



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:41 PM BST

PDB ID : 6TMU
Title : Crystal structure of the chaperonin gp146 from the bacteriophage EL 2 (Pseudomonas aeruginosa) in presence of ATP-BeFx, crystal form II
Authors : Bracher, A.; Paul, S.S.; Wang, H.; Wischnewski, N.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on : 2019-12-05
Resolution : 3.54 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	:	2.13
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)	:	2.13

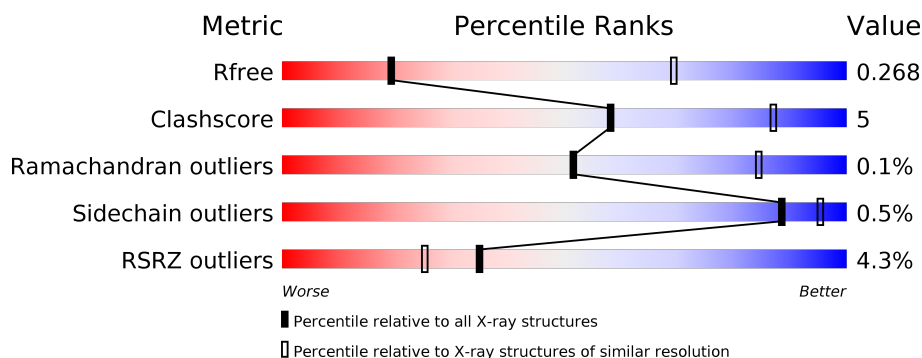
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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.



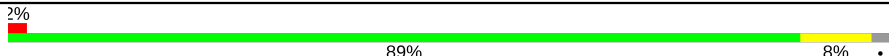
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	558	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>
1	B	558	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>
1	C	558	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	D	558	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	E	558	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	F	558	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	558	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	B	600	-	-	-	X
5	ADP	F	600	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 29306 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 Putative GroEL-like chaperonine protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4179	2620	729	819	11			
1	B	545	Total	C	N	O	S	0	0	0
			4149	2597	723	818	11			
1	C	550	Total	C	N	O	S	0	0	0
			4161	2605	726	819	11			
1	D	545	Total	C	N	O	S	0	0	0
			4157	2601	724	821	11			
1	E	549	Total	C	N	O	S	0	0	0
			4166	2610	726	819	11			
1	F	544	Total	C	N	O	S	0	0	0
			4134	2589	719	815	11			
1	G	545	Total	C	N	O	S	0	0	0
			4147	2598	722	816	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

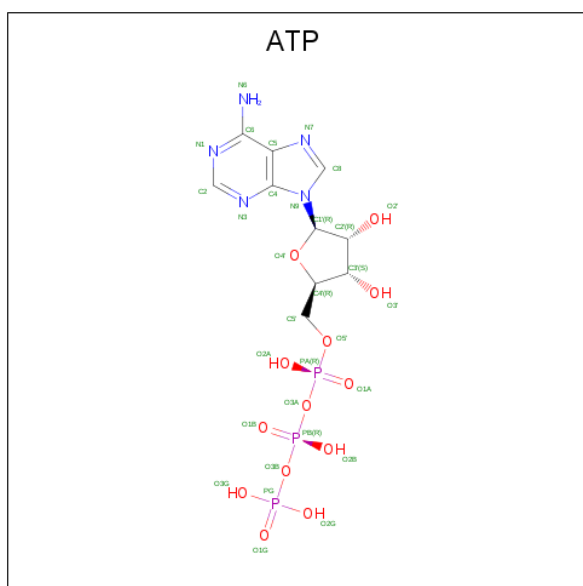
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		

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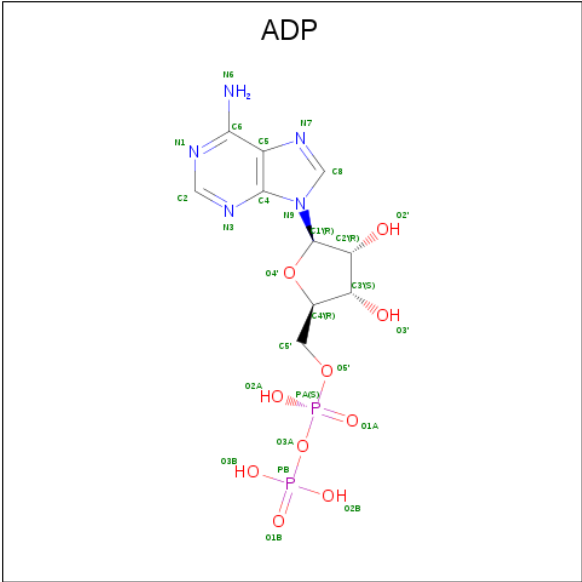
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

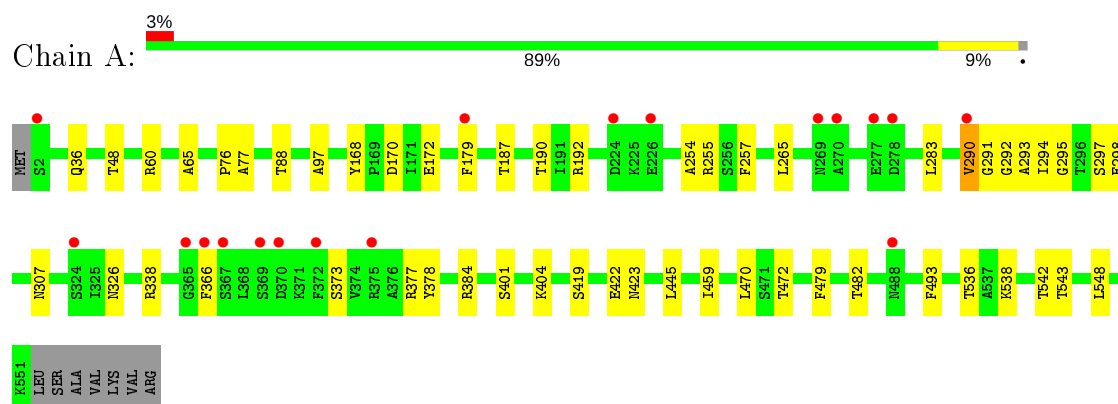


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

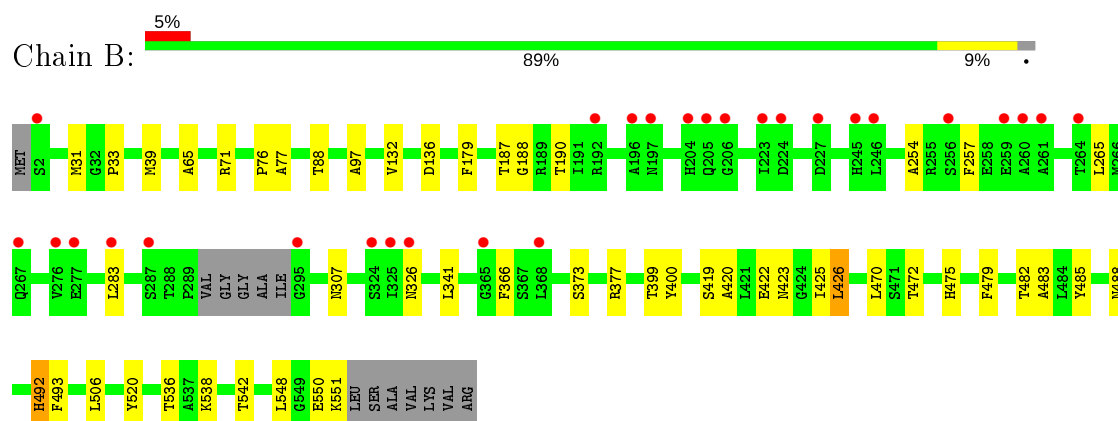
3 Residue-property plots [i](#)

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

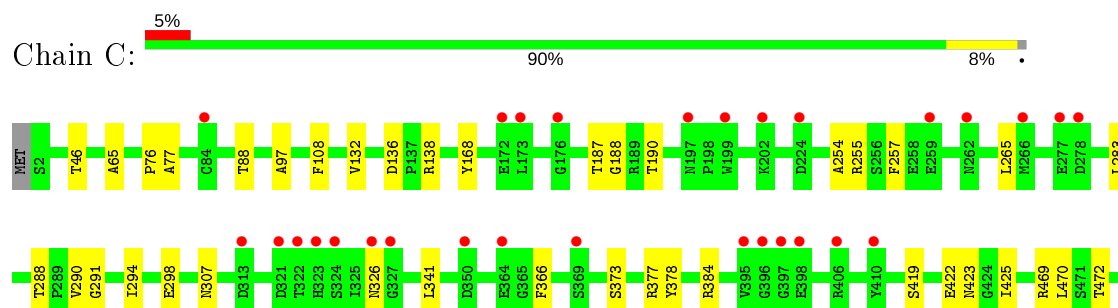
- Molecule 1: Putative GroEL-like chaperonine protein



- Molecule 1: Putative GroEL-like chaperonine protein

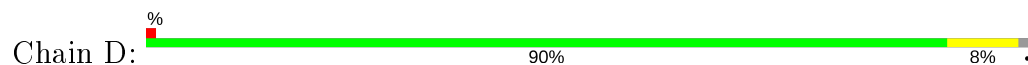


- Molecule 1: Putative GroEL-like chaperonine protein

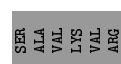
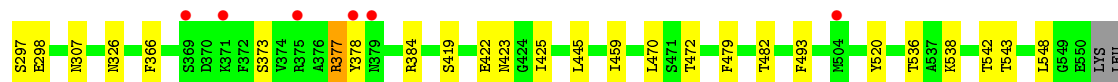
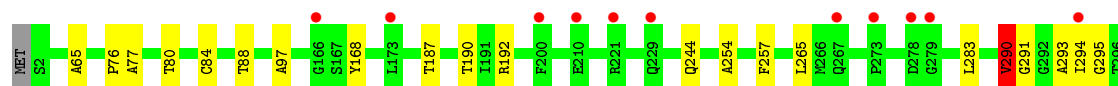
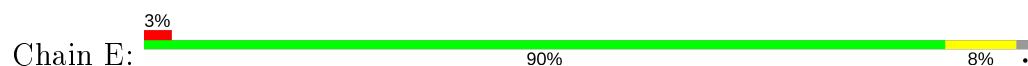




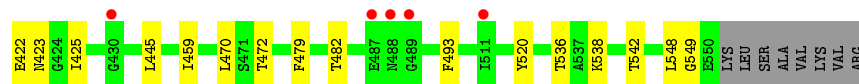
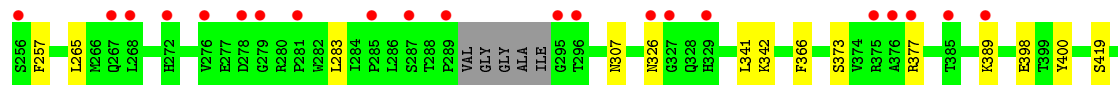
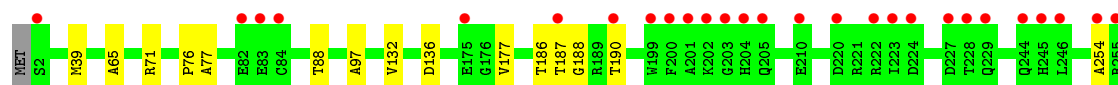
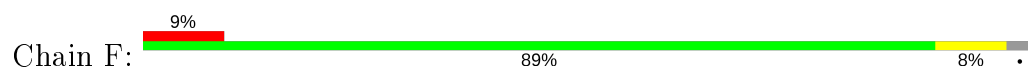
- Molecule 1: Putative GroEL-like chaperonine protein



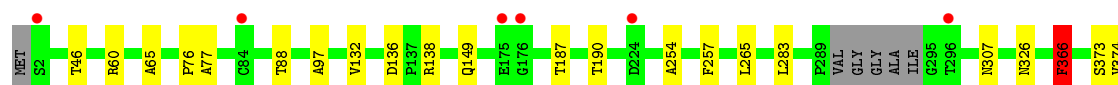
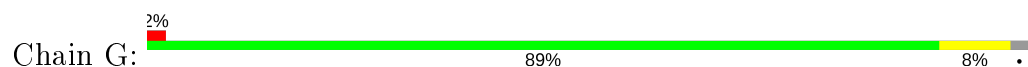
- Molecule 1: Putative GroEL-like chaperonine protein

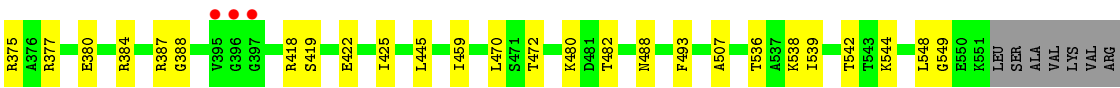


- Molecule 1: Putative GroEL-like chaperonine protein



- Molecule 1: Putative GroEL-like chaperonine protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.52Å 151.46Å 261.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.54 30.00 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.54) 99.7 (30.00-3.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.56Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.250 , 0.275 0.242 , 0.268	Depositor DCC
R_{free} test set	3576 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	130.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 98.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29306	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/4245	0.51	0/5765
1	B	0.33	1/4213 (0.0%)	0.53	1/5721 (0.0%)
1	C	0.30	0/4226	0.50	0/5744
1	D	0.30	0/4221	0.53	1/5731 (0.0%)
1	E	0.29	0/4232	0.51	1/5751 (0.0%)
1	F	0.30	0/4199	0.49	0/5706
1	G	0.33	1/4212 (0.0%)	0.53	2/5721 (0.0%)
All	All	0.31	2/29548 (0.0%)	0.52	5/40139 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	388	GLY	N-CA	-6.17	1.36	1.46
1	B	483	ALA	C-N	5.28	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	548	LEU	CA-CB-CG	10.42	139.26	115.30
1	B	426	LEU	CA-CB-CG	7.84	133.34	115.30
1	G	387	ARG	C-N-CA	-7.15	107.28	122.30
1	G	366	PHE	CB-CG-CD2	-5.79	116.74	120.80
1	E	377	ARG	NE-CZ-NH2	-5.15	117.73	120.30

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	4179	0	4102	59	0
1	B	4149	0	4060	45	0
1	C	4161	0	4062	44	1
1	D	4157	0	4070	36	0
1	E	4166	0	4073	44	1
1	F	4134	0	4028	34	0
1	G	4147	0	4052	37	2
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
4	E	31	0	12	0	0
4	G	31	0	12	0	0
5	B	27	0	12	0	0
5	D	27	0	12	0	0
5	F	27	0	12	0	0
All	All	29306	0	28531	275	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (275) 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:E:192:ARG:NH1	1:E:298:GLU:OE2	1.67	1.25
1:C:290:VAL:HG22	1:C:298:GLU:OE2	1.61	1.01
1:A:377:ARG:NH2	1:A:422:GLU:O	2.04	0.91
1:E:192:ARG:NH1	1:E:298:GLU:CD	2.27	0.88
1:E:290:VAL:CG1	1:E:295:GLY:HA2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HB3	1:B:179:PHE:CE1	2.14	0.83
1:C:377:ARG:NH2	1:C:422:GLU:O	2.12	0.82
1:E:377:ARG:NH2	1:E:422:GLU:O	2.13	0.82
1:E:290:VAL:HG12	1:E:295:GLY:HA2	1.62	0.80
1:B:420:ALA:HB1	1:B:425:ILE:HD11	1.65	0.78
1:D:132:VAL:HG21	1:D:425:ILE:HD12	1.66	0.77
1:A:290:VAL:HB	1:A:295:GLY:HA2	1.66	0.77
1:A:290:VAL:HG12	1:A:298:GLU:OE1	1.84	0.76
1:E:290:VAL:HG13	1:E:298:GLU:OE1	1.86	0.75
1:F:132:VAL:HG21	1:F:425:ILE:HD12	1.67	0.75
1:A:255:ARG:CD	1:A:290:VAL:HG23	2.19	0.73
1:E:168:TYR:CD1	1:E:384:ARG:HG2	2.22	0.73
1:C:255:ARG:CD	1:C:290:VAL:HB	2.19	0.72
1:B:479:PHE:O	1:B:485:TYR:CD1	2.42	0.72
1:E:294:ILE:HG23	1:E:378:TYR:CE2	2.25	0.72
1:C:168:TYR:CD1	1:C:384:ARG:HG2	2.25	0.71
1:C:255:ARG:HD3	1:C:290:VAL:HB	1.72	0.70
1:E:290:VAL:HG11	1:E:295:GLY:HA2	1.74	0.69
1:B:488:ASN:OD1	1:B:492:HIS:HB3	1.93	0.69
1:A:290:VAL:HB	1:A:295:GLY:CA	2.22	0.69
1:F:549:GLY:HA3	1:G:60:ARG:HD2	1.73	0.68
1:F:265:LEU:HD22	1:F:283:LEU:HD21	1.76	0.68
1:B:265:LEU:HD22	1:B:283:LEU:HD21	1.76	0.67
1:E:265:LEU:HD22	1:E:283:LEU:HD21	1.76	0.67
1:A:192:ARG:HH11	1:A:298:GLU:CD	1.97	0.67
1:G:265:LEU:HD22	1:G:283:LEU:HD21	1.76	0.67
1:A:265:LEU:HD22	1:A:283:LEU:HD21	1.76	0.67
1:A:172:GLU:OE2	1:A:338:ARG:NH2	2.26	0.67
1:D:265:LEU:HD22	1:D:283:LEU:HD21	1.76	0.66
1:G:380:GLU:OE1	1:G:422:GLU:HG3	1.95	0.66
1:C:265:LEU:HD22	1:C:283:LEU:HD21	1.76	0.66
1:A:255:ARG:HD3	1:A:290:VAL:HG23	1.76	0.65
1:B:33:PRO:HD3	1:B:506:LEU:HD13	1.79	0.65
1:D:33:PRO:HD3	1:D:506:LEU:HD13	1.79	0.64
1:E:298:GLU:HG3	1:E:378:TYR:OH	1.98	0.63
1:G:366:PHE:CZ	1:G:375:ARG:HD3	2.34	0.62
1:A:170:ASP:OD2	1:A:190:THR:HB	2.00	0.62
1:G:366:PHE:HZ	1:G:375:ARG:HD3	1.65	0.61
1:B:488:ASN:CG	1:B:492:HIS:HB3	2.22	0.60
1:A:192:ARG:CD	1:A:298:GLU:OE2	2.50	0.60
1:B:475:HIS:HD2	1:B:485:TYR:OH	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:PHE:O	1:C:482:THR:HG22	2.02	0.60
1:E:479:PHE:O	1:E:482:THR:HG22	2.02	0.59
1:A:479:PHE:O	1:A:482:THR:HG22	2.02	0.59
1:E:192:ARG:HH11	1:E:298:GLU:CD	2.03	0.59
1:F:479:PHE:O	1:F:482:THR:HG22	2.02	0.59
1:D:479:PHE:O	1:D:482:THR:HG22	2.02	0.59
1:B:420:ALA:CB	1:B:425:ILE:HD11	2.31	0.59
1:B:479:PHE:O	1:B:482:THR:HG22	2.02	0.59
1:F:132:VAL:CG2	1:F:425:ILE:HD12	2.31	0.59
1:D:132:VAL:CG2	1:D:425:ILE:HD12	2.32	0.59
1:C:294:ILE:HG23	1:C:378:TYR:CE2	2.39	0.57
1:B:492:HIS:CG	1:B:492:HIS:O	2.54	0.57
1:A:179:PHE:CE2	1:G:375:ARG:HA	2.41	0.56
1:A:255:ARG:HD3	1:A:290:VAL:CG2	2.35	0.56
1:G:77:ALA:HB1	1:G:88:THR:HB	1.88	0.56
1:A:192:ARG:HD3	1:A:298:GLU:OE2	2.06	0.56
1:A:77:ALA:HB1	1:A:88:THR:HB	1.88	0.56
1:C:290:VAL:CG2	1:C:298:GLU:OE2	2.47	0.55
1:C:108:PHE:HZ	1:D:36:GLN:HE22	1.50	0.55
1:C:255:ARG:HD2	1:C:290:VAL:HB	1.88	0.55
1:C:77:ALA:HB1	1:C:88:THR:HB	1.89	0.55
1:A:293:ALA:CB	1:B:179:PHE:CE1	2.87	0.54
1:A:48:THR:HG21	1:G:539:ILE:HG23	1.89	0.54
1:F:77:ALA:HB1	1:F:88:THR:HB	1.89	0.54
1:D:550:GLU:O	1:D:551:LYS:HB2	2.08	0.54
1:E:77:ALA:HB1	1:E:88:THR:HB	1.89	0.54
1:B:550:GLU:O	1:B:551:LYS:HB2	2.07	0.53
1:B:77:ALA:HB1	1:B:88:THR:HB	1.89	0.53
1:E:291:GLY:HA3	1:F:400:TYR:HD2	1.73	0.53
1:A:291:GLY:HA3	1:B:400:TYR:HD2	1.74	0.53
1:A:172:GLU:CG	1:A:338:ARG:HH22	2.20	0.53
1:D:77:ALA:HB1	1:D:88:THR:HB	1.89	0.53
1:C:187:THR:O	1:C:187:THR:HG22	2.09	0.53
1:F:377:ARG:NH2	1:F:423:ASN:OD1	2.29	0.52
1:D:377:ARG:NH2	1:D:423:ASN:OD1	2.30	0.52
1:C:543:THR:HG21	1:D:39:MET:HE3	1.91	0.52
1:A:172:GLU:HG2	1:A:338:ARG:HH22	1.74	0.52
1:C:294:ILE:HB	1:D:398:GLU:O	2.10	0.52
1:E:373:SER:O	1:E:377:ARG:HG3	2.10	0.52
1:G:187:THR:HG22	1:G:187:THR:O	2.10	0.52
1:C:290:VAL:HG12	1:C:291:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:SER:O	1:C:377:ARG:HG3	2.10	0.51
1:A:294:ILE:HG23	1:A:378:TYR:CZ	2.45	0.51
1:C:543:THR:HG21	1:D:39:MET:CE	2.39	0.51
1:F:187:THR:HG22	1:F:187:THR:O	2.11	0.51
1:E:294:ILE:HG23	1:E:378:TYR:CZ	2.45	0.51
1:A:172:GLU:CD	1:A:338:ARG:HH22	2.13	0.51
1:C:108:PHE:CZ	1:D:36:GLN:NE2	2.79	0.51
1:G:384:ARG:NH1	1:G:422:GLU:OE1	2.43	0.51
1:A:60:ARG:HB2	1:G:549:GLY:HA3	1.92	0.51
1:A:168:TYR:CD1	1:A:384:ARG:HG2	2.45	0.51
1:B:187:THR:O	1:B:187:THR:HG22	2.11	0.51
1:E:290:VAL:HG12	1:E:295:GLY:CA	2.37	0.51
1:A:168:TYR:CG	1:A:384:ARG:HD2	2.46	0.51
1:B:33:PRO:HD3	1:B:506:LEU:CD1	2.40	0.51
1:E:187:THR:HG22	1:E:187:THR:O	2.10	0.51
1:A:192:ARG:HD2	1:A:298:GLU:OE2	2.11	0.50
1:E:290:VAL:CG1	1:E:295:GLY:CA	2.85	0.50
1:A:290:VAL:HG11	1:A:298:GLU:HB3	1.93	0.50
1:F:265:LEU:HD22	1:F:283:LEU:CD2	2.41	0.50
1:A:543:THR:HG21	1:B:39:MET:CE	2.41	0.50
1:D:187:THR:O	1:D:187:THR:HG22	2.11	0.50
1:C:265:LEU:HD22	1:C:283:LEU:CD2	2.41	0.50
1:A:187:THR:HG22	1:A:187:THR:O	2.11	0.50
1:D:33:PRO:HD3	1:D:506:LEU:CD1	2.40	0.50
1:B:265:LEU:HD22	1:B:283:LEU:CD2	2.41	0.50
1:G:373:SER:O	1:G:377:ARG:HG3	2.12	0.50
1:A:265:LEU:HD22	1:A:283:LEU:CD2	2.42	0.50
1:D:373:SER:O	1:D:377:ARG:HG3	2.12	0.50
1:E:294:ILE:HD12	1:F:398:GLU:O	2.12	0.50
1:C:377:ARG:HH21	1:C:423:ASN:HA	1.77	0.49
1:F:373:SER:O	1:F:377:ARG:HG3	2.12	0.49
1:A:190:THR:HG23	1:A:190:THR:O	2.13	0.49
1:B:373:SER:O	1:B:377:ARG:HG3	2.12	0.49
1:F:71:ARG:NH1	1:G:46:THR:OG1	2.43	0.49
1:B:377:ARG:NH2	1:B:423:ASN:OD1	2.29	0.49
1:G:132:VAL:HG13	1:G:136:ASP:CB	2.42	0.49
1:D:132:VAL:HG13	1:D:136:ASP:CB	2.42	0.49
1:A:290:VAL:HG12	1:A:298:GLU:CD	2.34	0.48
1:E:265:LEU:HD22	1:E:283:LEU:CD2	2.41	0.48
1:A:292:GLY:HA3	1:B:399:THR:O	2.13	0.48
1:F:190:THR:HG23	1:F:190:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH1	1:A:298:GLU:CD	2.65	0.48
1:F:132:VAL:HG13	1:F:136:ASP:CB	2.43	0.48
1:B:132:VAL:HG13	1:B:136:ASP:CB	2.43	0.48
1:G:265:LEU:HD22	1:G:283:LEU:CD2	2.41	0.48
1:C:132:VAL:HG13	1:C:136:ASP:CB	2.43	0.48
1:C:190:THR:HG23	1:C:190:THR:O	2.14	0.48
1:G:190:THR:O	1:G:190:THR:HG23	2.14	0.48
1:A:172:GLU:HG2	1:A:338:ARG:NH2	2.29	0.47
1:A:290:VAL:HG23	1:A:291:GLY:H	1.79	0.47
1:G:384:ARG:NH1	1:G:418:ARG:HG2	2.29	0.47
1:D:76:PRO:HG2	1:D:536:THR:HG21	1.96	0.47
1:G:76:PRO:HG2	1:G:536:THR:HG21	1.96	0.47
1:A:373:SER:O	1:A:377:ARG:HG3	2.14	0.47
1:B:76:PRO:HG2	1:B:536:THR:HG21	1.96	0.47
1:E:293:ALA:HA	1:F:177:VAL:O	2.14	0.47
1:F:188:GLY:O	1:F:389:LYS:HA	2.15	0.47
1:G:472:THR:HG23	1:G:493:PHE:CE1	2.49	0.47
1:B:190:THR:HG23	1:B:190:THR:O	2.15	0.47
1:C:419:SER:HA	1:C:422:GLU:HB3	1.97	0.47
1:F:188:GLY:HA2	1:F:341:LEU:O	2.15	0.47
1:A:36:GLN:OE1	1:G:544:LYS:HG3	2.15	0.47
1:D:265:LEU:HD22	1:D:283:LEU:CD2	2.41	0.47
1:B:425:ILE:CG2	1:B:520:TYR:CD1	2.98	0.47
1:E:377:ARG:HH21	1:E:423:ASN:HA	1.80	0.47
1:E:190:THR:O	1:E:190:THR:HG23	2.14	0.47
1:G:419:SER:HA	1:G:422:GLU:HB3	1.97	0.47
1:G:480:LYS:O	1:G:482:THR:HG23	2.15	0.47
1:G:149:GLN:HG3	1:G:507:ALA:HB2	1.97	0.47
1:E:76:PRO:HG2	1:E:536:THR:HG21	1.97	0.46
1:C:472:THR:HG23	1:C:493:PHE:CE1	2.50	0.46
1:A:76:PRO:CG	1:A:536:THR:HG21	2.46	0.46
1:C:76:PRO:HG2	1:C:536:THR:HG21	1.97	0.46
1:D:190:THR:O	1:D:190:THR:HG23	2.16	0.46
1:B:538:LYS:O	1:B:542:THR:HG22	2.16	0.46
1:E:377:ARG:NH2	1:E:423:ASN:OD1	2.49	0.46
1:A:401:SER:HA	1:A:404:LYS:HG2	1.98	0.46
1:E:472:THR:HG23	1:E:493:PHE:CE1	2.50	0.46
1:F:76:PRO:HG2	1:F:536:THR:HG21	1.97	0.46
1:A:76:PRO:HG2	1:A:536:THR:HG21	1.96	0.46
1:A:543:THR:HG21	1:B:39:MET:HE3	1.97	0.46
1:C:538:LYS:O	1:C:542:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ALA:HB2	1:C:548:LEU:HD11	1.98	0.46
1:D:538:LYS:O	1:D:542:THR:HG22	2.15	0.46
1:F:472:THR:HG23	1:F:493:PHE:CE1	2.51	0.46
1:F:538:LYS:O	1:F:542:THR:HG22	2.16	0.46
1:G:472:THR:HG23	1:G:493:PHE:CZ	2.51	0.46
1:G:538:LYS:O	1:G:542:THR:HG22	2.16	0.46
1:D:472:THR:HG23	1:D:493:PHE:CE1	2.50	0.46
1:A:472:THR:HG23	1:A:493:PHE:CE1	2.50	0.45
1:A:65:ALA:HB2	1:A:548:LEU:HD11	1.98	0.45
1:E:419:SER:HA	1:E:422:GLU:HB3	1.97	0.45
1:F:186:THR:HG21	1:F:342:LYS:HE3	1.98	0.45
1:B:65:ALA:HB2	1:B:548:LEU:HD11	1.99	0.45
1:C:377:ARG:NH2	1:C:423:ASN:HA	2.31	0.45
1:D:76:PRO:CG	1:D:536:THR:HG21	2.47	0.45
1:F:419:SER:HA	1:F:422:GLU:HB3	1.98	0.45
1:G:76:PRO:CG	1:G:536:THR:HG21	2.46	0.45
1:D:472:THR:HG23	1:D:493:PHE:CZ	2.52	0.45
1:E:538:LYS:O	1:E:542:THR:HG22	2.16	0.45
1:E:76:PRO:CG	1:E:536:THR:HG21	2.46	0.45
1:A:472:THR:HG23	1:A:493:PHE:CZ	2.52	0.45
1:A:538:LYS:O	1:A:542:THR:HG22	2.16	0.45
1:B:420:ALA:CA	1:B:425:ILE:HD11	2.47	0.45
1:C:294:ILE:HG23	1:C:378:TYR:CD2	2.52	0.45
1:E:472:THR:HG23	1:E:493:PHE:CZ	2.52	0.45
1:D:419:SER:HA	1:D:422:GLU:HB3	1.99	0.45
1:C:472:THR:HG23	1:C:493:PHE:CZ	2.52	0.45
1:C:76:PRO:CG	1:C:536:THR:HG21	2.46	0.45
1:E:65:ALA:HB2	1:E:548:LEU:HD11	1.99	0.45
1:G:307:ASN:ND2	1:G:326:ASN:HB3	2.32	0.44
1:A:419:SER:HA	1:A:422:GLU:HB3	1.98	0.44
1:B:419:SER:HA	1:B:422:GLU:HB3	1.99	0.44
1:F:472:THR:HG23	1:F:493:PHE:CZ	2.52	0.44
1:F:65:ALA:HB2	1:F:548:LEU:HD11	1.99	0.44
1:D:64:GLU:OE1	1:D:548:LEU:HD23	2.17	0.44
1:B:76:PRO:CG	1:B:536:THR:HG21	2.47	0.44
1:A:377:ARG:HH21	1:A:423:ASN:HA	1.83	0.44
1:E:307:ASN:ND2	1:E:326:ASN:HB3	2.33	0.44
1:F:76:PRO:CG	1:F:536:THR:HG21	2.47	0.43
1:B:472:THR:HG23	1:B:493:PHE:CZ	2.53	0.43
1:D:425:ILE:CG2	1:D:520:TYR:CD1	3.01	0.43
1:F:425:ILE:CG2	1:F:520:TYR:CD1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ARG:HD2	1:C:425:ILE:HD11	2.01	0.43
1:G:65:ALA:HB2	1:G:548:LEU:HD11	1.99	0.43
1:C:377:ARG:NH2	1:C:423:ASN:OD1	2.52	0.43
1:G:132:VAL:HG13	1:G:136:ASP:HB3	2.01	0.43
1:B:479:PHE:O	1:B:485:TYR:HD1	1.99	0.43
1:B:425:ILE:HG23	1:B:520:TYR:HB3	2.01	0.43
1:B:550:GLU:O	1:B:551:LYS:CB	2.66	0.43
1:C:307:ASN:ND2	1:C:326:ASN:HB3	2.33	0.43
1:G:384:ARG:NH1	1:G:418:ARG:HD2	2.33	0.43
1:E:543:THR:HG21	1:F:39:MET:CE	2.49	0.43
1:D:307:ASN:ND2	1:D:326:ASN:HB3	2.34	0.43
1:G:77:ALA:O	1:G:88:THR:HG22	2.19	0.43
1:C:132:VAL:HG13	1:C:136:ASP:HB3	2.01	0.42
1:F:307:ASN:ND2	1:F:326:ASN:HB3	2.33	0.42
1:A:307:ASN:ND2	1:A:326:ASN:HB3	2.34	0.42
1:C:168:TYR:CE1	1:C:384:ARG:HG2	2.53	0.42
1:B:71:ARG:NH1	1:C:46:THR:OG1	2.51	0.42
1:B:307:ASN:ND2	1:B:326:ASN:HB3	2.34	0.42
1:C:77:ALA:O	1:C:88:THR:HG22	2.20	0.42
1:E:97:ALA:HB1	1:E:470:LEU:HD22	2.01	0.42
1:C:384:ARG:HH12	1:C:422:GLU:HA	1.84	0.42
1:F:77:ALA:O	1:F:88:THR:HG22	2.19	0.42
1:B:132:VAL:HG13	1:B:136:ASP:HB3	2.02	0.42
1:B:77:ALA:O	1:B:88:THR:HG22	2.19	0.42
1:F:132:VAL:HG13	1:F:136:ASP:HB3	2.01	0.42
1:D:97:ALA:HB1	1:D:470:LEU:HD22	2.02	0.42
1:G:366:PHE:CZ	1:G:375:ARG:CD	3.01	0.42
1:A:77:ALA:O	1:A:88:THR:HG22	2.20	0.42
1:D:33:PRO:HG3	1:D:506:LEU:HD22	2.02	0.42
1:E:168:TYR:CE1	1:E:384:ARG:HG2	2.54	0.42
1:A:254:ALA:HB3	1:A:257:PHE:CE1	2.55	0.42
1:B:254:ALA:HB3	1:B:257:PHE:CE1	2.55	0.42
1:F:445:LEU:HD13	1:F:459:ILE:HD13	2.02	0.42
1:D:132:VAL:HG13	1:D:136:ASP:HB3	2.01	0.41
1:D:77:ALA:O	1:D:88:THR:HG22	2.19	0.41
1:A:97:ALA:HB1	1:A:470:LEU:HD22	2.02	0.41
1:C:188:GLY:HA2	1:C:341:LEU:O	2.21	0.41
1:B:97:ALA:HB1	1:B:470:LEU:HD22	2.01	0.41
1:C:254:ALA:HB3	1:C:257:PHE:CE1	2.56	0.41
1:A:179:PHE:HE1	1:G:374:VAL:HB	1.85	0.41
1:C:97:ALA:HB1	1:C:470:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ALA:HB3	1:D:257:PHE:CE1	2.56	0.41
1:D:368:LEU:HA	1:D:371:LYS:HD2	2.03	0.41
1:E:254:ALA:HB3	1:E:257:PHE:CE1	2.56	0.41
1:E:425:ILE:CG2	1:E:520:TYR:CD1	3.03	0.41
1:E:77:ALA:O	1:E:88:THR:HG22	2.19	0.41
1:F:97:ALA:HB1	1:F:470:LEU:HD22	2.02	0.41
1:A:172:GLU:CG	1:A:338:ARG:NH2	2.83	0.41
1:A:291:GLY:HA3	1:B:400:TYR:CD2	2.56	0.41
1:D:425:ILE:HG23	1:D:520:TYR:HB3	2.02	0.41
1:E:377:ARG:NH2	1:E:423:ASN:HA	2.36	0.41
1:G:254:ALA:HB3	1:G:257:PHE:CE1	2.56	0.41
1:C:288:THR:O	1:C:290:VAL:HG23	2.21	0.41
1:E:290:VAL:HB	1:E:291:GLY:H	1.75	0.41
1:G:445:LEU:HD13	1:G:459:ILE:HD13	2.03	0.41
1:D:33:PRO:CG	1:D:506:LEU:HD22	2.51	0.41
1:E:445:LEU:HD13	1:E:459:ILE:HD13	2.03	0.41
1:F:254:ALA:HB3	1:F:257:PHE:CE1	2.56	0.40
1:A:445:LEU:HD13	1:A:459:ILE:HD13	2.02	0.40
1:G:97:ALA:HB1	1:G:470:LEU:HD22	2.02	0.40
1:B:33:PRO:HG3	1:B:506:LEU:HD22	2.02	0.40
1:E:80:THR:O	1:E:84:CYS:N	2.50	0.40
1:A:294:ILE:HG23	1:A:378:TYR:CE1	2.56	0.40
1:B:188:GLY:HA2	1:B:341:LEU:O	2.22	0.40
1:G:138:ARG:HD2	1:G:425:ILE:HD11	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ARG:NH2	1:G:488:ASN:O[3_544]	1.93	0.27
1:E:244:GLN:NE2	1:G:445:LEU:O[2_444]	2.14	0.06

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	548/558 (98%)	521 (95%)	26 (5%)	1 (0%)	47	80
1	B	541/558 (97%)	513 (95%)	27 (5%)	1 (0%)	47	80
1	C	548/558 (98%)	523 (95%)	25 (5%)	0	100	100
1	D	541/558 (97%)	517 (96%)	24 (4%)	0	100	100
1	E	547/558 (98%)	520 (95%)	26 (5%)	1 (0%)	47	80
1	F	540/558 (97%)	515 (95%)	25 (5%)	0	100	100
1	G	541/558 (97%)	515 (95%)	26 (5%)	0	100	100
All	All	3806/3906 (97%)	3624 (95%)	179 (5%)	3 (0%)	51	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	VAL
1	B	492	HIS
1	E	290	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	442/473 (93%)	440 (100%)	2 (0%)	88	95
1	B	440/473 (93%)	437 (99%)	3 (1%)	84	93
1	C	438/473 (93%)	437 (100%)	1 (0%)	93	98
1	D	442/473 (93%)	439 (99%)	3 (1%)	84	93
1	E	440/473 (93%)	437 (99%)	3 (1%)	84	93
1	F	437/473 (92%)	436 (100%)	1 (0%)	93	98
1	G	439/473 (93%)	438 (100%)	1 (0%)	93	98
All	All	3078/3311 (93%)	3064 (100%)	14 (0%)	88	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	A	366	PHE
1	B	31	MET
1	B	366	PHE
1	B	426	LEU
1	C	366	PHE
1	D	31	MET
1	D	366	PHE
1	D	526	SER
1	E	290	VAL
1	E	297	SER
1	E	366	PHE
1	F	366	PHE
1	G	366	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	HIS
1	B	475	HIS
1	C	475	HIS
1	D	475	HIS
1	E	475	HIS
1	F	475	HIS
1	G	475	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	ATP	A	603	3,2	26,33,33	0.92	1 (3%)	31,52,52	1.49	6 (19%)
4	ATP	C	603	3,2	26,33,33	0.97	2 (7%)	31,52,52	1.50	4 (12%)
5	ADP	D	600	-	24,29,29	0.98	1 (4%)	29,45,45	1.46	5 (17%)
5	ADP	B	600	-	24,29,29	0.98	1 (4%)	29,45,45	1.41	5 (17%)
4	ATP	E	603	3,2	26,33,33	0.93	1 (3%)	31,52,52	1.53	6 (19%)
5	ADP	F	600	-	24,29,29	0.96	1 (4%)	29,45,45	1.55	4 (13%)
4	ATP	G	603	3,2	26,33,33	0.97	1 (3%)	31,52,52	1.47	5 (16%)

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
4	ATP	A	603	3,2	-	5/18/38/38	0/3/3/3
4	ATP	C	603	3,2	-	5/18/38/38	0/3/3/3
5	ADP	D	600	-	-	3/12/32/32	0/3/3/3
5	ADP	B	600	-	-	6/12/32/32	0/3/3/3
4	ATP	E	603	3,2	-	4/18/38/38	0/3/3/3
5	ADP	F	600	-	-	7/12/32/32	0/3/3/3
4	ATP	G	603	3,2	-	5/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	ADP	C5-C4	2.52	1.47	1.40
5	B	600	ADP	C5-C4	2.47	1.47	1.40
5	F	600	ADP	C5-C4	2.33	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	603	ATP	C5-C4	2.29	1.47	1.40
4	C	603	ATP	C5-C4	2.26	1.46	1.40
4	A	603	ATP	C5-C4	2.20	1.46	1.40
4	E	603	ATP	C5-C4	2.19	1.46	1.40
4	C	603	ATP	O4'-C1'	2.06	1.44	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	ATP	N3-C2-N1	-3.90	122.58	128.68
4	A	603	ATP	N3-C2-N1	-3.88	122.61	128.68
4	C	603	ATP	PA-O3A-PB	-3.83	119.70	132.83
5	F	600	ADP	N3-C2-N1	-3.71	122.89	128.68
5	B	600	ADP	N3-C2-N1	-3.68	122.92	128.68
5	D	600	ADP	N3-C2-N1	-3.58	123.09	128.68
4	C	603	ATP	N3-C2-N1	-3.58	123.09	128.68
4	G	603	ATP	N3-C2-N1	-3.50	123.21	128.68
5	F	600	ADP	C3'-C2'-C1'	3.40	106.10	100.98
4	C	603	ATP	C4-C5-N7	-3.40	105.86	109.40
4	G	603	ATP	PB-O3B-PG	-3.31	121.47	132.83
4	A	603	ATP	PB-O3B-PG	-3.26	121.63	132.83
4	E	603	ATP	PA-O3A-PB	-3.24	121.71	132.83
4	E	603	ATP	PB-O3B-PG	-3.19	121.88	132.83
4	G	603	ATP	C4-C5-N7	-3.17	106.10	109.40
4	A	603	ATP	PA-O3A-PB	-3.10	122.19	132.83
5	D	600	ADP	C3'-C2'-C1'	3.07	105.59	100.98
4	E	603	ATP	C1'-N9-C4	-3.00	121.38	126.64
5	F	600	ADP	PA-O3A-PB	-2.97	122.65	132.83
4	G	603	ATP	PA-O3A-PB	-2.90	122.88	132.83
5	B	600	ADP	PA-O3A-PB	-2.85	123.05	132.83
5	B	600	ADP	C3'-C2'-C1'	2.83	105.24	100.98
4	C	603	ATP	PB-O3B-PG	-2.80	123.21	132.83
4	E	603	ATP	C4-C5-N7	-2.78	106.50	109.40
4	A	603	ATP	C4-C5-N7	-2.75	106.53	109.40
5	D	600	ADP	C4-C5-N7	-2.73	106.55	109.40
5	F	600	ADP	C4-C5-N7	-2.72	106.56	109.40
4	A	603	ATP	C1'-N9-C4	-2.61	122.05	126.64
5	B	600	ADP	C4-C5-N7	-2.58	106.71	109.40
5	D	600	ADP	PA-O3A-PB	-2.57	124.02	132.83
4	G	603	ATP	C1'-N9-C4	-2.38	122.47	126.64
4	A	603	ATP	C2-N1-C6	2.13	122.39	118.75
4	E	603	ATP	C2-N1-C6	2.12	122.38	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ADP	C2-N1-C6	2.07	122.30	118.75
5	D	600	ADP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

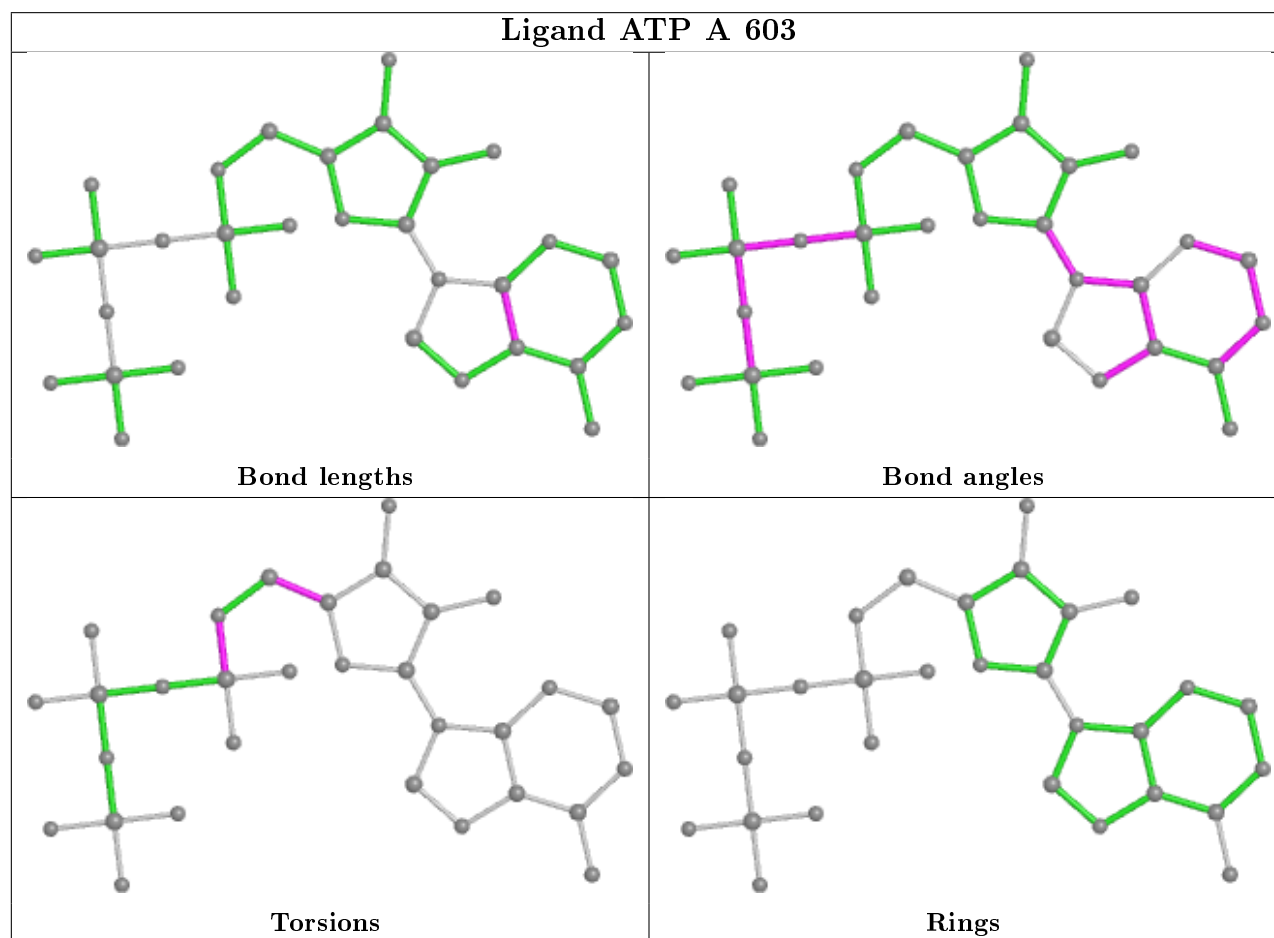
All (35) torsion outliers are listed below:

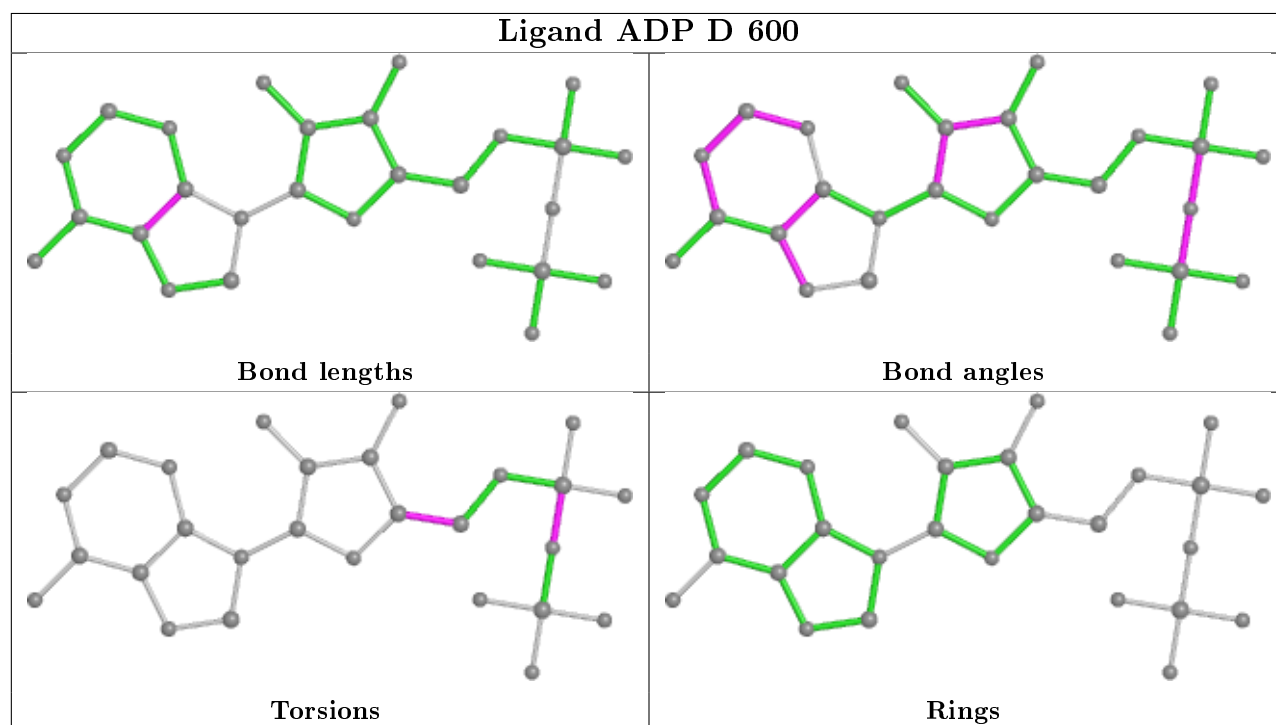
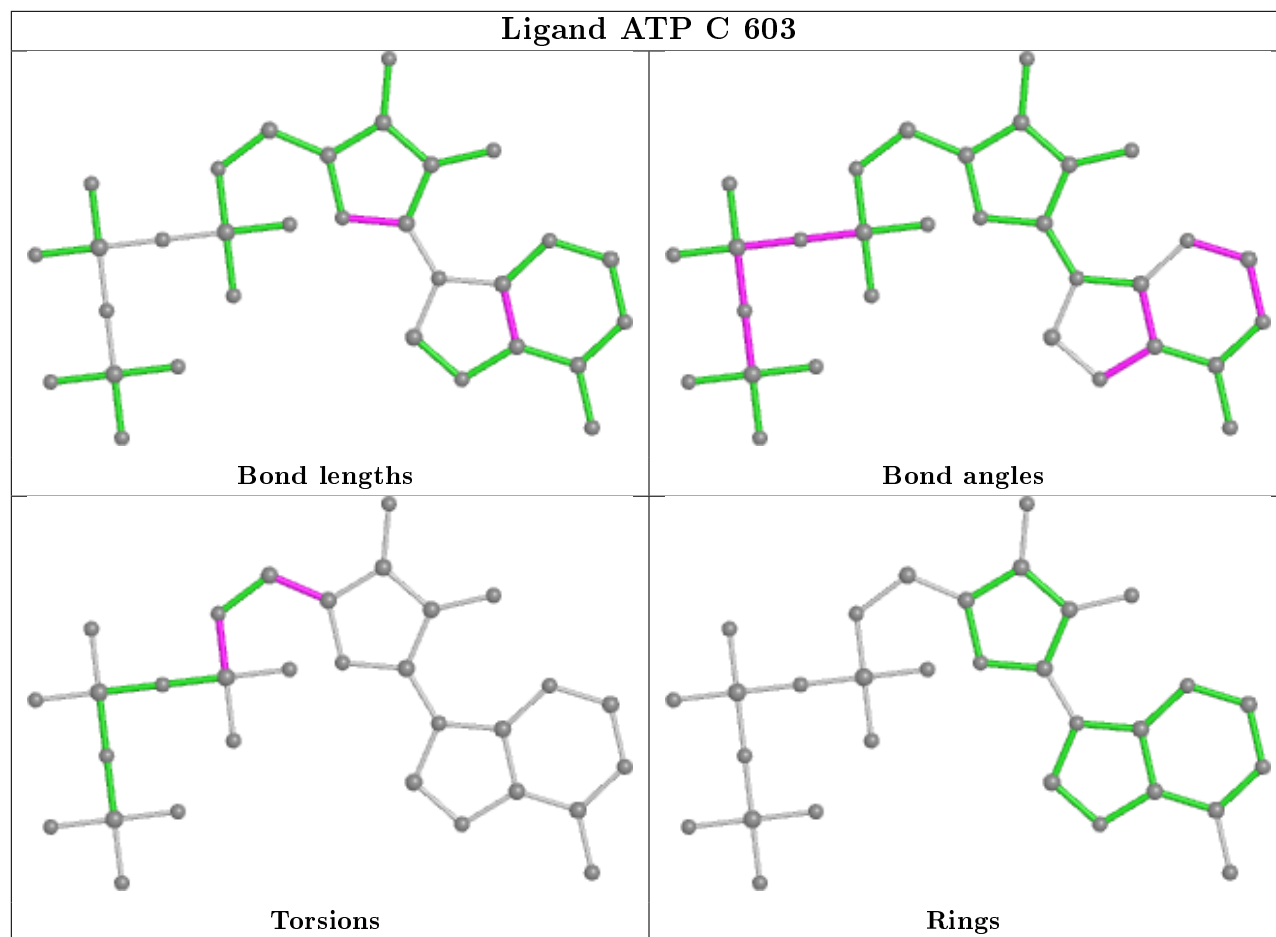
Mol	Chain	Res	Type	Atoms
4	A	603	ATP	C5'-O5'-PA-O2A
5	D	600	ADP	O4'-C4'-C5'-O5'
4	E	603	ATP	C5'-O5'-PA-O2A
4	C	603	ATP	C5'-O5'-PA-O1A
4	C	603	ATP	C5'-O5'-PA-O2A
5	B	600	ADP	C5'-O5'-PA-O2A
5	B	600	ADP	O4'-C4'-C5'-O5'
5	F	600	ADP	C5'-O5'-PA-O2A
4	G	603	ATP	C5'-O5'-PA-O1A
4	G	603	ATP	C5'-O5'-PA-O2A
4	A	603	ATP	C3'-C4'-C5'-O5'
4	C	603	ATP	C3'-C4'-C5'-O5'
5	F	600	ADP	O4'-C4'-C5'-O5'
4	G	603	ATP	C3'-C4'-C5'-O5'
5	D	600	ADP	C3'-C4'-C5'-O5'
4	A	603	ATP	O4'-C4'-C5'-O5'
4	C	603	ATP	O4'-C4'-C5'-O5'
4	G	603	ATP	O4'-C4'-C5'-O5'
5	F	600	ADP	C3'-C4'-C5'-O5'
4	A	603	ATP	C5'-O5'-PA-O3A
4	E	603	ATP	C5'-O5'-PA-O3A
5	B	600	ADP	C5'-O5'-PA-O3A
5	F	600	ADP	C5'-O5'-PA-O3A
5	B	600	ADP	PB-O3A-PA-O1A
5	F	600	ADP	PB-O3A-PA-O1A
4	A	603	ATP	C5'-O5'-PA-O1A
4	E	603	ATP	C5'-O5'-PA-O1A
4	C	603	ATP	C5'-O5'-PA-O3A
4	G	603	ATP	C5'-O5'-PA-O3A
4	E	603	ATP	C3'-C4'-C5'-O5'
5	D	600	ADP	PB-O3A-PA-O1A
5	B	600	ADP	PB-O3A-PA-O2A
5	F	600	ADP	PB-O3A-PA-O2A
5	B	600	ADP	C5'-O5'-PA-O1A
5	F	600	ADP	C5'-O5'-PA-O1A

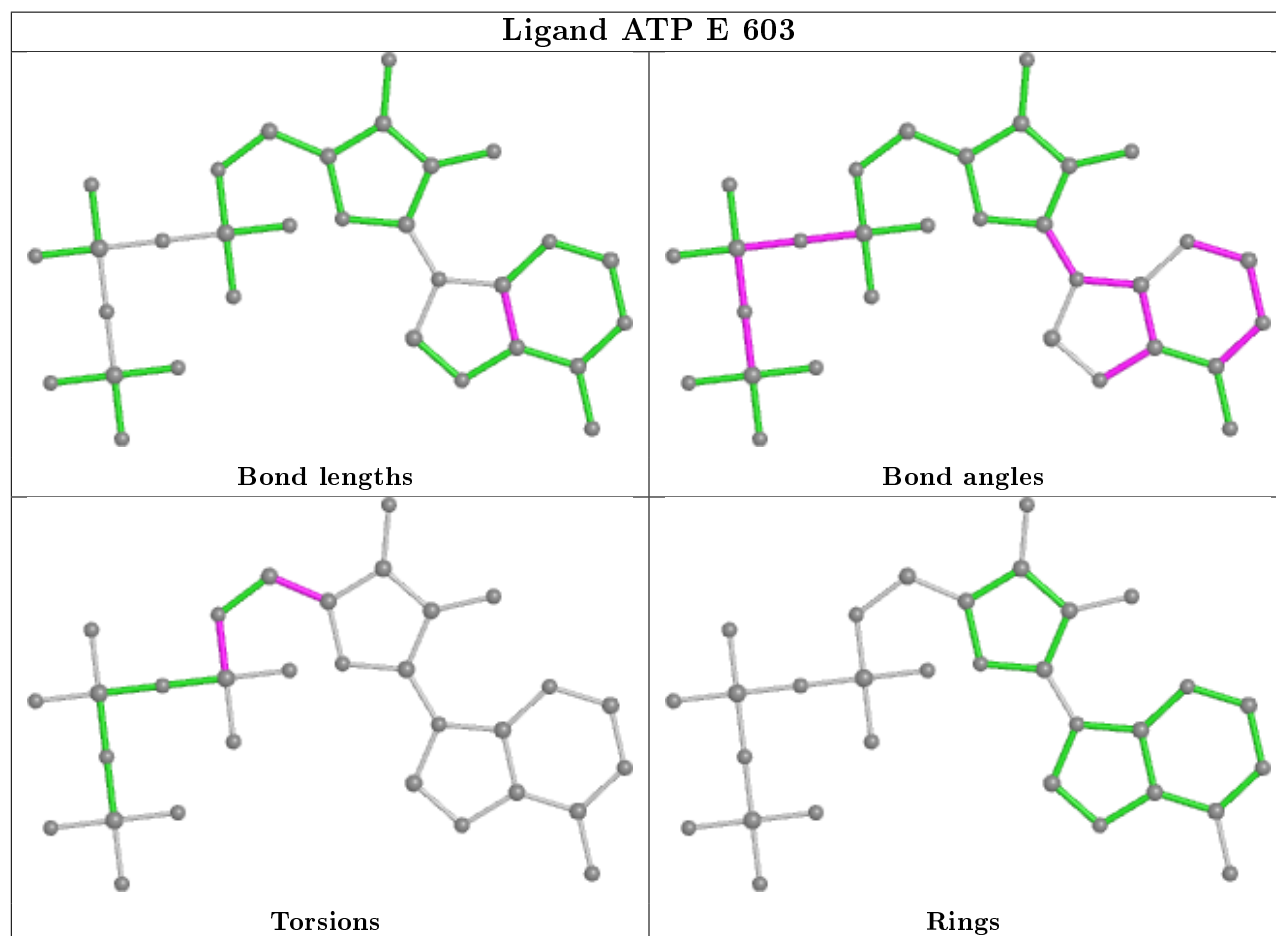
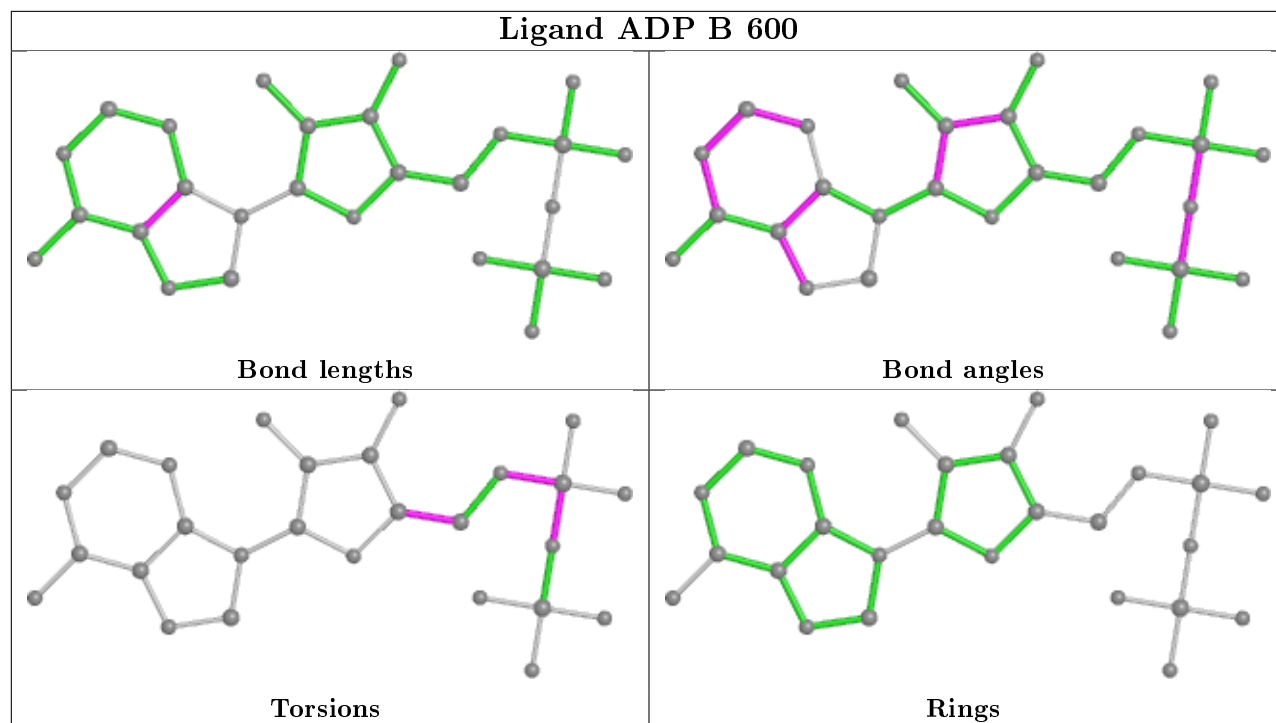
There are no ring outliers.

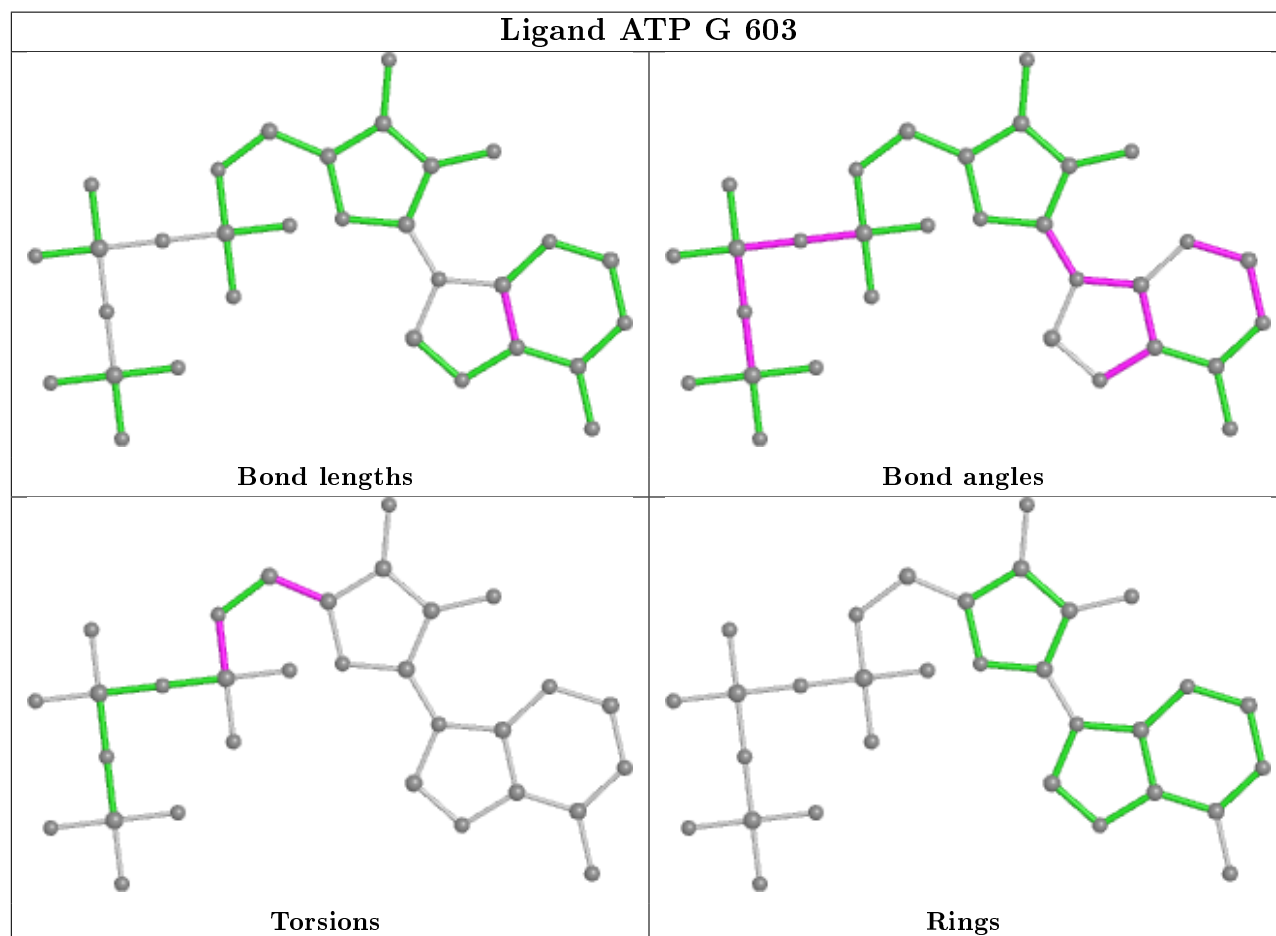
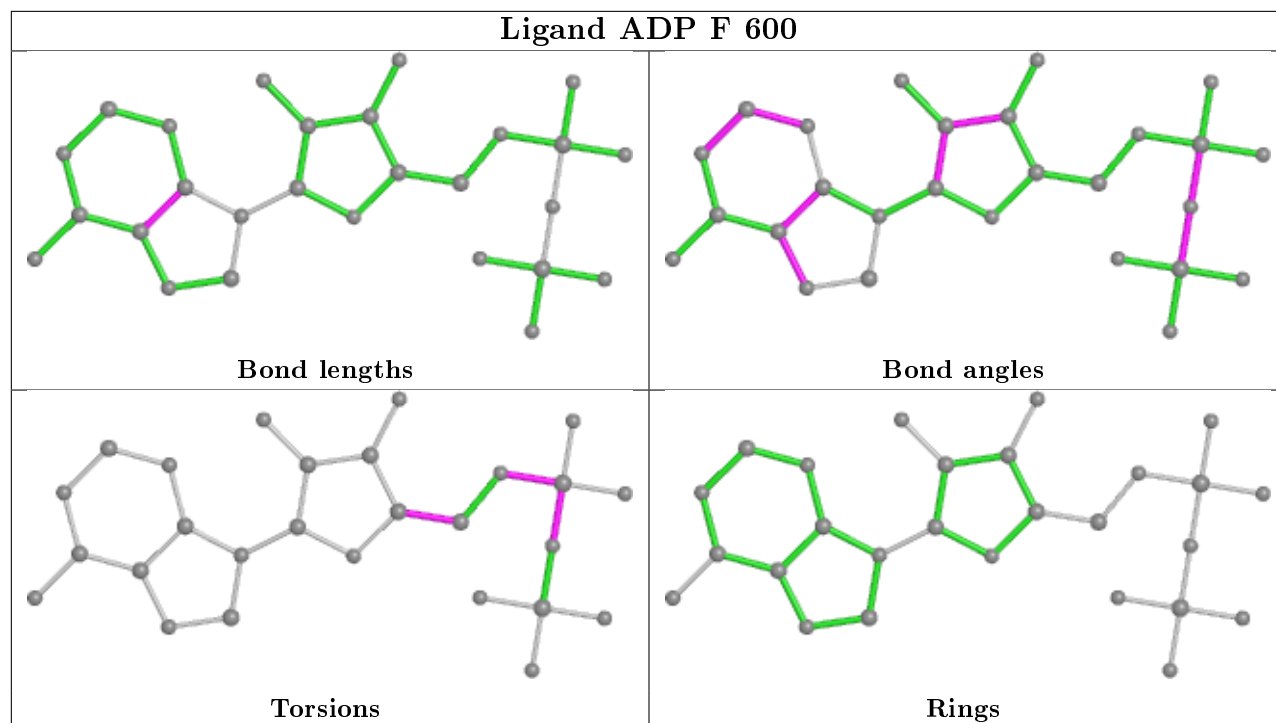
No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	550/558 (98%)	0.02	18 (3%)	46	34	92, 178, 285, 316	0
1	B	545/558 (97%)	0.10	28 (5%)	28	20	97, 175, 272, 299	0
1	C	550/558 (98%)	0.10	30 (5%)	25	18	97, 175, 247, 272	0
1	D	545/558 (97%)	-0.20	8 (1%)	73	61	89, 143, 195, 253	0
1	E	549/558 (98%)	-0.01	17 (3%)	49	36	93, 170, 273, 303	0
1	F	544/558 (97%)	0.40	53 (9%)	7	6	100, 212, 309, 341	0
1	G	545/558 (97%)	-0.16	9 (1%)	70	57	89, 155, 211, 243	0
All	All	3828/3906 (98%)	0.03	163 (4%)	35	25	89, 166, 279, 341	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	255	ARG	7.3
1	D	84	CYS	7.2
1	B	224	ASP	6.8
1	F	244	GLN	6.7
1	C	262	ASN	6.6
1	F	295	GLY	5.8
1	B	276	VAL	5.5
1	F	488	ASN	5.5
1	E	369	SER	5.2
1	F	200	PHE	5.1
1	F	281	PRO	5.0
1	G	224	ASP	4.5
1	F	227	ASP	4.4
1	A	370	ASP	4.4
1	F	83	GLU	4.3
1	F	84	CYS	4.3
1	F	204	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	487	GLU	4.1
1	F	289	PRO	4.1
1	B	2	SER	4.1
1	A	278	ASP	4.1
1	F	256	SER	3.9
1	F	222	ARG	3.9
1	F	187	THR	3.9
1	C	322	THR	3.9
1	B	325	ILE	3.9
1	C	259	GLU	3.9
1	F	385	THR	3.9
1	A	375	ARG	3.8
1	C	173	LEU	3.8
1	F	203	GLY	3.8
1	B	246	LEU	3.7
1	A	2	SER	3.7
1	F	326	ASN	3.6
1	B	260	ALA	3.6
1	C	350	ASP	3.6
1	C	278	ASP	3.5
1	A	367	SER	3.5
1	F	327	GLY	3.5
1	F	296	THR	3.5
1	A	179	PHE	3.5
1	F	278	ASP	3.4
1	C	326	ASN	3.4
1	D	488	ASN	3.4
1	E	279	GLY	3.4
1	A	369	SER	3.4
1	C	397	GLY	3.3
1	F	487	GLU	3.3
1	F	229	GLN	3.3
1	F	376	ALA	3.3
1	F	2	SER	3.2
1	B	267	GLN	3.2
1	E	278	ASP	3.2
1	F	489	GLY	3.1
1	G	176	GLY	3.1
1	F	190	THR	3.1
1	B	261	ALA	3.1
1	G	396	GLY	3.1
1	A	366	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	287	SER	3.0
1	F	224	ASP	3.0
1	E	166	GLY	3.0
1	B	324	SER	3.0
1	G	395	VAL	3.0
1	E	294	ILE	3.0
1	F	220	ASP	3.0
1	F	279	GLY	2.9
1	D	2	SER	2.9
1	C	396	GLY	2.9
1	F	223	ILE	2.9
1	C	202	LYS	2.9
1	F	329	HIS	2.9
1	C	327	GLY	2.9
1	C	197	ASN	2.9
1	E	210	GLU	2.9
1	D	489	GLY	2.8
1	C	172	GLU	2.8
1	E	378	TYR	2.8
1	A	270	ALA	2.8
1	F	430	GLY	2.8
1	B	192	ARG	2.8
1	B	196	ALA	2.8
1	C	313	ASP	2.7
1	C	395	VAL	2.7
1	C	369	SER	2.7
1	F	175	GLU	2.7
1	C	84	CYS	2.7
1	F	287	SER	2.7
1	B	326	ASN	2.7
1	F	228	THR	2.6
1	F	246	LEU	2.6
1	F	389	LYS	2.6
1	A	324	SER	2.6
1	F	272	HIS	2.6
1	F	267	GLN	2.6
1	F	276	VAL	2.6
1	B	205	GLN	2.6
1	C	199	TRP	2.6
1	E	221	ARG	2.6
1	B	227	ASP	2.6
1	F	245	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	375	ARG	2.5
1	A	277	GLU	2.5
1	F	375	ARG	2.5
1	F	285	PRO	2.5
1	C	398	GLU	2.5
1	G	175	GLU	2.5
1	F	205	GLN	2.5
1	A	226	GLU	2.5
1	F	201	ALA	2.5
1	G	2	SER	2.5
1	D	83	GLU	2.4
1	E	267	GLN	2.4
1	C	324	SER	2.4
1	F	377	ARG	2.4
1	A	224	ASP	2.4
1	F	210	GLU	2.4
1	E	379	ASN	2.4
1	B	368	LEU	2.4
1	B	197	ASN	2.4
1	B	277	GLU	2.3
1	E	229	GLN	2.3
1	F	202	LYS	2.3
1	B	365	GLY	2.3
1	C	321	ASP	2.3
1	A	488	ASN	2.3
1	G	397	GLY	2.3
1	A	269	ASN	2.3
1	B	256	SER	2.3
1	B	264	THR	2.3
1	C	406	ARG	2.3
1	F	82	GLU	2.2
1	C	266	MET	2.2
1	E	200	PHE	2.2
1	D	509	GLY	2.2
1	C	511	ILE	2.2
1	F	199	TRP	2.2
1	C	323	HIS	2.2
1	B	206	GLY	2.2
1	F	254	ALA	2.2
1	A	290	VAL	2.2
1	C	224	ASP	2.2
1	E	371	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	176	GLY	2.2
1	C	277	GLU	2.2
1	E	273	PRO	2.2
1	B	259	GLU	2.2
1	B	245	HIS	2.2
1	A	365	GLY	2.2
1	G	296	THR	2.2
1	F	511	ILE	2.1
1	B	295	GLY	2.1
1	B	283	LEU	2.1
1	A	372	PHE	2.1
1	E	504	MET	2.1
1	C	410	TYR	2.1
1	C	364	GLU	2.1
1	D	483	ALA	2.0
1	B	204	HIS	2.0
1	B	223	ILE	2.0
1	E	173	LEU	2.0
1	F	268	LEU	2.0
1	G	84	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

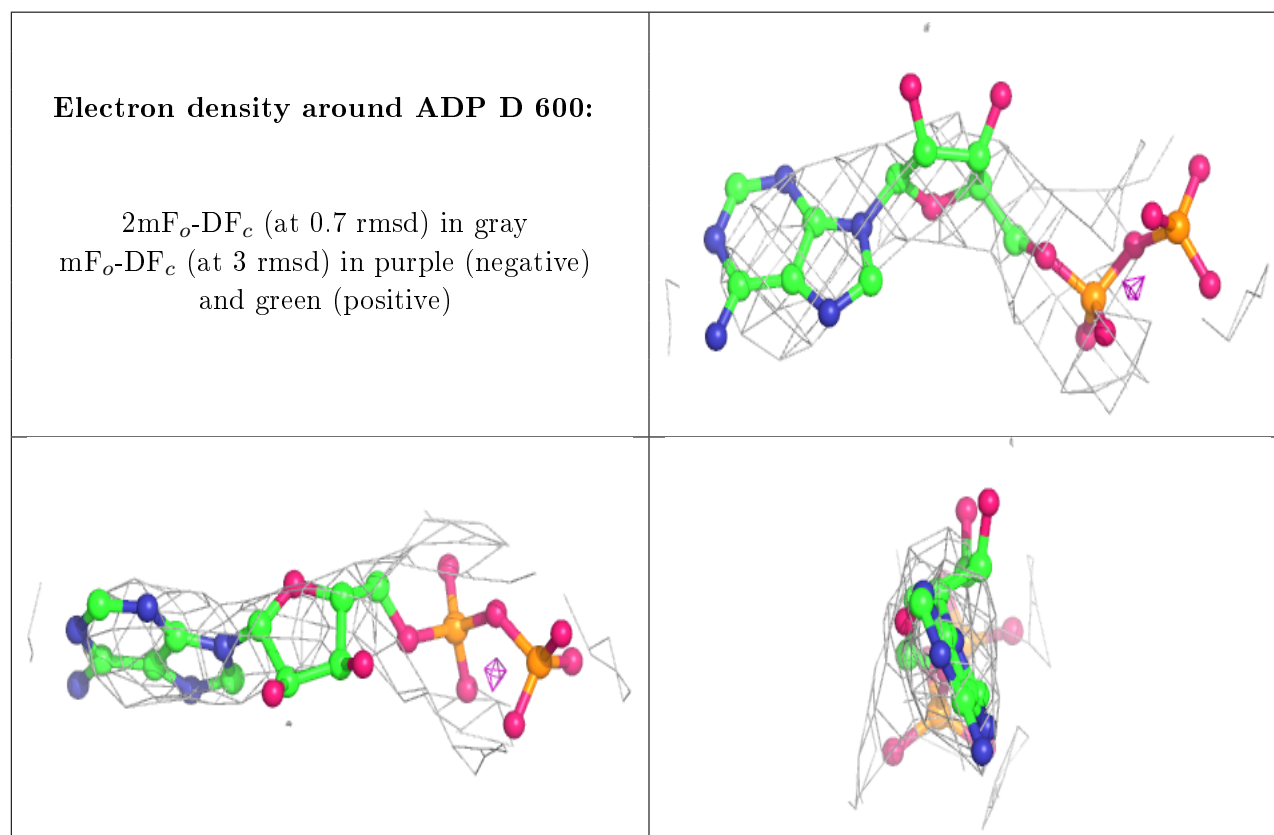
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ADP	D	600	27/27	0.75	0.33	181,192,210,213	0
5	ADP	B	600	27/27	0.75	0.42	175,190,200,206	0
5	ADP	F	600	27/27	0.77	0.43	176,187,197,199	0

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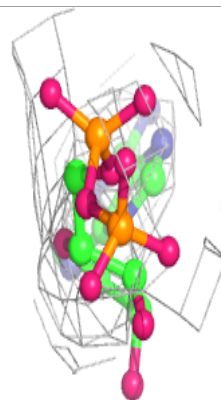
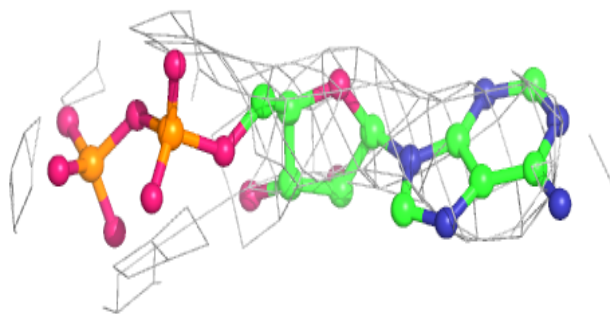
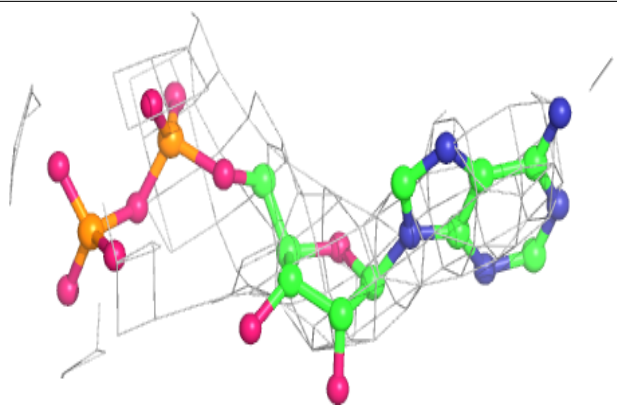
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	C	603	31/31	0.88	0.32	106,115,155,157	0
4	ATP	E	603	31/31	0.89	0.31	110,119,144,146	0
3	K	G	602	1/1	0.91	0.40	157,157,157,157	0
4	ATP	G	603	31/31	0.91	0.26	101,111,155,160	0
4	ATP	A	603	31/31	0.92	0.26	108,121,147,150	0
3	K	C	602	1/1	0.94	0.57	164,164,164,164	0
2	MG	A	601	1/1	0.95	0.77	124,124,124,124	0
2	MG	E	601	1/1	0.96	0.71	126,126,126,126	0
2	MG	C	601	1/1	0.96	0.44	133,133,133,133	0
3	K	E	602	1/1	0.97	0.37	148,148,148,148	0
3	K	A	602	1/1	0.97	0.32	150,150,150,150	0
2	MG	G	601	1/1	0.99	0.28	107,107,107,107	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.

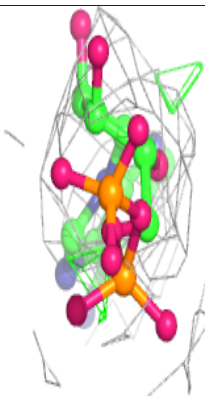
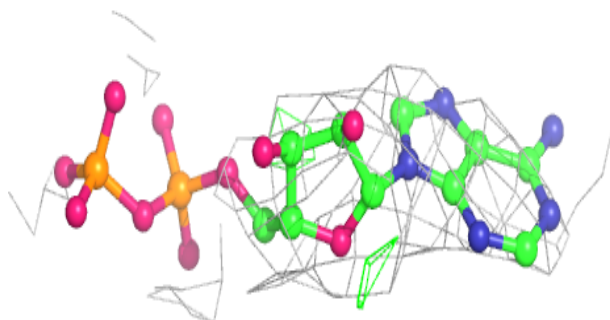
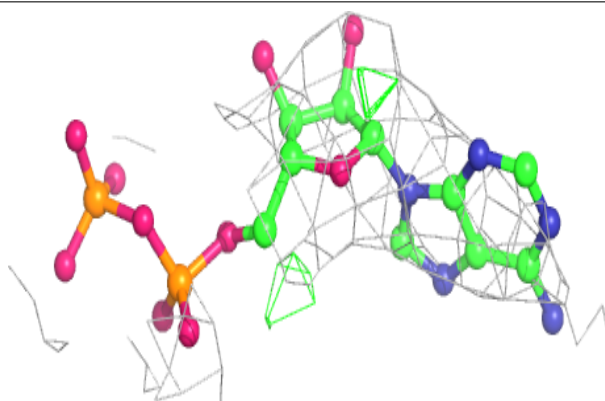


Electron density around ADP B 600:

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

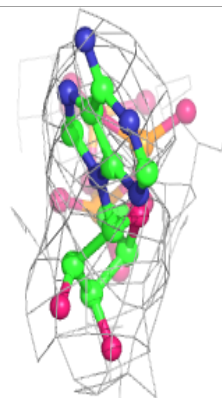
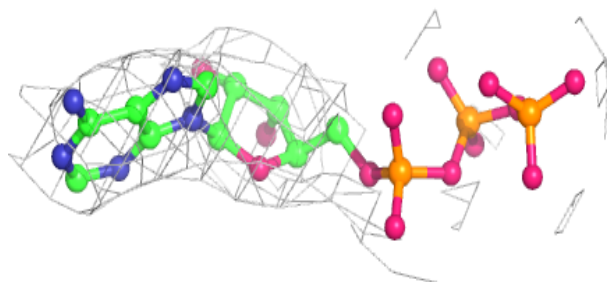
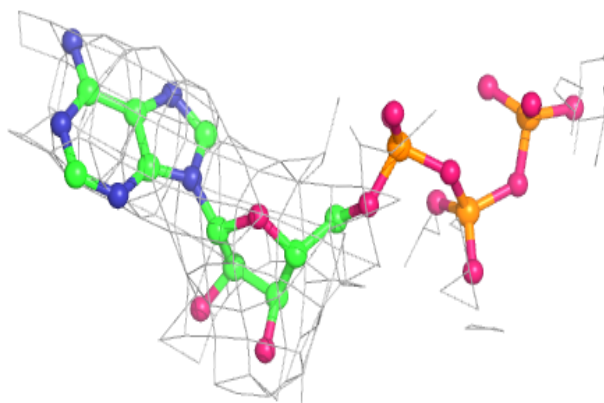
**Electron density around ADP F 600:**

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

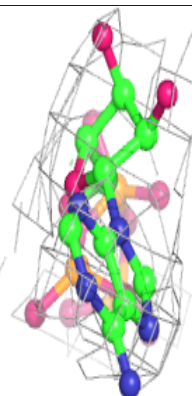
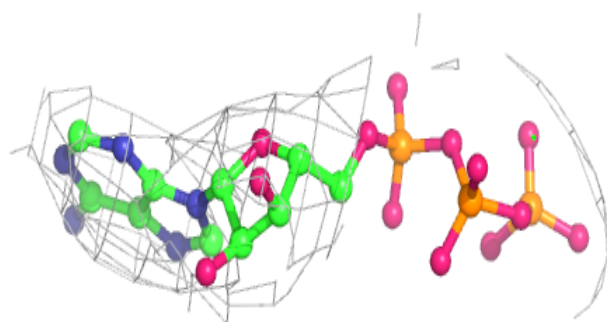
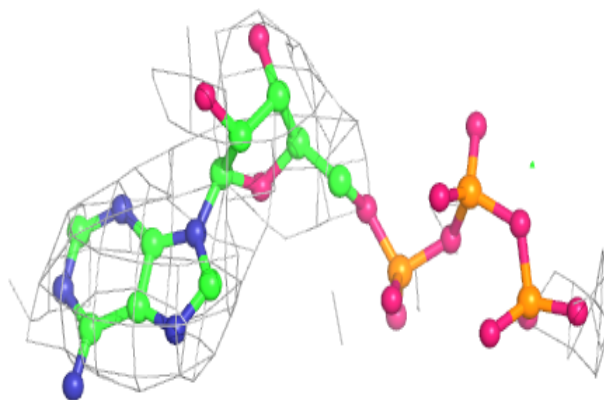


Electron density around ATP C 603:

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

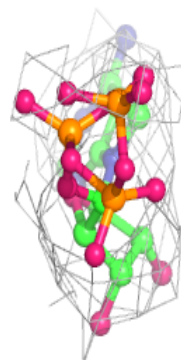
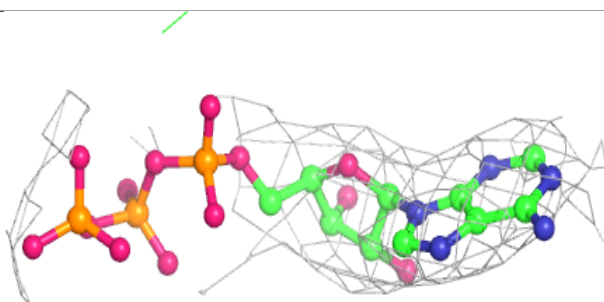
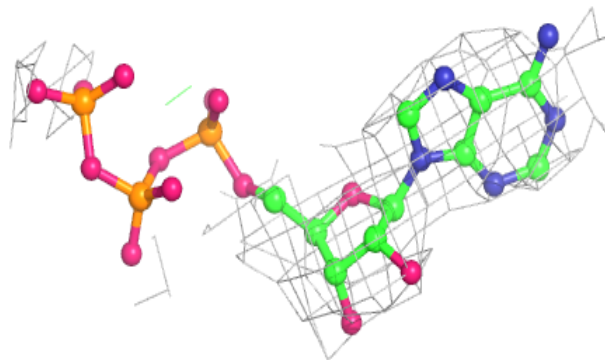
**Electron density around ATP E 603:**

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

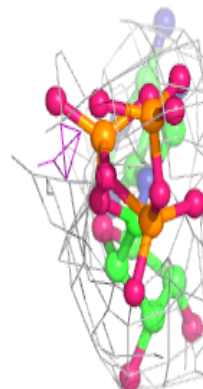
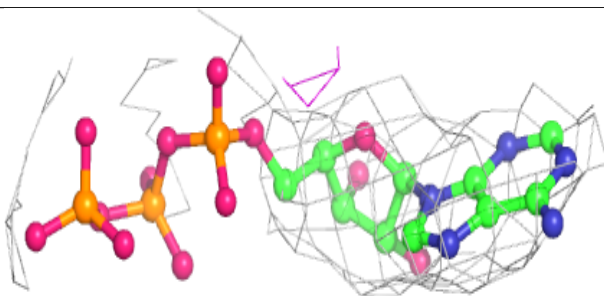
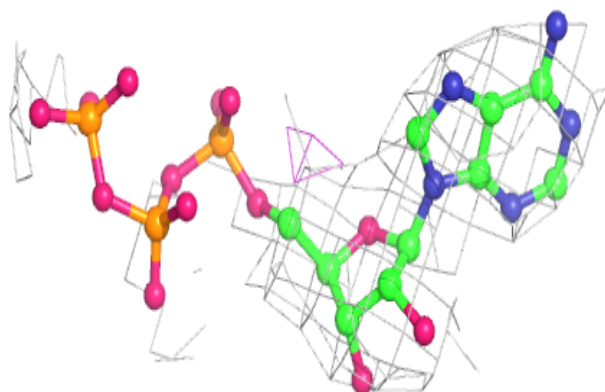


Electron density around ATP G 603:

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

**Electron density around ATP A 603:**

$2mF_o-DF_c$ (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.