



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 6QV0 / pdb_00006qv0
Title : Structure of ATP-bound outward-facing TM287/288 in complex with sybody
Sb_TM35
Authors : Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.
Deposited on : 2019-03-01
Resolution : 3.12 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:

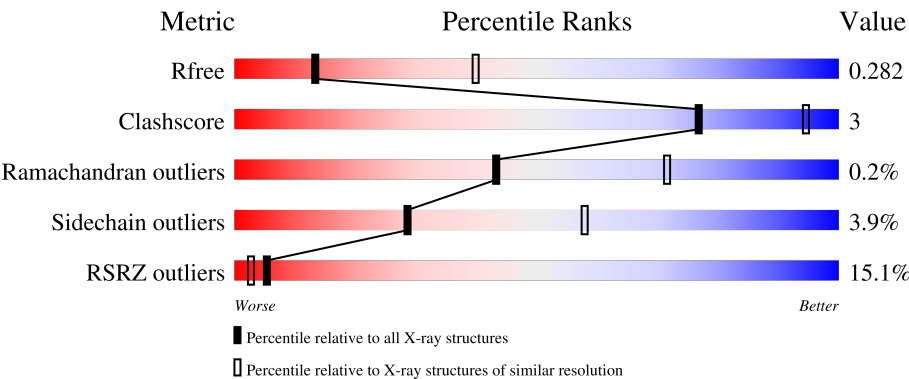
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.12 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	587	12% 83% 13% ..
1	C	587	13% 84% 12% .
2	B	599	12% 84% 10% . 5%
2	D	599	9% 84% 11% ..
3	E	128	45% 84% 10% ..

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Mol	Chain	Length	Quality of chain
3	F	128	41% 92% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20086 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 ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			
1	C	569	Total	C	N	O	S	0	0	0
			4470	2882	769	800	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3
A	41	ALA	ASP	engineered mutation	UNP Q9WYC3
C	-9	GLY	-	expression tag	UNP Q9WYC3
C	-8	PRO	-	expression tag	UNP Q9WYC3
C	-7	SER	-	expression tag	UNP Q9WYC3
C	-6	GLY	-	expression tag	UNP Q9WYC3
C	-5	SER	-	expression tag	UNP Q9WYC3
C	-4	GLY	-	expression tag	UNP Q9WYC3
C	-3	GLY	-	expression tag	UNP Q9WYC3
C	-2	GLY	-	expression tag	UNP Q9WYC3
C	-1	GLY	-	expression tag	UNP Q9WYC3
C	0	GLY	-	expression tag	UNP Q9WYC3
C	1	SER	-	expression tag	UNP Q9WYC3
C	41	ALA	ASP	engineered mutation	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			
2	D	574	Total	C	N	O	S	0	0	0
			4573	2957	772	830	14			

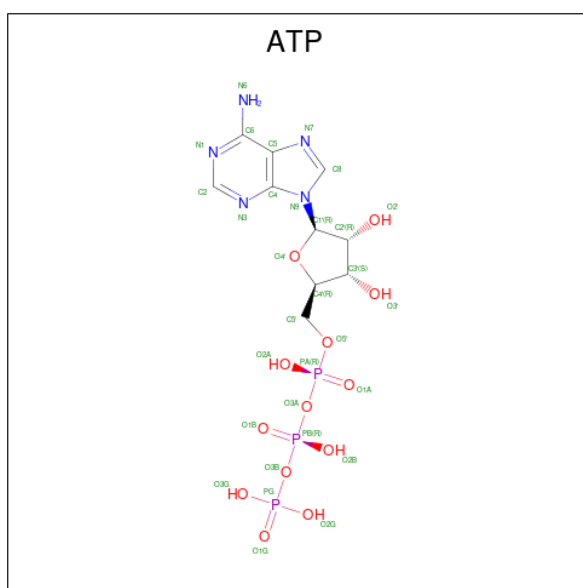
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ALA	ASP	engineered mutation	UNP Q9WYC4
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	65	ALA	ASP	engineered mutation	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Sb_TM35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			955	603	163	186	3			
3	F	124	Total	C	N	O	S	0	0	0
			955	603	163	186	3			

- 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	B	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	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

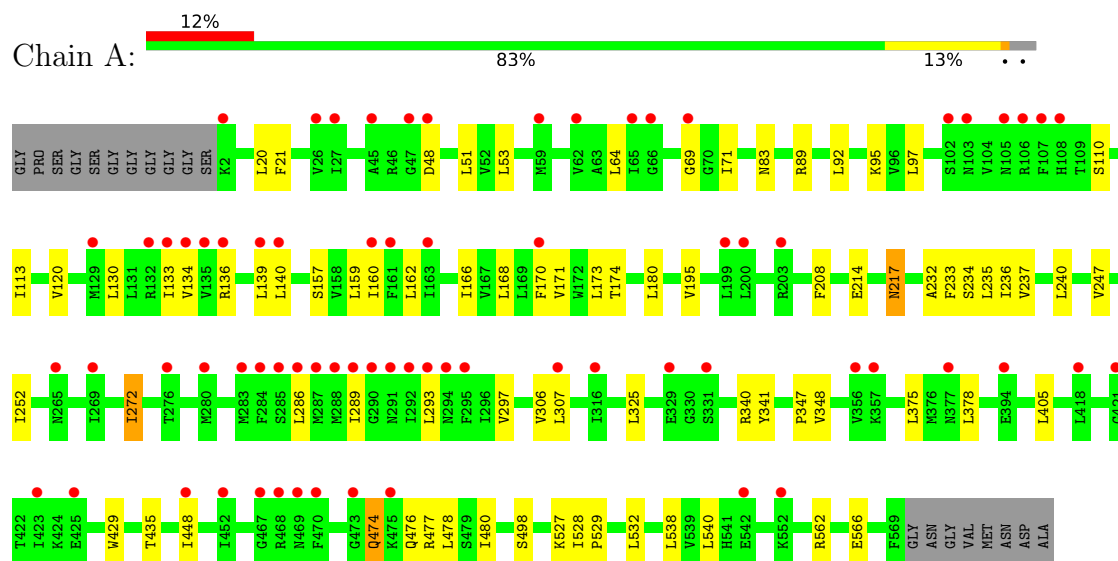
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

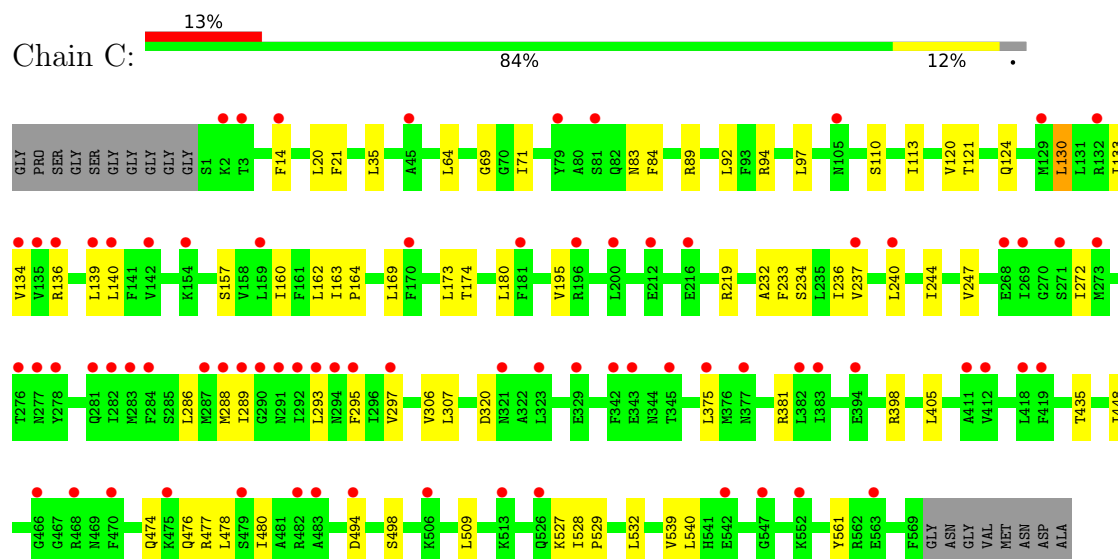
3 Residue-property plots [i](#)

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: ABC transporter, ATP-binding protein

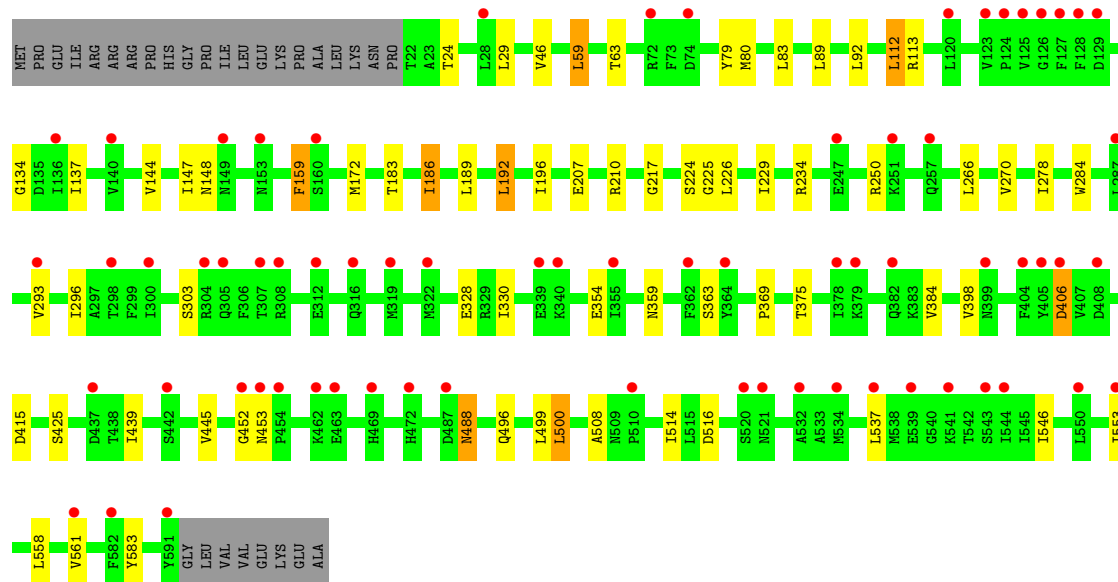


- Molecule 1: ABC transporter, ATP-binding protein



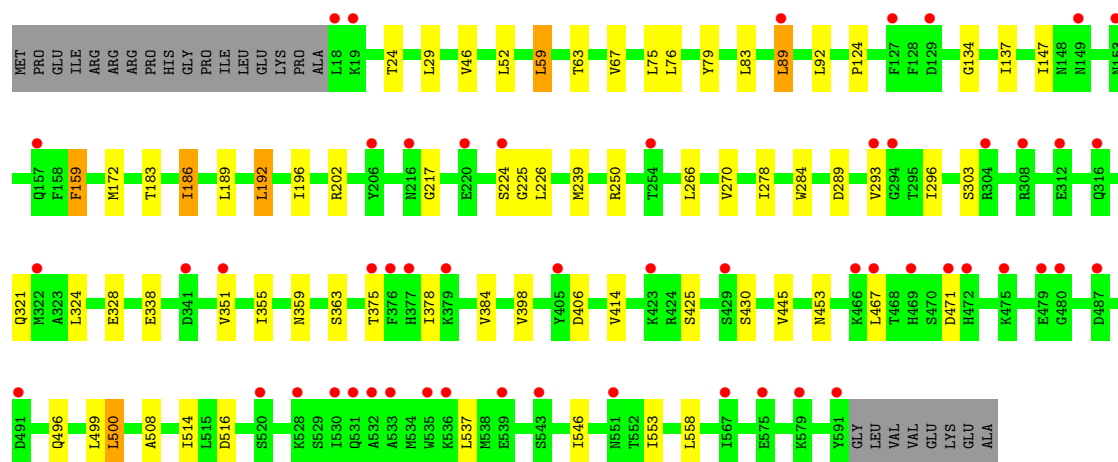
- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain B: 12% 84% 10% 5%



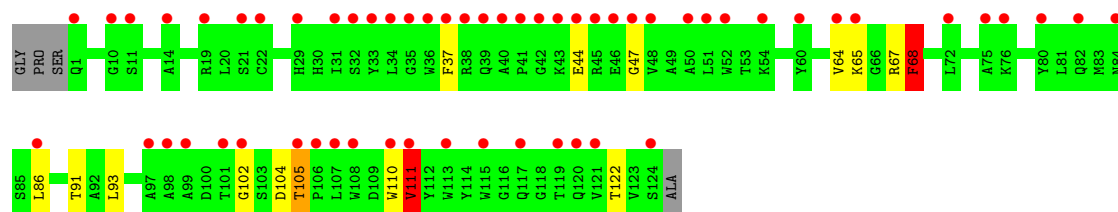
- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain D: 9% 84% 11% ..

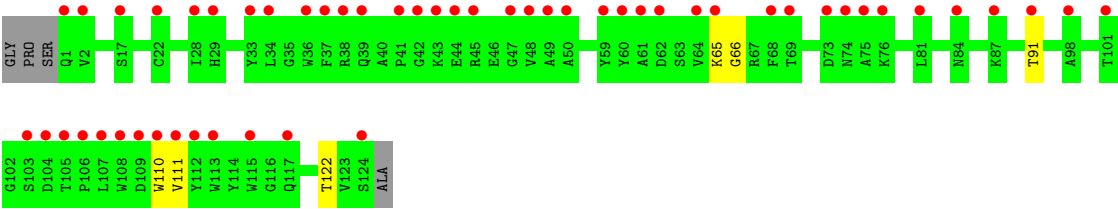
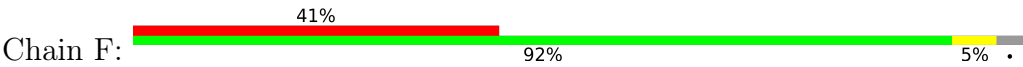


- Molecule 3: Sb_TM35

Chain E: 45% 84% 10% ..



- Molecule 3: Sb_TM35



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	166.28Å 77.29Å 207.18Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	49.19 – 3.12 49.19 – 3.12	Depositor EDS
% Data completeness (in resolution range)	62.9 (49.19-3.12) 63.1 (49.19-3.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.244 , 0.264 0.262 , 0.282	Depositor DCC
R_{free} test set	2797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	20086	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	1/4539 (0.0%)	1.37	9/6139 (0.1%)
1	C	0.77	1/4545 (0.0%)	1.36	5/6147 (0.1%)
2	B	0.76	0/4619	1.37	5/6245 (0.1%)
2	D	0.76	0/4652	1.39	8/6290 (0.1%)
3	E	0.70	0/981	1.04	1/1337 (0.1%)
3	F	0.70	0/981	1.05	0/1337
All	All	0.76	2/20317 (0.0%)	1.34	28/27495 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	ILE	CA-CB	5.21	1.57	1.54
1	C	528	ILE	CA-CB	5.19	1.57	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186	ILE	CA-C-N	6.92	125.87	120.33
2	B	186	ILE	C-N-CA	6.92	125.87	120.33
2	D	186	ILE	CA-C-N	6.89	125.84	120.33
2	D	186	ILE	C-N-CA	6.89	125.84	120.33
1	C	527	LYS	CA-C-N	6.85	125.81	120.33
1	C	527	LYS	C-N-CA	6.85	125.81	120.33
1	A	527	LYS	CA-C-N	6.80	125.77	120.33
1	A	527	LYS	C-N-CA	6.80	125.77	120.33
1	A	378	LEU	CA-C-N	6.75	125.73	120.33
1	A	378	LEU	C-N-CA	6.75	125.73	120.33
3	E	68	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	171	VAL	N-CA-C	-6.15	106.52	111.81
1	A	170	PHE	CA-CB-CG	5.79	119.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	471	ASP	CA-C-N	5.76	128.31	120.54
2	D	471	ASP	C-N-CA	5.76	128.31	120.54
2	D	406	ASP	CA-C-N	5.64	128.28	120.49
2	D	406	ASP	C-N-CA	5.64	128.28	120.49
2	B	406	ASP	CA-C-N	5.63	128.26	120.49
2	B	406	ASP	C-N-CA	5.63	128.26	120.49
1	A	48	ASP	CA-CB-CG	5.49	118.09	112.60
2	D	289	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	48	ASP	CA-C-N	5.14	127.68	120.28
1	A	48	ASP	C-N-CA	5.14	127.68	120.28
2	D	159	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	164	PRO	N-CA-C	5.09	116.92	110.70
1	C	84	PHE	CA-C-N	5.07	125.57	119.94
1	C	84	PHE	C-N-CA	5.07	125.57	119.94
2	B	159	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4464	0	4666	32	0
1	C	4470	0	4674	25	0
2	B	4541	0	4725	33	0
2	D	4573	0	4762	31	0
3	E	955	0	895	7	0
3	F	955	0	895	3	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20086	0	20665	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (118) 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)
3:E:102:GLY:H	3:E:111:VAL:HG11	1.51	0.73
2:B:46:VAL:HG11	2:B:159:PHE:HB3	1.72	0.71
2:D:46:VAL:HG11	2:D:159:PHE:HB3	1.72	0.71
2:D:284:TRP:HH2	3:F:110:TRP:HA	1.65	0.62
1:A:562:ARG:O	1:A:566:GLU:HG2	2.03	0.59
1:C:130:LEU:O	1:C:134:VAL:HB	2.04	0.57
1:A:83:ASN:HD21	2:B:250:ARG:HH21	1.53	0.56
3:F:91:THR:HG23	3:F:122:THR:HA	1.87	0.56
3:E:91:THR:HG23	3:E:122:THR:HA	1.88	0.56
2:B:359:ASN:H	2:B:375:THR:HB	1.71	0.54
2:B:439:ILE:HG23	2:B:488:ASN:HD21	1.72	0.54
2:D:359:ASN:H	2:D:375:THR:HB	1.72	0.54
1:A:133:ILE:HG22	1:A:136:ARG:HD3	1.89	0.53
2:B:112:LEU:HD23	2:B:330:ILE:HG21	1.90	0.53
2:B:384:VAL:HG22	2:B:558:LEU:HB3	1.91	0.53
2:D:384:VAL:HG22	2:D:558:LEU:HB3	1.91	0.53
3:E:37:PHE:HD1	3:E:47:GLY:HA2	1.74	0.53
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.90	0.52
1:C:21:PHE:HD2	1:C:69:GLY:HA2	1.74	0.52
1:A:234:SER:HA	1:A:237:VAL:HG22	1.91	0.52
2:B:284:TRP:HE1	3:E:110:TRP:HB3	1.74	0.51
1:A:21:PHE:HD1	1:A:69:GLY:HA2	1.76	0.51
1:C:133:ILE:HG22	1:C:136:ARG:HD3	1.93	0.51
2:D:445:VAL:HG13	2:D:500:LEU:HD21	1.93	0.51
1:A:341:TYR:HD1	1:A:348:VAL:HG21	1.76	0.50
1:C:234:SER:HA	1:C:237:VAL:HG22	1.92	0.50
2:D:516:ASP:HA	2:D:546:ILE:HB	1.95	0.49
1:A:180:LEU:HB3	1:A:232:ALA:HB2	1.93	0.49
1:A:474:GLN:HE22	4:B:600:ATP:H3'	1.78	0.49
1:C:160:ILE:HA	1:C:163:ILE:HD12	1.94	0.49
2:B:59:LEU:HB3	2:B:83:LEU:HD13	1.95	0.49
1:C:180:LEU:HB3	1:C:232:ALA:HB2	1.93	0.49
2:D:59:LEU:HB3	2:D:83:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.94	0.49
2:D:355:ILE:HG13	2:D:378:ILE:HB	1.94	0.49
1:A:476:GLN:HE22	1:A:498:SER:H	1.61	0.48
2:B:516:ASP:HA	2:B:546:ILE:HB	1.95	0.48
1:C:83:ASN:HD21	2:D:250:ARG:HH21	1.61	0.48
2:B:172:MET:HE3	2:B:303:SER:HA	1.95	0.48
2:D:172:MET:HE3	2:D:303:SER:HA	1.94	0.48
1:A:340:ARG:HG3	1:A:347:PRO:HA	1.95	0.48
1:A:477:ARG:HA	1:A:480:ILE:HD12	1.95	0.48
1:C:477:ARG:HA	1:C:480:ILE:HD12	1.95	0.48
2:B:113:ARG:HG3	2:B:144:VAL:HG11	1.96	0.47
1:C:195:VAL:HG13	2:D:137:ILE:HG12	1.94	0.47
1:A:97:LEU:HA	2:B:226:LEU:HD11	1.96	0.47
1:A:162:LEU:O	1:A:166:ILE:HG12	2.15	0.47
1:A:195:VAL:HG13	2:B:137:ILE:HG12	1.96	0.47
1:C:97:LEU:HA	2:D:226:LEU:HD11	1.95	0.47
1:C:539:VAL:HG21	1:C:561:TYR:HD2	1.80	0.47
1:C:94:ARG:HE	2:D:239:MET:HE2	1.80	0.47
1:A:208:PHE:HB3	2:B:452:GLY:HA2	1.98	0.46
2:B:398:VAL:HG13	2:B:514:ILE:HD13	1.96	0.46
2:D:398:VAL:HG13	2:D:514:ILE:HD13	1.97	0.46
1:C:529:PRO:HA	1:C:532:LEU:HD12	1.98	0.46
2:D:202:ARG:HB2	2:D:321:GLN:HE21	1.81	0.46
1:C:157:SER:HA	1:C:160:ILE:HD12	1.98	0.45
1:A:529:PRO:HA	1:A:532:LEU:HD12	1.98	0.45
2:B:63:THR:HG22	2:B:79:TYR:HB3	1.99	0.45
3:E:105:THR:HG21	3:E:111:VAL:HG22	1.99	0.44
1:A:92:LEU:HD11	1:A:306:VAL:HG13	1.98	0.44
1:C:110:SER:HA	1:C:113:ILE:HD12	1.99	0.44
2:D:496:GLN:HA	2:D:499:LEU:HD12	2.00	0.44
2:B:207:GLU:HA	2:B:210:ARG:HG2	2.00	0.44
1:A:286:LEU:HA	1:A:289:ILE:HD12	1.99	0.43
2:B:445:VAL:HG13	2:B:500:LEU:HD21	1.99	0.43
1:A:130:LEU:O	1:A:134:VAL:HB	2.18	0.43
2:B:144:VAL:O	2:B:147:ILE:HG13	2.18	0.43
1:A:341:TYR:CD1	1:A:348:VAL:HG21	2.53	0.43
1:A:429:TRP:HH2	2:B:229:ILE:HG12	1.83	0.43
2:B:192:LEU:O	2:B:196:ILE:HG12	2.18	0.43
1:C:286:LEU:HA	1:C:289:ILE:HD12	1.99	0.43
2:D:183:THR:HG23	2:D:278:ILE:HG21	2.01	0.43
1:A:375:LEU:HD22	1:A:540:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:THR:HG21	2:B:328:GLU:HG2	2.00	0.43
2:B:496:GLN:HA	2:B:499:LEU:HD12	2.00	0.43
2:D:63:THR:HG22	2:D:79:TYR:HB3	2.00	0.43
1:A:110:SER:HA	1:A:113:ILE:HD12	2.00	0.43
1:A:429:TRP:CE3	2:B:234:ARG:HG3	2.54	0.43
2:D:355:ILE:HG22	2:D:414:VAL:HG22	2.00	0.43
1:A:89:ARG:HG3	1:A:120:VAL:HG11	2.01	0.42
1:A:252:ILE:HG23	2:B:80:MET:HG2	2.01	0.42
1:C:476:GLN:HE22	1:C:498:SER:H	1.66	0.42
2:D:192:LEU:O	2:D:196:ILE:HG12	2.19	0.42
2:D:67:VAL:HG11	2:D:76:LEU:HB2	2.00	0.42
1:C:89:ARG:HG3	1:C:120:VAL:HG11	2.01	0.42
2:B:183:THR:HG23	2:B:278:ILE:HG21	2.01	0.42
1:C:92:LEU:HD11	1:C:306:VAL:HG13	2.00	0.42
2:B:134:GLY:HA3	2:B:217:GLY:HA2	2.02	0.42
3:E:64:VAL:HG13	3:E:68:PHE:H	1.84	0.42
2:D:189:LEU:HD23	2:D:270:VAL:HG13	2.02	0.42
2:D:24:THR:HG21	2:D:328:GLU:HG2	2.00	0.42
1:A:214:GLU:HA	1:A:217:ASN:HB2	2.02	0.41
1:A:272:ILE:H	1:A:272:ILE:HG13	1.62	0.41
2:B:189:LEU:HD23	2:B:270:VAL:HG13	2.02	0.41
2:B:354:GLU:HB3	2:B:415:ASP:HA	2.02	0.41
1:C:381:ARG:HH11	1:C:398:ARG:HD2	1.85	0.41
1:C:448:ILE:HG12	1:C:478:LEU:HG	2.02	0.41
3:E:67:ARG:HH21	3:E:86:LEU:HA	1.85	0.41
2:D:134:GLY:HA3	2:D:217:GLY:HA2	2.02	0.41
2:D:293:VAL:HA	2:D:296:ILE:HD12	2.03	0.41
2:B:293:VAL:HA	2:B:296:ILE:HD12	2.03	0.41
1:A:157:SER:HA	1:A:160:ILE:HD12	2.03	0.41
1:A:448:ILE:HG12	1:A:478:LEU:HG	2.02	0.41
2:B:453:ASN:HB2	2:B:508:ALA:HA	2.03	0.41
1:C:174:THR:HA	1:C:297:VAL:HG11	2.02	0.41
2:D:52:LEU:HD11	2:D:89:LEU:HD23	2.03	0.41
2:D:351:VAL:HG11	2:D:430:SER:HB3	2.03	0.41
1:C:121:THR:HA	1:C:124:GLN:HG2	2.02	0.40
2:D:124:PRO:HD3	2:D:338:GLU:HA	2.03	0.40
2:D:202:ARG:HH22	2:D:324:LEU:HD22	1.86	0.40
2:D:378:ILE:HG12	2:D:384:VAL:HG21	2.02	0.40
2:B:363:SER:HB2	2:B:369:PRO:HA	2.03	0.40
2:B:561:VAL:HG21	2:B:583:TYR:HB2	2.04	0.40
1:C:375:LEU:HD22	1:C:540:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:ASN:HB2	2:D:508:ALA:HA	2.02	0.40
3:F:65:LYS:HB3	3:F:66:GLY:H	1.74	0.40
1:A:174:THR:HA	1:A:297:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

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	566/587 (96%)	549 (97%)	17 (3%)	0	100	100
1	C	567/587 (97%)	548 (97%)	19 (3%)	0	100	100
2	B	568/599 (95%)	551 (97%)	16 (3%)	1 (0%)	43	71
2	D	572/599 (96%)	558 (98%)	13 (2%)	1 (0%)	43	71
3	E	122/128 (95%)	108 (88%)	10 (8%)	4 (3%)	3	16
3	F	122/128 (95%)	117 (96%)	5 (4%)	0	100	100
All	All	2517/2628 (96%)	2431 (97%)	80 (3%)	6 (0%)	43	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	111	VAL
3	E	44	GLU
3	E	65	LYS
3	E	104	ASP
2	B	225	GLY
2	D	225	GLY

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	494/503 (98%)	471 (95%)	23 (5%)	23	52
1	C	495/503 (98%)	469 (95%)	26 (5%)	20	49
2	B	506/531 (95%)	490 (97%)	16 (3%)	34	61
2	D	510/531 (96%)	494 (97%)	16 (3%)	35	62
3	E	97/99 (98%)	93 (96%)	4 (4%)	27	57
3	F	97/99 (98%)	96 (99%)	1 (1%)	68	77
All	All	2199/2266 (97%)	2113 (96%)	86 (4%)	28	58

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	51	LEU
1	A	53	LEU
1	A	64	LEU
1	A	71	ILE
1	A	95	LYS
1	A	139	LEU
1	A	140	LEU
1	A	159	LEU
1	A	168	LEU
1	A	173	LEU
1	A	217	ASN
1	A	235	LEU
1	A	240	LEU
1	A	247	VAL
1	A	272	ILE
1	A	293	LEU
1	A	307	LEU
1	A	325	LEU
1	A	405	LEU
1	A	435	THR
1	A	474	GLN

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Mol	Chain	Res	Type
1	A	538	LEU
2	B	29	LEU
2	B	59	LEU
2	B	89	LEU
2	B	92	LEU
2	B	112	LEU
2	B	148	ASN
2	B	186	ILE
2	B	192	LEU
2	B	224	SER
2	B	266	LEU
2	B	406	ASP
2	B	425	SER
2	B	488	ASN
2	B	500	LEU
2	B	537	LEU
2	B	553	ILE
1	C	14	PHE
1	C	20	LEU
1	C	35	LEU
1	C	64	LEU
1	C	71	ILE
1	C	130	LEU
1	C	139	LEU
1	C	140	LEU
1	C	162	LEU
1	C	169	LEU
1	C	173	LEU
1	C	219	ARG
1	C	240	LEU
1	C	244	ILE
1	C	247	VAL
1	C	272	ILE
1	C	288	MET
1	C	293	LEU
1	C	295	PHE
1	C	307	LEU
1	C	320	ASP
1	C	405	LEU
1	C	435	THR
1	C	474	GLN
1	C	494	ASP

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Mol	Chain	Res	Type
1	C	509	LEU
2	D	29	LEU
2	D	59	LEU
2	D	75	LEU
2	D	89	LEU
2	D	92	LEU
2	D	147	ILE
2	D	186	ILE
2	D	192	LEU
2	D	224	SER
2	D	266	LEU
2	D	363	SER
2	D	425	SER
2	D	467	LEU
2	D	500	LEU
2	D	537	LEU
2	D	553	ILE
3	E	68	PHE
3	E	93	LEU
3	E	105	THR
3	E	111	VAL
3	F	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	185	GLN
1	A	215	ASN
1	A	217	ASN
1	A	277	ASN
1	A	294	ASN
1	A	344	ASN
1	A	447	GLN
1	A	474	GLN
2	B	133	HIS
2	B	146	ASN
2	B	149	ASN
2	B	200	GLN
2	B	271	ASN
2	B	305	GLN
2	B	315	ASN

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Mol	Chain	Res	Type
2	B	590	GLN
1	C	83	ASN
1	C	264	ASN
1	C	277	ASN
1	C	294	ASN
2	D	20	ASN
2	D	133	HIS
2	D	146	ASN
2	D	149	ASN
2	D	208	ASN
2	D	257	GLN
2	D	268	ASN
2	D	271	ASN
2	D	315	ASN
2	D	321	GLN
2	D	453	ASN
2	D	494	GLN
2	D	590	GLN
3	E	27	ASN
3	E	39	GLN
3	E	77	ASN
3	E	84	ASN
3	F	27	ASN
3	F	82	GLN
3	F	84	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	600	5	32,33,33	0.31	0	48,52,52	0.38	0
4	ATP	B	600	5	32,33,33	0.27	0	48,52,52	0.42	0
4	ATP	D	600	5	32,33,33	0.26	0	48,52,52	0.44	0
4	ATP	C	600	5	32,33,33	0.28	0	48,52,52	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	600	5	-	9/22/38/38	0/3/3/3
4	ATP	B	600	5	-	4/22/38/38	0/3/3/3
4	ATP	D	600	5	-	3/22/38/38	0/3/3/3
4	ATP	C	600	5	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ATP	C5'-O5'-PA-O2A
4	C	600	ATP	PB-O3B-PG-O2G
4	A	600	ATP	O4'-C4'-C5'-O5'
4	A	600	ATP	C3'-C4'-C5'-O5'
4	C	600	ATP	PB-O3B-PG-O3G
4	B	600	ATP	PG-O3B-PB-O1B
4	B	600	ATP	PA-O3A-PB-O1B

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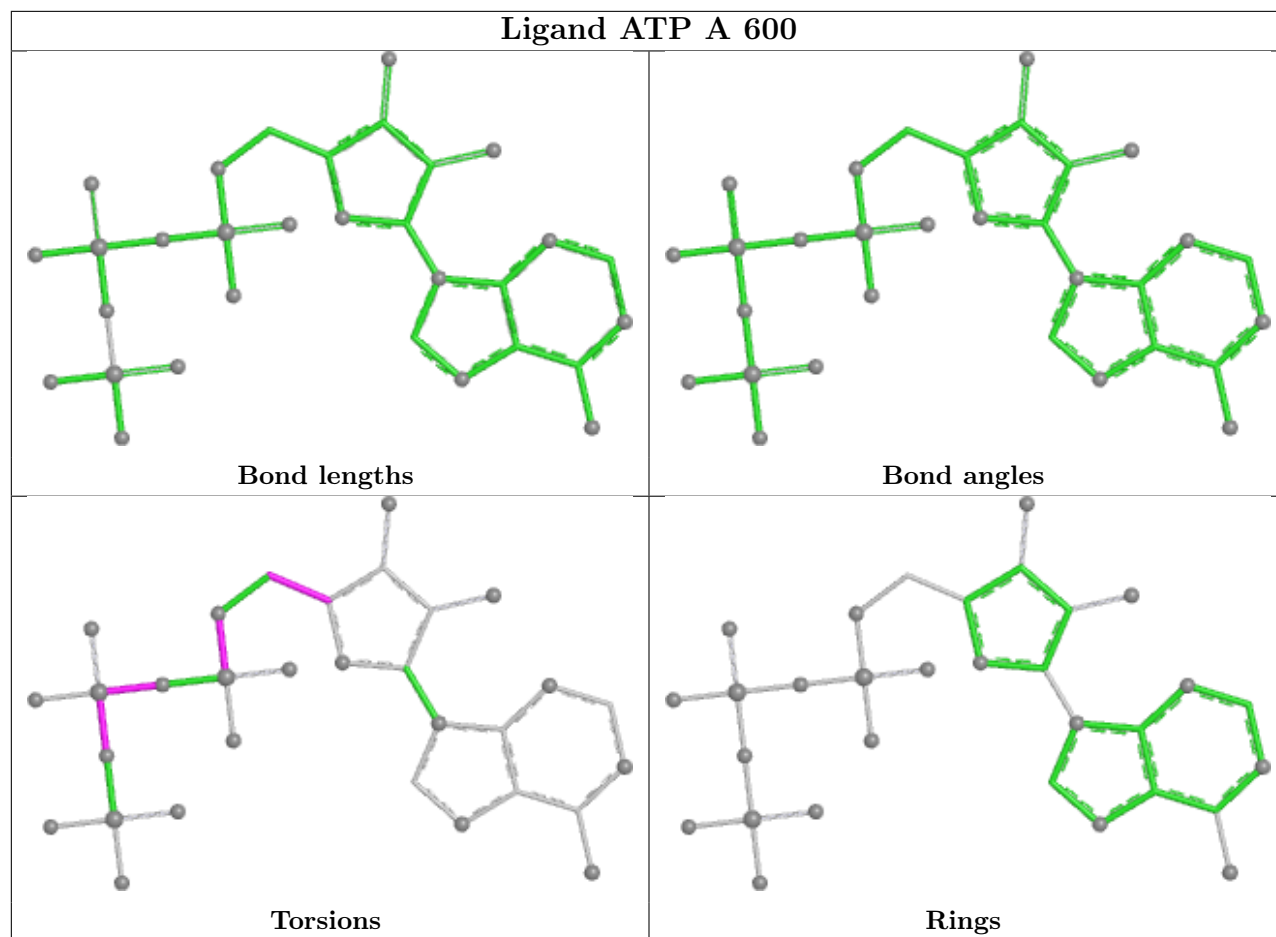
Mol	Chain	Res	Type	Atoms
4	C	600	ATP	PG-O3B-PB-O2B
4	D	600	ATP	PG-O3B-PB-O2B
4	A	600	ATP	C5'-O5'-PA-O1A
4	A	600	ATP	C5'-O5'-PA-O3A
4	A	600	ATP	PG-O3B-PB-O2B
4	D	600	ATP	PA-O3A-PB-O2B
4	A	600	ATP	PA-O3A-PB-O2B
4	C	600	ATP	PA-O3A-PB-O1B
4	C	600	ATP	PA-O3A-PB-O2B
4	D	600	ATP	PA-O3A-PB-O1B
4	C	600	ATP	PB-O3B-PG-O1G
4	A	600	ATP	PG-O3B-PB-O1B
4	A	600	ATP	PA-O3A-PB-O1B
4	B	600	ATP	PG-O3B-PB-O2B
4	B	600	ATP	PA-O3A-PB-O2B

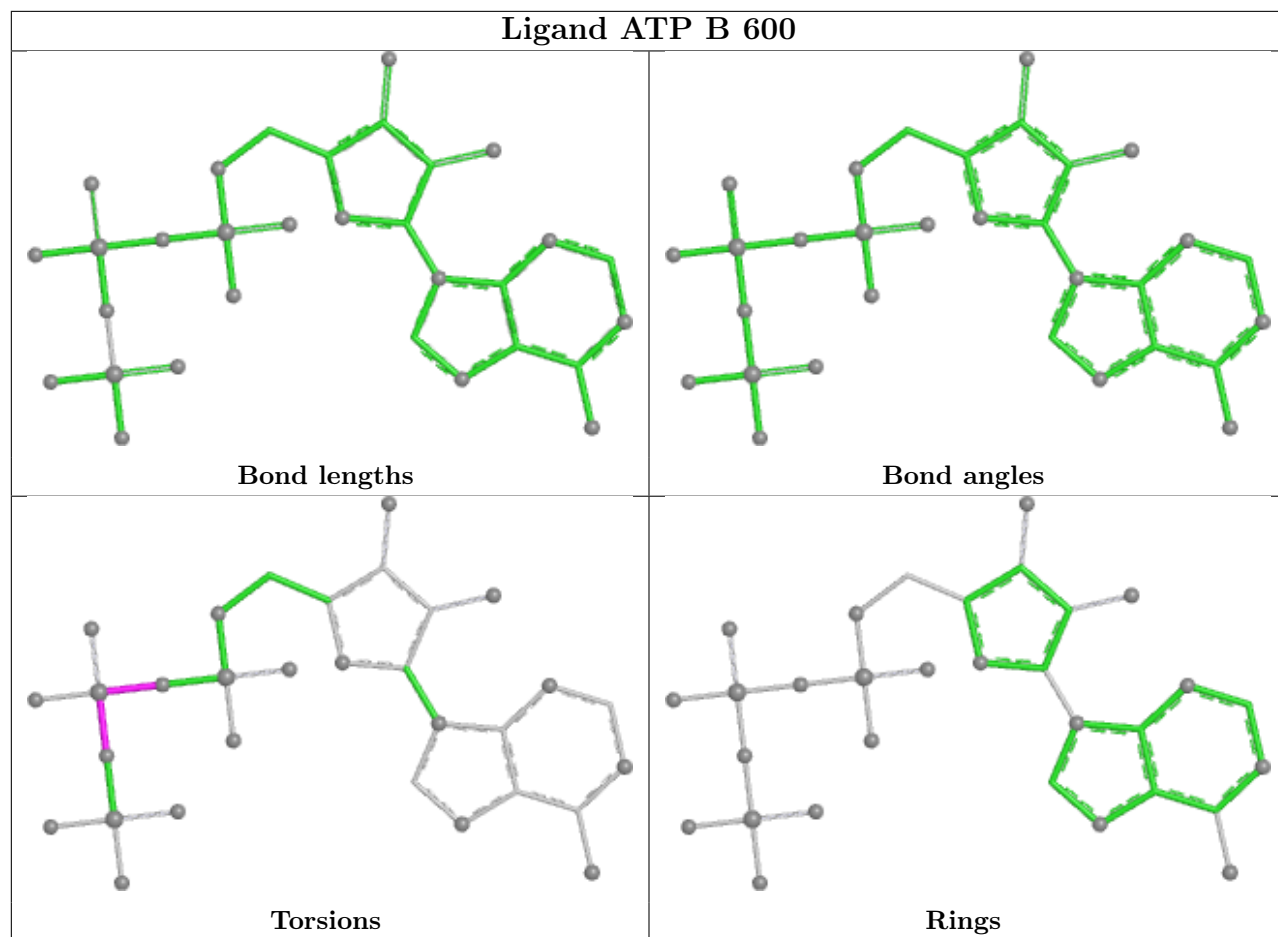
There are no ring outliers.

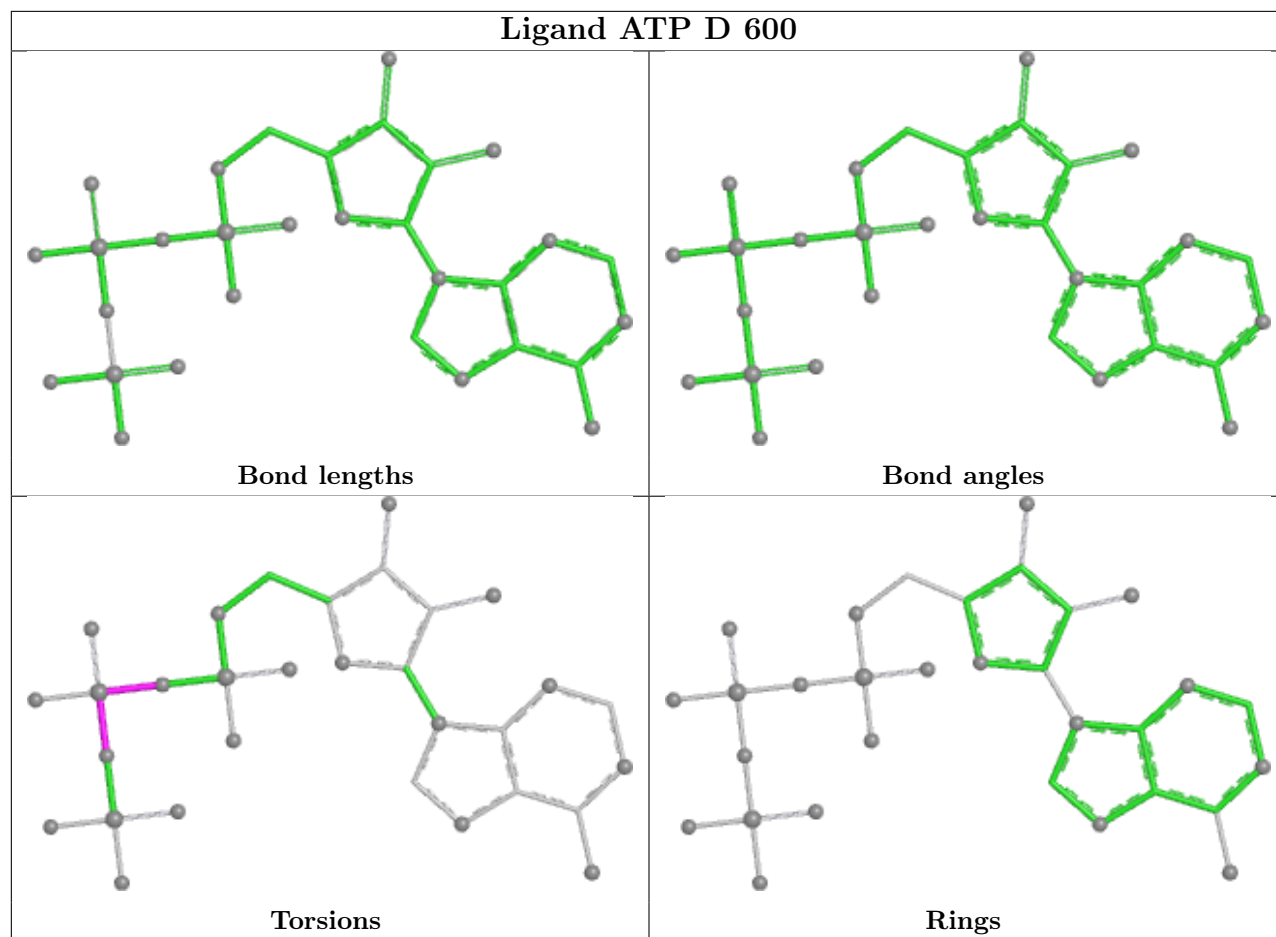
1 monomer is involved in 1 short contact:

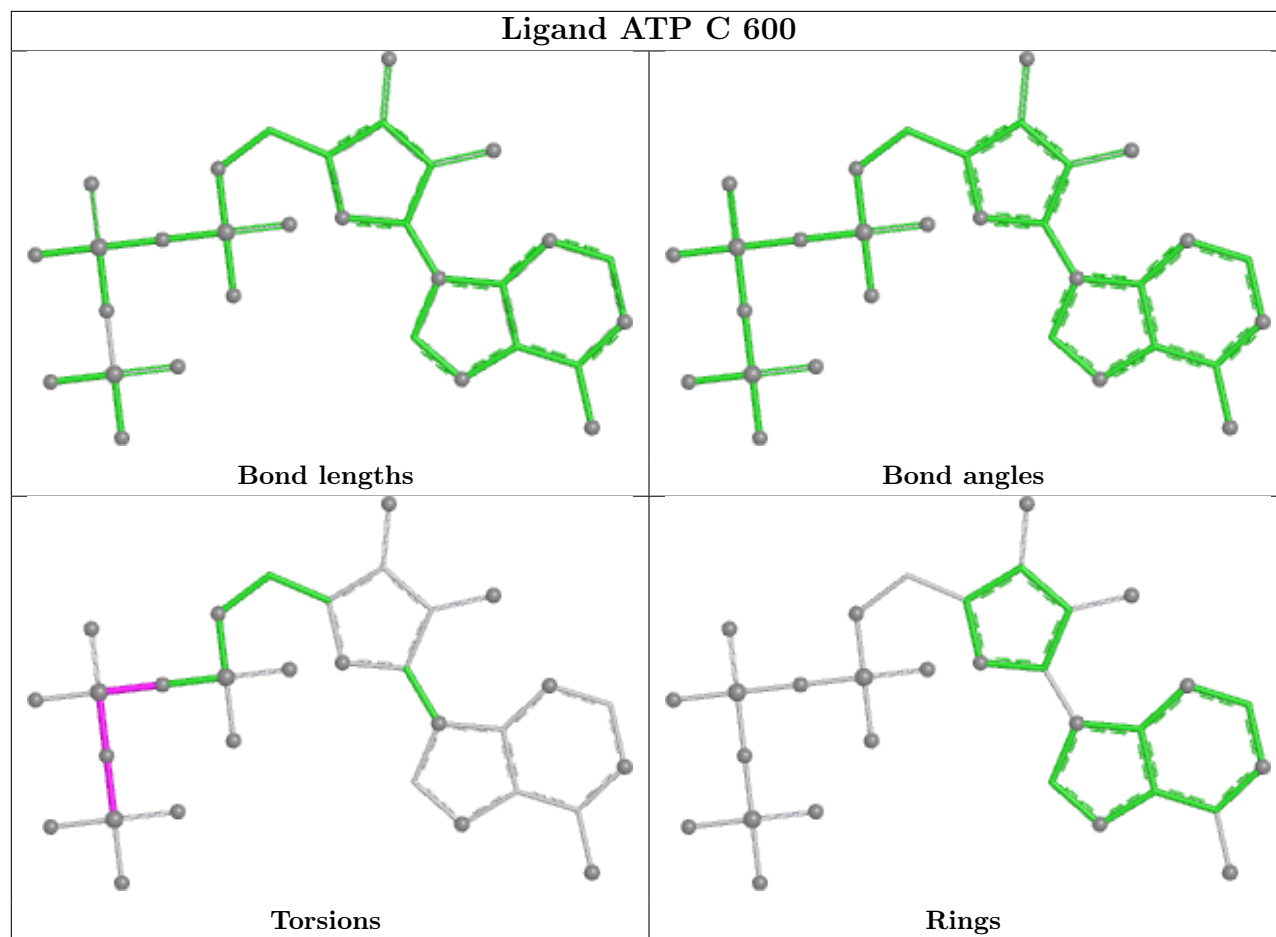
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	ATP	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	568/587 (96%)	0.85	71 (12%) 8 5	26, 54, 102, 126	0
1	C	569/587 (96%)	0.94	76 (13%) 7 4	33, 69, 113, 132	0
2	B	570/599 (95%)	0.86	69 (12%) 8 5	26, 63, 100, 129	0
2	D	574/599 (95%)	0.83	54 (9%) 14 8	32, 64, 91, 119	0
3	E	124/128 (96%)	2.21	58 (46%) 0 0	101, 131, 168, 180	0
3	F	124/128 (96%)	1.98	53 (42%) 0 0	89, 118, 147, 159	0
All	All	2529/2628 (96%)	0.99	381 (15%) 5 3	26, 66, 126, 180	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	42	GLY	7.5
3	F	60	TYR	7.3
1	A	105	ASN	6.9
3	E	11	SER	6.6
3	E	33	TYR	6.6
1	A	200	LEU	6.2
3	E	47	GLY	6.2
1	A	283	MET	6.2
2	D	153	ASN	6.1
3	F	111	VAL	6.1
3	E	43	LYS	6.1
1	A	293	LEU	6.0
1	C	200	LEU	5.9
1	A	292	ILE	5.9
1	A	470	PHE	5.7
2	B	339	GLU	5.7
1	C	294	ASN	5.7
1	A	475	LYS	5.6
1	A	288	MET	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	5.5
1	A	329	GLU	5.3
3	E	37	PHE	5.3
1	C	105	ASN	5.3
3	F	75	ALA	5.3
3	E	113	TRP	5.2
3	E	65	LYS	5.2
2	B	305	GLN	5.2
1	C	343	GLU	5.1
1	C	291	ASN	5.1
1	C	79	TYR	5.1
1	C	377	ASN	5.0
3	E	107	LEU	4.9
2	D	535	TRP	4.9
3	E	44	GLU	4.8
2	B	127	PHE	4.8
3	F	110	TRP	4.8
3	F	50	ALA	4.7
3	F	109	ASP	4.6
2	D	18	LEU	4.6
3	E	45	ARG	4.5
3	E	115	TRP	4.5
3	E	40	ALA	4.5
2	B	304	ARG	4.5
1	A	394	GLU	4.5
1	A	468	ARG	4.5
2	B	129	ASP	4.4
1	C	468	ARG	4.4
1	A	291	ASN	4.3
1	A	357	LYS	4.3
3	E	124	SER	4.3
2	D	591	TYR	4.2
2	B	399	ASN	4.2
3	F	68	PHE	4.2
3	E	14	ALA	4.2
3	F	108	TRP	4.2
1	A	542	GLU	4.1
1	C	212	GLU	4.1
2	B	308	ARG	4.1
3	E	46	GLU	4.1
1	C	329	GLU	4.1
2	B	442	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	102	SER	4.0
2	B	405	TYR	4.0
3	F	107	LEU	4.0
1	C	287	MET	3.8
2	D	157	GLN	3.8
2	B	406	ASP	3.8
2	D	528	LYS	3.8
2	B	463	GLU	3.8
2	B	553	ILE	3.8
1	A	467	GLY	3.8
1	C	479	SER	3.7
2	B	582	PHE	3.7
3	F	17	SER	3.7
1	C	2	LYS	3.7
2	B	307	THR	3.7
3	F	87	LYS	3.7
1	A	331	SER	3.7
2	B	469	HIS	3.6
2	B	251	LYS	3.6
3	F	59	TYR	3.6
1	C	283	MET	3.6
1	A	47	GLY	3.6
2	B	126	GLY	3.6
1	C	81	SER	3.6
1	A	45	ALA	3.6
3	F	124	SER	3.6
1	C	295	PHE	3.6
2	D	532	ALA	3.6
1	A	377	ASN	3.6
2	D	536	LYS	3.6
2	B	312	GLU	3.5
2	D	475	LYS	3.5
1	C	293	LEU	3.5
3	F	48	VAL	3.5
3	F	39	GLN	3.5
2	D	312	GLU	3.5
3	E	41	PRO	3.5
1	A	136	ARG	3.5
2	B	300	ILE	3.5
3	E	36	TRP	3.5
1	C	139	LEU	3.4
1	C	411	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	112	TYR	3.4
1	C	136	ARG	3.4
3	E	76	LYS	3.4
2	D	129	ASP	3.4
3	F	74	ASN	3.4
3	F	34	LEU	3.4
1	A	129	MET	3.4
1	A	161	PHE	3.3
3	F	76	LYS	3.3
1	A	289	ILE	3.3
1	A	469	ASN	3.3
2	B	520	SER	3.3
2	D	294	GLY	3.3
2	B	120	LEU	3.3
1	C	552	LYS	3.3
1	C	289	ILE	3.3
2	D	575	GLU	3.3
1	A	66	GLY	3.3
1	A	290	GLY	3.3
3	E	106	PRO	3.3
1	C	470	PHE	3.3
1	A	132	ARG	3.2
3	F	105	THR	3.2
3	E	80	TYR	3.2
3	E	34	LEU	3.2
1	A	134	VAL	3.2
2	D	375	THR	3.2
2	B	404	PHE	3.2
3	E	39	GLN	3.2
2	D	567	ILE	3.2
2	D	531	GLN	3.2
1	A	280	MET	3.2
1	C	269	ILE	3.2
2	D	149	ASN	3.1
2	B	322	MET	3.1
2	B	153	ASN	3.1
1	A	160	ILE	3.1
2	B	408	ASP	3.1
1	A	135	VAL	3.1
2	D	351	VAL	3.1
3	E	22	CYS	3.1
3	E	111	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	294	ASN	3.1
3	F	49	ALA	3.1
3	E	64	VAL	3.1
2	B	247	GLU	3.0
1	A	140	LEU	3.0
3	E	38	ARG	3.0
2	B	379	LYS	3.0
2	B	561	VAL	3.0
3	F	69	THR	3.0
2	B	534	MET	3.0
1	C	412	VAL	3.0
3	E	101	THR	3.0
1	C	382	LEU	3.0
1	C	132	ARG	3.0
3	E	50	ALA	3.0
1	A	448	ILE	3.0
2	B	298	THR	3.0
3	F	36	TRP	2.9
2	D	224	SER	2.9
2	B	437	ASP	2.9
2	B	123	VAL	2.9
1	C	342	PHE	2.9
1	A	106	ARG	2.9
1	C	45	ALA	2.9
3	F	106	PRO	2.9
3	F	84	ASN	2.9
1	C	284	PHE	2.9
1	A	2	LYS	2.9
1	C	129	MET	2.9
1	C	418	LEU	2.9
2	D	530	ILE	2.9
2	B	382	GLN	2.8
3	F	61	ALA	2.8
2	D	127	PHE	2.8
3	F	47	GLY	2.8
2	B	355	ILE	2.8
2	B	140	VAL	2.8
1	A	423	ILE	2.8
3	F	22	CYS	2.8
1	A	26	VAL	2.8
1	C	135	VAL	2.8
1	A	452	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	277	ASN	2.8
2	D	376	PHE	2.8
2	D	322	MET	2.8
2	B	454	PRO	2.8
1	C	375	LEU	2.8
3	E	31	ILE	2.8
2	D	533	ALA	2.7
3	E	97	ALA	2.7
2	B	125	VAL	2.7
1	C	288	MET	2.7
3	F	103	SER	2.7
2	B	452	GLY	2.7
1	C	278	TYR	2.7
1	A	287	MET	2.7
3	F	42	GLY	2.7
2	B	543	SER	2.7
2	B	287	LEU	2.7
1	A	203	ARG	2.7
2	D	304	ARG	2.7
2	B	462	LYS	2.7
2	D	543	SER	2.7
3	E	121	VAL	2.7
3	F	29	HIS	2.7
1	C	14	PHE	2.6
2	B	257	GLN	2.6
3	F	98	ALA	2.6
1	A	107	PHE	2.6
1	A	295	PHE	2.6
3	F	45	ARG	2.6
3	E	10	GLY	2.6
3	E	102	GLY	2.6
3	E	99	ALA	2.6
3	F	2	VAL	2.6
3	F	33	TYR	2.6
3	E	1	GLN	2.6
2	B	378	ILE	2.6
2	D	405	TYR	2.6
3	E	82	GLN	2.6
3	F	117	GLN	2.6
1	A	425	GLU	2.6
1	A	265	ASN	2.6
1	C	323	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	506	LYS	2.6
1	A	269	ILE	2.5
1	A	284	PHE	2.5
2	D	520	SER	2.5
1	A	552	LYS	2.5
1	C	513	LYS	2.5
3	E	84	ASN	2.5
1	C	181	PHE	2.5
2	D	466	LYS	2.5
1	C	273	MET	2.5
3	F	113	TRP	2.5
3	F	115	TRP	2.5
2	D	429	SER	2.5
2	D	293	VAL	2.5
2	B	149	ASN	2.5
2	B	544	ILE	2.5
2	D	487	ASP	2.5
3	F	101	THR	2.5
1	C	383	ILE	2.5
2	D	539	GLU	2.5
3	E	48	VAL	2.5
1	C	482	ARG	2.4
2	D	491	ASP	2.4
3	E	21	SER	2.4
1	C	170	PHE	2.4
1	A	139	LEU	2.4
1	A	103	ASN	2.4
1	C	3	THR	2.4
2	D	579	LYS	2.4
2	B	521	ASN	2.4
1	A	418	LEU	2.4
2	D	467	LEU	2.4
2	B	539	GLU	2.4
1	A	69	GLY	2.3
1	C	466	GLY	2.3
2	D	551	ASN	2.3
3	E	98	ALA	2.3
1	C	140	LEU	2.3
1	C	563	GLU	2.3
2	B	453	ASN	2.3
1	C	475	LYS	2.3
3	E	32	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	550	LEU	2.3
1	A	170	PHE	2.3
1	C	237	VAL	2.3
3	F	43	LYS	2.3
1	C	196	ARG	2.3
1	A	27	ILE	2.3
1	A	286	LEU	2.3
3	F	81	LEU	2.3
2	B	487	ASP	2.3
2	D	471	ASP	2.3
2	B	541	LYS	2.3
1	C	134	VAL	2.3
2	B	124	PRO	2.3
1	A	59	MET	2.3
3	E	108	TRP	2.3
2	D	89	LEU	2.3
1	A	108	HIS	2.3
3	E	29	HIS	2.3
2	B	364	TYR	2.3
1	C	321	ASN	2.3
1	C	297	VAL	2.3
3	E	35	GLY	2.2
1	C	159	LEU	2.2
2	B	128	PHE	2.2
2	D	254	THR	2.2
2	D	377	HIS	2.2
3	F	37	PHE	2.2
2	B	591	TYR	2.2
1	C	526	GLN	2.2
2	B	293	VAL	2.2
2	D	216	ASN	2.2
1	C	216	GLU	2.2
3	F	73	ASP	2.2
2	B	532	ALA	2.2
3	E	51	LEU	2.2
2	B	340	LYS	2.2
2	B	72	ARG	2.2
2	B	136	ILE	2.2
3	F	28	ILE	2.2
3	F	62	ASP	2.2
2	D	423	LYS	2.2
1	C	276	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	285	SER	2.2
1	C	281	GLN	2.2
3	F	44	GLU	2.2
1	C	547	GLY	2.2
3	F	65	LYS	2.2
3	F	104	ASP	2.2
1	A	65	ILE	2.2
1	C	282	ILE	2.2
3	E	86	LEU	2.2
1	C	394	GLU	2.2
3	E	52	TRP	2.2
3	E	119	THR	2.1
1	A	133	ILE	2.1
3	E	120	GLN	2.1
1	C	154	LYS	2.1
2	D	19	LYS	2.1
1	C	483	ALA	2.1
2	D	220	GLU	2.1
2	D	480	GLY	2.1
2	B	472	HIS	2.1
1	A	199	LEU	2.1
1	C	240	LEU	2.1
3	E	54	LYS	2.1
2	B	316	GLN	2.1
3	F	1	GLN	2.1
1	C	271	SER	2.1
2	B	160	SER	2.1
2	B	362	PHE	2.1
3	E	110	TRP	2.1
1	A	276	THR	2.1
1	A	307	LEU	2.1
1	C	345	THR	2.1
2	B	537	LEU	2.1
3	F	91	THR	2.1
1	A	421	GLY	2.1
1	A	473	GLY	2.1
1	C	290	GLY	2.1
1	C	542	GLU	2.1
1	C	292	ILE	2.1
2	D	341	ASP	2.1
3	E	60	TYR	2.1
3	E	105	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	38	ARG	2.1
2	B	319	MET	2.1
3	E	117	GLN	2.1
1	A	62	VAL	2.1
2	D	308	ARG	2.1
2	D	469	HIS	2.1
2	B	74	ASP	2.1
2	D	206	TYR	2.1
1	C	268	GLU	2.1
1	C	419	PHE	2.1
2	B	510	PRO	2.1
1	C	142	VAL	2.0
1	A	163	ILE	2.0
1	C	494	ASP	2.0
3	E	75	ALA	2.0
2	D	379	LYS	2.0
2	D	479	GLU	2.0
1	A	356	VAL	2.0
3	F	64	VAL	2.0
3	E	19	ARG	2.0
1	A	316	ILE	2.0
2	D	472	HIS	2.0
2	D	316	GLN	2.0
3	F	41	PRO	2.0
2	B	28	LEU	2.0
3	E	72	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

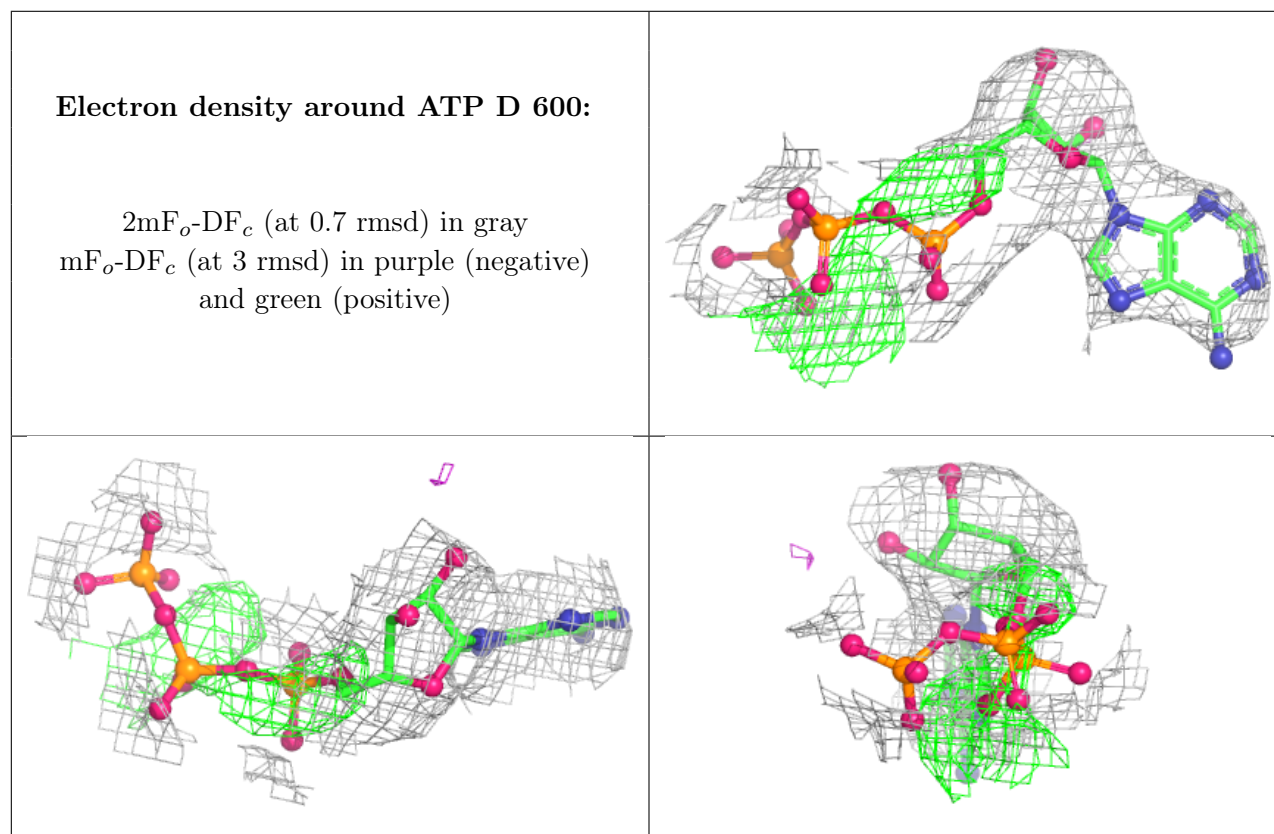
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

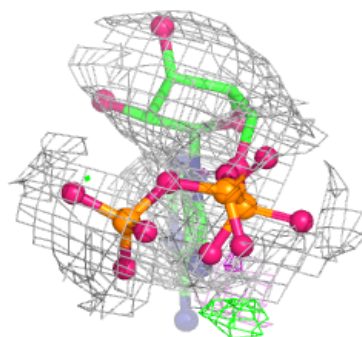
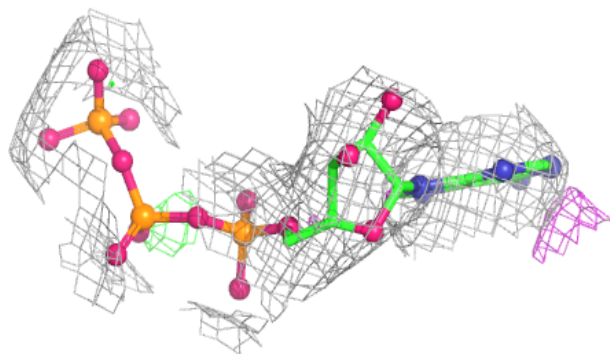
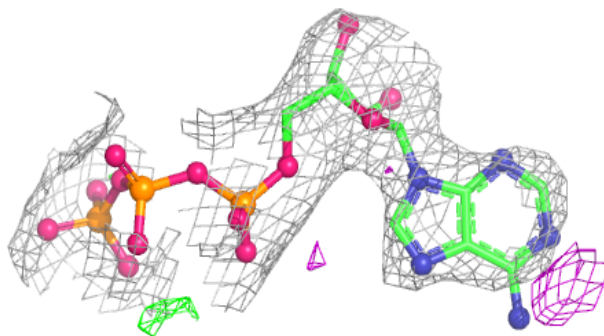
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	D	600	31/31	0.93	0.14	43,49,55,55	0
5	MG	A	601	1/1	0.93	0.20	13,13,13,13	0
4	ATP	B	600	31/31	0.94	0.12	47,52,58,58	0
4	ATP	C	600	31/31	0.95	0.10	65,67,70,70	0
4	ATP	A	600	31/31	0.96	0.09	32,36,38,39	0
5	MG	B	601	1/1	0.97	0.15	34,34,34,34	0
5	MG	C	601	1/1	0.97	0.17	43,43,43,43	0
5	MG	D	601	1/1	0.98	0.17	20,20,20,20	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.

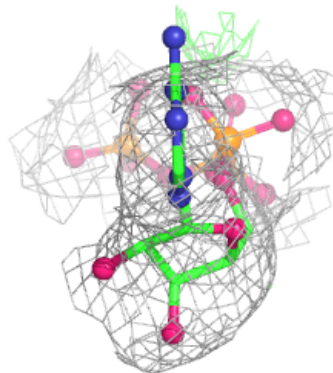
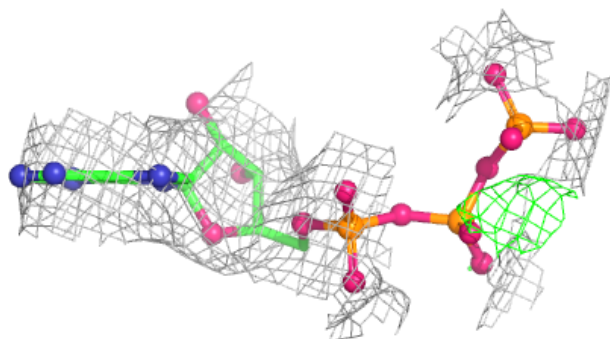
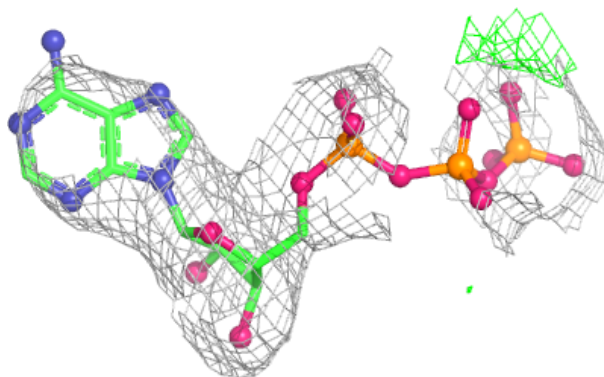


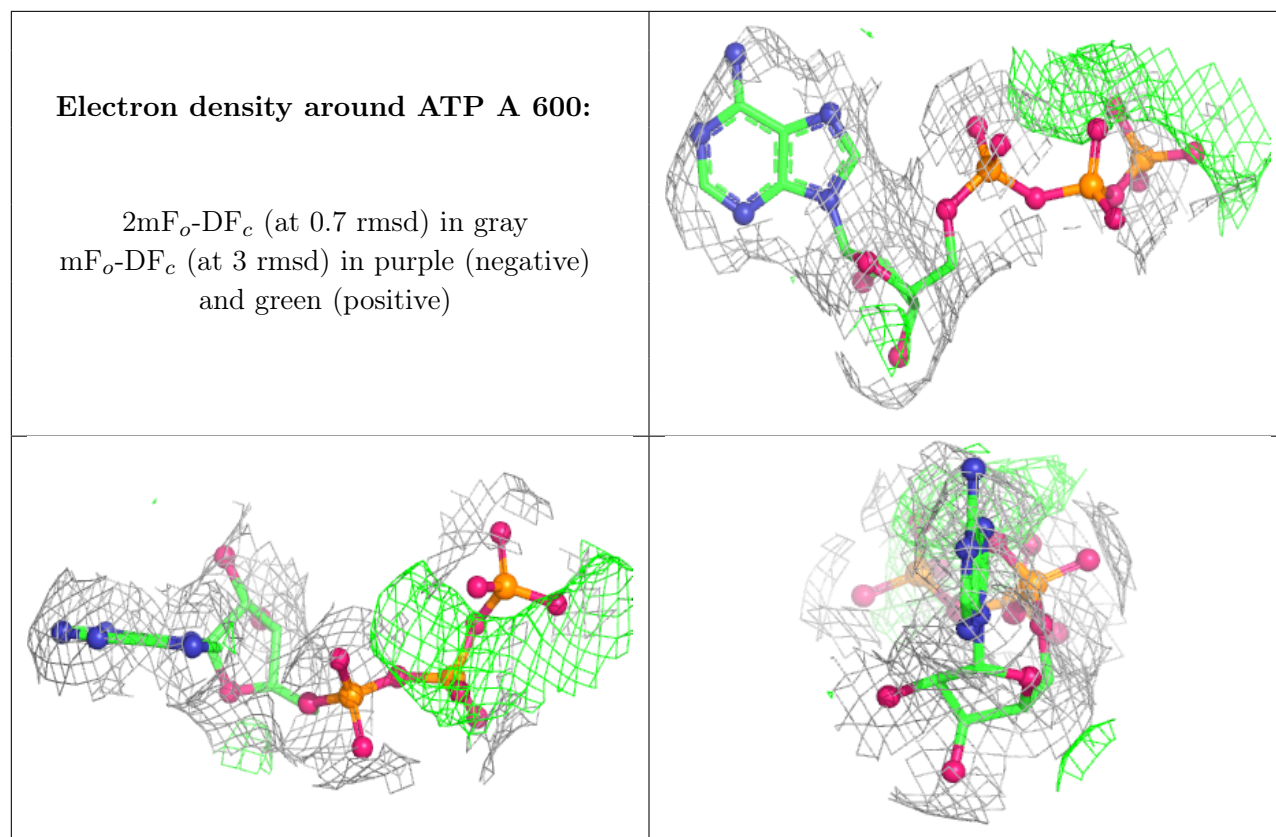
Electron density around ATP B 600:

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

**Electron density around ATP C 600:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.