



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:21 PM UTC

PDB ID : 6TMU / pdb_00006tmu
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 types of validation reports are described at

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

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

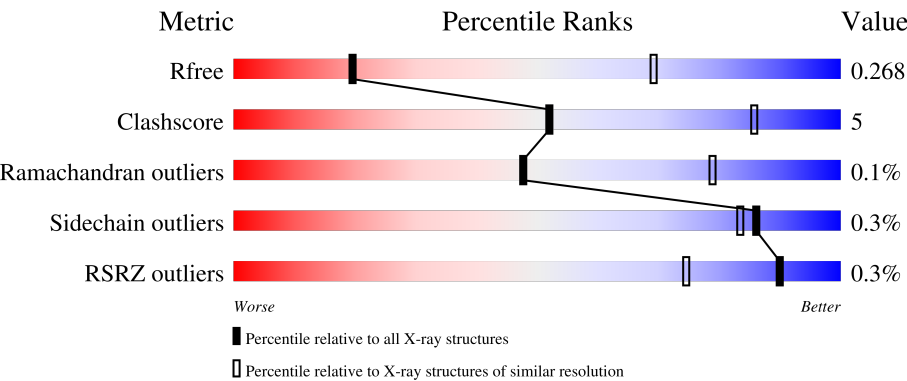
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	558	88%10%.
1	B	558	88%10%.
1	C	558	89%9%.
1	D	558	89%8%.

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Mol	Chain	Length	Quality of chain
1	E	558	 89%9%•
1	F	558	 88%9%•
1	G	558	 88%9%•

2 Entry composition

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

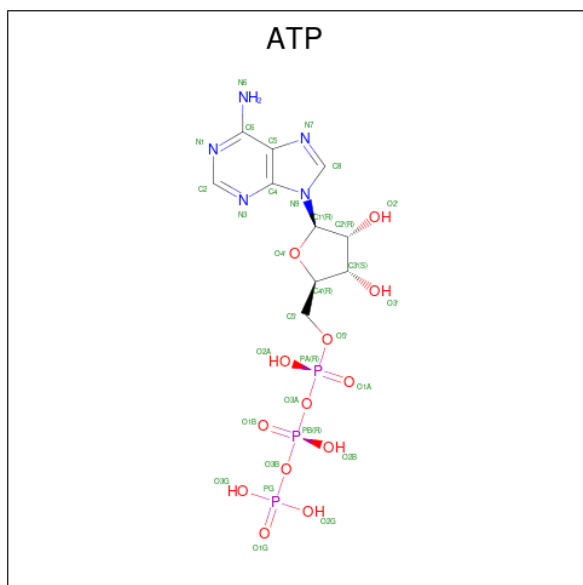
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

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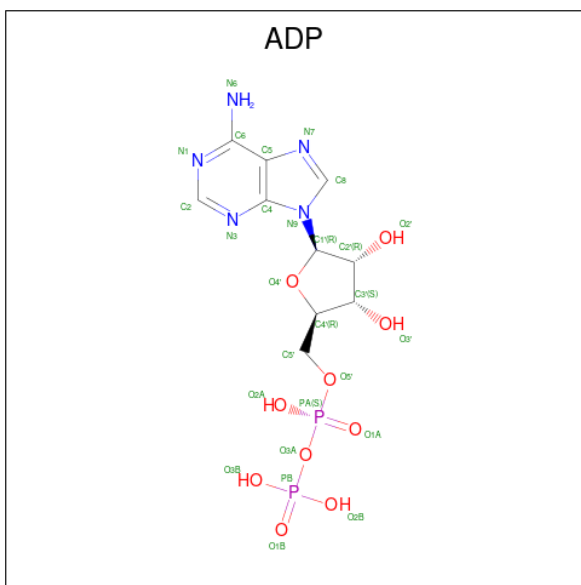
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	G	1	Total	K	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

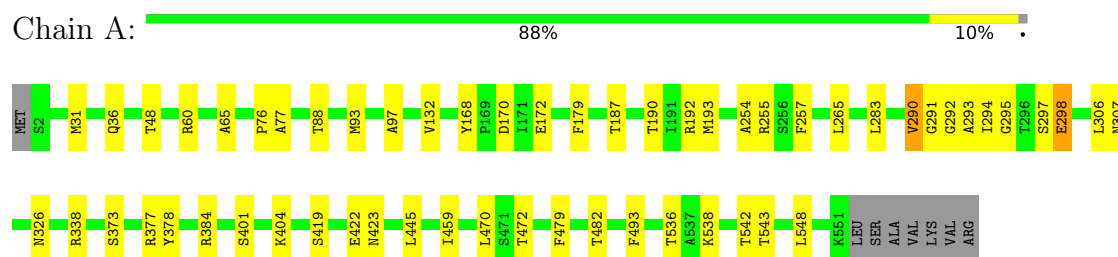


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

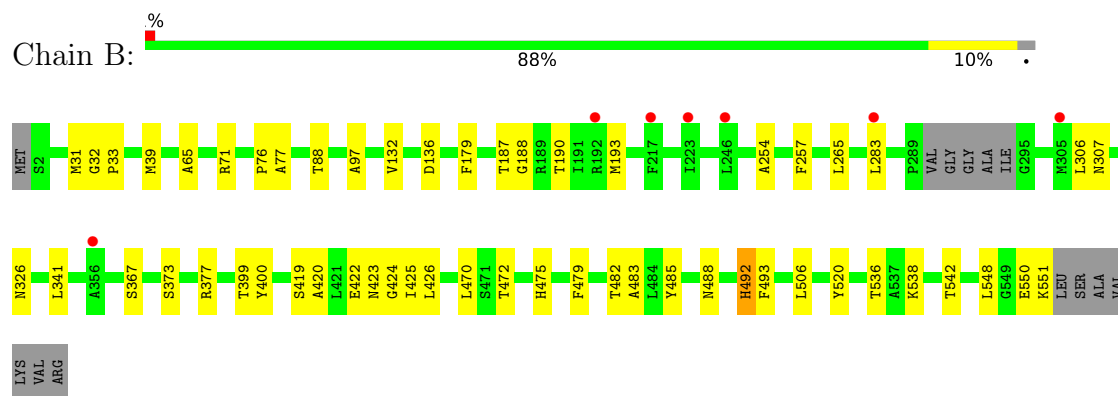
3 Residue-property plots

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.

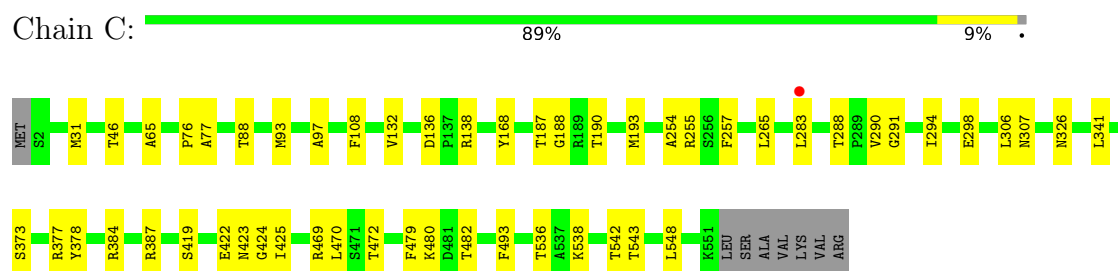
- Molecule 1: Putative GroEL-like chaperonine protein



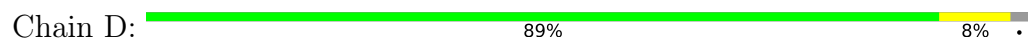
- Molecule 1: Putative GroEL-like chaperonine protein

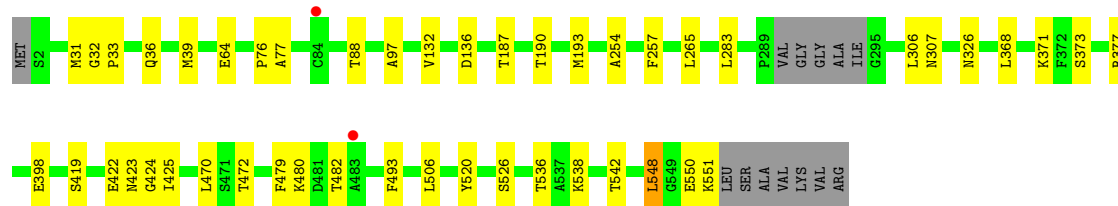


- Molecule 1: Putative GroEL-like chaperonine protein



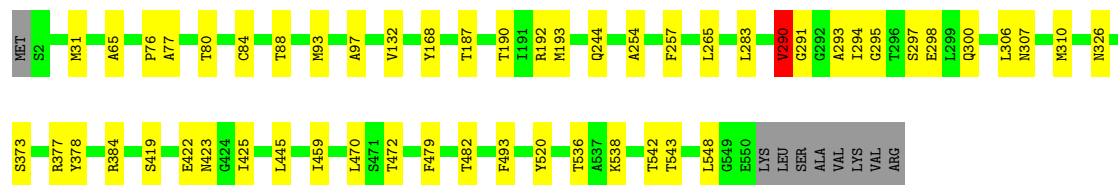
- Molecule 1: Putative GroEL-like chaperonine protein





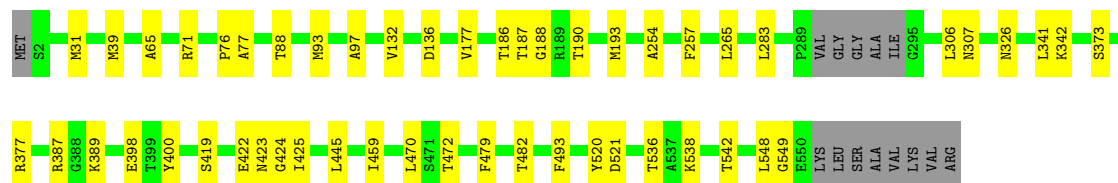
- Molecule 1: Putative GroEL-like chaperonine protein

Chain E: 89% 9% .



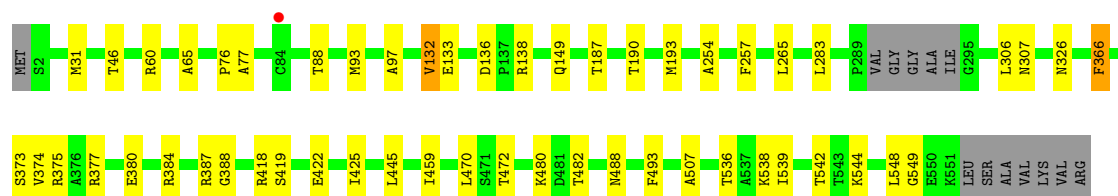
- Molecule 1: Putative GroEL-like chaperonine protein

Chain F: 88% 9% .



- Molecule 1: Putative GroEL-like chaperonine protein

Chain G: 88% 9% .



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) 99.5 (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 (5.04%)	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)	0.30 , 102.5	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

5.1 Standard geometry

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

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	0.45	0/4245	0.74	2/5765 (0.0%)
1	B	0.48	1/4213 (0.0%)	0.76	3/5721 (0.1%)
1	C	0.44	0/4226	0.75	4/5744 (0.1%)
1	D	0.44	0/4221	0.75	4/5731 (0.1%)
1	E	0.44	0/4232	0.74	1/5751 (0.0%)
1	F	0.45	0/4199	0.75	3/5706 (0.1%)
1	G	0.47	1/4212 (0.0%)	0.76	3/5721 (0.1%)
All	All	0.45	2/29548 (0.0%)	0.75	20/40139 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	483	ALA	C-N	9.07	1.46	1.33
1	G	388	GLY	N-CA	-8.24	1.36	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	387	ARG	CA-C-N	-8.36	107.28	121.17
1	G	387	ARG	C-N-CA	-8.36	107.28	121.17
1	B	424	GLY	N-CA-C	-7.57	103.14	112.68
1	F	424	GLY	N-CA-C	-7.56	103.16	112.68
1	D	424	GLY	N-CA-C	-7.00	103.87	112.68
1	D	548	LEU	CA-CB-CG	6.56	139.26	116.30
1	A	132	VAL	N-CA-C	6.29	119.00	108.81
1	E	132	VAL	N-CA-C	6.22	118.89	108.81
1	C	424	GLY	N-CA-C	6.19	119.22	112.29
1	B	32	GLY	N-CA-C	6.16	124.90	112.34
1	D	32	GLY	N-CA-C	6.15	124.89	112.34
1	C	387	ARG	CA-C-N	5.97	126.21	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	ARG	C-N-CA	5.97	126.21	121.61
1	F	387	ARG	CA-C-N	5.80	126.57	121.58
1	F	387	ARG	C-N-CA	5.80	126.57	121.58
1	C	480	LYS	N-CA-C	-5.27	103.43	110.55
1	D	480	LYS	N-CA-C	-5.21	103.65	110.53
1	A	298	GLU	CA-CB-CG	5.14	124.39	114.10
1	G	132	VAL	N-CA-C	5.09	116.04	108.46
1	B	367	SER	N-CA-C	5.03	117.01	110.43

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	63	0
1	B	4149	0	4060	46	0
1	C	4161	0	4062	47	1
1	D	4157	0	4070	37	0
1	E	4166	0	4073	47	1
1	F	4134	0	4028	37	0
1	G	4147	0	4052	39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	27	0	12	1	0
All	All	29306	0	28531	292	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 (292) 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:E:192:ARG:NH1	1:E:298:GLU:CD	2.27	0.93
1:A:377:ARG:NH2	1:A:422:GLU:O	2.04	0.91
1:E:290:VAL:CG1	1:E:295:GLY:HA2	2.04	0.87
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:A:192:ARG:HH11	1:A:298:GLU:CD	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:192:ARG:HH11	1:E:298:GLU:CD	2.03	0.65
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:B:488:ASN:CG	1:B:492:HIS:HB3	2.22	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: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
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: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:A:172:GLU:CD	1:A:338:ARG:HH22	2.13	0.56
1:G:77:ALA:HB1	1:G:88:THR:HB	1.88	0.56
1:A:77:ALA:HB1	1:A:88:THR:HB	1.88	0.56
1:A:192:ARG:HD3	1:A:298:GLU:OE2	2.06	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:48:THR:HG21	1:G:539:ILE:HG23	1.89	0.54
1:A:293:ALA:CB	1:B:179:PHE:CE1	2.87	0.54
1:F:77:ALA:HB1	1:F:88:THR:HB	1.89	0.54
1:A:192:ARG:NH1	1:A:298:GLU:CD	2.65	0.54
1:D:550:GLU:O	1:D:551:LYS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ALA:HB1	1:E:88:THR:HB	1.89	0.54
1:B:77:ALA:HB1	1:B:88:THR:HB	1.89	0.53
1:B:550:GLU:O	1:B:551:LYS:HB2	2.07	0.53
1:A:290:VAL:HG12	1:A:298:GLU:CD	2.34	0.53
1:E:291:GLY:HA3	1:F:400:TYR:HD2	1.73	0.53
1:A:172:GLU:CG	1:A:338:ARG:HH22	2.20	0.53
1:A:291:GLY:HA3	1:B:400:TYR:HD2	1.74	0.53
1:D:77:ALA:HB1	1:D:88:THR:HB	1.89	0.53
1:C:187:THR:HG22	1:C:187:THR:O	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: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:O	1:G:187:THR:HG22	2.10	0.52
1:C:290:VAL:HG12	1:C:291:GLY:N	2.26	0.51
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: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:C:543:THR:HG21	1:D:39:MET:HE3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:193:MET:HE1	1:G:306:LEU:HD11	1.95	0.49
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:B:193:MET:HE1	1:B:306:LEU:HD11	1.95	0.48
1:F:190:THR:HG23	1:F:190:THR:O	2.13	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:F:193:MET:HE1	1:F:306:LEU:HD11	1.96	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:D:193:MET:HE1	1:D:306:LEU:HD11	1.96	0.48
1:A:193:MET:HE1	1:A:306:LEU:HD11	1.96	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:O	1:B:190:THR:HG23	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:B:425:ILE:CG2	1:B:520:TYR:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:MET:HE1	1:C:306:LEU:HD11	1.95	0.47
1:D:265:LEU:HD22	1:D:283:LEU:CD2	2.41	0.47
1:E:377:ARG:HH21	1:E:423:ASN:HA	1.80	0.47
1:E:190:THR:HG23	1:E:190:THR:O	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:E:193:MET:HE1	1:E:306:LEU:HD11	1.96	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:HG23	1:D:190:THR:O	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:C:65:ALA:HB2	1:C:548:LEU:HD11	1.98	0.46
1:C:538:LYS:O	1:C:542:THR:HG22	2.16	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:E:300:GLN:HG3	1:E:310:MET:HE3	1.98	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:76:PRO:CG	1:E:536:THR:HG21	2.46	0.45
1:E:538:LYS:O	1:E:542:THR:HG22	2.16	0.45
1:A:472:THR:HG23	1:A:493:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:PRO:CG	1:C:536:THR:HG21	2.46	0.45
1:C:472:THR:HG23	1:C:493:PHE:CZ	2.52	0.45
1:E:65:ALA:HB2	1:E:548:LEU:HD11	1.99	0.45
1:A:543:THR:HG21	1:B:39:MET:HE3	1.98	0.44
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:294:ILE:O	1:A:378:TYR:OH	2.32	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
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:A:290:VAL:CG1	1:A:298:GLU:CD	2.91	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:F:521:ASP:OD1	5:F:600:ADP:O2'	2.28	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:B:71:ARG:NH1	1:C:46:THR:OG1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TYR:CE1	1:C:384:ARG:HG2	2.53	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:77:ALA:O	1:B:88:THR:HG22	2.19	0.42
1:B:132:VAL:HG13	1:B:136:ASP:HB3	2.02	0.42
1:C:288:THR:C	1:C:290:VAL:HG23	2.45	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:77:ALA:O	1:D:88:THR:HG22	2.19	0.41
1:D:132:VAL:HG13	1:D:136:ASP:HB3	2.01	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:G:31:MET:HE1	1:G:93:MET:HE2	2.02	0.41
1:A:179:PHE:HE1	1:G:374:VAL:HB	1.85	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:C:97:ALA:HB1	1:C:470:LEU:HD22	2.02	0.41
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:77:ALA:O	1:E:88:THR:HG22	2.19	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:F:97:ALA:HB1	1:F:470:LEU:HD22	2.02	0.41
1:A:31:MET:HE1	1:A:93:MET:HE2	2.03	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:C:288:THR:O	1:C:290:VAL:HG23	2.21	0.41
1:D:425:ILE:HG23	1:D:520:TYR:HB3	2.02	0.41
1:E:290:VAL:HB	1:E:291:GLY:H	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:MET:HE1	1:E:93:MET:HE2	2.03	0.40
1:E:80:THR:O	1:E:84:CYS:N	2.50	0.40
1:F:31:MET:HE1	1:F:93:MET:HE2	2.03	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:C:31:MET:HE1	1:C:93:MET:HE2	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	548/558 (98%)	521 (95%)	26 (5%)	1 (0%)	43 73
1	B	541/558 (97%)	513 (95%)	27 (5%)	1 (0%)	43 73
1	C	548/558 (98%)	523 (95%)	25 (5%)	0	100 100
1	D	541/558 (97%)	517 (96%)	24 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	547/558 (98%)	520 (95%)	26 (5%)	1 (0%)	43	73
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%)	48	79

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%)	441 (100%)	1 (0%)	87	85
1	B	440/473 (93%)	438 (100%)	2 (0%)	81	81
1	C	438/473 (93%)	438 (100%)	0	100	100
1	D	442/473 (93%)	440 (100%)	2 (0%)	81	81
1	E	440/473 (93%)	438 (100%)	2 (0%)	81	81
1	F	437/473 (92%)	437 (100%)	0	100	100
1	G	439/473 (93%)	437 (100%)	2 (0%)	81	81
All	All	3078/3311 (93%)	3069 (100%)	9 (0%)	86	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	31	MET
1	B	426	LEU
1	D	31	MET

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Mol	Chain	Res	Type
1	D	526	SER
1	E	290	VAL
1	E	297	SER
1	G	133	GLU
1	G	366	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	178	ASN
1	A	355	HIS
1	A	475	HIS
1	B	8	HIS
1	B	178	ASN
1	B	307	ASN
1	B	355	HIS
1	B	475	HIS
1	C	8	HIS
1	C	178	ASN
1	C	307	ASN
1	C	355	HIS
1	C	475	HIS
1	D	8	HIS
1	D	36	GLN
1	D	178	ASN
1	D	307	ASN
1	D	355	HIS
1	D	475	HIS
1	E	8	HIS
1	E	178	ASN
1	E	307	ASN
1	E	355	HIS
1	E	475	HIS
1	F	8	HIS
1	F	178	ASN
1	F	307	ASN
1	F	355	HIS
1	F	475	HIS
1	G	8	HIS
1	G	178	ASN
1	G	307	ASN

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Mol	Chain	Res	Type
1	G	355	HIS
1	G	475	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	603	3,2	32,33,33	1.36	6 (18%)	48,52,52	1.75	12 (25%)
4	ATP	A	603	3,2	32,33,33	1.37	6 (18%)	48,52,52	1.71	10 (20%)
5	ADP	D	600	-	28,29,29	1.49	6 (21%)	43,45,45	1.85	11 (25%)
5	ADP	F	600	-	28,29,29	1.42	6 (21%)	43,45,45	1.88	11 (25%)
4	ATP	C	603	3,2	32,33,33	1.43	6 (18%)	48,52,52	1.79	9 (18%)
4	ATP	G	603	3,2	32,33,33	1.41	5 (15%)	48,52,52	1.74	11 (22%)
5	ADP	B	600	-	28,29,29	1.44	6 (21%)	43,45,45	1.78	10 (23%)

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	E	603	3,2	-	6/22/38/38	0/3/3/3
4	ATP	A	603	3,2	-	5/22/38/38	0/3/3/3
5	ADP	D	600	-	-	4/16/32/32	0/3/3/3
5	ADP	F	600	-	-	6/16/32/32	0/3/3/3
4	ATP	C	603	3,2	-	5/22/38/38	0/3/3/3
4	ATP	G	603	3,2	-	6/22/38/38	0/3/3/3
5	ADP	B	600	-	-	5/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	ADP	C5-C4	4.76	1.47	1.39
5	B	600	ADP	C5-C4	4.70	1.47	1.39
5	F	600	ADP	C5-C4	4.50	1.47	1.39
4	G	603	ATP	C5-C4	4.43	1.47	1.39
4	C	603	ATP	C5-C4	4.39	1.46	1.39
4	A	603	ATP	C5-C4	4.30	1.46	1.39
4	E	603	ATP	C5-C4	4.28	1.46	1.39
4	G	603	ATP	C5-C6	2.83	1.48	1.41
4	C	603	ATP	PB-O3B	2.81	1.62	1.59
4	C	603	ATP	C5-C6	2.80	1.48	1.41
5	D	600	ADP	C5-C6	2.79	1.48	1.41
5	F	600	ADP	C5-C6	2.73	1.48	1.41
4	C	603	ATP	C8-N7	2.69	1.36	1.31
4	E	603	ATP	C5-C6	2.60	1.48	1.41
5	D	600	ADP	PA-O3A	2.59	1.62	1.59
4	A	603	ATP	C4-N9	-2.57	1.32	1.37
4	A	603	ATP	C5-C6	2.55	1.48	1.41
5	B	600	ADP	C5-C6	2.55	1.48	1.41
4	G	603	ATP	C8-N7	2.55	1.36	1.31
4	E	603	ATP	C8-N7	2.53	1.36	1.31
4	E	603	ATP	C4-N9	-2.52	1.32	1.37
4	C	603	ATP	C5-N7	-2.51	1.34	1.39
5	B	600	ADP	C5-N7	-2.51	1.34	1.39
4	A	603	ATP	C8-N7	2.48	1.36	1.31
4	G	603	ATP	C4-N9	-2.42	1.32	1.37
4	E	603	ATP	C5-N7	-2.42	1.34	1.39
5	B	600	ADP	C8-N7	2.40	1.36	1.31
5	D	600	ADP	C8-N7	2.40	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	600	ADP	C8-N7	2.39	1.36	1.31
4	A	603	ATP	C5-N7	-2.36	1.34	1.39
4	G	603	ATP	C5-N7	-2.34	1.34	1.39
5	F	600	ADP	C5-N7	-2.32	1.34	1.39
5	D	600	ADP	C5-N7	-2.30	1.34	1.39
4	A	603	ATP	PB-O3B	2.18	1.61	1.59
5	F	600	ADP	C4-N9	-2.17	1.33	1.37
4	E	603	ATP	PB-O3B	2.13	1.61	1.59
5	B	600	ADP	C4-N9	-2.06	1.33	1.37
4	C	603	ATP	C4-N9	-2.03	1.33	1.37
5	D	600	ADP	C4-N9	-2.03	1.33	1.37
5	F	600	ADP	PA-O3A	2.01	1.61	1.59
5	B	600	ADP	PA-O3A	2.01	1.61	1.59

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	ATP	C5-C4-N3	-5.99	118.47	126.72
5	D	600	ADP	C5-C4-N3	-5.60	119.01	126.72
5	B	600	ADP	C5-C4-N3	-5.49	119.16	126.72
5	F	600	ADP	C5-C4-N3	-5.42	119.25	126.72
4	G	603	ATP	C5-C4-N3	-5.23	119.51	126.72
4	A	603	ATP	C5-C4-N3	-4.87	120.02	126.72
4	E	603	ATP	C5-C4-N3	-4.81	120.09	126.72
5	D	600	ADP	N3-C4-N9	4.37	134.60	127.17
5	F	600	ADP	N3-C4-N9	4.21	134.33	127.17
5	B	600	ADP	N3-C4-N9	4.21	134.32	127.17
4	C	603	ATP	C4-C5-N7	-4.13	105.86	110.58
4	C	603	ATP	C2-N3-C4	4.06	121.74	111.83
4	C	603	ATP	N3-C4-N9	4.00	133.97	127.17
4	E	603	ATP	N3-C2-N1	-3.96	122.58	128.58
4	A	603	ATP	N3-C2-N1	-3.94	122.61	128.58
4	G	603	ATP	C4-C5-N7	-3.92	106.10	110.58
5	F	600	ADP	C2-N3-C4	3.78	121.06	111.83
5	F	600	ADP	N3-C2-N1	-3.76	122.89	128.58
5	D	600	ADP	C2-N3-C4	3.75	120.99	111.83
4	A	603	ATP	C2-N3-C4	3.74	120.97	111.83
5	B	600	ADP	N3-C2-N1	-3.74	122.92	128.58
4	E	603	ATP	C2-N3-C4	3.73	120.94	111.83
4	G	603	ATP	C2-N3-C4	3.72	120.91	111.83
5	B	600	ADP	C2-N3-C4	3.71	120.89	111.83
4	G	603	ATP	N3-C4-N9	3.70	133.46	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	ADP	N3-C2-N1	-3.63	123.09	128.58
4	C	603	ATP	N3-C2-N1	-3.63	123.09	128.58
4	A	603	ATP	N3-C4-N9	3.58	133.26	127.17
4	E	603	ATP	C4-C5-N7	-3.57	106.50	110.58
4	G	603	ATP	N3-C2-N1	-3.55	123.21	128.58
4	A	603	ATP	C4-C5-N7	-3.54	106.53	110.58
5	D	600	ADP	C4-C5-N7	-3.53	106.55	110.58
5	F	600	ADP	C4-C5-N7	-3.52	106.56	110.58
4	E	603	ATP	N3-C4-N9	3.51	133.13	127.17
5	B	600	ADP	C4-C5-N7	-3.38	106.71	110.58
5	F	600	ADP	C4-N9-C8	2.98	108.87	105.74
4	A	603	ATP	C4-N9-C8	2.96	108.85	105.74
4	E	603	ATP	C4-N9-C8	2.91	108.79	105.74
4	G	603	ATP	O4'-C1'-N9	2.91	113.68	108.09
4	E	603	ATP	C6-C5-N7	2.84	137.57	132.09
4	C	603	ATP	C5-N7-C8	2.83	107.89	103.45
5	D	600	ADP	C4-N9-C8	2.76	108.64	105.74
4	G	603	ATP	C4-N9-C8	2.72	108.60	105.74
4	A	603	ATP	C6-C5-N7	2.71	137.32	132.09
4	G	603	ATP	C6-C5-N7	2.70	137.29	132.09
5	F	600	ADP	C5-N7-C8	2.70	107.69	103.45
4	G	603	ATP	C5-N7-C8	2.69	107.68	103.45
5	D	600	ADP	C5-N7-C8	2.64	107.60	103.45
4	C	603	ATP	C6-C5-N7	2.60	137.10	132.09
4	E	603	ATP	C5-N7-C8	2.59	107.52	103.45
4	A	603	ATP	C5-N7-C8	2.55	107.46	103.45
4	E	603	ATP	O4'-C1'-N9	2.52	112.93	108.09
5	B	600	ADP	C5-N7-C8	2.51	107.40	103.45
4	E	603	ATP	N9-C8-N7	-2.49	110.41	113.94
4	A	603	ATP	N9-C8-N7	-2.47	110.44	113.94
5	F	600	ADP	C3'-C2'-C1'	2.45	106.10	101.46
5	F	600	ADP	N9-C8-N7	-2.44	110.47	113.94
5	B	600	ADP	C4-N9-C8	2.44	108.30	105.74
5	F	600	ADP	C6-C5-N7	2.36	136.65	132.09
4	G	603	ATP	N9-C8-N7	-2.36	110.59	113.94
4	E	603	ATP	C4-N9-C1'	-2.25	121.38	126.63
4	A	603	ATP	C2-N1-C6	2.23	122.39	118.73
4	E	603	ATP	C2-N1-C6	2.22	122.38	118.73
5	D	600	ADP	C6-C5-N7	2.21	136.35	132.09
5	D	600	ADP	N9-C8-N7	-2.20	110.82	113.94
5	D	600	ADP	C3'-C2'-C1'	2.18	105.59	101.46
4	C	603	ATP	O4'-C1'-N9	2.18	112.28	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ADP	C2-N1-C6	2.17	122.30	118.73
5	B	600	ADP	C6-C5-N7	2.15	136.23	132.09
4	C	603	ATP	N9-C8-N7	-2.14	110.90	113.94
5	D	600	ADP	C2-N1-C6	2.12	122.21	118.73
5	F	600	ADP	C2-N1-C6	2.06	122.11	118.73
4	G	603	ATP	C2-N1-C6	2.02	122.04	118.73
5	B	600	ADP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (37) torsion outliers are listed below:

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

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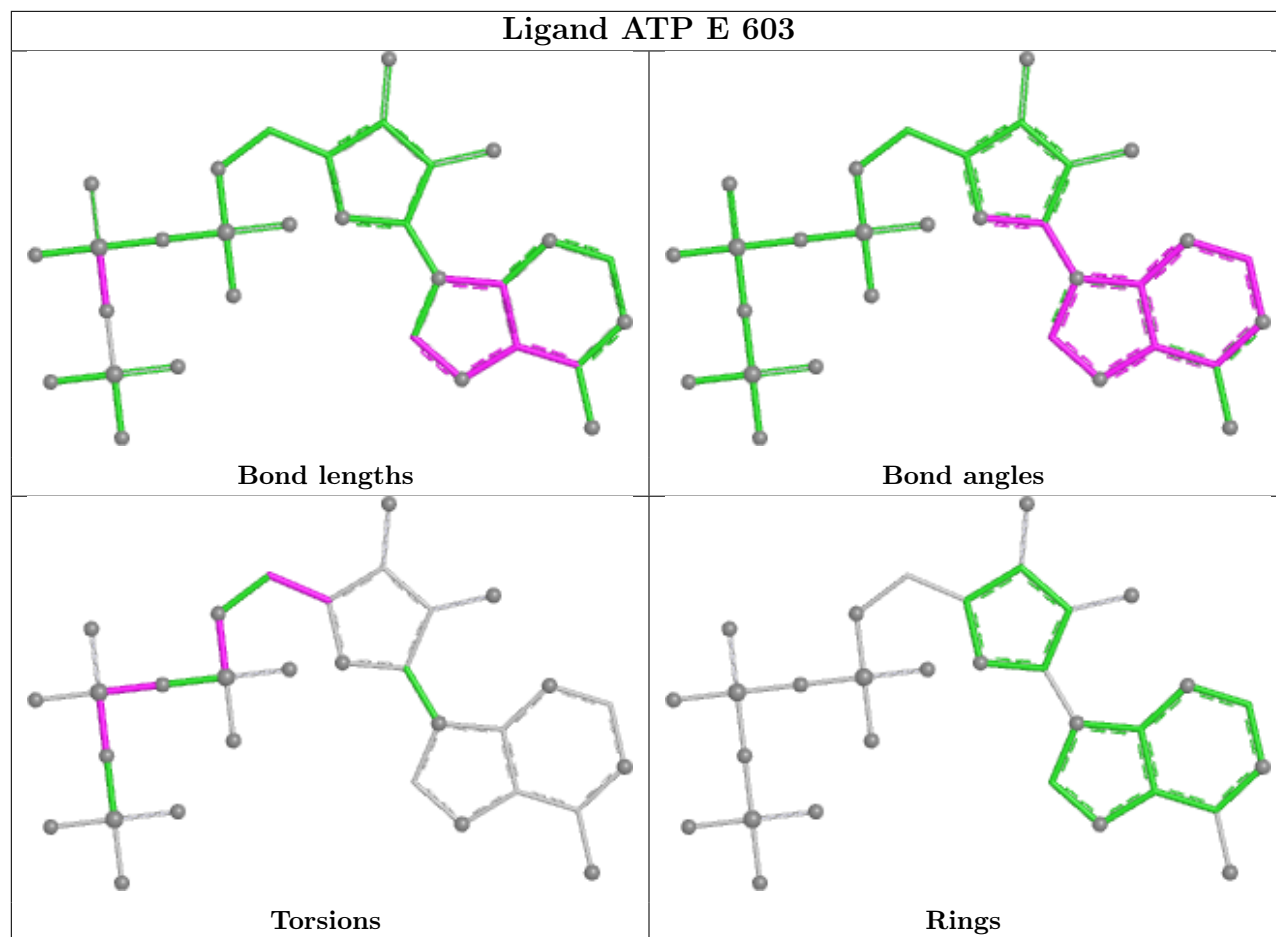
Mol	Chain	Res	Type	Atoms
5	B	600	ADP	PB-O3A-PA-O2A
5	D	600	ADP	PB-O3A-PA-O1A
5	F	600	ADP	PB-O3A-PA-O2A
4	E	603	ATP	PG-O3B-PB-O2B
4	E	603	ATP	PA-O3A-PB-O2B
4	G	603	ATP	PA-O3A-PB-O2B
5	D	600	ADP	PB-O3A-PA-O2A

There are no ring outliers.

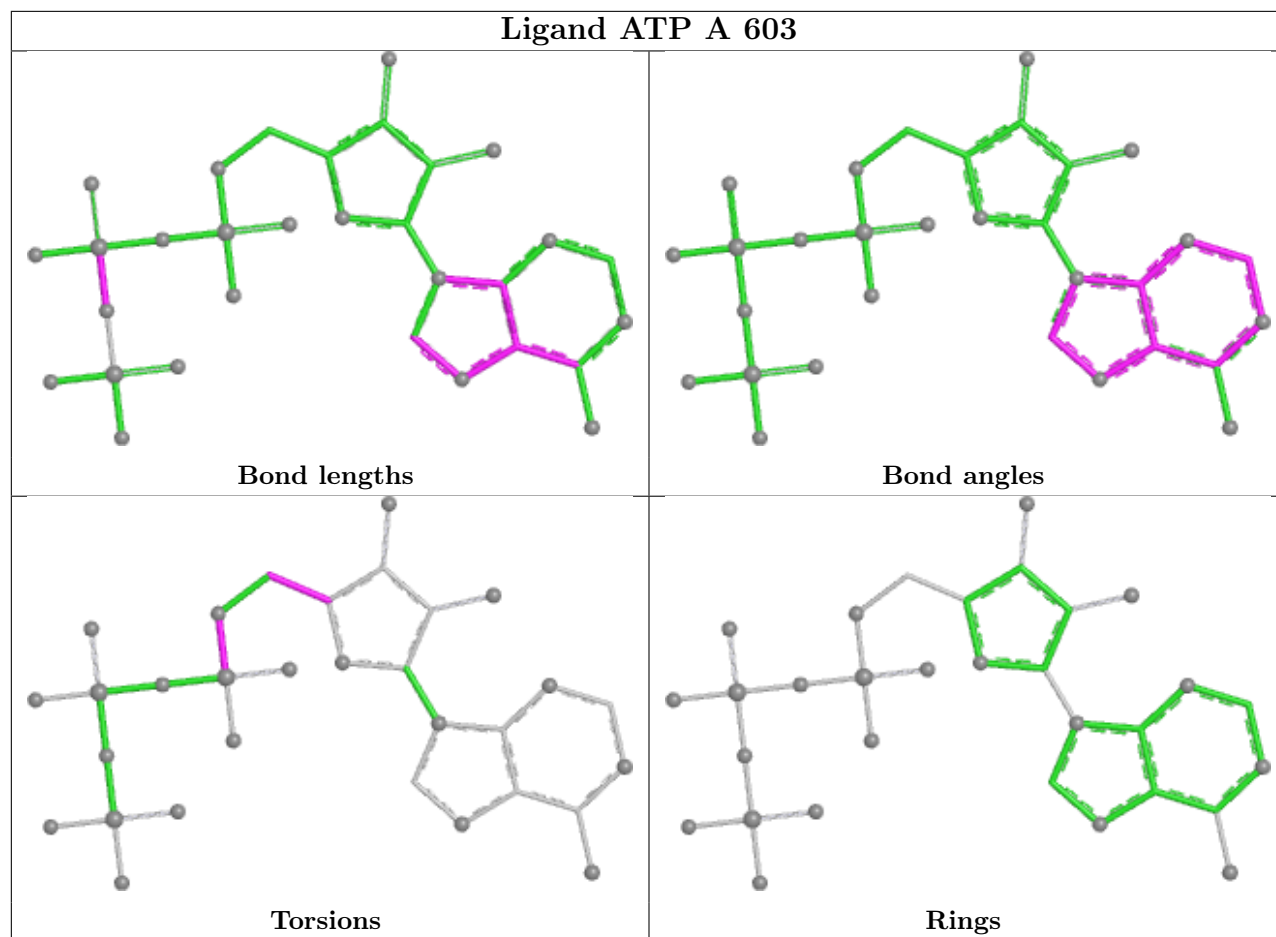
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	600	ADP	1	0

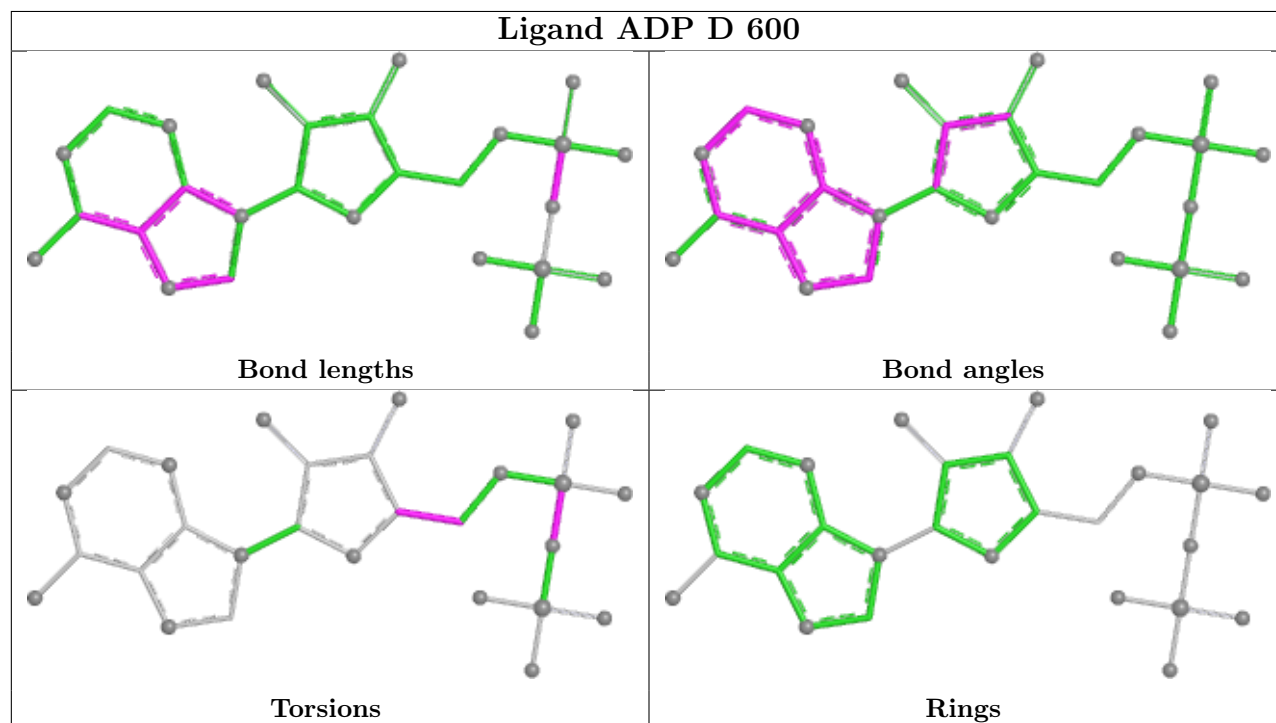
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

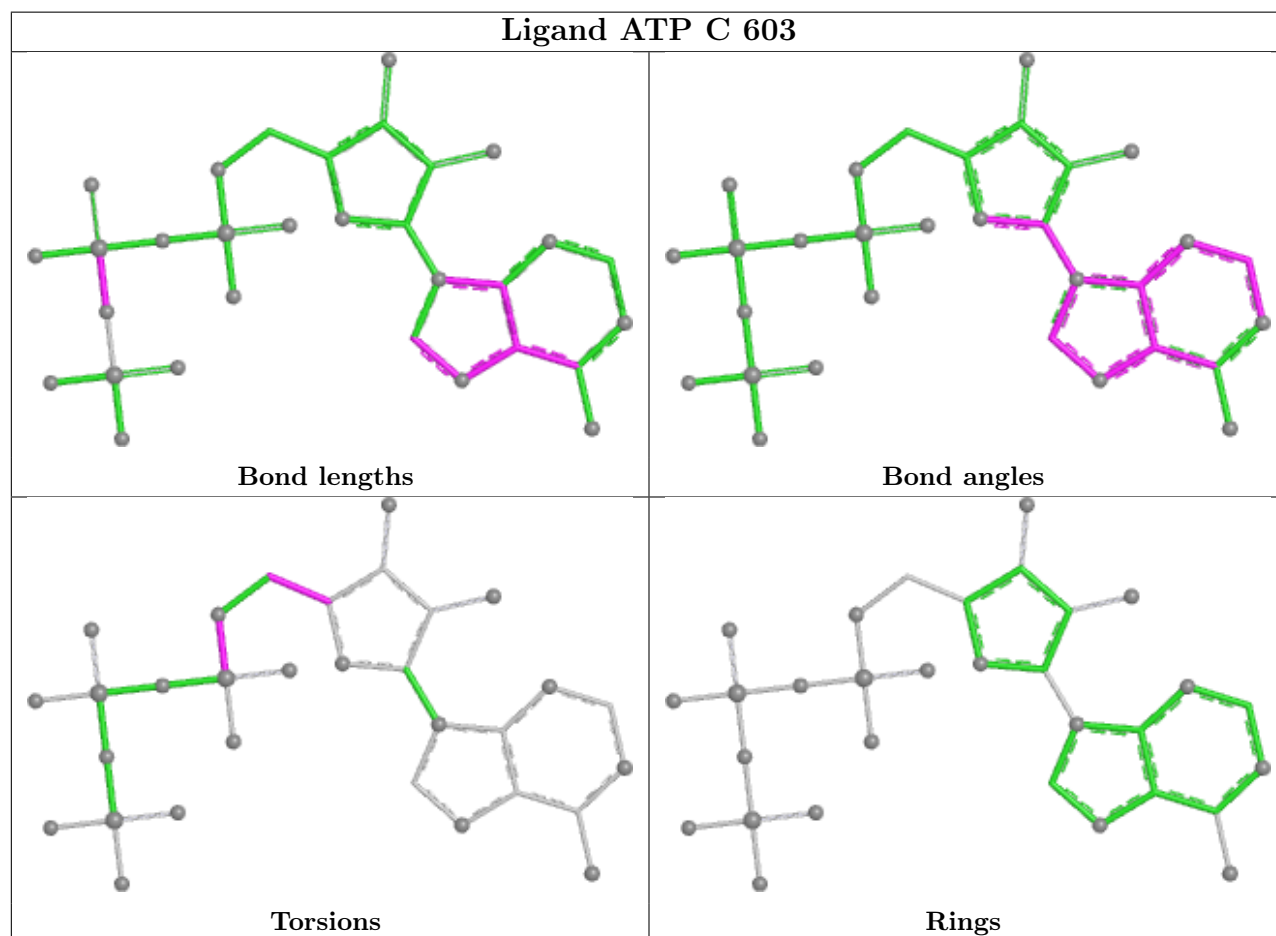
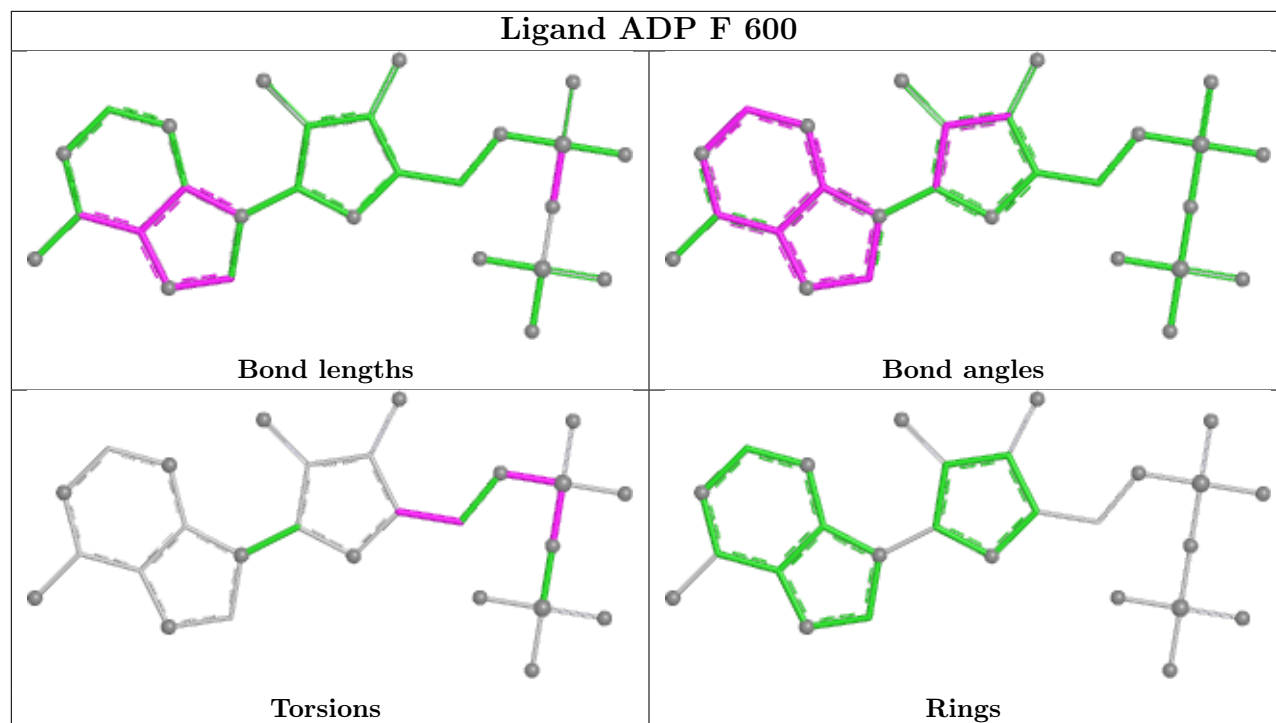


Ligand ATP A 603

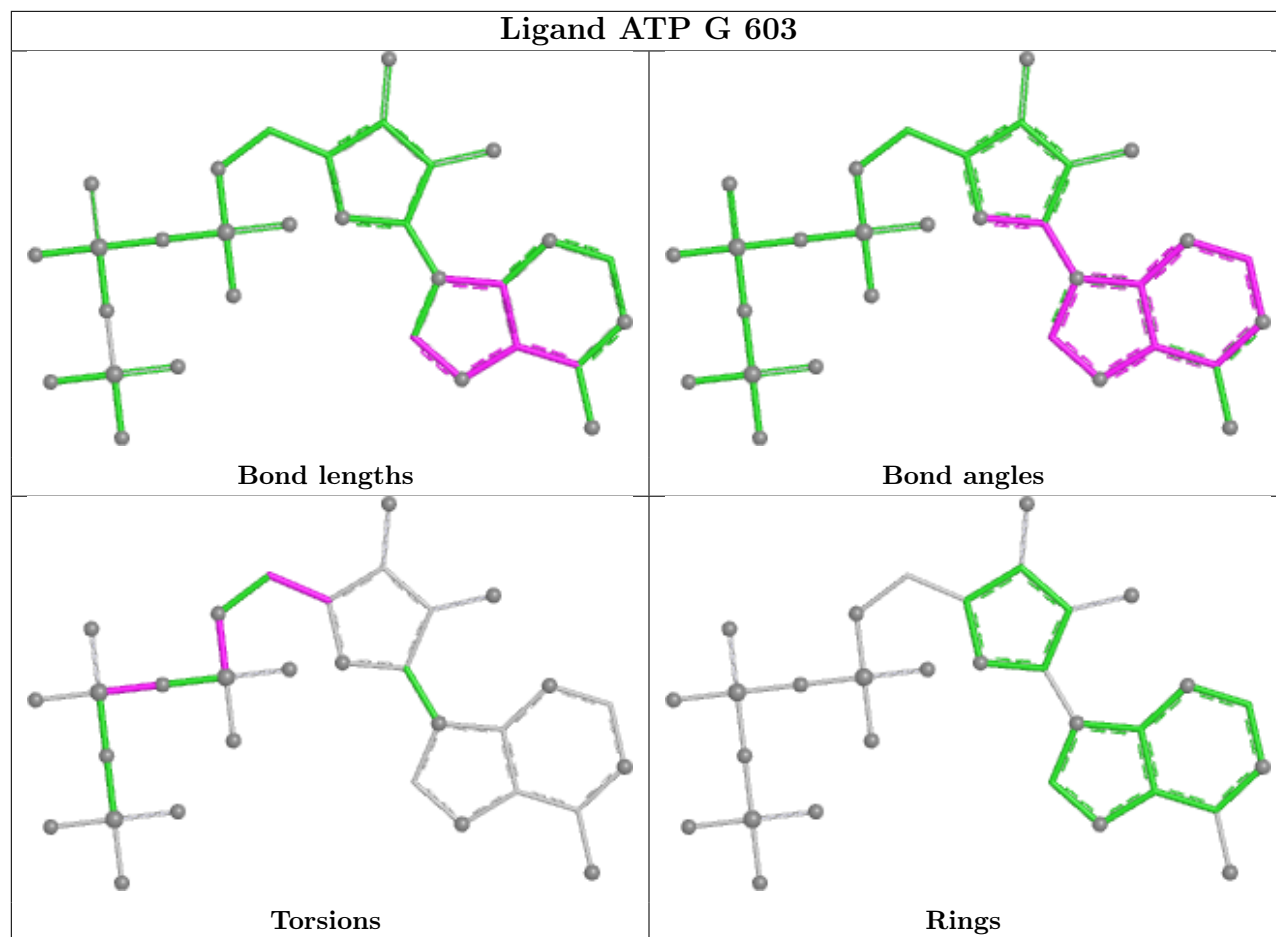


Ligand ADP D 600

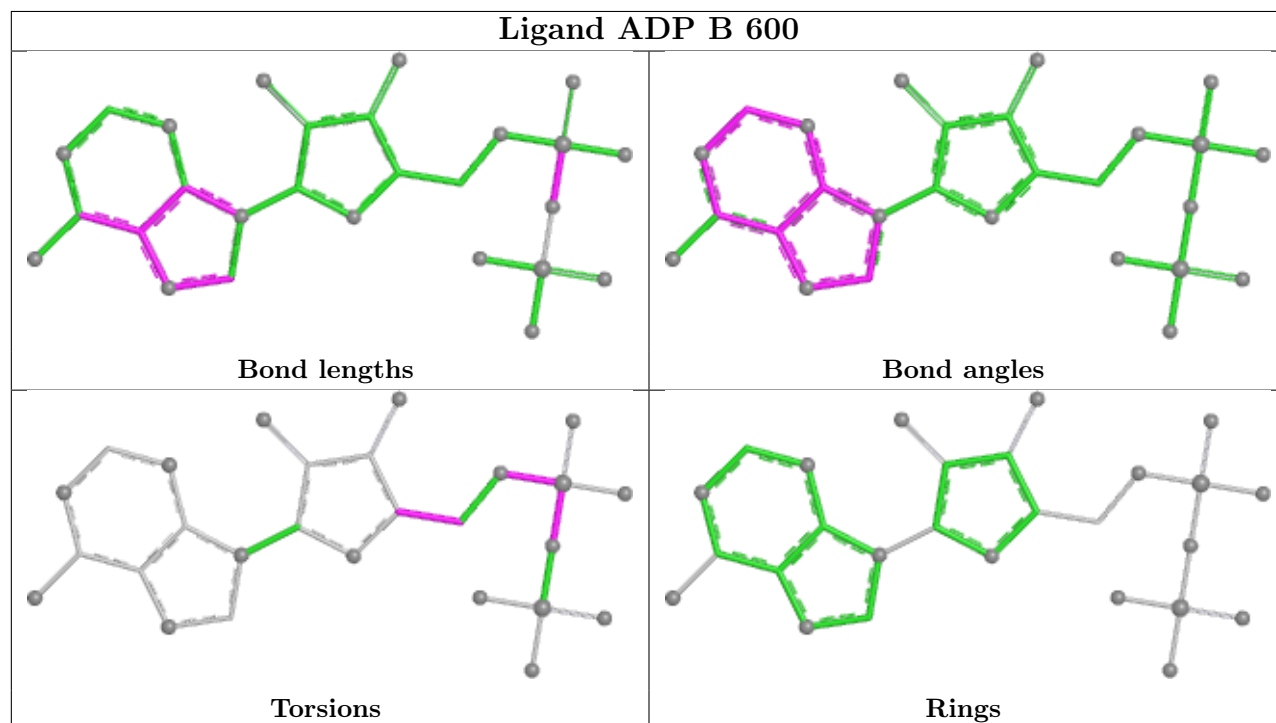




Ligand ATP G 603



Ligand ADP B 600



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%)	-0.37	0 100 100	92, 178, 285, 316	0
1	B	545/558 (97%)	-0.24	7 (1%) 75 47	97, 175, 272, 299	0
1	C	550/558 (98%)	-0.31	1 (0%) 91 80	97, 175, 247, 272	0
1	D	545/558 (97%)	-0.37	2 (0%) 88 69	89, 143, 195, 253	0
1	E	549/558 (98%)	-0.34	0 100 100	93, 170, 273, 303	0
1	F	544/558 (97%)	-0.29	0 100 100	100, 212, 309, 341	0
1	G	545/558 (97%)	-0.33	1 (0%) 91 80	89, 155, 211, 243	0
All	All	3828/3906 (98%)	-0.32	11 (0%) 90 74	89, 166, 279, 341	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	LEU	4.5
1	D	84	CYS	4.0
1	B	305	MET	3.6
1	B	217	PHE	2.9
1	D	483	ALA	2.6
1	G	84	CYS	2.6
1	B	192	ARG	2.6
1	B	283	LEU	2.5
1	B	223	ILE	2.2
1	C	283	LEU	2.1
1	B	356	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

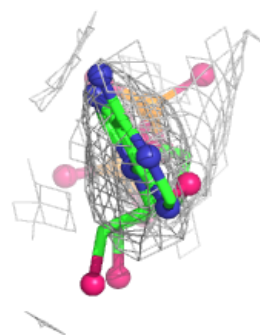
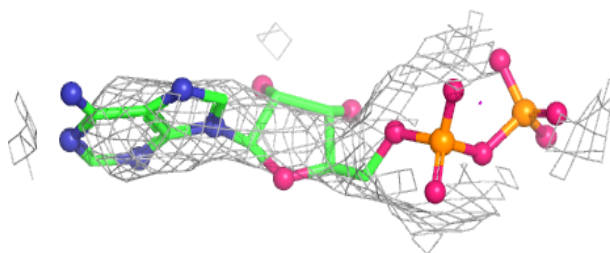
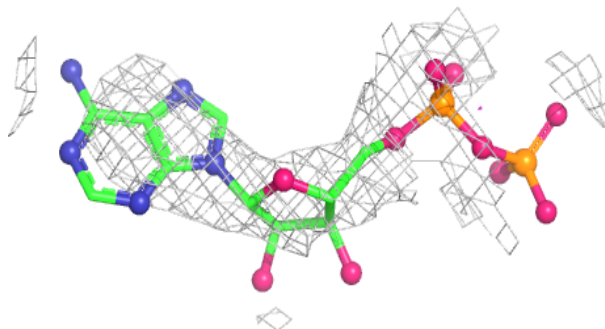
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	K	C	602	1/1	0.80	0.11	164,164,164,164	0
2	MG	A	601	1/1	0.83	0.13	124,124,124,124	0
3	K	G	602	1/1	0.83	0.11	157,157,157,157	0
5	ADP	D	600	27/27	0.87	0.08	181,192,210,213	0
5	ADP	F	600	27/27	0.88	0.10	176,187,197,199	0
5	ADP	B	600	27/27	0.91	0.08	175,190,200,206	0
2	MG	G	601	1/1	0.92	0.05	107,107,107,107	0
2	MG	E	601	1/1	0.92	0.07	126,126,126,126	0
3	K	A	602	1/1	0.94	0.12	150,150,150,150	0
2	MG	C	601	1/1	0.94	0.03	133,133,133,133	0
4	ATP	G	603	31/31	0.95	0.07	101,111,155,160	0
4	ATP	A	603	31/31	0.95	0.06	108,121,147,150	0
4	ATP	C	603	31/31	0.95	0.07	106,115,155,157	0
4	ATP	E	603	31/31	0.95	0.06	110,119,144,146	0
3	K	E	602	1/1	0.97	0.04	148,148,148,148	0

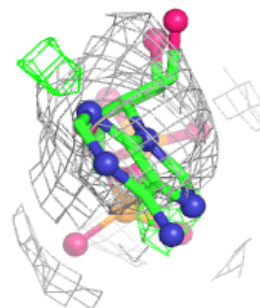
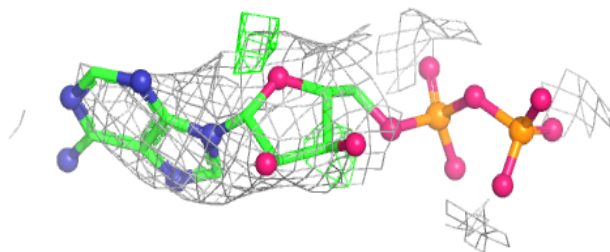
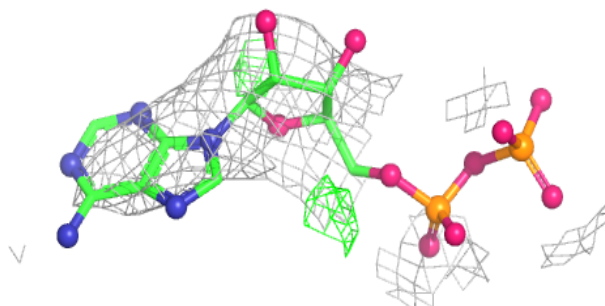
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

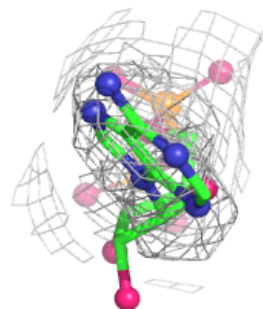
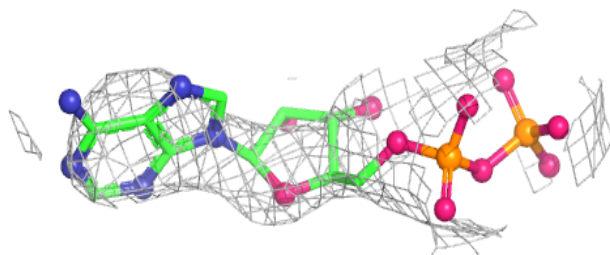
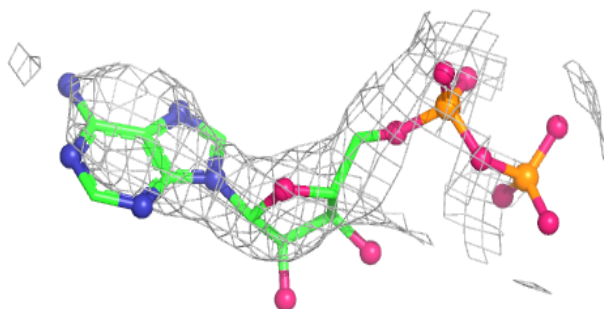
**Electron density around ADP F 600:**

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

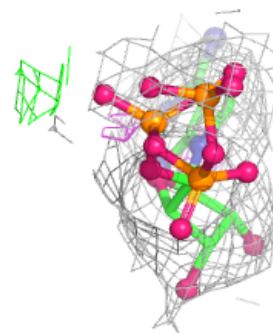
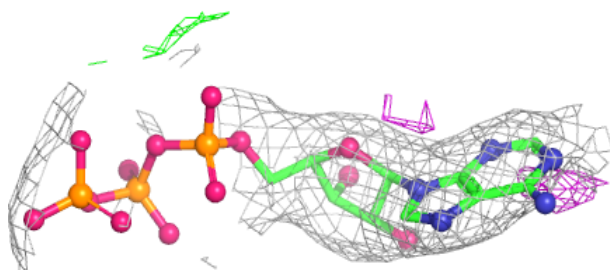
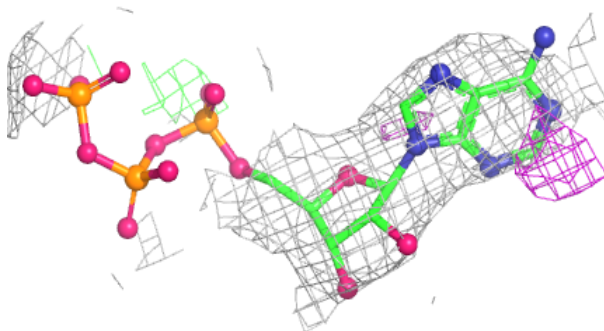


Electron density around ADP B 600:

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

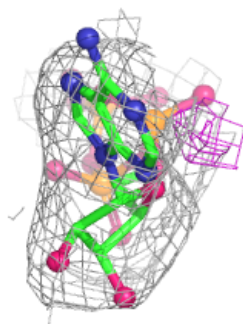
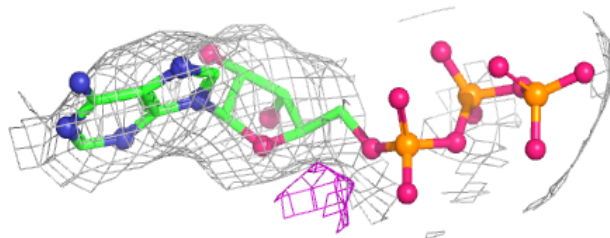
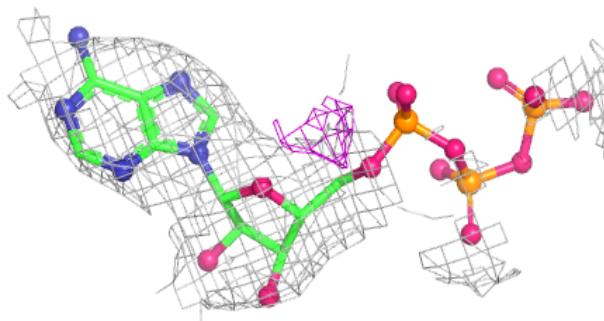
**Electron density around ATP G 603:**

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

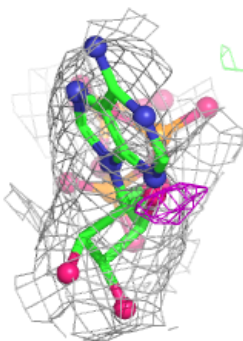
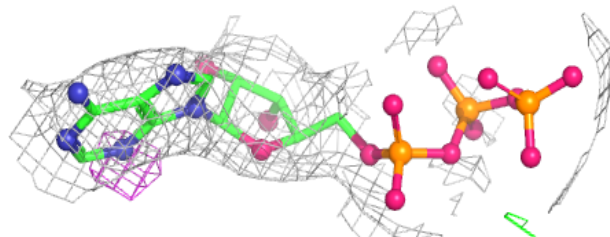
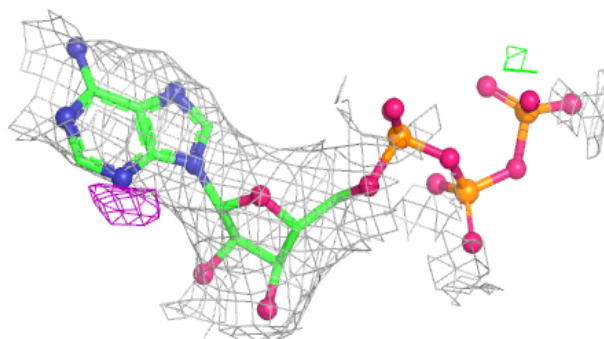


Electron density around ATP A 603:

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

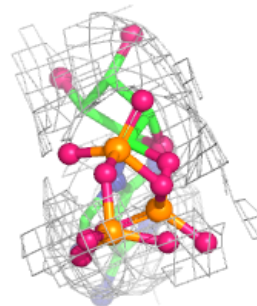
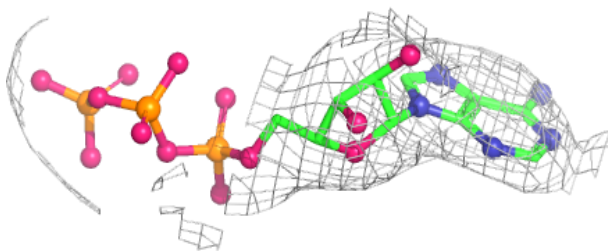
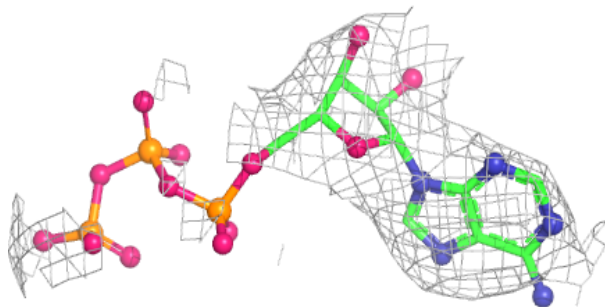
**Electron density around ATP C 603:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.