	0	0
9	F	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	27	0	12	0	0
9	M	27	0	12	1	0
9	N	27	0	12	0	0
9	O	27	0	12	0	0
9	P	27	0	12	0	0
10	C	4	0	6	0	0
10	L	8	0	12	0	0
10	M	4	0	6	2	0
10	O	4	0	6	0	0
10	P	4	0	6	1	0
11	A	18	0	0	0	0
11	B	90	0	0	4	0
11	C	94	0	0	1	0
11	D	37	0	0	0	0
11	E	20	0	0	0	0
11	F	81	0	0	3	0
11	G	11	0	0	1	0
11	H	1	0	0	1	0
11	I	1	0	0	1	0
11	K	27	0	0	0	0
11	L	156	0	0	3	0
11	M	76	0	0	0	0
11	N	32	0	0	0	0
11	O	52	0	0	2	0
11	P	68	0	0	0	0
11	Q	8	0	0	0	0
11	R	1	0	0	0	0
All	All	51906	0	52051	617	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (617) 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)
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.30	1.11
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.30	1.09
3:Q:96:ARG:HE	3:Q:121:THR:HG21	1.18	1.08
3:G:96:ARG:HE	3:G:121:THR:HG21	1.18	1.08
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.36	1.07
2:P:85:VAL:HG11	2:P:235:THR:HG23	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:422:ARG:HH12	1:K:453:GLY:HA2	1.27	0.98
4:R:93:LEU:HD22	4:R:93:LEU:H	1.26	0.96
4:H:93:LEU:HD22	4:H:93:LEU:H	1.27	0.96
5:S:59:ILE:HG22	5:S:60:THR:H	1.30	0.96
6:T:30:ARG:HG2	6:T:30:ARG:HH11	1.30	0.96
6:J:30:ARG:HG2	6:J:30:ARG:HH11	1.29	0.96
1:A:422:ARG:HH12	1:A:453:GLY:HA2	1.28	0.96
5:I:59:ILE:HG22	5:I:60:THR:H	1.31	0.94
2:O:221:GLN:HG3	2:O:223:ASN:OD1	1.70	0.91
5:S:3:TRP:HB2	5:S:8:ILE:HB	1.52	0.90
5:I:3:TRP:HB2	5:I:8:ILE:HB	1.52	0.90
2:E:221:GLN:HG3	2:E:223:ASN:OD1	1.72	0.89
2:E:319:ASP:OD1	2:E:320:PRO:HD2	1.74	0.87
1:B:387:GLN:HE22	1:B:491:LEU:H	1.21	0.87
1:L:387:GLN:HE22	1:L:491:LEU:H	1.21	0.86
2:P:351:LEU:O	2:P:352:ASP:HB2	1.74	0.86
2:O:319:ASP:OD1	2:O:320:PRO:HD2	1.75	0.85
1:M:142:ARG:HG2	1:M:142:ARG:HH11	1.41	0.85
2:D:201:MET:CE	2:D:217:LEU:HD21	2.07	0.85
2:N:201:MET:CE	2:N:217:LEU:HD21	2.07	0.84
2:F:351:LEU:O	2:F:352:ASP:HB2	1.75	0.84
1:C:142:ARG:HH11	1:C:142:ARG:HG2	1.43	0.84
2:D:41:THR:HB	2:D:42:PRO:HD2	1.60	0.82
2:N:41:THR:HB	2:N:42:PRO:HD2	1.60	0.82
1:M:363:ILE:HG13	1:M:363:ILE:O	1.84	0.78
1:C:363:ILE:HG13	1:C:363:ILE:O	1.85	0.77
3:G:96:ARG:NE	3:G:121:THR:HG21	2.00	0.76
1:A:444:VAL:HG23	1:A:445:PRO:HD3	1.67	0.75
1:M:283:LEU:HD23	1:M:284:SER:N	2.01	0.74
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.68	0.74
1:M:303:LEU:HA	10:M:602:EDO:H22	1.70	0.73
2:N:201:MET:HE3	2:N:217:LEU:HD21	1.71	0.72
1:A:112:ALA:O	1:A:251:THR:HG21	1.90	0.72
2:O:220:GLY:HA3	2:O:232:VAL:HG11	1.71	0.72
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.71	0.72
2:P:351:LEU:O	2:P:352:ASP:CB	2.37	0.72
4:H:67:LYS:HB3	4:H:93:LEU:HD21	1.71	0.72
6:J:30:ARG:CG	6:J:30:ARG:HH11	2.01	0.72
1:K:112:ALA:O	1:K:251:THR:HG21	1.90	0.72
2:E:390:ILE:HD11	3:G:24:LYS:HE3	1.71	0.72
4:R:67:LYS:HB3	4:R:93:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:96:ARG:NE	3:Q:121:THR:HG21	2.00	0.71
2:F:351:LEU:O	2:F:352:ASP:CB	2.38	0.71
6:T:30:ARG:CG	6:T:30:ARG:HH11	2.01	0.71
1:M:336:VAL:HG11	1:M:353:PHE:CE1	2.26	0.70
1:C:283:LEU:HD23	1:C:284:SER:N	2.06	0.70
2:N:26:GLU:O	2:N:29:GLU:HG3	1.92	0.69
4:H:37:GLY:O	4:H:39:ILE:HG12	1.91	0.69
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.28	0.69
2:D:26:GLU:O	2:D:29:GLU:HG3	1.93	0.68
2:D:382:LYS:HG2	6:J:7:THR:HG21	1.75	0.68
4:R:37:GLY:O	4:R:39:ILE:HG12	1.92	0.68
1:B:54:LEU:O	1:B:93:THR:HB	1.94	0.68
2:N:237:LEU:HD13	2:N:296:ILE:HG12	1.75	0.68
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.75	0.68
1:L:54:LEU:O	1:L:93:THR:HB	1.94	0.68
4:H:93:LEU:H	4:H:93:LEU:CD2	2.04	0.67
2:F:351:LEU:HD23	11:F:2076:HOH:O	1.93	0.67
4:R:93:LEU:H	4:R:93:LEU:CD2	2.04	0.67
6:J:20:ARG:O	6:J:24:THR:HG23	1.94	0.67
2:N:197:LEU:O	2:N:201:MET:HG2	1.93	0.67
6:T:20:ARG:O	6:T:24:THR:HG23	1.95	0.67
2:N:382:LYS:HG2	6:T:7:THR:HG21	1.77	0.67
2:D:197:LEU:O	2:D:201:MET:HG2	1.94	0.66
1:C:413:ASP:CB	1:C:416:THR:HB	2.25	0.66
1:M:413:ASP:CB	1:M:416:THR:HB	2.25	0.66
1:L:220:GLN:HE21	1:L:224:GLN:HE21	1.42	0.66
2:O:313:PRO:HG2	2:O:319:ASP:OD2	1.96	0.66
1:B:220:GLN:HE21	1:B:224:GLN:HE21	1.43	0.65
1:L:335:ASP:OD2	3:Q:257:ARG:HD3	1.97	0.65
2:E:316:ASP:OD2	3:G:256:ASN:HB3	1.97	0.65
2:D:201:MET:HE3	2:D:217:LEU:HD21	1.78	0.65
1:B:417:LYS:O	1:B:421:VAL:HG23	1.96	0.64
1:L:417:LYS:O	1:L:421:VAL:HG23	1.96	0.64
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.77	0.64
2:E:384:LEU:O	2:E:388:ILE:HG12	1.98	0.64
1:K:42:ARG:HD2	1:K:72:GLN:HE22	1.62	0.64
4:H:35:LYS:HD2	4:H:51:GLN:NE2	2.12	0.63
3:Q:14:LYS:HA	3:Q:248:ILE:HD11	1.79	0.63
4:R:35:LYS:HD2	4:R:51:GLN:NE2	2.12	0.63
4:R:48:THR:H	4:R:77:VAL:HB	1.64	0.63
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:384:LEU:O	2:O:388:ILE:HG12	1.99	0.63
1:A:42:ARG:HD2	1:A:72:GLN:HE22	1.64	0.63
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.28	0.63
4:H:48:THR:H	4:H:77:VAL:HB	1.64	0.63
3:Q:24:LYS:HB2	3:Q:237:MET:HB3	1.81	0.62
1:A:52:GLU:O	1:A:97:VAL:HG23	1.99	0.62
1:K:248:ALA:HB3	1:K:249:PRO:HD3	1.81	0.62
1:K:52:GLU:O	1:K:97:VAL:HG23	1.99	0.62
3:G:115:LYS:O	3:G:119:LEU:HB2	2.00	0.62
4:R:118:ARG:NH1	5:S:8:ILE:HG13	2.14	0.62
3:G:24:LYS:HB2	3:G:237:MET:HB3	1.82	0.62
2:O:220:GLY:CA	2:O:232:VAL:HG11	2.29	0.62
2:D:85:VAL:HG22	2:D:117:ILE:HG22	1.81	0.62
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.82	0.62
1:B:55:VAL:HG21	1:B:75:ILE:HD13	1.82	0.61
5:S:59:ILE:HG22	5:S:60:THR:N	2.09	0.61
4:H:111:ASN:HA	4:H:114:SER:HB3	1.83	0.61
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.83	0.61
1:C:64:MET:HE1	11:C:2008:HOH:O	1.99	0.61
2:E:313:PRO:HG2	2:E:319:ASP:OD2	2.01	0.61
3:Q:78:THR:HG23	3:Q:114:ILE:HB	1.81	0.61
1:C:413:ASP:O	1:C:416:THR:HB	2.01	0.61
5:I:59:ILE:HG22	5:I:60:THR:N	2.09	0.61
6:J:30:ARG:HG2	6:J:30:ARG:NH1	2.07	0.61
2:N:85:VAL:HG22	2:N:117:ILE:HG22	1.82	0.61
4:R:111:ASN:HA	4:R:114:SER:HB3	1.83	0.61
3:G:78:THR:HG23	3:G:114:ILE:HB	1.81	0.60
4:H:93:LEU:HD22	4:H:93:LEU:N	2.10	0.60
3:Q:115:LYS:O	3:Q:119:LEU:HB2	2.02	0.60
6:T:30:ARG:HG2	6:T:30:ARG:NH1	2.08	0.60
11:B:2086:HOH:O	2:F:192:ARG:HD3	2.01	0.60
1:M:413:ASP:O	1:M:416:THR:HB	2.02	0.60
2:N:85:VAL:HG13	2:N:235:THR:HG23	1.83	0.60
4:R:93:LEU:N	4:R:93:LEU:HD22	2.09	0.60
1:A:444:VAL:CG2	1:A:445:PRO:HD3	2.32	0.60
1:C:413:ASP:HB2	1:C:416:THR:HB	1.83	0.60
3:Q:15:ASN:O	3:Q:19:ILE:HG12	2.02	0.60
2:N:130:SER:O	2:N:356:ARG:NH2	2.35	0.59
2:D:130:SER:O	2:D:356:ARG:NH2	2.35	0.59
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.32	0.59
3:Q:78:THR:CG2	3:Q:114:ILE:HB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:THR:HG22	1:L:95:ASN:H	1.67	0.59
2:O:410:ILE:HG23	2:O:441:PHE:HE2	1.68	0.59
2:F:371:ALA:O	2:F:375:GLN:HG3	2.03	0.59
1:M:413:ASP:HB2	1:M:416:THR:HB	1.84	0.59
1:A:243:PRO:HG3	1:A:283:LEU:HD21	1.83	0.59
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.68	0.59
3:G:78:THR:CG2	3:G:114:ILE:HB	2.33	0.59
3:G:15:ASN:O	3:G:19:ILE:HG12	2.02	0.59
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.83	0.59
1:M:142:ARG:HH11	1:M:142:ARG:CG	2.13	0.59
2:D:85:VAL:HG13	2:D:235:THR:HG23	1.84	0.59
5:S:59:ILE:CG2	5:S:60:THR:H	2.12	0.59
1:M:291:PRO:HB2	1:M:295:ALA:HA	1.85	0.59
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.85	0.58
3:G:262:VAL:O	3:G:266:GLU:HG3	2.02	0.58
3:Q:75:VAL:HG22	3:Q:108:VAL:HB	1.85	0.58
1:C:280:TYR:O	1:C:283:LEU:HD23	2.03	0.58
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.33	0.58
2:D:41:THR:HB	2:D:42:PRO:CD	2.28	0.58
1:L:377:GLY:N	11:L:2148:HOH:O	2.36	0.58
4:R:116:ASP:O	4:R:117:ALA:CB	2.52	0.58
1:C:142:ARG:CG	1:C:142:ARG:HH11	2.14	0.58
2:O:98:VAL:HB	2:O:232:VAL:HG13	1.86	0.58
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.33	0.58
5:I:59:ILE:CG2	5:I:60:THR:H	2.13	0.58
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.85	0.57
5:I:46:GLN:O	5:I:55:GLU:HB2	2.04	0.57
4:H:116:ASP:O	4:H:117:ALA:CB	2.52	0.57
3:Q:78:THR:OG1	3:Q:79:SER:N	2.37	0.57
5:S:46:GLN:O	5:S:55:GLU:HB2	2.04	0.57
2:E:319:ASP:OD1	2:E:320:PRO:CD	2.51	0.57
3:G:78:THR:OG1	3:G:79:SER:N	2.37	0.57
3:Q:75:VAL:HB	3:Q:164:ILE:HD13	1.87	0.57
3:G:75:VAL:HG22	3:G:108:VAL:HB	1.86	0.57
2:N:41:THR:HB	2:N:42:PRO:CD	2.28	0.57
1:B:93:THR:HG22	1:B:95:ASN:H	1.69	0.57
2:N:201:MET:HE2	2:N:217:LEU:HD21	1.85	0.57
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.85	0.57
1:K:138:ILE:HD13	2:O:191:THR:HG23	1.87	0.56
1:C:291:PRO:HB2	1:C:295:ALA:HA	1.88	0.56
2:O:140:VAL:HG21	2:O:348:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ARG:HD2	1:B:465:GLU:OE1	2.06	0.56
2:E:140:VAL:HG21	2:E:348:VAL:HG11	1.88	0.56
3:Q:77:ILE:HG21	3:Q:222:MET:HG2	1.87	0.56
3:G:205:VAL:H	3:G:206:PRO:HD3	1.71	0.56
1:M:173:ARG:HG2	1:M:174:GLN:HG2	1.88	0.56
3:Q:205:VAL:H	3:Q:206:PRO:HD3	1.70	0.56
1:B:138:ILE:HD12	11:B:2027:HOH:O	2.04	0.56
1:B:332:GLN:HB3	2:E:318:THR:HB	1.88	0.56
2:P:371:ALA:O	2:P:375:GLN:HG3	2.05	0.56
1:L:335:ASP:HB2	3:Q:257:ARG:NH1	2.22	0.55
2:P:189:GLU:O	2:P:221:GLN:HB3	2.06	0.55
1:L:462:ARG:HD2	1:L:465:GLU:OE1	2.07	0.55
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.89	0.55
1:C:173:ARG:HG2	1:C:174:GLN:HG2	1.89	0.55
3:Q:205:VAL:N	3:Q:206:PRO:CD	2.70	0.55
11:L:2142:HOH:O	2:P:192:ARG:HD3	2.07	0.55
1:A:302:TYR:O	1:A:306:ARG:HB2	2.06	0.55
3:G:205:VAL:N	3:G:206:PRO:CD	2.70	0.55
1:M:77:LEU:HD12	1:M:81:ASP:HB3	1.88	0.55
1:L:211:LYS:HD2	2:O:328:HIS:HA	1.87	0.55
2:F:189:GLU:O	2:F:221:GLN:HB3	2.07	0.54
2:F:289[B]:MET:CE	2:F:325:THR:HG23	2.37	0.54
3:G:49:GLN:HG2	3:G:52:TYR:HB2	1.88	0.54
6:J:3:GLY:CA	6:J:7:THR:HG23	2.38	0.54
1:K:42:ARG:HD2	1:K:72:GLN:NE2	2.23	0.54
3:Q:49:GLN:HG2	3:Q:52:TYR:HB2	1.88	0.54
6:T:3:GLY:CA	6:T:7:THR:HG23	2.38	0.54
2:O:158:GLY:O	2:O:161:VAL:HG22	2.08	0.54
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.90	0.54
1:A:42:ARG:HD2	1:A:72:GLN:NE2	2.23	0.54
1:M:170:ILE:HG23	1:M:353:PHE:HD1	1.73	0.54
3:Q:108:VAL:HG22	3:Q:128:LEU:HB3	1.90	0.53
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.89	0.53
2:E:158:GLY:O	2:E:161:VAL:HG22	2.09	0.53
1:M:336:VAL:HG11	1:M:353:PHE:HE1	1.73	0.53
1:C:222:LEU:HB2	1:C:228:MET:CE	2.38	0.53
1:C:170:ILE:HG23	1:C:353:PHE:HD1	1.73	0.53
2:D:204:THR:CG2	2:D:206:VAL:HG23	2.38	0.53
2:F:289[B]:MET:CE	2:F:293:GLN:HE21	2.22	0.53
3:G:203:ALA:HB1	4:H:35:LYS:NZ	2.24	0.53
1:K:302:TYR:O	1:K:306:ARG:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:440:SER:HB3	2:N:463:ILE:HB	1.90	0.53
2:N:204:THR:CG2	2:N:206:VAL:HG23	2.38	0.53
1:L:399:TYR:OH	1:L:424:GLU:HG3	2.09	0.53
1:C:138:ILE:H	1:C:138:ILE:HD12	1.74	0.53
2:O:133:ILE:HD12	2:O:146:PRO:HB2	1.90	0.53
4:R:118:ARG:HH11	5:S:8:ILE:HG13	1.74	0.53
1:B:399:TYR:OH	1:B:424:GLU:HG3	2.09	0.52
2:P:289[B]:MET:CE	2:P:293:GLN:HE21	2.21	0.52
2:E:33:ILE:O	2:E:34:LEU:HB2	2.09	0.52
4:R:13:GLN:HG2	4:R:23:SER:HA	1.91	0.52
1:M:222:LEU:HB2	1:M:228:MET:CE	2.39	0.52
2:N:396:LEU:HD13	2:N:400:ASP:HB3	1.90	0.52
3:Q:219:LEU:HD21	4:R:17:PRO:HB3	1.92	0.52
2:P:289[B]:MET:CE	2:P:325:THR:HG23	2.40	0.52
1:C:358:LEU:HB3	1:C:363:ILE:HG12	1.92	0.52
1:C:402:VAL:HG12	1:C:420:LEU:HD13	1.92	0.52
2:D:440:SER:HB3	2:D:463:ILE:HB	1.91	0.52
1:A:174:GLN:HG3	2:D:354:LYS:HG3	1.90	0.52
2:D:242:TYR:CD1	2:D:246:GLU:HG3	2.45	0.52
1:M:358:LEU:HB3	1:M:363:ILE:HG12	1.91	0.52
1:C:336:VAL:HG11	1:C:353:PHE:HE1	1.74	0.52
5:I:4:ARG:HD2	5:I:4:ARG:N	2.25	0.52
1:M:402:VAL:HG12	1:M:420:LEU:HD13	1.92	0.52
2:P:152:LYS:NZ	2:P:293:GLN:HB3	2.25	0.52
1:L:220:GLN:HE21	1:L:224:GLN:NE2	2.08	0.52
1:M:389:ALA:HB2	1:M:447:ILE:HG21	1.92	0.52
1:C:283:LEU:HD23	1:C:284:SER:H	1.73	0.51
1:C:389:ALA:HB2	1:C:447:ILE:HG21	1.91	0.51
4:H:13:GLN:HG2	4:H:23:SER:HA	1.92	0.51
2:N:218:VAL:HG21	2:N:236:GLY:HA2	1.91	0.51
2:O:456:ALA:HA	2:O:469:LYS:HD3	1.92	0.51
4:R:118:ARG:NH1	5:S:8:ILE:HA	2.25	0.51
2:N:242:TYR:CD1	2:N:246:GLU:HG3	2.45	0.51
2:O:344:ILE:HG23	2:O:415:SER:HB3	1.92	0.51
1:B:154:ALA:HB1	1:B:367:ILE:HD12	1.93	0.51
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.93	0.51
2:N:189:GLU:O	2:N:221:GLN:HB3	2.11	0.51
1:B:444:VAL:HG22	1:B:445:PRO:HD3	1.93	0.51
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.93	0.51
4:H:116:ASP:O	4:H:117:ALA:HB3	2.11	0.51
1:M:302:TYR:CE1	1:M:306:ARG:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:319:ASP:OD1	2:O:320:PRO:CD	2.54	0.51
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.93	0.51
2:F:449:TYR:HD1	2:F:452:ILE:CD1	2.23	0.51
1:M:414:ALA:HA	1:M:417:LYS:HE3	1.92	0.51
2:O:204:THR:HG23	2:O:206:VAL:HG13	1.92	0.51
4:R:116:ASP:O	4:R:117:ALA:HB3	2.10	0.51
1:C:414:ALA:HA	1:C:417:LYS:HE3	1.93	0.51
3:G:207:ARG:HH12	5:I:4:ARG:HH21	1.59	0.51
1:K:404:ALA:HB2	3:Q:18:LYS:HE3	1.92	0.51
1:M:283:LEU:HD23	1:M:284:SER:H	1.76	0.51
5:S:4:ARG:N	5:S:4:ARG:HD2	2.25	0.51
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.92	0.50
2:D:396:LEU:HD13	2:D:400:ASP:HB3	1.91	0.50
2:E:152:LYS:HE3	2:E:296:ILE:HB	1.94	0.50
1:B:478:HIS:O	1:B:481:LEU:HB2	2.11	0.50
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.93	0.50
2:F:242:TYR:CE2	2:F:246:GLU:HG3	2.46	0.50
1:L:478:HIS:O	1:L:481:LEU:HB2	2.11	0.50
2:F:152:LYS:NZ	2:F:293:GLN:HB3	2.26	0.50
2:F:384:LEU:O	2:F:388:ILE:HG12	2.12	0.50
2:P:449:TYR:HD1	2:P:452:ILE:CD1	2.24	0.50
1:M:404:ALA:HB1	6:T:23:ALA:HB2	1.92	0.50
1:B:220:GLN:HE21	1:B:224:GLN:NE2	2.10	0.50
1:C:364:ARG:HA	1:C:365:PRO:C	2.31	0.50
2:P:242:TYR:CE2	2:P:246:GLU:HG3	2.47	0.50
1:K:187:ASN:OD1	1:K:437:PRO:HB2	2.11	0.50
1:M:138:ILE:HD12	1:M:138:ILE:H	1.77	0.50
2:O:340:SER:HB3	2:O:347:ALA:CB	2.42	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.32	0.50
2:O:33:ILE:O	2:O:34:LEU:HB2	2.12	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.93	0.49
1:L:243:PRO:HG3	1:L:283:LEU:HD21	1.94	0.49
1:C:413:ASP:HB3	1:C:416:THR:HB	1.94	0.49
2:D:152:LYS:HD2	2:D:296:ILE:O	2.12	0.49
2:P:15:ALA:HB3	2:P:22:ASP:HB2	1.92	0.49
1:L:444:VAL:HG22	1:L:445:PRO:HD3	1.94	0.49
1:K:211:LYS:HD3	2:N:328:HIS:HA	1.94	0.49
2:P:384:LEU:O	2:P:388:ILE:HG12	2.13	0.49
1:B:421:VAL:O	1:B:425:ARG:HG2	2.13	0.49
1:C:302:TYR:CE1	1:C:306:ARG:HB3	2.48	0.49
1:M:413:ASP:HB3	1:M:416:THR:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:413:ASP:HB3	1:M:416:THR:HB	1.93	0.49
2:O:340:SER:HB3	2:O:347:ALA:HB2	1.94	0.49
1:C:413:ASP:HB3	1:C:416:THR:CB	2.43	0.49
1:A:187:ASN:OD1	1:A:437:PRO:HB2	2.11	0.49
1:C:280:TYR:O	1:C:283:LEU:CD2	2.61	0.49
2:F:375:GLN:HG2	11:F:2076:HOH:O	2.11	0.49
2:N:449:TYR:HD1	2:N:452:ILE:HD12	1.76	0.49
3:Q:99:LEU:HD21	3:Q:107:ILE:HD11	1.95	0.49
2:D:449:TYR:HD1	2:D:452:ILE:HD12	1.77	0.49
3:G:99:LEU:HD21	3:G:107:ILE:HD11	1.95	0.49
1:L:421:VAL:O	1:L:425:ARG:HG2	2.13	0.49
1:M:364:ARG:HA	1:M:365:PRO:C	2.33	0.49
1:A:28:ASN:HB3	1:A:48:ASN:ND2	2.28	0.49
2:E:204:THR:HG23	2:E:206:VAL:HG13	1.94	0.49
2:O:152:LYS:HE3	2:O:296:ILE:HB	1.95	0.49
1:C:222:LEU:CB	1:C:228:MET:HE2	2.43	0.49
2:E:340:SER:HB3	2:E:347:ALA:CB	2.43	0.49
2:E:140:VAL:HG21	2:E:348:VAL:CG1	2.42	0.49
1:M:142:ARG:HG2	1:M:142:ARG:NH1	2.19	0.49
2:P:345:TYR:HA	2:P:346:PRO:C	2.33	0.48
4:R:116:ASP:N	4:R:116:ASP:OD1	2.45	0.48
3:G:75:VAL:HB	3:G:164:ILE:CD1	2.42	0.48
4:H:54:PRO:HD3	5:I:13:TYR:OH	2.12	0.48
4:H:94:GLU:O	5:I:26:LYS:HD2	2.13	0.48
2:N:178:HIS:HE1	2:N:250:ASP:O	1.96	0.48
2:O:140:VAL:HG21	2:O:348:VAL:CG1	2.42	0.48
1:A:478:HIS:HB3	1:A:481:LEU:HG	1.94	0.48
1:B:299:ASP:HA	11:B:2075:HOH:O	2.13	0.48
4:H:116:ASP:OD1	4:H:116:ASP:N	2.46	0.48
1:L:154:ALA:HB1	1:L:367:ILE:HD12	1.96	0.48
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.95	0.48
5:I:4:ARG:HD2	5:I:4:ARG:H	1.79	0.48
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.96	0.48
1:C:363:ILE:CG1	1:C:363:ILE:O	2.60	0.48
2:P:152:LYS:HZ1	2:P:293:GLN:HB3	1.78	0.48
1:B:243:PRO:HG3	1:B:283:LEU:HD21	1.95	0.48
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.49	0.48
11:H:2001:HOH:O	5:I:13:TYR:HE2	1.97	0.48
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.94	0.48
2:P:333:THR:HA	2:P:353:SER:HB3	1.94	0.48
3:Q:75:VAL:HB	3:Q:164:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.28	0.48
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.94	0.48
2:D:189:GLU:O	2:D:221:GLN:HB3	2.14	0.48
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.96	0.48
2:E:340:SER:HB3	2:E:347:ALA:HB2	1.96	0.48
2:F:333:THR:HA	2:F:353:SER:HB3	1.95	0.48
3:G:119:LEU:HD11	5:I:53:ALA:HB1	1.95	0.48
1:K:174:GLN:HG3	2:N:354:LYS:HG3	1.95	0.48
1:K:28:ASN:HB3	1:K:48:ASN:ND2	2.29	0.48
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.96	0.48
1:M:336:VAL:HG11	1:M:353:PHE:CZ	2.48	0.47
5:S:4:ARG:H	5:S:4:ARG:HD2	1.79	0.47
2:D:64:MET:CE	2:D:228:ALA:HA	2.43	0.47
5:I:15:ASN:ND2	11:I:2001:HOH:O	2.27	0.47
1:M:280:TYR:O	1:M:283:LEU:CD2	2.62	0.47
1:M:306:ARG:HE	10:M:602:EDO:H21	1.78	0.47
2:N:152:LYS:HD2	2:N:296:ILE:O	2.14	0.47
3:Q:184:ASN:HA	3:Q:210:PHE:CD1	2.49	0.47
1:A:444:VAL:HG23	1:A:445:PRO:CD	2.42	0.47
2:F:289[B]:MET:HE3	2:F:293:GLN:HE21	1.79	0.47
1:M:280:TYR:O	1:M:283:LEU:HD23	2.15	0.47
1:K:421:VAL:O	1:K:425:ARG:HD2	2.15	0.47
2:N:64:MET:CE	2:N:228:ALA:HA	2.44	0.47
5:S:61:LYS:HE3	5:S:61:LYS:HB3	1.60	0.47
1:B:211:LYS:HD2	2:E:328:HIS:HA	1.96	0.47
2:N:224:GLU:O	2:N:229:ARG:HD3	2.15	0.47
2:P:65:ASP:HB2	10:P:603:EDO:H21	1.96	0.47
1:K:301:PHE:HB3	2:O:267:GLU:OE2	2.15	0.47
2:O:339:ILE:HG22	2:O:340:SER:H	1.79	0.47
4:R:30:VAL:HG21	4:R:83:LEU:CD2	2.45	0.47
2:D:200:GLU:O	2:D:204:THR:HB	2.15	0.47
2:D:178:HIS:HE1	2:D:250:ASP:O	1.97	0.47
2:F:152:LYS:HZ1	2:F:293:GLN:HB3	1.79	0.47
4:H:30:VAL:HG21	4:H:83:LEU:CD2	2.45	0.47
2:N:200:GLU:O	2:N:204:THR:HB	2.15	0.47
1:K:239:SER:HB3	2:N:294:GLU:HG3	1.96	0.47
2:N:64:MET:HE1	2:N:228:ALA:HA	1.97	0.47
3:Q:91:LEU:HD23	3:Q:114:ILE:HD13	1.96	0.47
2:E:336:SER:HB3	2:E:339:ILE:HG12	1.97	0.47
1:A:280:TYR:CE2	1:A:297:PRO:HG2	2.49	0.47
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:LEU:CB	1:M:228:MET:HE2	2.45	0.46
1:A:64:MET:SD	1:A:97:VAL:HG21	2.55	0.46
3:G:205:VAL:H	3:G:206:PRO:CD	2.28	0.46
1:K:55:VAL:HG21	1:K:75:ILE:HD13	1.96	0.46
1:M:192:ASN:HA	1:M:200:LYS:HG2	1.97	0.46
2:D:64:MET:HE1	2:D:231:ARG:HB2	1.97	0.46
2:O:417:PRO:HG2	2:O:430:LYS:HG2	1.98	0.46
5:S:4:ARG:N	5:S:4:ARG:CD	2.79	0.46
2:N:385:GLN:OE1	6:T:7:THR:HG22	2.15	0.46
1:A:421:VAL:O	1:A:425:ARG:HD2	2.16	0.46
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.97	0.46
1:A:346:SER:CB	2:E:260:ARG:HH22	2.29	0.46
1:K:444:VAL:HG23	1:K:445:PRO:CD	2.43	0.46
1:B:384:ALA:HA	1:B:387:GLN:HE21	1.81	0.46
1:C:336:VAL:HG11	1:C:353:PHE:CZ	2.49	0.46
2:F:349:ASP:OD1	2:F:351:LEU:O	2.34	0.46
1:K:108:ARG:NH1	1:K:123:ILE:HD13	2.31	0.46
2:P:289[B]:MET:HE3	2:P:293:GLN:HE21	1.81	0.46
4:R:118:ARG:HH12	5:S:8:ILE:HA	1.80	0.46
1:A:108:ARG:NH1	1:A:123:ILE:HD13	2.31	0.46
2:D:244:ARG:HD3	2:D:304:VAL:HG23	1.98	0.46
2:E:339:ILE:HG22	2:E:340:SER:H	1.81	0.46
3:G:91:LEU:HD23	3:G:114:ILE:HD13	1.97	0.46
3:G:125:ASN:N	3:G:125:ASN:HD22	2.14	0.46
1:M:43:VAL:HG21	1:M:75:ILE:HD12	1.98	0.46
3:Q:125:ASN:HD22	3:Q:125:ASN:N	2.13	0.46
3:Q:205:VAL:H	3:Q:206:PRO:CD	2.28	0.46
6:T:15:ASP:HB2	6:T:18:VAL:H	1.81	0.46
2:D:224:GLU:O	2:D:229:ARG:HD3	2.16	0.46
1:L:384:ALA:HA	1:L:387:GLN:HE21	1.81	0.46
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.98	0.45
1:B:197:GLU:HB2	11:B:2049:HOH:O	2.16	0.45
1:A:139:LEU:HD22	2:E:105:GLU:HB2	1.97	0.45
2:E:67:THR:HB	2:E:70:LEU:HD12	1.98	0.45
2:O:336:SER:HB3	2:O:339:ILE:HG12	1.98	0.45
2:E:417:PRO:HG2	2:E:430:LYS:HG2	1.99	0.45
1:K:64:MET:SD	1:K:97:VAL:HG21	2.56	0.45
2:N:253:LEU:O	2:N:306:SER:HA	2.15	0.45
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.98	0.45
1:L:402:VAL:O	1:L:405:PHE:CD1	2.69	0.45
2:E:168:GLN:HA	2:E:171:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.99	0.45
6:J:15:ASP:HB2	6:J:18:VAL:H	1.82	0.45
1:K:124:ASP:N	1:K:124:ASP:OD1	2.49	0.45
1:K:280:TYR:CE2	1:K:297:PRO:HG2	2.51	0.45
1:K:361:LYS:HG3	2:N:379:GLN:HG2	1.98	0.45
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.99	0.45
1:B:402:VAL:O	1:B:405:PHE:CD1	2.69	0.45
6:J:29:VAL:O	6:J:33:GLU:HG3	2.15	0.45
1:M:222:LEU:HB2	1:M:228:MET:HE2	1.98	0.45
2:P:349:ASP:OD1	2:P:351:LEU:O	2.35	0.45
6:T:29:VAL:O	6:T:33:GLU:HG3	2.15	0.45
1:A:139:LEU:CD2	2:E:105:GLU:HB2	2.47	0.45
2:D:389:ALA:HB2	6:J:21:ALA:HB2	1.98	0.45
1:L:93:THR:HG22	1:L:95:ASN:N	2.31	0.45
2:O:443:ALA:HB1	2:O:449:TYR:HE2	1.82	0.45
3:Q:46:GLU:O	3:Q:50:LEU:HB2	2.17	0.45
1:A:124:ASP:OD1	1:A:124:ASP:N	2.49	0.44
1:C:107:GLY:HA2	1:C:228:MET:O	2.17	0.44
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.99	0.44
2:O:237:LEU:HD21	2:O:295:ARG:HB2	1.99	0.44
2:P:152:LYS:NZ	2:P:293:GLN:O	2.50	0.44
1:B:93:THR:HG22	1:B:95:ASN:N	2.32	0.44
2:P:244:ARG:HD3	2:P:304:VAL:HG23	1.99	0.44
2:P:279:VAL:O	2:P:279:VAL:HG12	2.17	0.44
1:B:364:ARG:HA	1:B:365:PRO:C	2.37	0.44
2:E:443:ALA:HB1	2:E:449:TYR:HE2	1.82	0.44
5:I:4:ARG:N	5:I:4:ARG:CD	2.78	0.44
1:L:364:ARG:HA	1:L:365:PRO:C	2.37	0.44
1:M:417:LYS:HA	1:M:420:LEU:HB3	2.00	0.44
2:D:64:MET:HE1	2:D:228:ALA:HA	2.00	0.44
2:P:237:LEU:HD13	2:P:296:ILE:HG12	1.99	0.44
2:P:377:THR:HG22	2:P:407:ALA:HB2	1.99	0.44
1:C:417:LYS:HA	1:C:420:LEU:HB3	2.00	0.44
2:F:292:LEU:HD12	2:F:292:LEU:C	2.38	0.44
2:F:244:ARG:HD3	2:F:304:VAL:HG23	1.99	0.44
2:N:64:MET:HE1	2:N:231:ARG:HB2	1.99	0.44
1:C:378:SER:HB2	1:C:386:LYS:HD2	2.00	0.44
1:A:309:GLU:HG3	2:E:223:ASN:HB3	2.00	0.44
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.99	0.44
2:O:67:THR:HB	2:O:70:LEU:HD12	1.99	0.44
5:S:55:GLU:OE1	5:S:55:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:HD3	1:B:490:GLU:HG3	2.00	0.44
1:C:413:ASP:CB	1:C:416:THR:CB	2.95	0.44
1:L:26:ASN:O	1:L:30:THR:HB	2.17	0.44
1:L:383:LYS:HD3	1:L:490:GLU:HG3	2.00	0.44
2:O:168:GLN:HA	2:O:171:ILE:HD12	2.00	0.44
4:R:94:GLU:O	5:S:26:LYS:HD2	2.18	0.44
1:B:422:ARG:HE	1:B:453:GLY:HA2	1.83	0.43
3:G:182:ILE:HD11	3:G:217:GLN:HG3	2.00	0.43
5:I:18:ALA:HA	5:I:21:ILE:HD12	2.00	0.43
2:O:97:ASN:HB2	11:O:2010:HOH:O	2.18	0.43
1:A:361:LYS:HG3	2:D:379:GLN:HG2	2.00	0.43
1:A:422:ARG:NH1	1:A:453:GLY:HA2	2.11	0.43
1:A:73:VAL:HG12	1:A:75:ILE:HG13	1.99	0.43
1:B:335:ASP:OD2	3:G:257:ARG:HD3	2.18	0.43
3:G:46:GLU:O	3:G:50:LEU:HB2	2.18	0.43
5:I:55:GLU:N	5:I:55:GLU:OE1	2.51	0.43
1:K:329:ILE:HD11	1:K:344:VAL:HG21	2.00	0.43
1:K:51:ALA:O	1:K:52:GLU:HB2	2.18	0.43
4:R:118:ARG:HD2	5:S:8:ILE:HD11	2.00	0.43
1:B:402:VAL:HA	1:B:405:PHE:CD1	2.52	0.43
1:C:413:ASP:HB3	1:C:416:THR:OG1	2.18	0.43
2:E:140:VAL:HG13	2:E:414:LEU:HB3	2.00	0.43
1:L:402:VAL:HA	1:L:405:PHE:CD1	2.52	0.43
1:L:440:THR:O	1:L:444:VAL:HG13	2.17	0.43
1:A:173:ARG:C	1:A:174:GLN:HG2	2.38	0.43
1:C:140:PRO:HB3	1:C:318:GLU:HG3	2.00	0.43
1:C:142:ARG:CG	1:C:142:ARG:NH1	2.75	0.43
2:F:84:SER:HB3	11:F:2015:HOH:O	2.19	0.43
1:K:444:VAL:HG21	1:K:485:ILE:HG21	2.00	0.43
2:O:300:LYS:HD3	2:O:300:LYS:HA	1.74	0.43
1:B:440:THR:O	1:B:444:VAL:HG13	2.18	0.43
2:D:390:ILE:HD13	3:G:19:ILE:HG13	1.99	0.43
2:E:300:LYS:HA	2:E:300:LYS:HD3	1.75	0.43
2:F:152:LYS:NZ	2:F:293:GLN:O	2.52	0.43
1:M:413:ASP:HB3	1:M:416:THR:OG1	2.18	0.43
1:M:140:PRO:HB3	1:M:318:GLU:HG3	2.01	0.43
2:N:98:VAL:HG23	2:N:232:VAL:HA	2.01	0.43
3:Q:182:ILE:HD11	3:Q:217:GLN:HG3	2.01	0.43
1:A:211:LYS:HD3	2:D:328:HIS:HA	1.99	0.43
1:A:492:SER:HB2	1:A:495:LEU:H	1.84	0.43
1:K:338:ALA:O	1:K:342:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:422:ARG:NH1	1:K:453:GLY:HA2	2.10	0.43
1:L:422:ARG:HE	1:L:453:GLY:HA2	1.84	0.43
5:S:18:ALA:HA	5:S:21:ILE:HD12	2.00	0.43
1:A:444:VAL:HG21	1:A:485:ILE:HG21	2.01	0.43
2:D:253:LEU:O	2:D:306:SER:HA	2.18	0.43
2:D:41:THR:CB	2:D:42:PRO:HD2	2.40	0.43
2:O:95:ILE:HD11	2:O:198:TYR:CD1	2.54	0.43
1:M:285:LEU:HD21	1:M:291:PRO:HB3	2.01	0.43
1:A:404:ALA:HB2	3:G:18:LYS:HE3	2.01	0.42
2:D:222:MET:HA	2:D:229:ARG:HD2	2.01	0.42
1:K:346:SER:CB	2:O:260:ARG:HH22	2.32	0.42
2:N:26:GLU:O	2:N:29:GLU:CG	2.66	0.42
2:O:367:HIS:CE1	2:O:434:LEU:HD11	2.54	0.42
1:C:399:TYR:CG	1:C:423:GLY:HA3	2.54	0.42
2:D:98:VAL:HG23	2:D:232:VAL:HA	2.01	0.42
2:F:374:VAL:HG13	2:F:410:ILE:HG21	2.01	0.42
3:G:149:LYS:HE2	5:I:44:TYR:CZ	2.53	0.42
1:K:170:ILE:HG23	1:K:353:PHE:HD1	1.84	0.42
2:O:140:VAL:HG13	2:O:414:LEU:HB3	2.01	0.42
1:M:107:GLY:HA2	1:M:228:MET:O	2.20	0.42
1:M:378:SER:HB2	1:M:386:LYS:HD2	2.01	0.42
1:M:399:TYR:CG	1:M:423:GLY:HA3	2.55	0.42
1:C:402:VAL:O	1:C:402:VAL:HG12	2.19	0.42
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.55	0.42
1:M:402:VAL:HG12	1:M:402:VAL:O	2.19	0.42
3:Q:55:ALA:O	3:Q:191:SER:HB2	2.20	0.42
2:E:152:LYS:HE2	2:E:293:GLN:HB3	2.02	0.42
1:K:492:SER:HB2	1:K:495:LEU:H	1.84	0.42
1:M:142:ARG:NH1	1:M:142:ARG:CG	2.74	0.42
1:M:434:GLN:OE1	9:M:600:ADP:H2'	2.19	0.42
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.49	0.42
1:B:26:ASN:O	1:B:30:THR:HB	2.19	0.42
1:K:173:ARG:C	1:K:174:GLN:HG2	2.39	0.42
2:P:258:ILE:O	2:P:258:ILE:HD13	2.20	0.42
1:K:73:VAL:HG12	1:K:75:ILE:HG13	2.01	0.42
1:L:99:VAL:HG21	1:L:251:THR:HB	2.02	0.42
2:N:158:GLY:O	2:N:161:VAL:HG22	2.19	0.42
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.50	0.42
2:P:97:ASN:C	2:P:97:ASN:HD22	2.23	0.42
1:A:349:ASP:OD1	2:E:192:ARG:NE	2.42	0.42
1:A:51:ALA:O	1:A:52:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:SER:O	2:D:215:VAL:HA	2.20	0.42
6:J:30:ARG:CG	6:J:30:ARG:NH1	2.70	0.42
1:M:400:ARG:HA	1:M:400:ARG:HD2	1.88	0.42
2:D:26:GLU:O	2:D:29:GLU:CG	2.67	0.41
2:E:95:ILE:HD11	2:E:198:TYR:CD1	2.55	0.41
5:I:43:PHE:CD2	5:I:59:ILE:O	2.74	0.41
1:K:260:ARG:O	1:K:321:GLY:HA3	2.20	0.41
2:O:253:LEU:O	2:O:306:SER:HA	2.20	0.41
6:T:7:THR:HA	6:T:8:PRO:HD3	1.92	0.41
1:A:170:ILE:HG23	1:A:353:PHE:HD1	1.85	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD12	1.85	0.41
3:G:159:TYR:HA	3:G:160:PRO:HD3	1.94	0.41
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.55	0.41
2:N:449:TYR:CD1	2:N:452:ILE:HD12	2.54	0.41
1:A:260:ARG:O	1:A:321:GLY:HA3	2.20	0.41
1:A:355:GLU:OE2	1:A:368:ASN:ND2	2.48	0.41
1:C:400:ARG:HA	1:C:400:ARG:HD2	1.88	0.41
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.55	0.41
1:L:38:ASP:HB3	1:L:286:LEU:HD22	2.02	0.41
2:N:222:MET:HA	2:N:229:ARG:HD2	2.02	0.41
2:O:300:LYS:HG2	11:O:2015:HOH:O	2.20	0.41
4:R:49:VAL:HG22	4:R:76:THR:HG23	2.02	0.41
1:K:242:ALA:N	1:K:243:PRO:CD	2.83	0.41
1:K:346:SER:HB2	2:O:260:ARG:HH22	1.85	0.41
2:P:374:VAL:HG13	2:P:410:ILE:HG21	2.03	0.41
2:P:449:TYR:HD1	2:P:452:ILE:HD12	1.85	0.41
1:A:338:ALA:O	1:A:342:THR:HB	2.20	0.41
3:G:55:ALA:O	3:G:191:SER:HB2	2.20	0.41
11:G:2007:HOH:O	5:I:36:ASN:HB3	2.21	0.41
1:L:192:ASN:HA	1:L:200:LYS:HG2	2.03	0.41
4:H:49:VAL:HG22	4:H:76:THR:HG23	2.03	0.41
1:L:299:ASP:HA	11:L:2125:HOH:O	2.21	0.41
1:M:413:ASP:CB	1:M:416:THR:CB	2.95	0.41
1:B:192:ASN:HA	1:B:200:LYS:HG2	2.03	0.41
2:D:449:TYR:CD1	2:D:452:ILE:HD12	2.55	0.41
2:E:98:VAL:HB	2:E:232:VAL:CG1	2.50	0.41
2:F:449:TYR:CD1	2:F:452:ILE:HD12	2.56	0.41
1:A:242:ALA:N	1:A:243:PRO:CD	2.83	0.41
1:C:434:GLN:OE1	9:C:600:ADP:H2'	2.20	0.41
4:R:35:LYS:HD2	4:R:51:GLN:HE22	1.84	0.41
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:203:CYS:O	1:L:231:SER:HA	2.21	0.41
1:K:349:ASP:O	1:K:375:ARG:HB2	2.21	0.41
2:P:449:TYR:CD1	2:P:452:ILE:HD12	2.56	0.41
2:E:221:GLN:H	2:E:221:GLN:HG2	1.66	0.41
2:F:237:LEU:HD13	2:F:296:ILE:HG12	2.02	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD11	1.85	0.41
3:G:193:SER:HB3	3:G:196:LYS:HE2	2.02	0.41
4:H:111:ASN:O	4:H:114:SER:HB3	2.21	0.41
2:N:33:ILE:O	2:N:34:LEU:HB2	2.21	0.41
5:S:43:PHE:CD2	5:S:59:ILE:O	2.74	0.41
1:A:349:ASP:O	1:A:375:ARG:HB2	2.22	0.40
1:B:203:CYS:O	1:B:231:SER:HA	2.22	0.40
1:B:399:TYR:CD1	1:B:423:GLY:HA3	2.57	0.40
6:J:7:THR:HA	6:J:8:PRO:HD3	1.92	0.40
2:P:256:ASP:HA	2:P:257:ASN:HA	1.88	0.40
1:B:99:VAL:HG21	1:B:251:THR:HB	2.04	0.40
1:C:85:LYS:O	1:C:88:GLU:HB3	2.20	0.40
5:I:55:GLU:HA	5:I:56:PRO:HD3	1.96	0.40
1:L:146:GLU:HA	1:L:147:PRO:HD3	1.95	0.40
2:N:404:VAL:O	2:N:408:ARG:HG3	2.22	0.40
3:Q:193:SER:HB3	3:Q:196:LYS:HE2	2.02	0.40
5:S:10:TYR:CE2	5:S:14:LEU:HD11	2.56	0.40
1:L:399:TYR:CD1	1:L:423:GLY:HA3	2.57	0.40
1:B:139:LEU:HD12	1:B:139:LEU:HA	1.89	0.40
2:D:158:GLY:O	2:D:161:VAL:HG22	2.21	0.40
2:E:109:ILE:HG22	2:E:111:SER:HB2	2.03	0.40
1:A:305:SER:HB2	2:E:222:MET:HB3	2.03	0.40
2:E:253:LEU:O	2:E:306:SER:HA	2.22	0.40
1:M:363:ILE:CG1	1:M:363:ILE:O	2.59	0.40
2:N:182:SER:O	2:N:215:VAL:HA	2.21	0.40
2:O:98:VAL:HB	2:O:232:VAL:CG1	2.50	0.40
1:B:38:ASP:HB3	1:B:286:LEU:HD22	2.04	0.40
1:C:399:TYR:CD1	1:C:423:GLY:HA3	2.57	0.40
2:N:396:LEU:CD1	2:N:400:ASP:HB3	2.50	0.40
3:Q:149:LYS:HE2	5:S:44:TYR:CZ	2.57	0.40
3:Q:191:SER:OG	3:Q:194:PHE:HB2	2.22	0.40
6:T:30:ARG:NH1	6:T:30:ARG:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	482/510 (94%)	462 (96%)	19 (4%)	1 (0%)	47	68
1	B	477/510 (94%)	464 (97%)	13 (3%)	0	100	100
1	C	482/510 (94%)	460 (95%)	22 (5%)	0	100	100
1	K	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	47	68
1	L	477/510 (94%)	463 (97%)	14 (3%)	0	100	100
1	M	482/510 (94%)	460 (95%)	22 (5%)	0	100	100
2	D	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	47	68
2	E	466/478 (98%)	444 (95%)	20 (4%)	2 (0%)	34	54
2	F	468/478 (98%)	445 (95%)	21 (4%)	2 (0%)	34	54
2	N	468/478 (98%)	449 (96%)	18 (4%)	1 (0%)	47	68
2	O	466/478 (98%)	445 (96%)	19 (4%)	2 (0%)	34	54
2	P	470/478 (98%)	446 (95%)	22 (5%)	2 (0%)	34	54
3	G	261/278 (94%)	251 (96%)	10 (4%)	0	100	100
3	Q	262/278 (94%)	252 (96%)	10 (4%)	0	100	100
4	H	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	9	16
4	R	120/138 (87%)	104 (87%)	14 (12%)	2 (2%)	9	16
5	I	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	8	13
5	S	54/61 (88%)	51 (94%)	2 (4%)	1 (2%)	8	13
6	J	34/63 (54%)	33 (97%)	1 (3%)	0	100	100
6	T	34/63 (54%)	33 (97%)	1 (3%)	0	100	100
All	All	6627/7008 (95%)	6326 (96%)	283 (4%)	18 (0%)	41	61

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	117	ALA

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Mol	Chain	Res	Type
5	I	57	THR
4	R	117	ALA
5	S	57	THR
2	F	352	ASP
4	H	115	SER
2	P	352	ASP
4	R	115	SER
2	O	448	LYS
2	E	448	LYS
1	K	339	TYR
2	O	279	VAL
1	A	339	TYR
2	E	279	VAL
2	D	42	PRO
2	N	42	PRO
2	F	279	VAL
2	P	279	VAL

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	390/412 (95%)	381 (98%)	9 (2%)	50	76
1	B	387/412 (94%)	367 (95%)	20 (5%)	23	44
1	C	390/412 (95%)	376 (96%)	14 (4%)	35	61
1	K	390/412 (95%)	380 (97%)	10 (3%)	46	72
1	L	387/412 (94%)	366 (95%)	21 (5%)	22	42
1	M	390/412 (95%)	375 (96%)	15 (4%)	33	58
2	D	380/384 (99%)	365 (96%)	15 (4%)	32	57
2	E	378/384 (98%)	367 (97%)	11 (3%)	42	69
2	F	380/384 (99%)	369 (97%)	11 (3%)	42	69
2	N	380/384 (99%)	365 (96%)	15 (4%)	32	57
2	O	378/384 (98%)	366 (97%)	12 (3%)	39	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	382/384 (100%)	372 (97%)	10 (3%)	46	72
3	G	227/236 (96%)	215 (95%)	12 (5%)	22	43
3	Q	228/236 (97%)	215 (94%)	13 (6%)	20	39
4	H	105/112 (94%)	100 (95%)	5 (5%)	25	48
4	R	105/112 (94%)	100 (95%)	5 (5%)	25	48
5	I	47/48 (98%)	43 (92%)	4 (8%)	10	21
5	S	47/48 (98%)	43 (92%)	4 (8%)	10	21
6	J	30/57 (53%)	28 (93%)	2 (7%)	16	31
6	T	30/57 (53%)	28 (93%)	2 (7%)	16	31
All	All	5431/5682 (96%)	5221 (96%)	210 (4%)	32	57

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	81	ASP
1	A	124	ASP
1	A	174	GLN
1	A	251	THR
1	A	342	THR
1	A	383	LYS
1	A	429	LEU
1	A	495	LEU
1	B	30	THR
1	B	36	VAL
1	B	67	ASN
1	B	93	THR
1	B	106	LEU
1	B	139	LEU
1	B	142	ARG
1	B	144	VAL
1	B	166	ARG
1	B	223	GLU
1	B	246	TYR
1	B	378	SER
1	B	385	LEU
1	B	412	LEU
1	B	415	SER
1	B	418	GLN

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Mol	Chain	Res	Type
1	B	444	VAL
1	B	472	SER
1	B	481	LEU
1	B	494	GLU
1	C	59	SER
1	C	142	ARG
1	C	159	VAL
1	C	166	ARG
1	C	220	GLN
1	C	283	LEU
1	C	293	ARG
1	C	320	SER
1	C	351	GLN
1	C	363	ILE
1	C	440	THR
1	C	481	LEU
1	C	496	LEU
1	C	501	SER
2	D	74	GLU
2	D	85	VAL
2	D	89	ARG
2	D	129	THR
2	D	133	ILE
2	D	149	ARG
2	D	204	THR
2	D	246	GLU
2	D	250	ASP
2	D	303	SER
2	D	336	SER
2	D	396	LEU
2	D	436	ASP
2	D	455	HIS
2	D	464	GLU
2	E	10	THR
2	E	112	LYS
2	E	140	VAL
2	E	163	LYS
2	E	204	THR
2	E	232	VAL
2	E	348	VAL
2	E	357	LEU
2	E	366	GLU

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Mol	Chain	Res	Type
2	E	436	ASP
2	E	460	VAL
2	F	26	GLU
2	F	45	LYS
2	F	68	GLU
2	F	97	ASN
2	F	113	LEU
2	F	208	ASN
2	F	258	ILE
2	F	274	ARG
2	F	292	LEU
2	F	353	SER
2	F	464	GLU
3	G	4	LYS
3	G	24	LYS
3	G	28	SER
3	G	77	ILE
3	G	78	THR
3	G	118	LEU
3	G	150	LEU
3	G	181	PRO
3	G	237	MET
3	G	247	MET
3	G	254	LEU
3	G	276	SER
4	H	51	GLN
4	H	60	MET
4	H	93	LEU
4	H	104	LEU
4	H	105	LEU
5	I	4	ARG
5	I	27	THR
5	I	55	GLU
5	I	61	LYS
6	J	9	ARG
6	J	30	ARG
1	K	59	SER
1	K	81	ASP
1	K	124	ASP
1	K	166	ARG
1	K	174	GLN
1	K	251	THR

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Mol	Chain	Res	Type
1	K	342	THR
1	K	383	LYS
1	K	429	LEU
1	K	495	LEU
1	L	30	THR
1	L	36	VAL
1	L	67	ASN
1	L	93	THR
1	L	106	LEU
1	L	139	LEU
1	L	142	ARG
1	L	144	VAL
1	L	166	ARG
1	L	223	GLU
1	L	246	TYR
1	L	337	SER
1	L	378	SER
1	L	385	LEU
1	L	412	LEU
1	L	415	SER
1	L	418	GLN
1	L	444	VAL
1	L	472	SER
1	L	481	LEU
1	L	494	GLU
1	M	59	SER
1	M	142	ARG
1	M	159	VAL
1	M	166	ARG
1	M	220	GLN
1	M	283	LEU
1	M	293	ARG
1	M	306	ARG
1	M	320	SER
1	M	351	GLN
1	M	363	ILE
1	M	440	THR
1	M	481	LEU
1	M	496	LEU
1	M	501	SER
2	N	74	GLU
2	N	85	VAL

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Mol	Chain	Res	Type
2	N	89	ARG
2	N	129	THR
2	N	133	ILE
2	N	149	ARG
2	N	204	THR
2	N	246	GLU
2	N	250	ASP
2	N	303	SER
2	N	336	SER
2	N	396	LEU
2	N	436	ASP
2	N	455	HIS
2	N	464	GLU
2	O	10	THR
2	O	112	LYS
2	O	132	GLU
2	O	140	VAL
2	O	163	LYS
2	O	204	THR
2	O	232	VAL
2	O	348	VAL
2	O	357	LEU
2	O	366	GLU
2	O	436	ASP
2	O	460	VAL
2	P	26	GLU
2	P	45	LYS
2	P	68	GLU
2	P	97	ASN
2	P	113	LEU
2	P	208	ASN
2	P	258	ILE
2	P	274	ARG
2	P	353	SER
2	P	464	GLU
3	Q	4	LYS
3	Q	24	LYS
3	Q	28	SER
3	Q	77	ILE
3	Q	78	THR
3	Q	118	LEU
3	Q	125	ASN

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Mol	Chain	Res	Type
3	Q	150	LEU
3	Q	181	PRO
3	Q	237	MET
3	Q	247	MET
3	Q	254	LEU
3	Q	276	SER
4	R	51	GLN
4	R	60	MET
4	R	93	LEU
4	R	104	LEU
4	R	105	LEU
5	S	4	ARG
5	S	27	THR
5	S	55	GLU
5	S	61	LYS
6	T	9	ARG
6	T	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	149	GLN
1	A	174	GLN
1	A	220	GLN
1	A	262	ASN
1	A	265	HIS
1	A	407	GLN
1	B	95	ASN
1	B	145	HIS
1	B	224	GLN
1	B	387	GLN
1	B	418	GLN
1	C	220	GLN
2	D	178	HIS
2	D	195	ASN
2	D	367	HIS
2	E	168	GLN
2	E	221	GLN
2	F	52	GLN
2	F	97	ASN
2	F	208	ASN

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Mol	Chain	Res	Type
3	G	90	GLN
3	G	125	ASN
4	H	103	ASN
5	I	19	GLN
5	I	36	ASN
6	J	36	GLN
1	K	72	GLN
1	K	149	GLN
1	K	174	GLN
1	K	220	GLN
1	K	262	ASN
1	K	265	HIS
1	K	407	GLN
1	L	95	ASN
1	L	224	GLN
1	L	387	GLN
1	L	418	GLN
1	M	220	GLN
2	N	178	HIS
2	N	195	ASN
2	N	367	HIS
2	O	168	GLN
2	O	221	GLN
2	P	52	GLN
2	P	97	ASN
2	P	208	ASN
3	Q	90	GLN
3	Q	125	ASN
4	R	51	GLN
5	S	19	GLN
5	S	36	ASN
6	T	36	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 10 are monoatomic - 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
9	ADP	O	600	-	24,29,29	1.43	3 (12%)	29,45,45	1.39	3 (10%)
9	ADP	M	600	8	24,29,29	1.14	2 (8%)	29,45,45	1.46	4 (13%)
9	ADP	N	600	8	24,29,29	1.29	2 (8%)	29,45,45	1.38	3 (10%)
9	ADP	C	600	8	24,29,29	1.16	2 (8%)	29,45,45	1.50	4 (13%)
9	ADP	L	600	8	24,29,29	1.18	2 (8%)	29,45,45	1.49	4 (13%)
7	ATP	A	600	8	26,33,33	1.10	2 (7%)	31,52,52	1.25	2 (6%)
9	ADP	P	600	8	24,29,29	1.21	2 (8%)	29,45,45	1.33	3 (10%)
10	EDO	P	603	-	3,3,3	0.69	0	2,2,2	0.44	0
10	EDO	C	603	-	3,3,3	0.33	0	2,2,2	0.45	0
10	EDO	M	602	-	3,3,3	0.38	0	2,2,2	0.30	0
10	EDO	L	602	-	3,3,3	0.59	0	2,2,2	0.21	0
10	EDO	O	602	-	3,3,3	0.46	0	2,2,2	0.40	0
9	ADP	B	600	8	24,29,29	1.37	3 (12%)	29,45,45	1.56	4 (13%)
9	ADP	E	600	-	24,29,29	1.31	2 (8%)	29,45,45	1.41	3 (10%)
9	ADP	F	600	8	24,29,29	1.16	3 (12%)	29,45,45	1.35	3 (10%)
7	ATP	K	600	8	26,33,33	1.03	1 (3%)	31,52,52	1.24	2 (6%)
9	ADP	D	600	8	24,29,29	1.33	3 (12%)	29,45,45	1.40	3 (10%)
10	EDO	L	604	-	3,3,3	0.52	0	2,2,2	0.27	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
9	ADP	O	600	-	-	0/12/32/32	0/3/3/3
9	ADP	M	600	8	-	4/12/32/32	0/3/3/3
9	ADP	N	600	8	-	1/12/32/32	0/3/3/3
9	ADP	C	600	8	-	4/12/32/32	0/3/3/3
9	ADP	L	600	8	-	0/12/32/32	0/3/3/3
7	ATP	A	600	8	-	2/18/38/38	0/3/3/3
9	ADP	P	600	8	-	1/12/32/32	0/3/3/3
10	EDO	P	603	-	-	0/1/1/1	-
10	EDO	C	603	-	-	0/1/1/1	-
10	EDO	M	602	-	-	0/1/1/1	-
10	EDO	L	602	-	-	0/1/1/1	-
10	EDO	O	602	-	-	0/1/1/1	-
9	ADP	B	600	8	-	0/12/32/32	0/3/3/3
9	ADP	E	600	-	-	0/12/32/32	0/3/3/3
9	ADP	F	600	8	-	1/12/32/32	0/3/3/3
7	ATP	K	600	8	-	2/18/38/38	0/3/3/3
9	ADP	D	600	8	-	1/12/32/32	0/3/3/3
10	EDO	L	604	-	-	0/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	600	ADP	PB-O1B	4.15	1.63	1.50
9	O	600	ADP	O4'-C1'	3.96	1.46	1.41
9	O	600	ADP	PB-O1B	3.83	1.62	1.50
9	E	600	ADP	O4'-C1'	3.83	1.46	1.41
9	D	600	ADP	O4'-C1'	3.81	1.46	1.41
9	N	600	ADP	O4'-C1'	3.61	1.46	1.41
9	P	600	ADP	O4'-C1'	3.61	1.46	1.41
9	M	600	ADP	O4'-C1'	3.39	1.45	1.41
9	E	600	ADP	PB-O1B	3.38	1.61	1.50
9	D	600	ADP	PB-O1B	3.35	1.61	1.50
9	C	600	ADP	O4'-C1'	3.31	1.45	1.41
9	L	600	ADP	PB-O1B	3.15	1.60	1.50
7	A	600	ATP	O4'-C1'	3.14	1.45	1.41
9	N	600	ADP	PB-O1B	3.13	1.60	1.50
9	B	600	ADP	O4'-C1'	3.01	1.45	1.41
9	F	600	ADP	O4'-C1'	2.97	1.45	1.41
9	L	600	ADP	O4'-C1'	2.64	1.44	1.41
9	M	600	ADP	PB-O1B	2.42	1.58	1.50
9	O	600	ADP	PB-O2B	2.33	1.63	1.54
9	C	600	ADP	PB-O1B	2.29	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	600	ATP	O4'-C1'	2.23	1.44	1.41
9	F	600	ADP	PB-O1B	2.19	1.57	1.50
9	F	600	ADP	PB-O2B	2.09	1.62	1.54
9	P	600	ADP	PB-O1B	2.07	1.57	1.50
9	B	600	ADP	PB-O2B	2.07	1.62	1.54
7	A	600	ATP	PG-O3G	2.03	1.62	1.54
9	D	600	ADP	PB-O2B	2.01	1.62	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	600	ADP	N3-C2-N1	-4.89	121.03	128.68
9	F	600	ADP	N3-C2-N1	-4.88	121.04	128.68
9	P	600	ADP	N3-C2-N1	-4.81	121.16	128.68
9	D	600	ADP	N3-C2-N1	-4.63	121.44	128.68
9	M	600	ADP	N3-C2-N1	-4.60	121.49	128.68
9	C	600	ADP	N3-C2-N1	-4.55	121.56	128.68
7	K	600	ATP	N3-C2-N1	-4.49	121.66	128.68
7	A	600	ATP	N3-C2-N1	-4.46	121.70	128.68
9	E	600	ADP	N3-C2-N1	-4.44	121.73	128.68
9	O	600	ADP	N3-C2-N1	-4.27	122.01	128.68
9	B	600	ADP	O3B-PB-O3A	4.24	118.86	104.64
9	B	600	ADP	N3-C2-N1	-4.00	122.42	128.68
9	L	600	ADP	N3-C2-N1	-3.98	122.46	128.68
9	L	600	ADP	O3B-PB-O3A	3.87	117.60	104.64
9	O	600	ADP	PA-O3A-PB	-3.44	121.02	132.83
9	M	600	ADP	O3B-PB-O3A	3.43	116.13	104.64
9	E	600	ADP	PA-O3A-PB	-3.42	121.09	132.83
9	C	600	ADP	O3B-PB-O3A	3.39	116.00	104.64
9	B	600	ADP	PA-O3A-PB	-3.25	121.69	132.83
9	D	600	ADP	PA-O3A-PB	-3.11	122.17	132.83
9	C	600	ADP	PA-O3A-PB	-3.10	122.20	132.83
9	L	600	ADP	PA-O3A-PB	-3.08	122.25	132.83
9	M	600	ADP	PA-O3A-PB	-2.85	123.06	132.83
9	P	600	ADP	PA-O3A-PB	-2.83	123.11	132.83
9	N	600	ADP	PA-O3A-PB	-2.80	123.23	132.83
9	O	600	ADP	O3B-PB-O3A	2.75	113.84	104.64
9	F	600	ADP	O3B-PB-O3A	2.60	113.36	104.64
9	E	600	ADP	O3B-PB-O3A	2.55	113.19	104.64
9	F	600	ADP	PA-O3A-PB	-2.49	124.27	132.83
7	K	600	ATP	O2G-PG-O3B	2.49	112.98	104.64
9	D	600	ADP	O3B-PB-O3A	2.40	112.69	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	600	ADP	C4-C5-N7	-2.39	106.91	109.40
9	P	600	ADP	O3B-PB-O3A	2.34	112.49	104.64
9	L	600	ADP	C4-C5-N7	-2.29	107.01	109.40
7	A	600	ATP	O2G-PG-O3B	2.28	112.29	104.64
9	M	600	ADP	C4-C5-N7	-2.25	107.05	109.40
9	B	600	ADP	C4-C5-N7	-2.12	107.19	109.40
9	N	600	ADP	O3B-PB-O3A	2.04	111.48	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	600	ATP	PB-O3B-PG-O2G
9	M	600	ADP	C5'-O5'-PA-O1A
7	K	600	ATP	PB-O3B-PG-O2G
9	D	600	ADP	PA-O3A-PB-O2B
9	N	600	ADP	PA-O3A-PB-O2B
9	C	600	ADP	C5'-O5'-PA-O1A
9	M	600	ADP	O4'-C4'-C5'-O5'
9	C	600	ADP	O4'-C4'-C5'-O5'
7	A	600	ATP	PB-O3B-PG-O1G
7	K	600	ATP	PB-O3B-PG-O1G
9	P	600	ADP	PA-O3A-PB-O2B
9	F	600	ADP	PA-O3A-PB-O2B
9	M	600	ADP	C5'-O5'-PA-O3A
9	C	600	ADP	C5'-O5'-PA-O3A
9	M	600	ADP	C5'-O5'-PA-O2A
9	C	600	ADP	C5'-O5'-PA-O2A

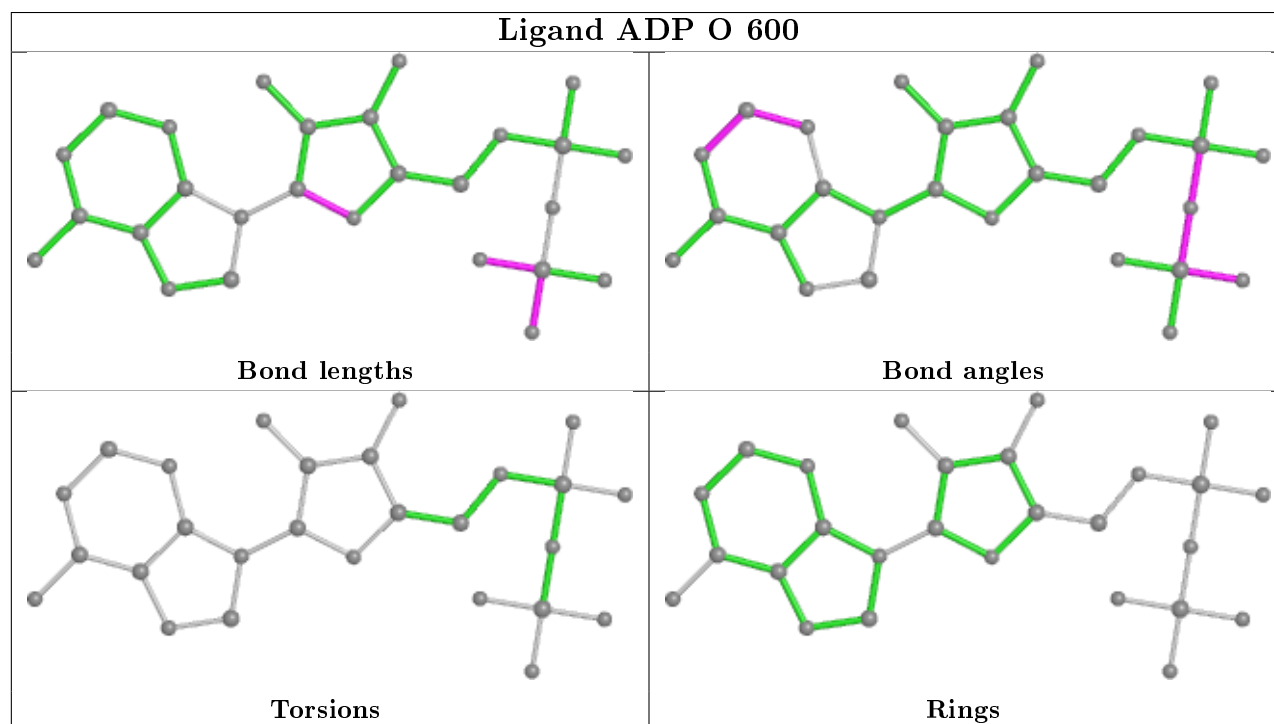
There are no ring outliers.

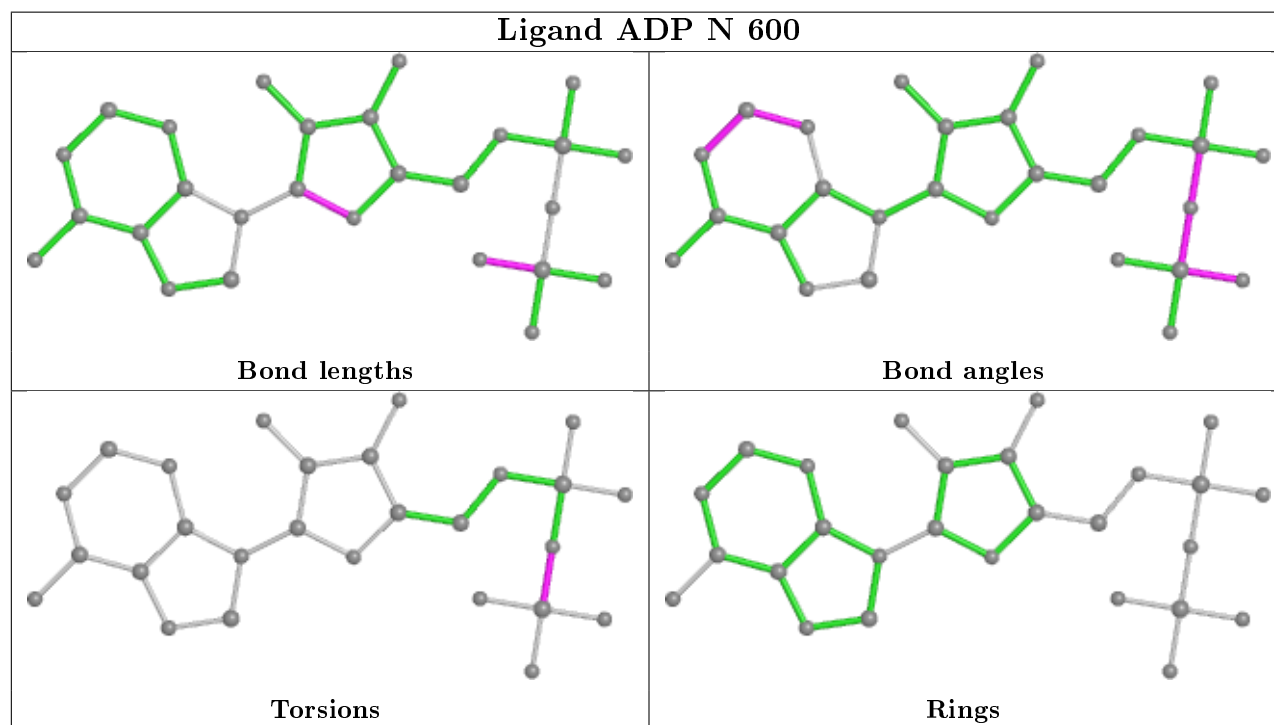
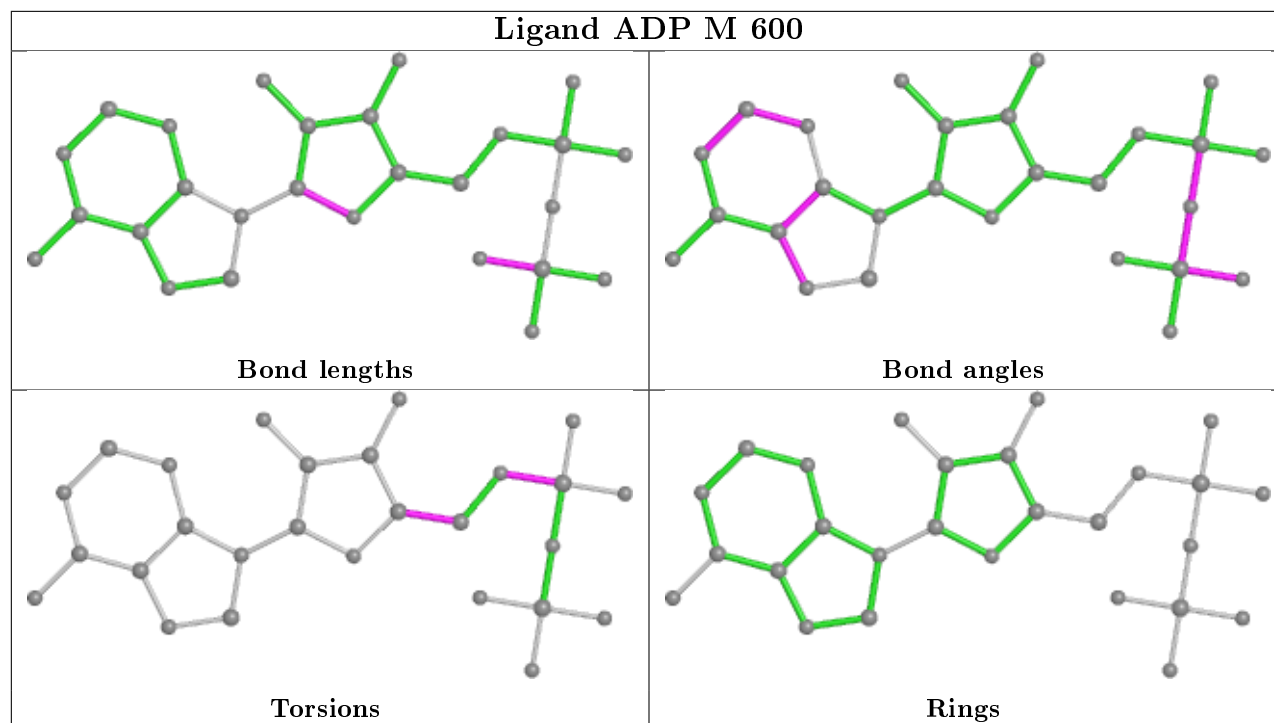
4 monomers are involved in 5 short contacts:

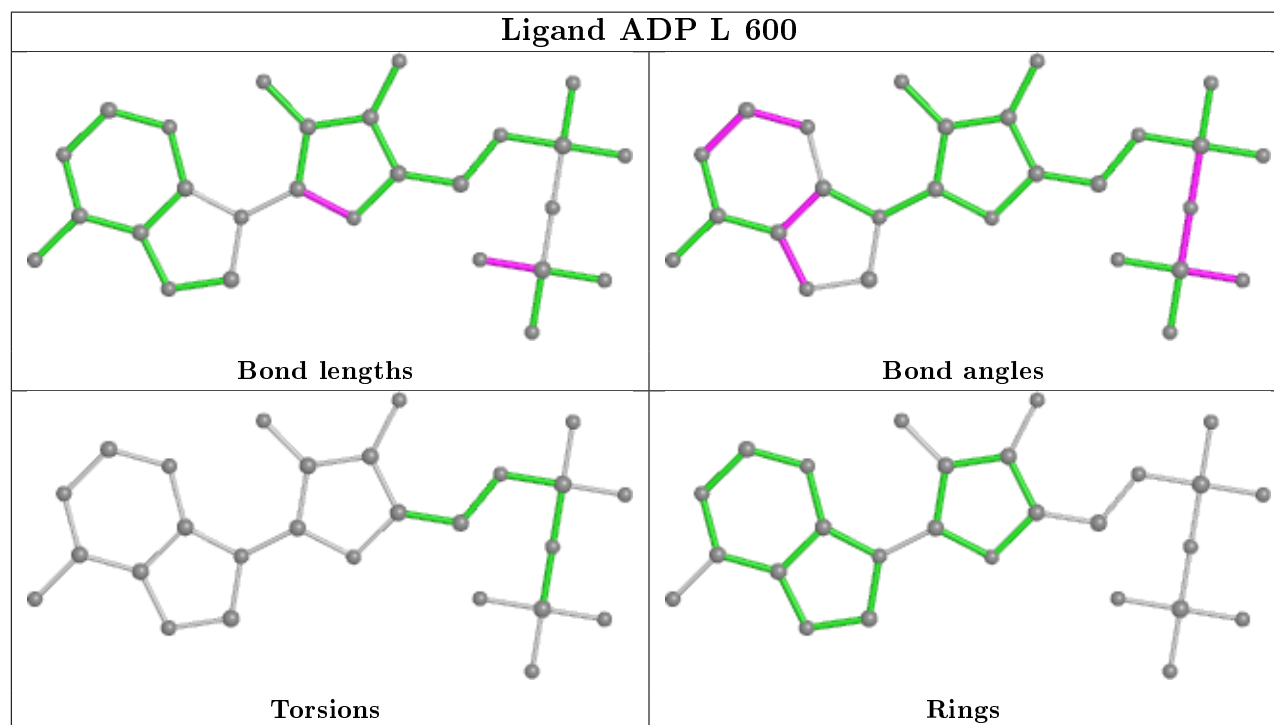
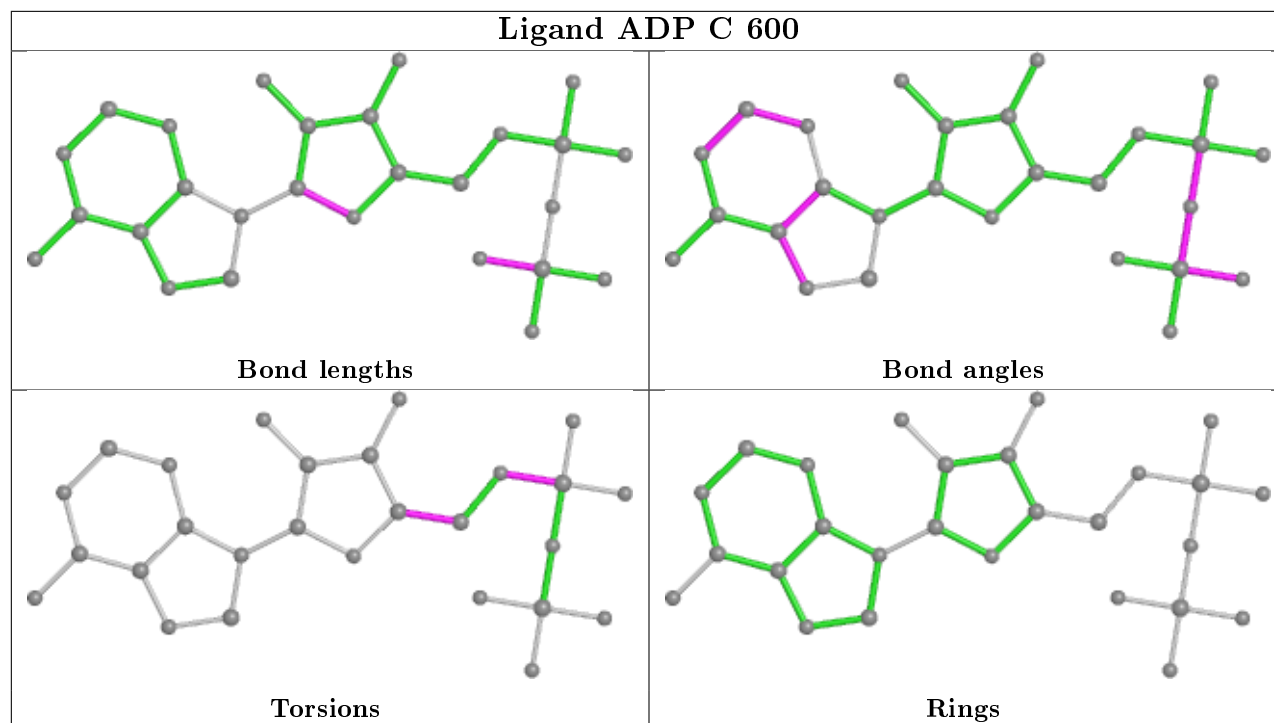
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	600	ADP	1	0
9	C	600	ADP	1	0
10	P	603	EDO	1	0
10	M	602	EDO	2	0

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

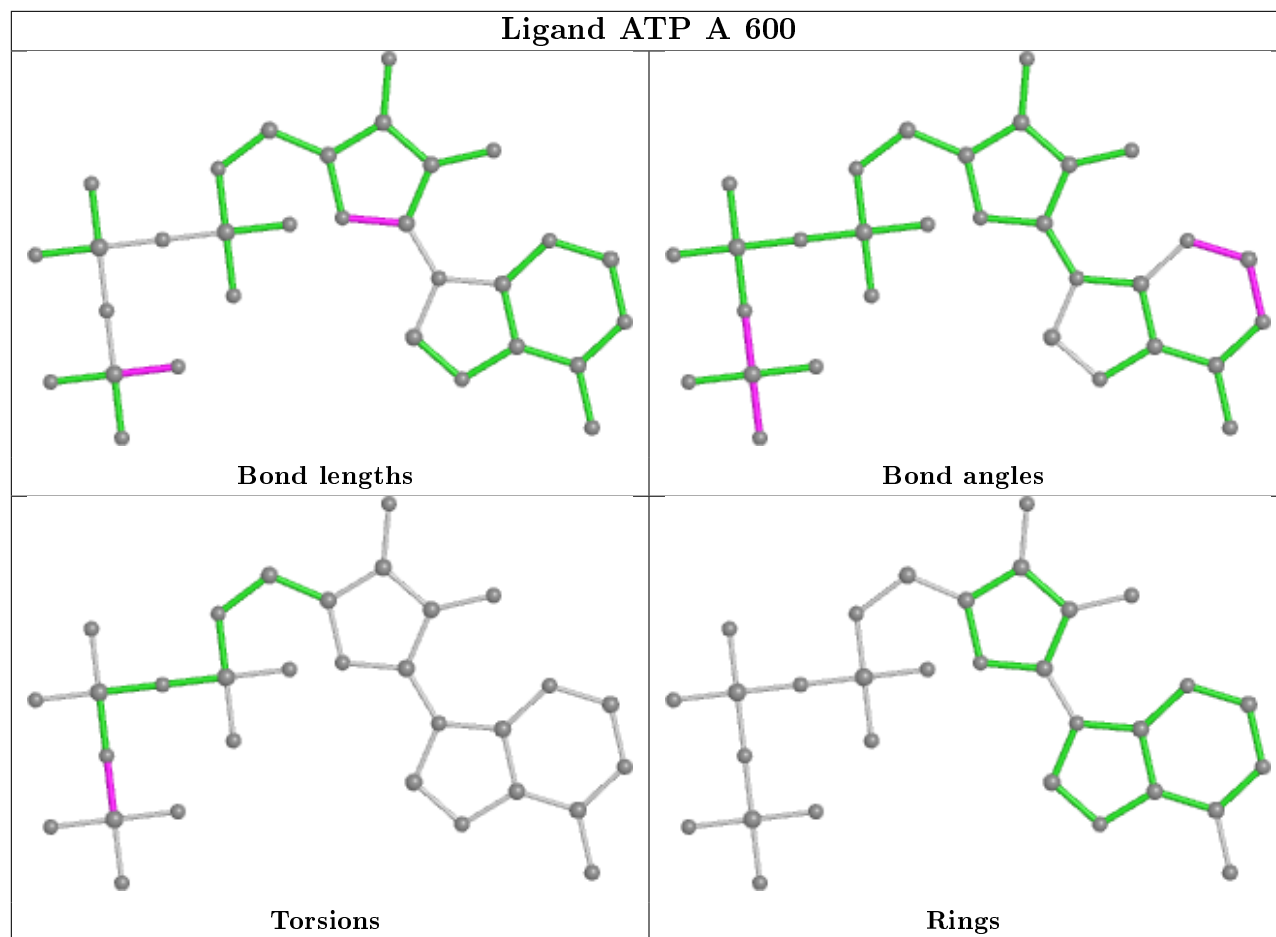
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



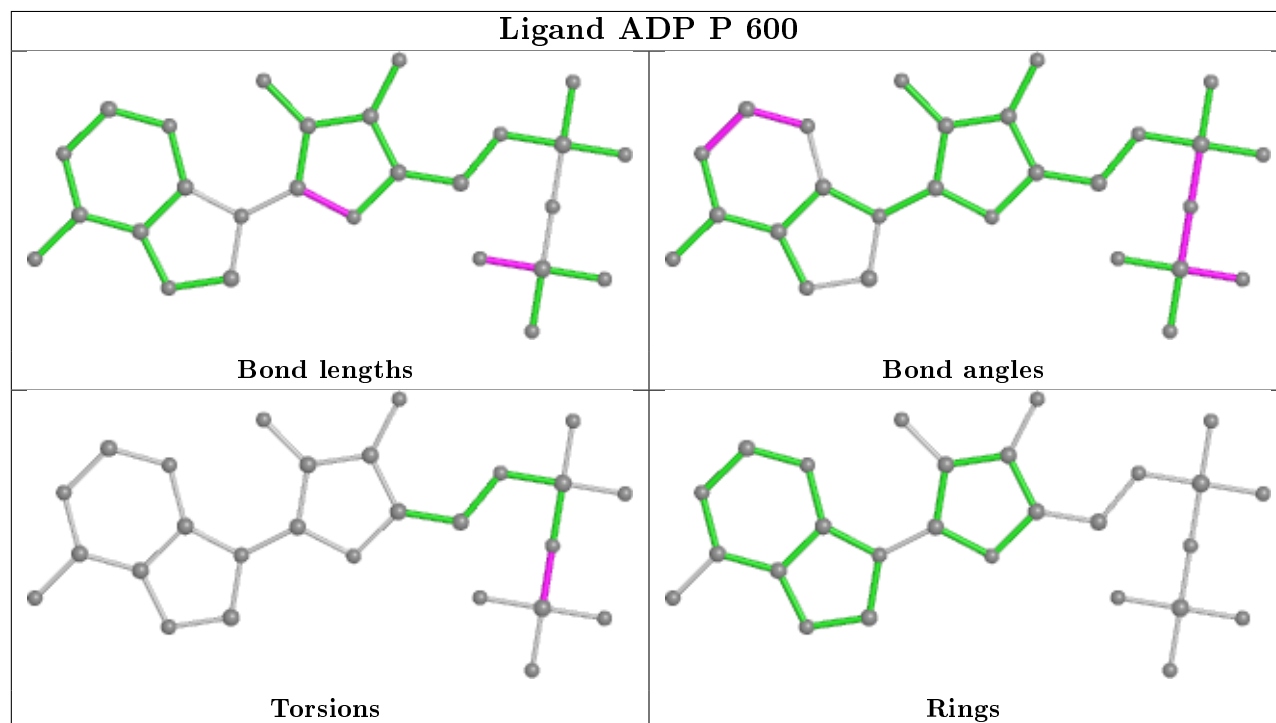


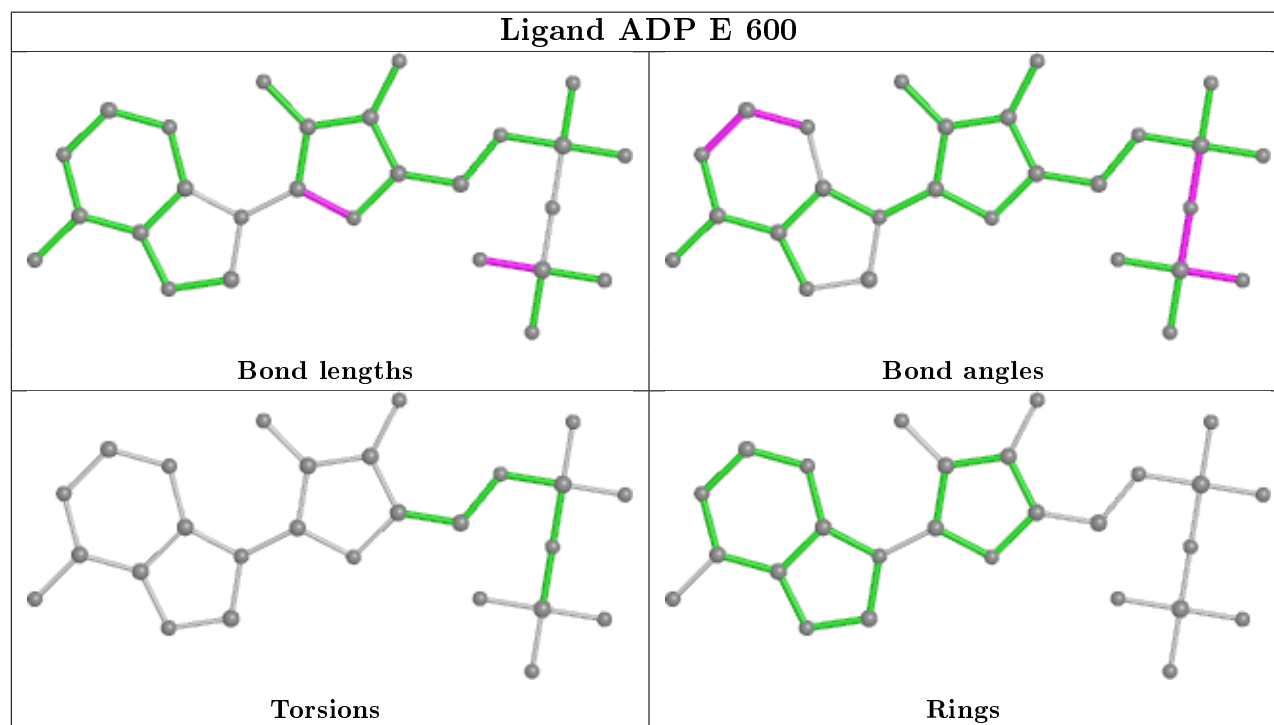
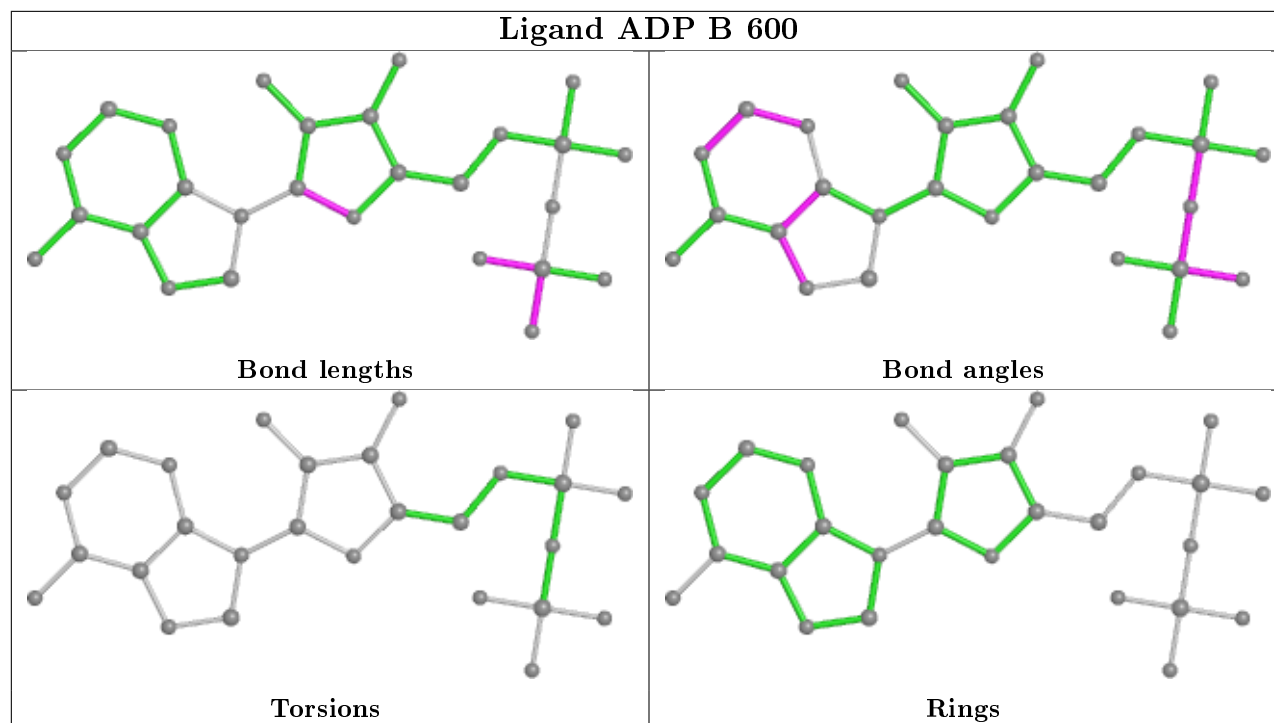


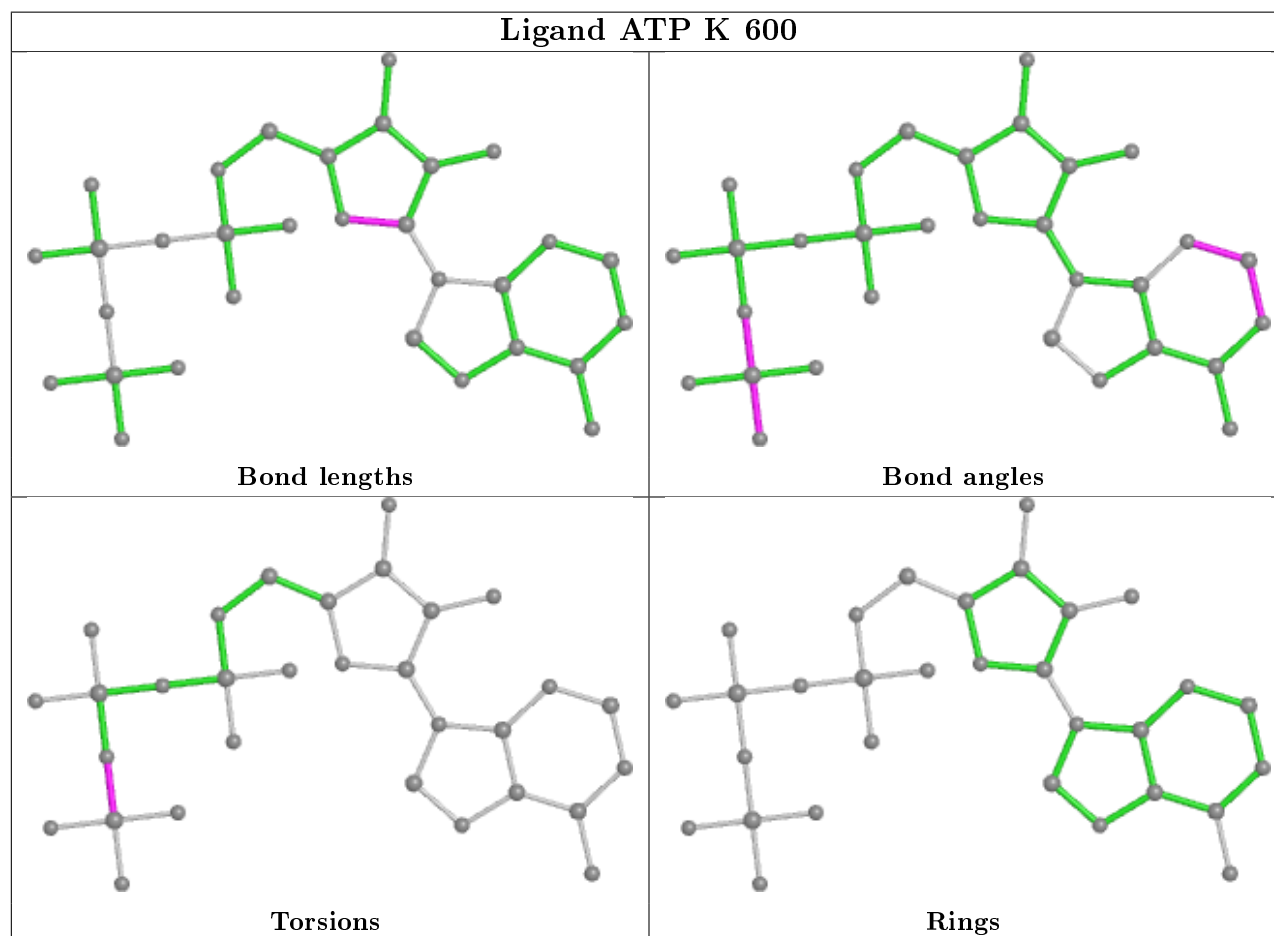
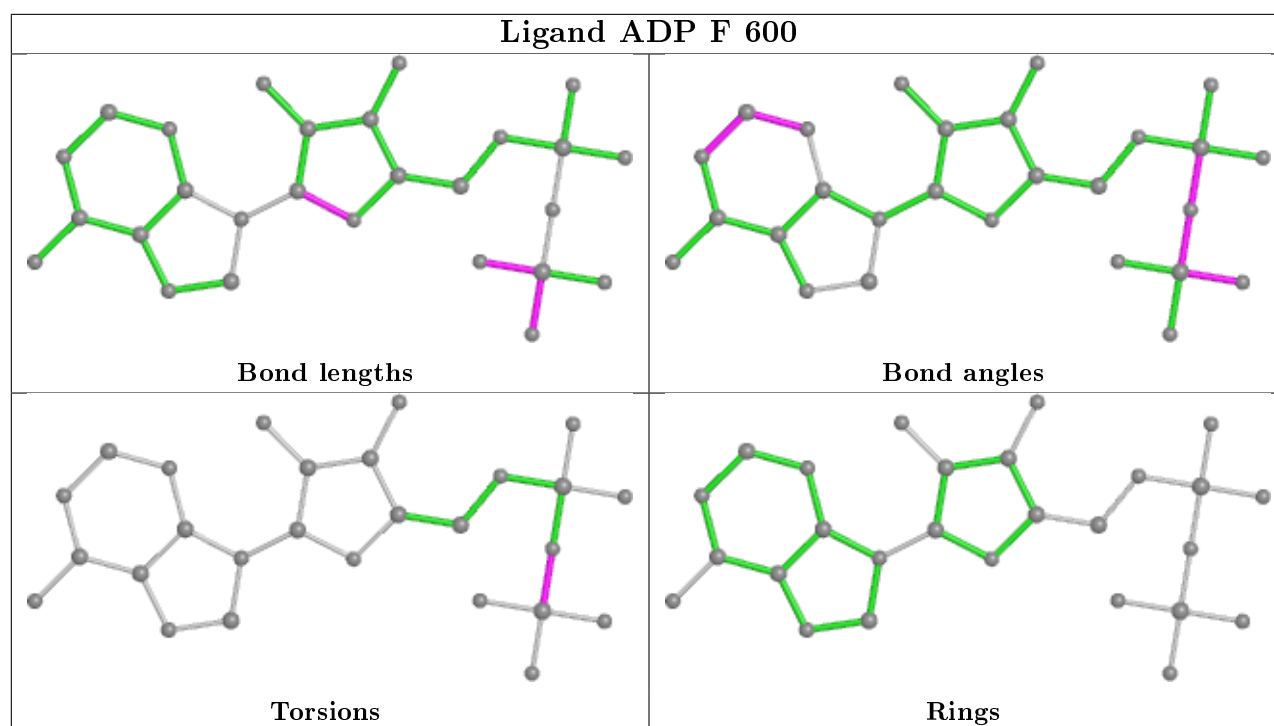
Ligand ATP A 600

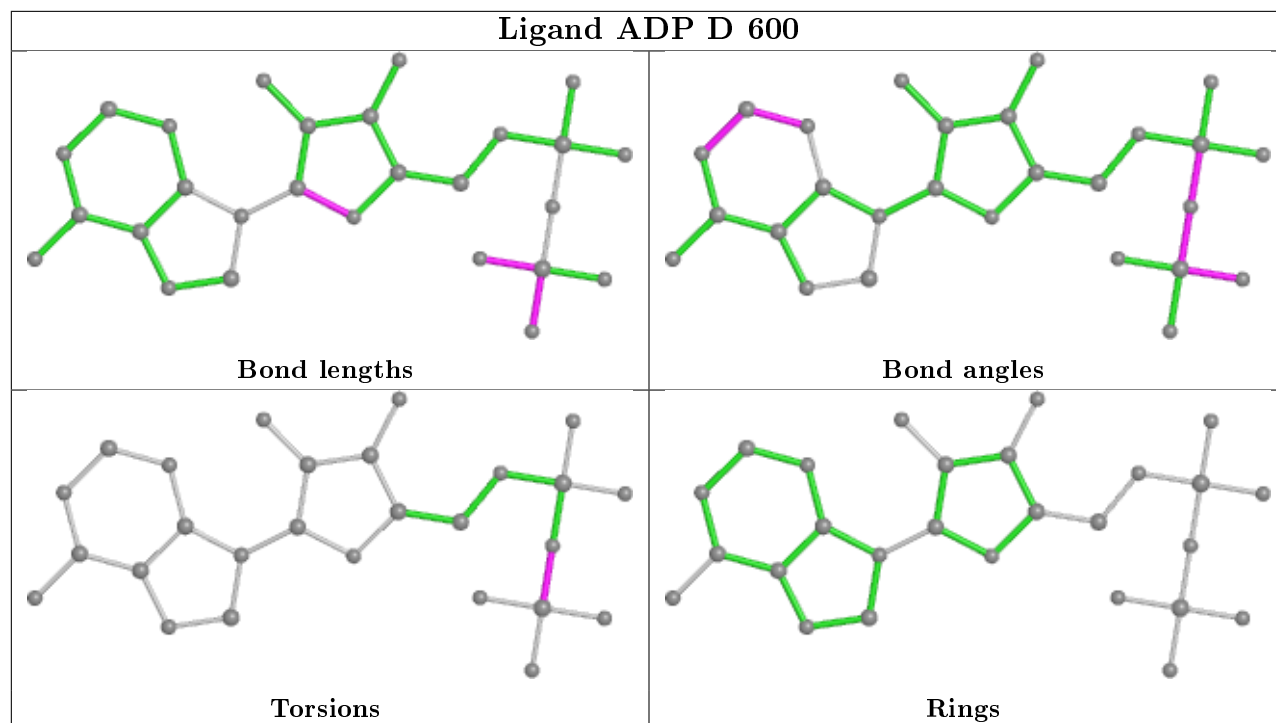


Ligand ADP P 600









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	484/510 (94%)	0.40	27 (5%) 24 25	34, 67, 108, 119	0
1	B	480/510 (94%)	0.16	27 (5%) 24 25	18, 42, 84, 104	0
1	C	484/510 (94%)	0.18	36 (7%) 14 15	22, 40, 112, 138	0
1	K	484/510 (94%)	0.43	34 (7%) 16 16	32, 60, 110, 119	0
1	L	480/510 (94%)	-0.18	3 (0%) 89 90	15, 31, 70, 100	0
1	M	484/510 (94%)	0.29	37 (7%) 13 14	23, 48, 116, 138	0
2	D	470/478 (98%)	0.21	18 (3%) 40 43	32, 55, 77, 100	0
2	E	468/478 (97%)	0.69	51 (10%) 5 5	34, 65, 118, 133	0
2	F	469/478 (98%)	-0.10	7 (1%) 73 75	19, 38, 64, 76	0
2	N	470/478 (98%)	0.29	20 (4%) 35 38	34, 60, 82, 103	0
2	O	468/478 (97%)	0.57	52 (11%) 5 5	20, 50, 119, 135	0
2	P	469/478 (98%)	0.07	17 (3%) 42 46	20, 43, 72, 79	0
3	G	265/278 (95%)	0.69	24 (9%) 9 9	36, 70, 120, 129	0
3	Q	265/278 (95%)	1.04	44 (16%) 1 1	30, 83, 122, 128	0
4	H	124/138 (89%)	1.77	46 (37%) 0 0	97, 110, 128, 133	0
4	R	124/138 (89%)	1.63	43 (34%) 0 0	96, 111, 127, 132	0
5	I	58/61 (95%)	0.98	5 (8%) 10 10	64, 84, 115, 117	0
5	S	58/61 (95%)	1.09	14 (24%) 0 0	65, 86, 121, 123	0
6	J	36/63 (57%)	0.62	2 (5%) 24 25	70, 84, 109, 110	0
6	T	36/63 (57%)	0.80	4 (11%) 5 5	76, 87, 112, 113	0
All	All	6676/7008 (95%)	0.37	511 (7%) 13 13	15, 57, 113, 138	0

All (511) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	389	ALA	10.0
2	O	396	LEU	9.0
2	O	386	ASP	8.5
2	O	387	ILE	8.2
2	O	404	VAL	8.2
2	O	391	LEU	7.8
2	D	6	SER	7.5
4	R	42	LEU	7.3
1	C	408	PHE	7.2
4	R	12	LEU	7.1
2	O	390	ILE	6.9
1	M	405	PHE	6.6
2	E	467	VAL	6.5
1	M	402	VAL	6.4
1	B	405	PHE	6.3
1	C	402	VAL	6.0
2	O	403	THR	6.0
1	C	406	ALA	6.0
2	E	402	LEU	5.7
2	O	467	VAL	5.7
1	B	25	ALA	5.6
3	Q	128	LEU	5.6
2	E	392	GLY	5.5
5	S	49	ASN	5.5
3	Q	105	ALA	5.4
3	G	195	GLY	5.4
1	A	499	LEU	5.4
4	H	77	VAL	5.3
1	C	409	GLY	5.3
5	S	57	THR	5.2
2	O	395	GLU	5.2
1	M	195	SER	5.2
1	C	457	GLY	5.2
1	B	499	LEU	5.2
3	Q	153	VAL	5.1
2	E	389	ALA	5.1
3	G	53	LYS	5.1
2	N	27	GLN	5.1
2	O	385	GLN	5.0
2	O	470	ALA	5.0
1	K	473	TYR	4.9
2	E	468	ALA	4.8
1	K	412	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	497	ALA	4.8
2	O	384	LEU	4.8
3	Q	202	ASP	4.7
2	D	7	THR	4.7
3	G	192	PRO	4.7
4	R	62	GLY	4.7
2	N	6	SER	4.7
2	O	474	ALA	4.7
2	E	475	ALA	4.7
5	I	49	ASN	4.7
2	O	473	LEU	4.7
2	O	27	GLN	4.6
1	M	415	SER	4.6
1	B	457	GLY	4.6
3	G	52	TYR	4.6
2	E	43	GLN	4.6
4	H	64	ASN	4.6
4	R	28	THR	4.6
5	S	54	SER	4.6
1	M	509	THR	4.6
2	O	392	GLY	4.6
3	G	197	PHE	4.6
3	G	1	ALA	4.5
4	R	27	VAL	4.5
2	E	29	GLU	4.5
2	E	393	MET	4.5
1	M	353	PHE	4.5
1	C	395	PHE	4.4
2	F	179	GLY	4.4
4	R	82	GLN	4.4
5	S	7	GLY	4.3
3	Q	127	LYS	4.3
5	S	55	GLU	4.3
4	H	41	VAL	4.3
3	Q	50	LEU	4.3
2	O	402	LEU	4.3
2	N	474	ALA	4.2
2	E	474	ALA	4.2
2	F	7	THR	4.1
4	R	59	VAL	4.1
2	N	473	LEU	4.1
2	E	27	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	28	SER	4.1
3	Q	197	PHE	4.1
1	C	448	TYR	4.0
2	O	393	MET	4.0
2	O	397	SER	4.0
3	G	206	PRO	3.9
4	R	60	MET	3.9
1	K	391	SER	3.9
5	I	57	THR	3.9
2	O	382	LYS	3.9
1	K	395	PHE	3.9
2	E	9	ILE	3.9
2	E	398	GLU	3.9
2	E	473	LEU	3.9
4	H	42	LEU	3.9
3	Q	172	SER	3.8
1	M	473	TYR	3.8
2	O	407	ALA	3.8
2	O	457	PHE	3.8
2	P	28	SER	3.8
3	Q	192	PRO	3.8
3	G	51	PHE	3.8
4	R	63	SER	3.8
1	B	460	LEU	3.8
4	H	46	VAL	3.8
1	A	502	ALA	3.7
4	H	79	PRO	3.7
2	O	388	ILE	3.7
2	O	383	SER	3.7
1	C	509	THR	3.7
2	E	394	ASP	3.7
1	C	399	TYR	3.7
2	D	473	LEU	3.7
2	O	394	ASP	3.7
2	O	344	ILE	3.7
3	Q	104	ASN	3.7
1	K	32	ARG	3.6
3	Q	49	GLN	3.6
1	A	507	VAL	3.6
1	C	414	ALA	3.6
2	E	390	ILE	3.6
1	M	503	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	506	PHE	3.6
3	G	202	ASP	3.6
1	A	497	ALA	3.6
1	C	195	SER	3.6
2	E	8	PRO	3.6
4	H	133	LEU	3.6
1	M	448	TYR	3.6
5	I	55	GLU	3.6
4	H	73	GLY	3.6
4	H	12	LEU	3.5
4	R	137	LEU	3.5
3	Q	154	MET	3.5
1	M	457	GLY	3.5
2	O	445	LEU	3.5
2	P	7	THR	3.5
2	E	452	ILE	3.5
1	B	503	THR	3.5
4	R	43	ALA	3.5
3	Q	161	LYS	3.5
1	M	476	SER	3.5
4	H	30	VAL	3.5
4	H	80	ASP	3.5
4	H	28	THR	3.5
1	A	501	SER	3.5
1	A	395	PHE	3.4
5	S	47	TYR	3.4
1	K	392	LEU	3.4
1	L	404	ALA	3.4
3	Q	126	ILE	3.4
5	I	5	LYS	3.4
4	R	61	GLU	3.4
3	Q	51	PHE	3.4
3	G	203	ALA	3.4
2	O	401	LYS	3.4
3	Q	173	LEU	3.4
1	C	449	ALA	3.4
4	H	82	GLN	3.4
4	H	113	SER	3.4
2	O	400	ASP	3.3
1	A	481	LEU	3.3
2	E	472	LYS	3.3
2	N	467	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	408	PHE	3.3
1	M	508	ALA	3.3
3	G	55	ALA	3.3
1	B	26	ASN	3.3
2	N	7	THR	3.3
4	H	29	GLN	3.3
2	O	338	GLY	3.3
2	E	112	LYS	3.3
1	K	494	GLU	3.2
2	O	430	LYS	3.2
1	B	507	VAL	3.2
1	B	412	LEU	3.2
2	O	410	ILE	3.2
2	E	401	LYS	3.2
1	C	499	LEU	3.2
2	O	425	THR	3.2
1	M	410	SER	3.2
2	F	27	GLN	3.2
4	H	56	VAL	3.2
1	A	448	TYR	3.1
1	B	463	ILE	3.1
1	A	465	GLU	3.1
5	S	8	ILE	3.1
2	E	391	LEU	3.1
1	A	202	TYR	3.1
4	H	116	ASP	3.1
1	B	404	ALA	3.1
6	T	31	GLN	3.1
4	H	44	ASN	3.1
1	B	454	HIS	3.1
1	C	353	PHE	3.1
1	A	389	ALA	3.1
1	M	497	ALA	3.1
4	R	65	SER	3.1
3	Q	195	GLY	3.1
1	C	501	SER	3.1
4	H	27	VAL	3.1
1	C	458	ILE	3.0
3	Q	100	ASN	3.0
2	D	28	SER	3.0
2	P	27	GLN	3.0
4	H	59	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	435	LYS	3.0
3	Q	203	ALA	3.0
1	K	492	SER	3.0
4	R	83	LEU	3.0
4	R	93	LEU	3.0
1	L	405	PHE	3.0
1	B	469	SER	3.0
1	K	421	VAL	3.0
2	D	43	GLN	3.0
4	R	13	GLN	3.0
1	B	456	ASP	3.0
4	H	61	GLU	3.0
4	R	99	GLU	2.9
1	K	476	SER	2.9
3	Q	171	SER	2.9
1	C	411	ASP	2.9
1	C	491	LEU	2.9
1	K	406	ALA	2.9
3	Q	160	PRO	2.9
1	C	418	GLN	2.9
1	A	124	ASP	2.9
1	K	457	GLY	2.9
3	Q	159	TYR	2.9
2	O	415	SER	2.9
4	R	31	ASN	2.9
3	Q	107	ILE	2.9
1	A	496	LEU	2.9
1	L	420	LEU	2.9
4	R	114	SER	2.8
2	E	409	LYS	2.8
2	N	452	ILE	2.8
1	A	454	HIS	2.8
4	R	116	ASP	2.8
1	M	505	SER	2.8
4	H	114	SER	2.8
2	O	444	VAL	2.8
4	R	41	VAL	2.8
1	M	480	GLU	2.8
2	E	210	GLU	2.8
3	Q	59	ASN	2.8
2	P	464	GLU	2.8
2	N	451	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	72	GLY	2.8
1	C	484	GLU	2.8
1	K	501	SER	2.8
1	M	378	SER	2.8
2	N	28	SER	2.8
1	C	412	LEU	2.8
4	H	49	VAL	2.7
4	H	62	GLY	2.7
3	Q	165	PHE	2.7
1	K	414	ALA	2.7
1	M	399	TYR	2.7
4	R	22	TYR	2.7
2	D	210	GLU	2.7
2	E	388	ILE	2.7
1	K	475	LYS	2.7
6	J	31	GLN	2.7
1	K	454	HIS	2.7
3	Q	103	PRO	2.7
2	E	451	ASN	2.7
1	B	403	ALA	2.7
2	E	399	GLN	2.7
4	H	74	PHE	2.7
5	S	46	GLN	2.7
1	B	502	ALA	2.7
2	D	456	ALA	2.7
1	M	481	LEU	2.7
2	O	458	TYR	2.7
1	A	421	VAL	2.7
4	R	30	VAL	2.7
3	Q	56	GLU	2.7
1	K	495	LEU	2.7
2	E	158	GLY	2.7
1	M	406	ALA	2.6
2	E	178	HIS	2.6
2	P	435	LYS	2.6
4	H	53	LEU	2.6
4	H	130	LEU	2.6
6	T	17	PHE	2.6
1	K	316	GLU	2.6
1	A	476	SER	2.6
2	E	396	LEU	2.6
1	C	398	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	43	GLN	2.6
3	G	194	PHE	2.6
1	M	506	PHE	2.6
5	S	44	TYR	2.6
1	K	480	GLU	2.6
2	N	210	GLU	2.6
1	A	489	GLY	2.6
1	K	389	ALA	2.6
4	H	17	PRO	2.6
4	R	54	PRO	2.6
2	E	395	GLU	2.6
1	K	496	LEU	2.6
1	B	466	PHE	2.6
2	E	42	PRO	2.6
2	O	9	ILE	2.6
2	E	301	LYS	2.6
4	R	23	SER	2.6
3	G	49	GLN	2.5
2	P	210	GLU	2.5
1	B	473	TYR	2.5
1	K	448	TYR	2.5
4	R	14	PHE	2.5
4	R	91	PHE	2.5
2	O	28	SER	2.5
4	R	11	LYS	2.5
1	B	482	LEU	2.5
1	C	495	LEU	2.5
1	K	405	PHE	2.5
4	R	88	ILE	2.5
4	R	79	PRO	2.5
4	R	131	GLU	2.5
2	P	391	LEU	2.5
4	R	113	SER	2.5
4	H	60	MET	2.5
1	C	503	THR	2.5
1	M	404	ALA	2.5
2	O	475	ALA	2.5
3	Q	240	ALA	2.5
4	R	80	ASP	2.5
3	G	3	LEU	2.5
4	H	83	LEU	2.5
2	N	468	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	455	HIS	2.4
1	K	499	LEU	2.4
4	R	77	VAL	2.4
4	H	81	SER	2.4
2	P	424	PHE	2.4
3	G	56	GLU	2.4
1	B	421	VAL	2.4
2	E	302	GLY	2.4
4	H	86	THR	2.4
1	C	474	LEU	2.4
4	H	137	LEU	2.4
3	G	44	MET	2.4
4	R	132	ASN	2.4
2	D	468	ALA	2.4
1	A	480	GLU	2.4
4	H	50	GLU	2.4
1	C	476	SER	2.4
4	H	129	VAL	2.4
5	S	5	LYS	2.4
2	D	29	GLU	2.4
1	C	502	ALA	2.4
3	Q	196	LYS	2.4
1	K	472	SER	2.4
1	M	491	LEU	2.4
2	E	244	ARG	2.4
1	C	421	VAL	2.4
2	D	27	GLN	2.4
3	G	235	ASN	2.4
4	H	88	ILE	2.4
2	D	436	ASP	2.4
2	E	405	GLU	2.4
2	P	212	GLU	2.4
2	E	344	ILE	2.4
2	E	453	PRO	2.4
2	O	380	THR	2.4
2	O	399	GLN	2.4
3	G	57	THR	2.4
2	E	212	GLU	2.4
2	O	398	GLU	2.4
2	N	112	LYS	2.3
2	O	210	GLU	2.3
4	H	65	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	180	VAL	2.3
2	P	26	GLU	2.3
1	M	488	LYS	2.3
1	B	415	SER	2.3
1	B	89	LEU	2.3
1	M	400	ARG	2.3
2	N	44	GLY	2.3
1	K	462	ARG	2.3
2	F	210	GLU	2.3
3	Q	150	LEU	2.3
1	K	408	PHE	2.3
3	G	54	ASN	2.3
1	C	480	GLU	2.3
4	H	71	SER	2.3
4	H	67	LYS	2.3
4	R	130	LEU	2.3
1	A	492	SER	2.3
2	F	474	ALA	2.3
4	R	67	LYS	2.3
4	H	31	ASN	2.3
2	D	462	GLY	2.3
3	Q	74	ILE	2.3
2	P	386	ASP	2.3
1	A	460	LEU	2.3
2	N	209	LEU	2.3
2	N	448	LYS	2.2
4	H	69	PHE	2.2
2	D	471	GLU	2.2
2	N	180	GLY	2.2
1	C	373	VAL	2.2
1	M	507	VAL	2.2
1	C	487	GLU	2.2
1	B	449	ALA	2.2
4	H	70	ILE	2.2
5	S	43	PHE	2.2
6	J	34	LYS	2.2
1	K	471	LEU	2.2
1	M	321	GLY	2.2
2	D	452	ILE	2.2
2	P	474	ALA	2.2
4	R	121	ALA	2.2
2	E	341	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	179	GLY	2.2
2	E	458	TYR	2.2
3	Q	4	LYS	2.2
1	M	421	VAL	2.2
2	P	455	HIS	2.2
3	Q	183	PHE	2.2
1	A	475	LYS	2.2
1	M	493	LYS	2.2
4	R	64	ASN	2.2
1	A	198	SER	2.2
2	E	246	GLU	2.2
2	F	26	GLU	2.2
4	R	29	GLN	2.2
1	C	493	LYS	2.2
2	O	463	ILE	2.2
3	Q	198	GLU	2.2
2	E	423	VAL	2.2
4	R	123	ALA	2.2
2	O	452	ILE	2.2
1	M	455	LEU	2.2
4	H	105	LEU	2.2
5	S	29	LEU	2.2
1	C	504	GLU	2.2
4	R	50	GLU	2.2
2	D	472	LYS	2.1
1	B	400	ARG	2.1
2	E	464	GLU	2.1
3	Q	179	GLU	2.1
1	C	396	LEU	2.1
1	K	493	LYS	2.1
2	P	451	ASN	2.1
3	Q	235	ASN	2.1
3	G	4	LYS	2.1
1	A	314	LEU	2.1
3	Q	3	LEU	2.1
1	C	452	ASN	2.1
3	G	198	GLU	2.1
2	O	112	LYS	2.1
3	Q	42	LYS	2.1
1	M	499	LEU	2.1
2	O	209	LEU	2.1
3	G	191	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	33	LYS	2.1
1	C	388	VAL	2.1
2	D	474	ALA	2.1
2	E	404	VAL	2.1
2	N	456	ALA	2.1
2	O	453	PRO	2.1
3	Q	201	THR	2.1
5	S	25	LEU	2.1
2	N	40	LYS	2.1
6	T	1	SER	2.1
2	E	187	VAL	2.1
5	S	53	ALA	2.1
1	A	498	SER	2.1
1	K	498	SER	2.1
4	H	104	LEU	2.1
2	O	341	GLU	2.1
1	B	475	LYS	2.1
3	Q	52	TYR	2.1
2	D	44	GLY	2.1
2	P	176	LYS	2.1
4	H	102	LYS	2.1
2	E	98	VAL	2.0
2	E	218	VAL	2.0
1	M	360	TYR	2.0
1	A	491	LEU	2.0
1	K	398	GLN	2.0
2	P	29	GLU	2.0
2	P	390	ILE	2.0
3	G	59	ASN	2.0
3	G	173	LEU	2.0
2	O	408	ARG	2.0
3	Q	44	MET	2.0
2	O	446	GLU	2.0
1	B	471	LEU	2.0
1	M	412	LEU	2.0
2	F	431	LEU	2.0
1	M	487	GLU	2.0
6	T	34	LYS	2.0
1	K	469	SER	2.0
1	M	362	GLY	2.0
3	Q	207	ARG	2.0
1	M	396	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	384	LEU	2.0
3	Q	31	LEU	2.0
4	R	53	LEU	2.0
1	A	353	PHE	2.0
1	A	487	GLU	2.0
5	I	39	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

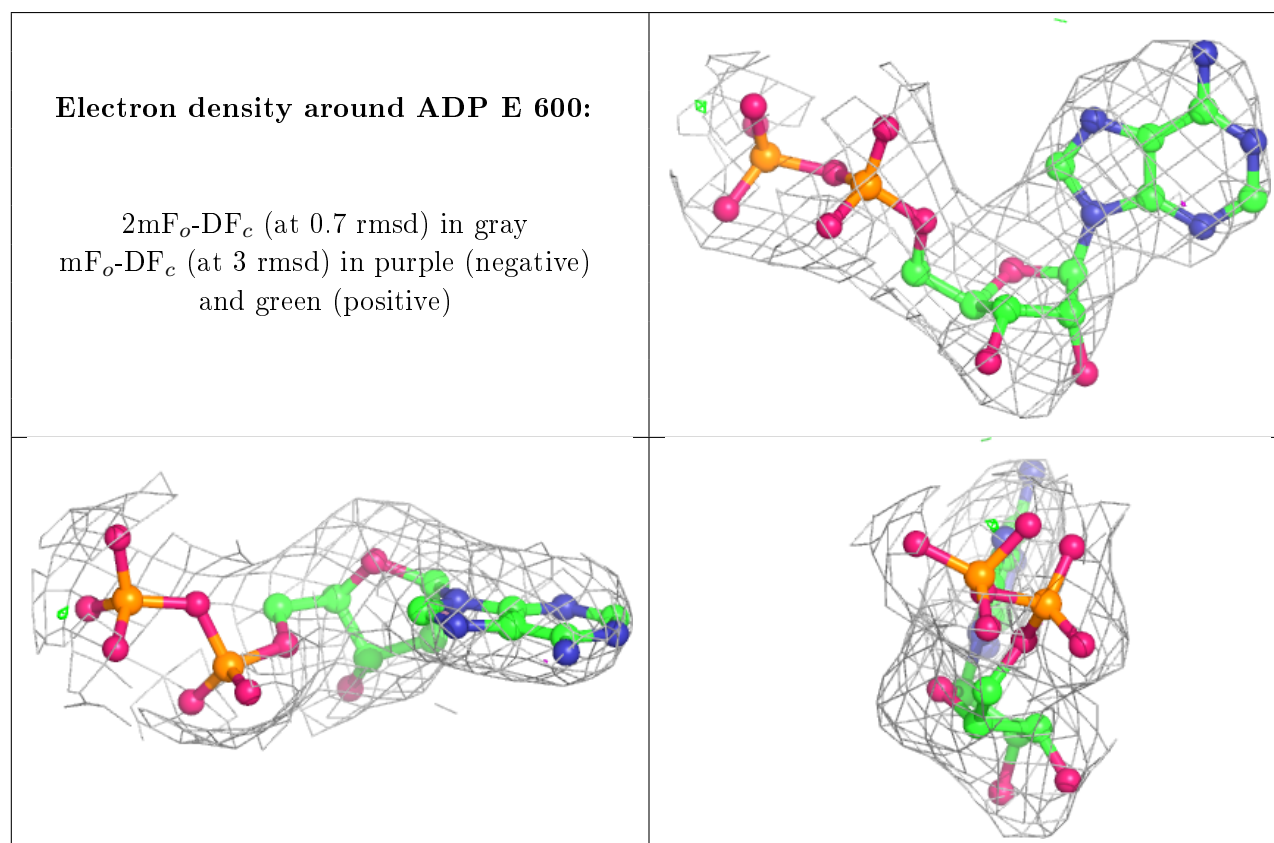
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	EDO	O	602	4/4	0.85	0.29	46,47,49,53	0
10	EDO	L	604	4/4	0.86	0.26	46,47,51,51	0
9	ADP	E	600	27/27	0.89	0.15	86,90,92,93	0
10	EDO	P	603	4/4	0.90	0.18	31,42,47,50	0
9	ADP	O	600	27/27	0.90	0.17	74,90,91,92	0
8	MG	A	601	1/1	0.92	0.18	50,50,50,50	0
8	MG	L	601	1/1	0.92	0.19	24,24,24,24	0
8	MG	B	601	1/1	0.93	0.15	40,40,40,40	0
8	MG	K	601	1/1	0.94	0.19	45,45,45,45	0
8	MG	P	601	1/1	0.95	0.22	25,25,25,25	0
9	ADP	M	600	27/27	0.96	0.13	36,65,72,73	0
9	ADP	N	600	27/27	0.96	0.15	37,46,55,57	0
9	ADP	C	600	27/27	0.96	0.16	28,53,65,65	0
10	EDO	L	602	4/4	0.96	0.12	28,28,31,32	0
7	ATP	A	600	31/31	0.96	0.16	45,53,57,58	4
7	ATP	K	600	31/31	0.96	0.19	38,54,59,60	4
10	EDO	C	603	4/4	0.97	0.20	33,35,36,39	0

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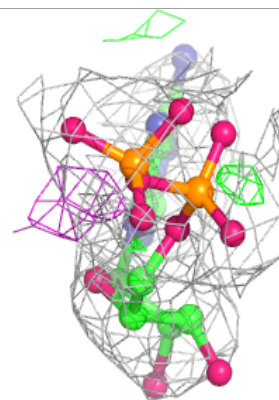
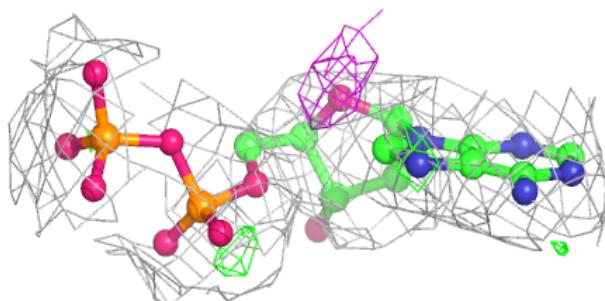
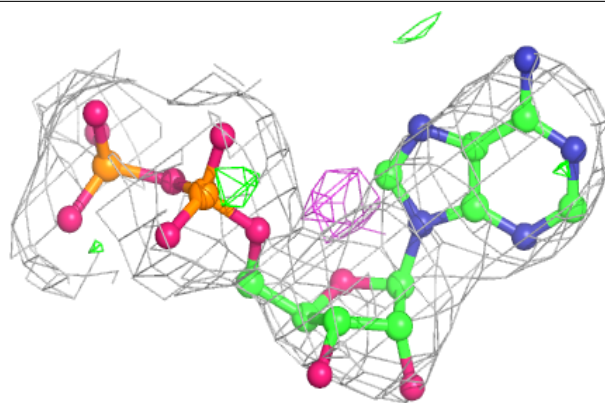
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	ADP	B	600	27/27	0.97	0.14	29,48,55,57	0
9	ADP	D	600	27/27	0.98	0.16	33,46,55,58	0
8	MG	F	601	1/1	0.98	0.20	24,24,24,24	0
8	MG	C	601	1/1	0.98	0.15	27,27,27,27	0
8	MG	M	601	1/1	0.98	0.15	34,34,34,34	0
8	MG	D	601	1/1	0.98	0.18	35,35,35,35	0
9	ADP	L	600	27/27	0.98	0.14	18,32,41,43	0
10	EDO	M	602	4/4	0.98	0.20	32,39,42,45	0
9	ADP	F	600	27/27	0.98	0.17	24,29,32,39	0
9	ADP	P	600	27/27	0.99	0.16	22,33,36,41	0
8	MG	N	601	1/1	0.99	0.15	40,40,40,40	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.

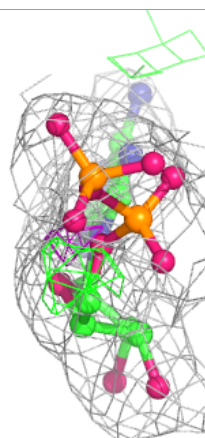
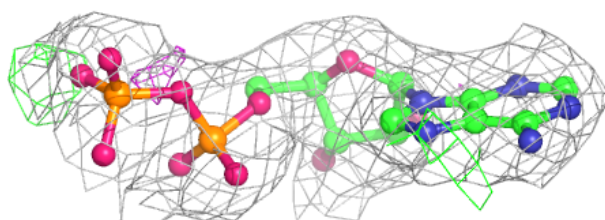
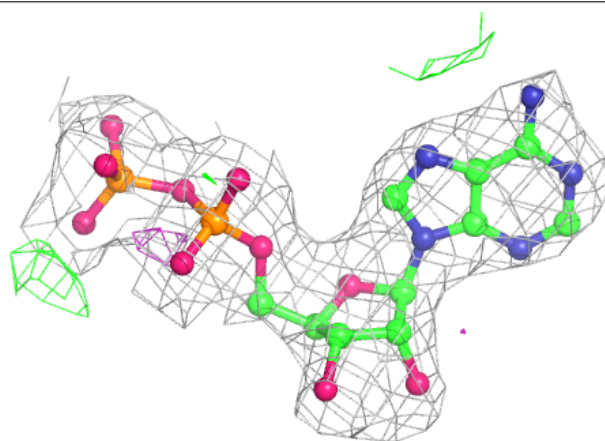


Electron density around ADP O 600:

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

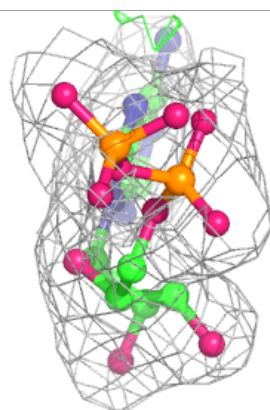
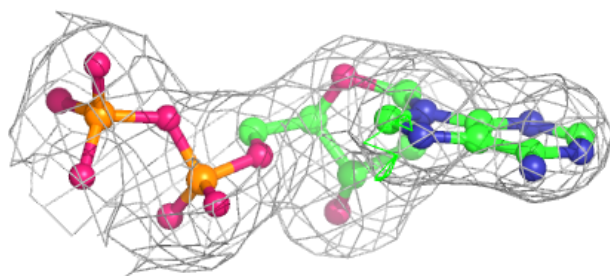
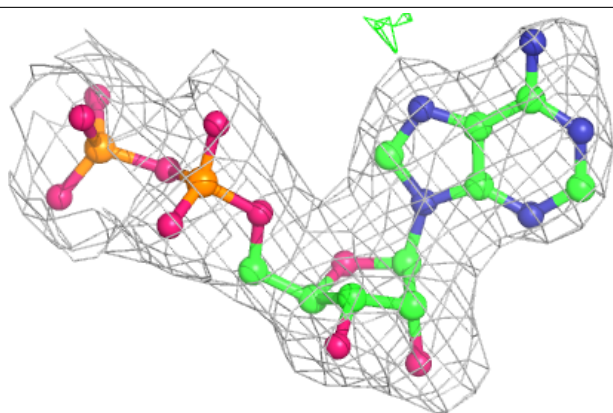
**Electron density around ADP M 600:**

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

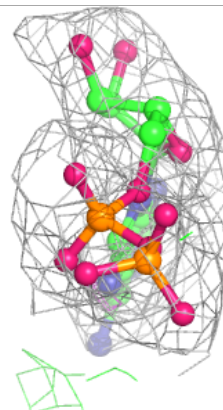
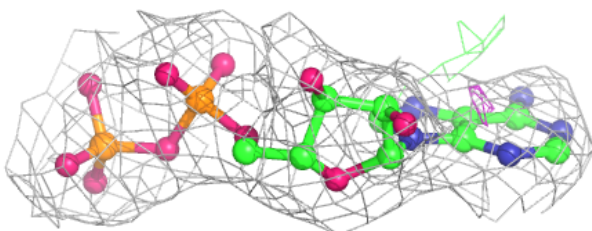
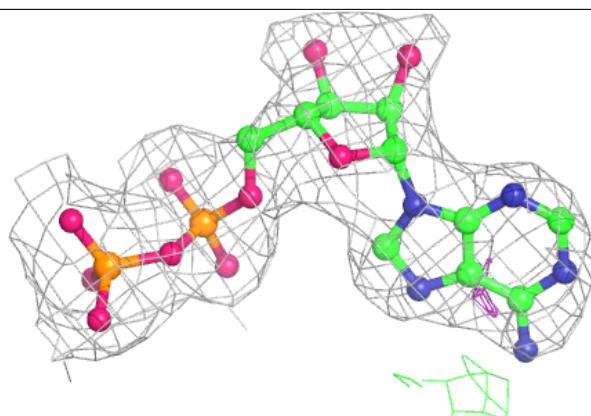


Electron density around ADP N 600:

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

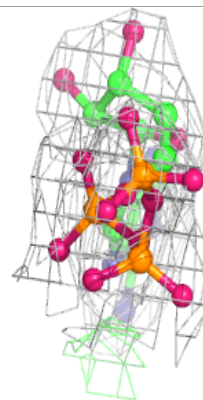
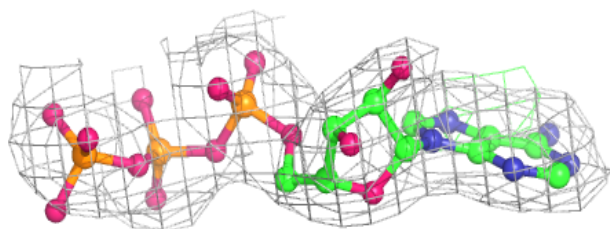
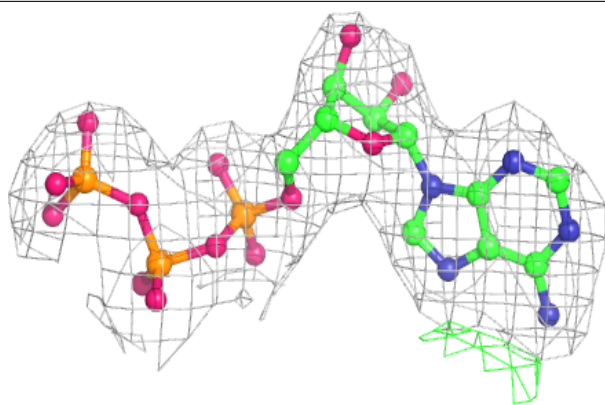
**Electron density around ADP C 600:**

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

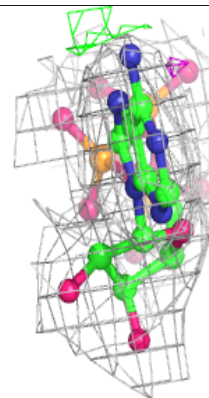
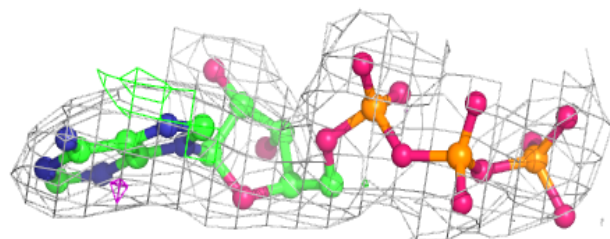
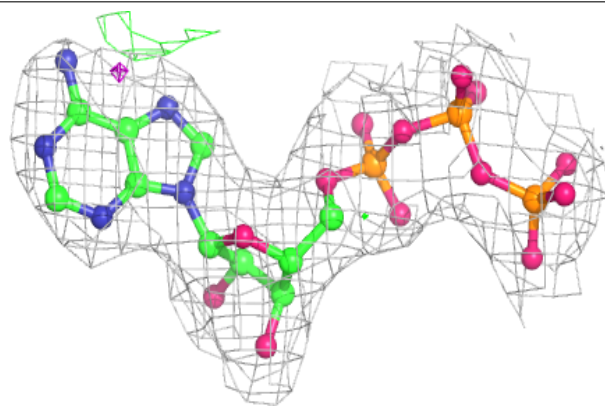


Electron density around ATP A 600:

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

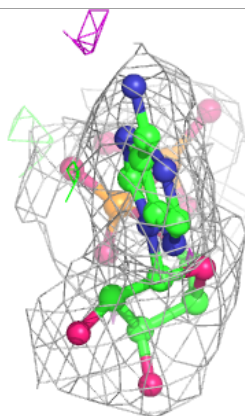
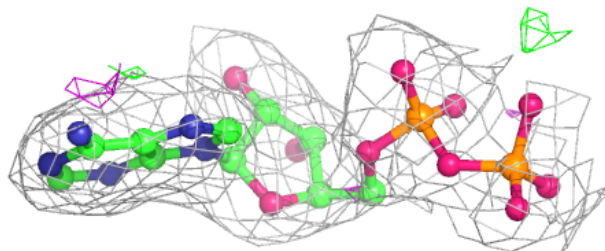
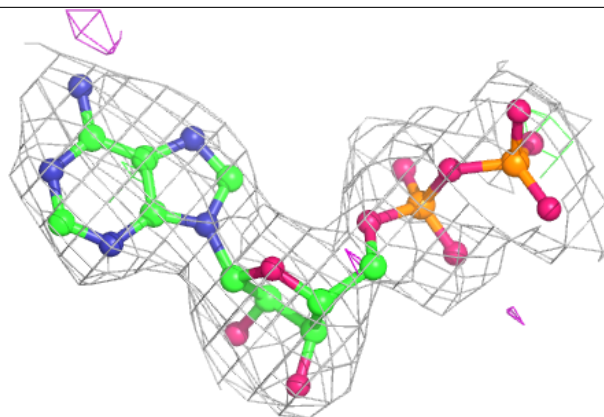
**Electron density around ATP K 600:**

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

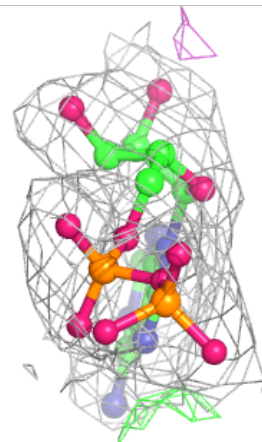
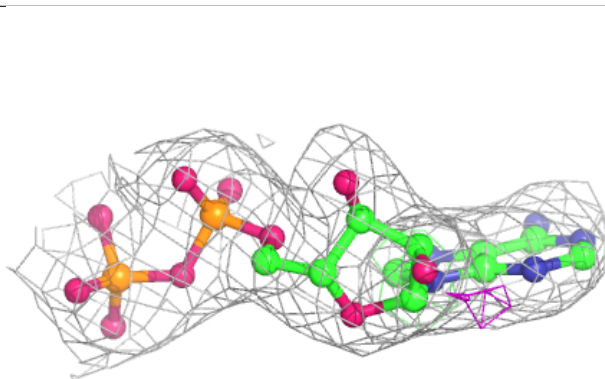
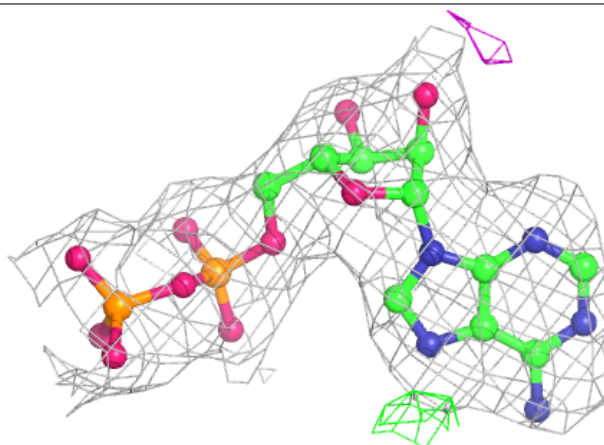


Electron density around ADP B 600:

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

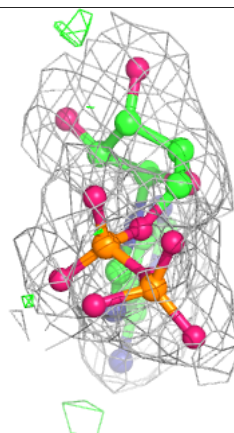
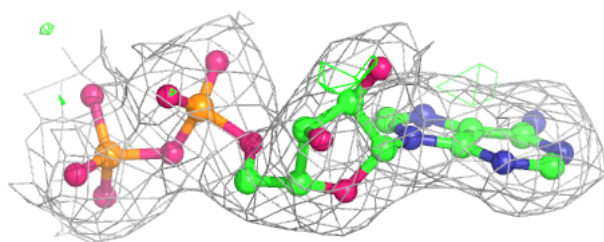
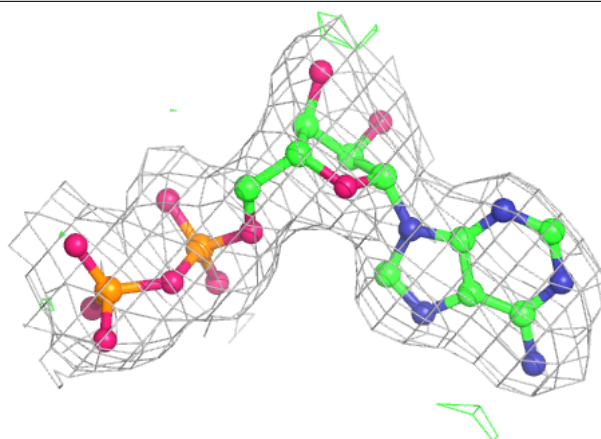
**Electron density around ADP D 600:**

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



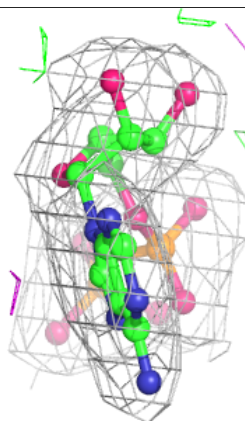
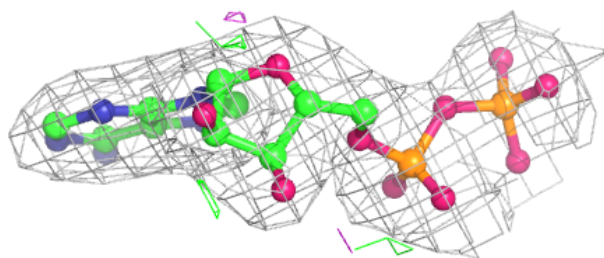
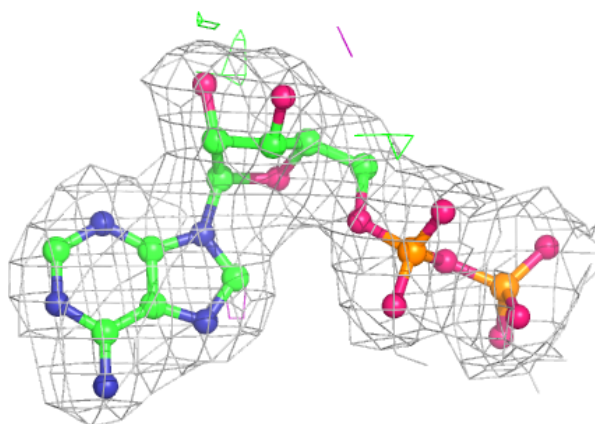
Electron density around ADP L 600:

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

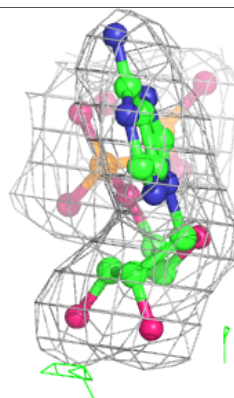
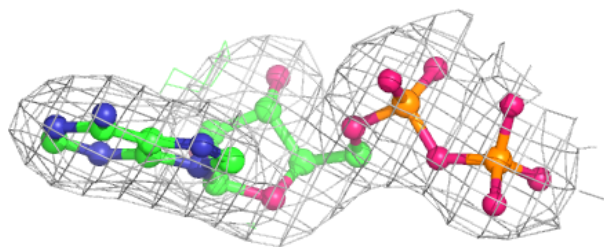
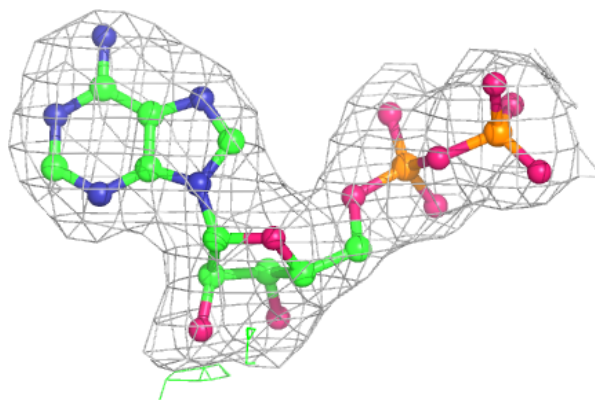


Electron density around ADP F 600:

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

**Electron density around ADP P 600:**

$2mF_o - DF_c$ (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.