



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:21 PM UTC

PDB ID : 5DN6 / pdb_00005dn6
Title : ATP synthase from *Paracoccus denitrificans*
Authors : Morales-Rios, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2015-09-09
Resolution : 3.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

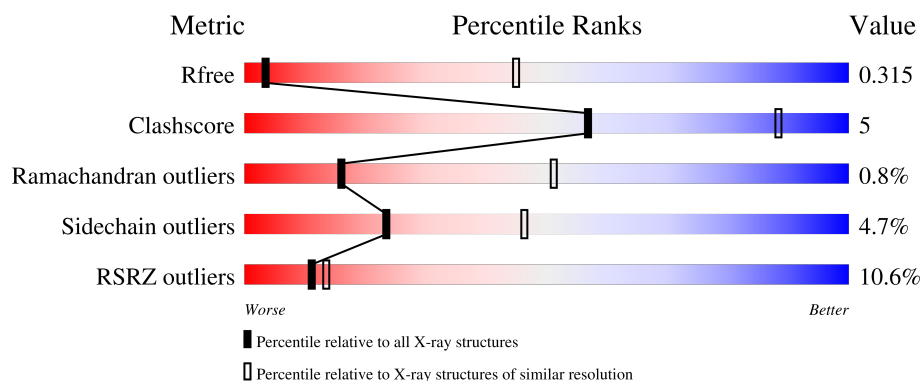
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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	1	20	100%
2	2	15	100%
3	3	19	100%
4	A	511	10% 83% 14% ..
4	B	511	8% 81% 14% ..

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Mol	Chain	Length	Quality of chain
4	C	511	
5	D	474	
5	E	474	
5	F	474	
6	G	290	
7	H	188	
8	I	148	
9	J	77	
9	K	77	
9	L	77	
9	M	77	
9	N	77	
9	O	77	
9	P	77	
9	Q	77	
9	R	77	
9	S	77	
9	T	77	
9	U	77	
10	V	78	
11	W	124	
12	X	283	
13	Y	54	
14	Z	104	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31527 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 Chain A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	1	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 2 is a protein called Chain B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	2	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 3 is a protein called Chain C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	3	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 4 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	505	Total	C	N	O	S	0	0	0
			3811	2395	665	735	16			
4	B	496	Total	C	N	O	S	0	0	0
			3754	2359	657	723	15			
4	C	484	Total	C	N	O	S	0	0	0
			3652	2293	640	703	16			

- Molecule 5 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	470	Total	C	N	O	S	0	0	0
			3508	2211	600	687	10			
5	E	466	Total	C	N	O	S	0	0	0
			3490	2198	596	686	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	466	Total	C	N	O	S	0	0	0
			3489	2199	596	684	10			

- Molecule 6 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	260	Total	C	N	O	S	0	0	0
			1978	1227	367	375	9			

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	110	Total	C	N	O	0	0	0
			544	324	110	110			

- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	75	Total	C	N	O	0	0	0
			366	216	75	75			

- Molecule 9 is a protein called ATP synthase F0 subcomplex C subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	K	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	L	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	M	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	N	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	O	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	P	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	Q	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	R	74	Total	C	N	O	0	0	0
			358	210	74	74			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	T	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	U	74	Total	C	N	O	0	0	0
			358	210	74	74			

- Molecule 10 is a protein called Chain V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	78	Total	C	N	O	0	0	0
			390	234	78	78			

- Molecule 11 is a protein called Chain W.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	W	124	Total	C	N	O	0	0	0
			620	372	124	124			

- Molecule 12 is a protein called ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	98	Total	C	N	O	0	0	0
			486	291	98	97			

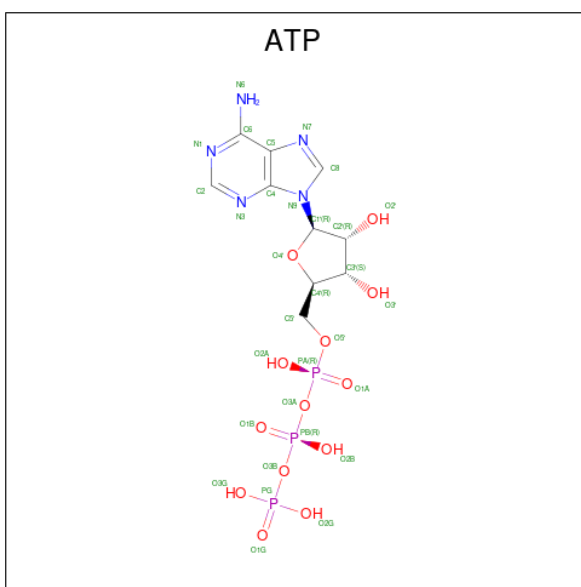
- Molecule 13 is a protein called Chain Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	Y	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 14 is a protein called Zeta inhibitor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Z	54	Total	C	N	O	S	0	0	0
			447	274	88	84	1			

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

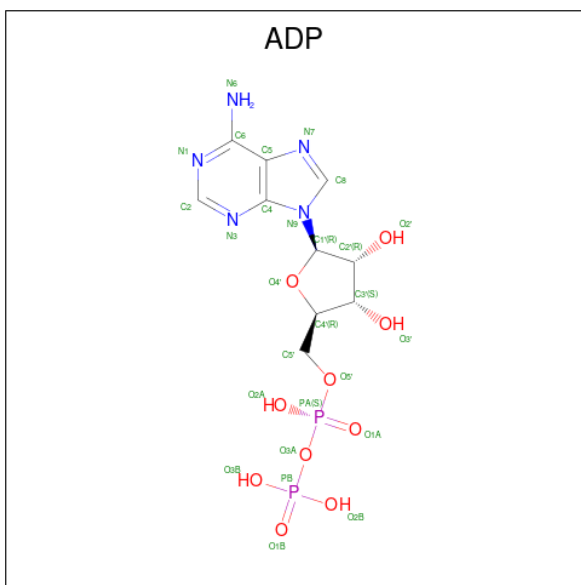


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	F	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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: Chain A

Chain 1:  100%

There are no outlier residues recorded for this chain.

• Molecule 2: Chain B

Chain 2:  100%

There are no outlier residues recorded for this chain.

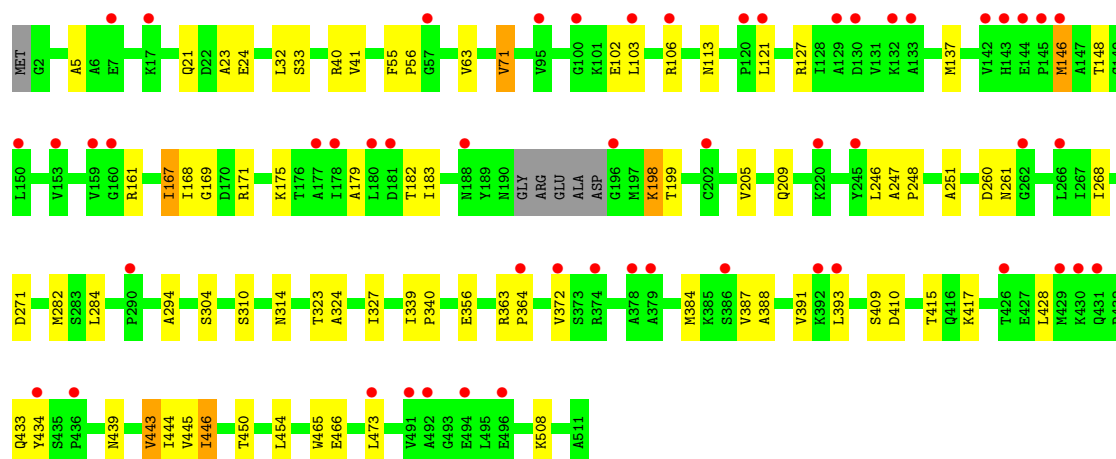
• Molecule 3: Chain C

Chain 3:  100%

There are no outlier residues recorded for this chain.

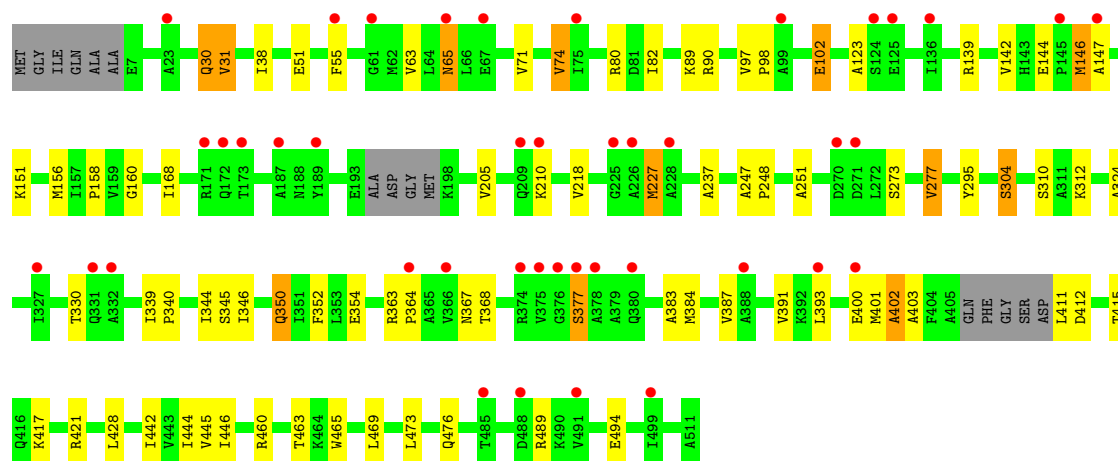
• Molecule 4: ATP synthase subunit alpha

Chain A:  10% 83% 14% ..

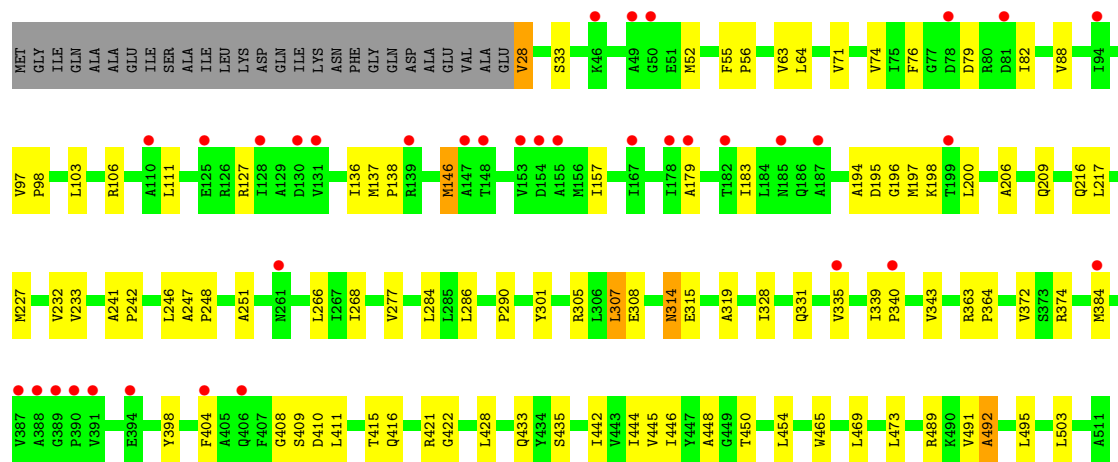
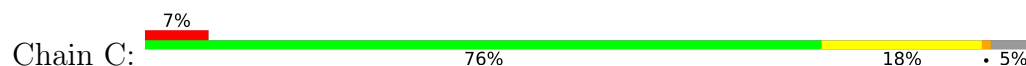


• Molecule 4: ATP synthase subunit alpha

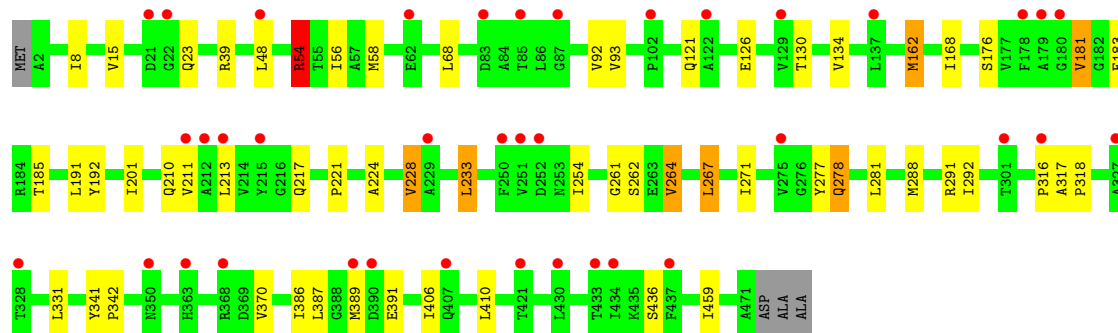
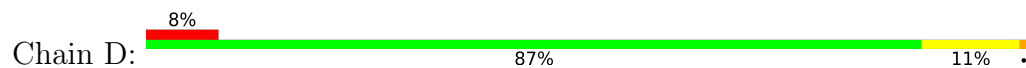
Chain B:  8% 81% 14% ..



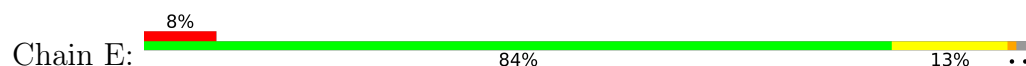
• Molecule 4: ATP synthase subunit alpha

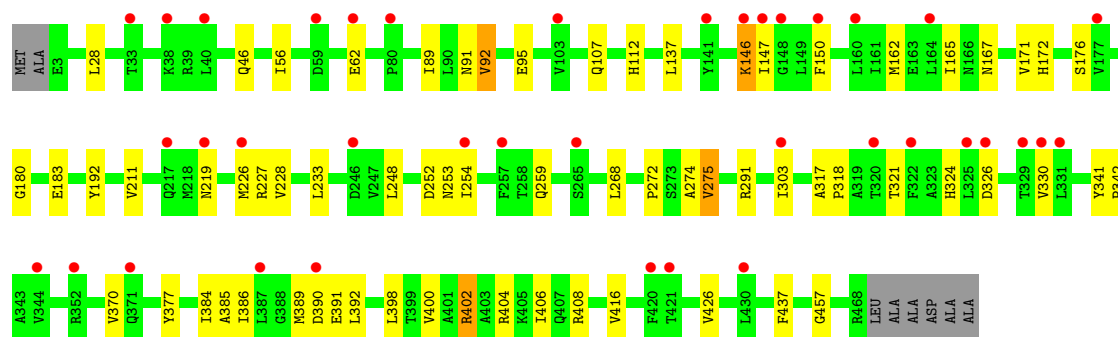


• Molecule 5: ATP synthase subunit beta

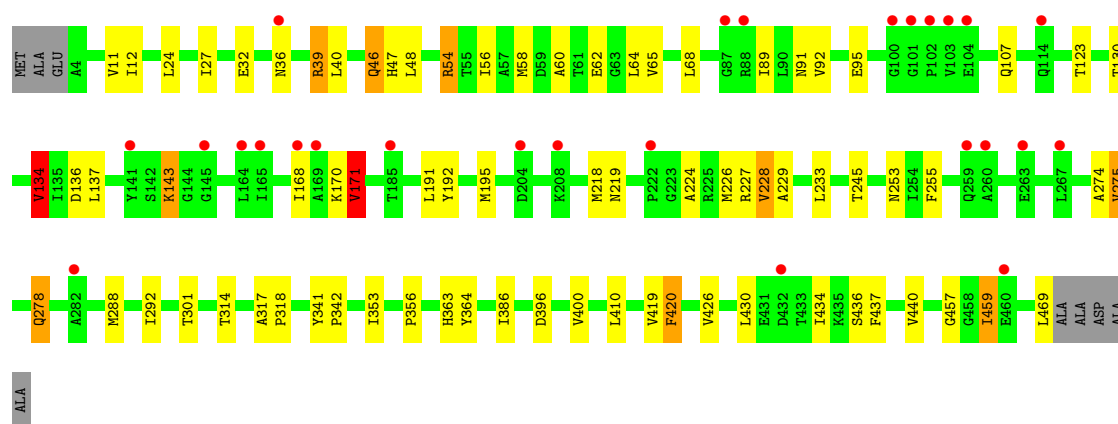
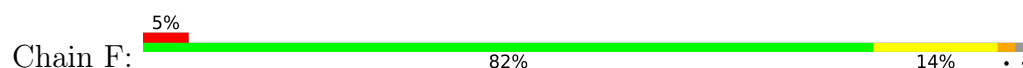


• Molecule 5: ATP synthase subunit beta

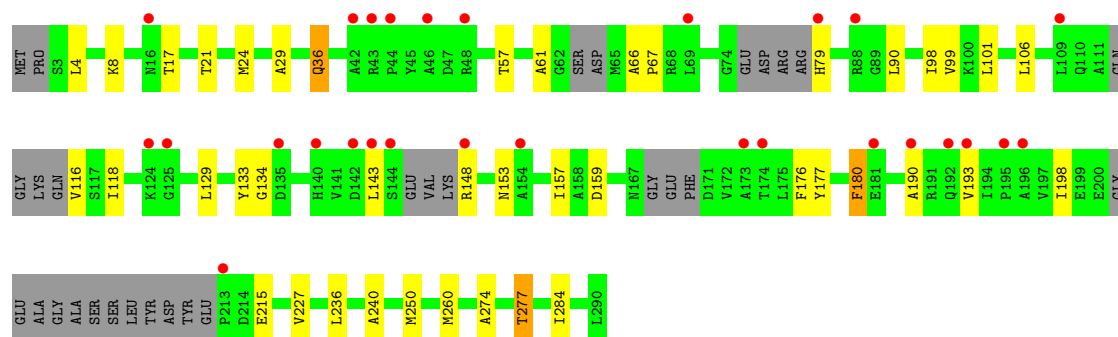
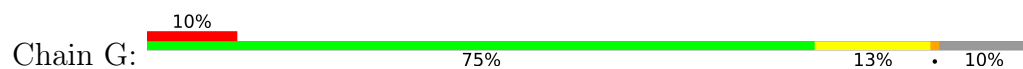




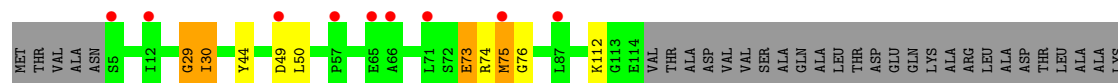
- Molecule 5: ATP synthase subunit beta



- Molecule 6: ATP synthase gamma chain



- Molecule 7: ATP synthase subunit delta



SER GLY LYS THR VAL LYS LEU ASN ALA ARG VAL ASP GLU SER LEU TLE GLY MET TLE VAL LYS LYS LEU SER GLN MET TLE VAL LYS LYS LEU SER ALA SER LEU GLN ASN ALA MET LYS GLU VAL GLY

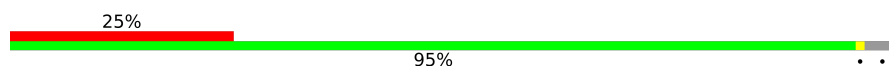
- Molecule 8: ATP synthase epsilon chain

Chain I: 

MET ALA ASP THR MET GLN PHE ASP LEU V9 S10 V62 G55 T60 N73 R82 G83 HIS PRO ARG ALA GLU MET THR GLN SER SER TLE ARG ASN SER LYS LEU ALA SER LEU GLN ASN ARG ARG VAL GLU ALA LYS ARG GLU SER GLY VAL ALA

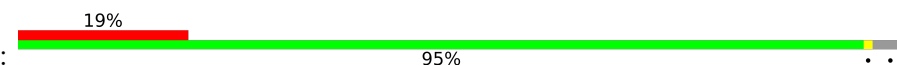
ALA LYS LEU ASP MET ALA GLY THR HIS TLE LEU ASP PRO HIS

- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain J: 

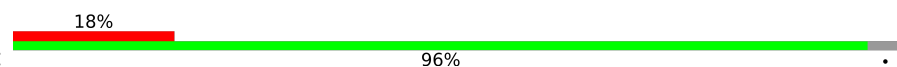
MET GLU N3 A21 G22 A23 A24 M25 N29 V30 A31 G32 N33 S47 Q48 T49 F63 I54 A57 F58 A59 E60 A61 L62 F65 L68 L71 L74 F75 A76 VAL

- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain K: 

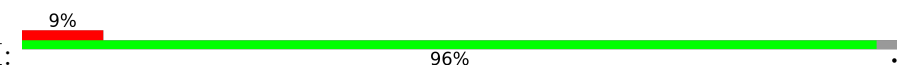
MET GLU N3 A21 G22 A23 A24 M25 N29 V30 A31 G32 N33 S47 Q48 T49 F63 I54 A57 F58 A59 E60 A61 L62 F65 L68 L71 A76 VAL

- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain L: 

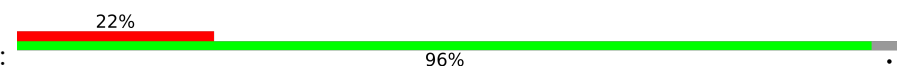
MET GLU N3 V18 A31 L35 A36 G37 A38 N41 P42 S43 S47 Q48 T49 F53 A57 L68 A76 VAL

- Molecule 9: ATP synthase F0 subcomplex C subunit

Chain M: 

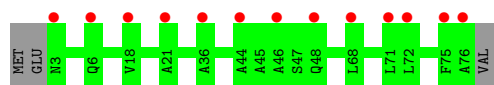
MET GLU N3 L16 V18 A31 V34 L35 A36 S43 L68 A76 VAL

- Molecule 9: ATP synthase F0 subcomplex C subunit

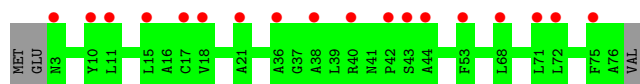
Chain N: 

MET GLU N3 V18 G19 W20 A21 V30 A38 N41 P42 S43 A44 A45 A46 S47 Q48 T49 A61 I64 F65 L68 A76 VAL

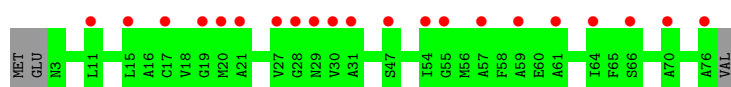
- Molecule 9: ATP synthase F0 subcomplex C subunit



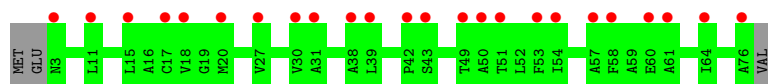
- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



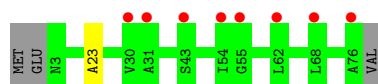
- Molecule 9: ATP synthase F0 subcomplex C subunit



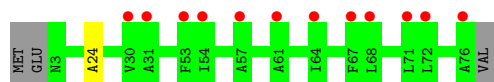
- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 10: Chain V

Chain V:  100%

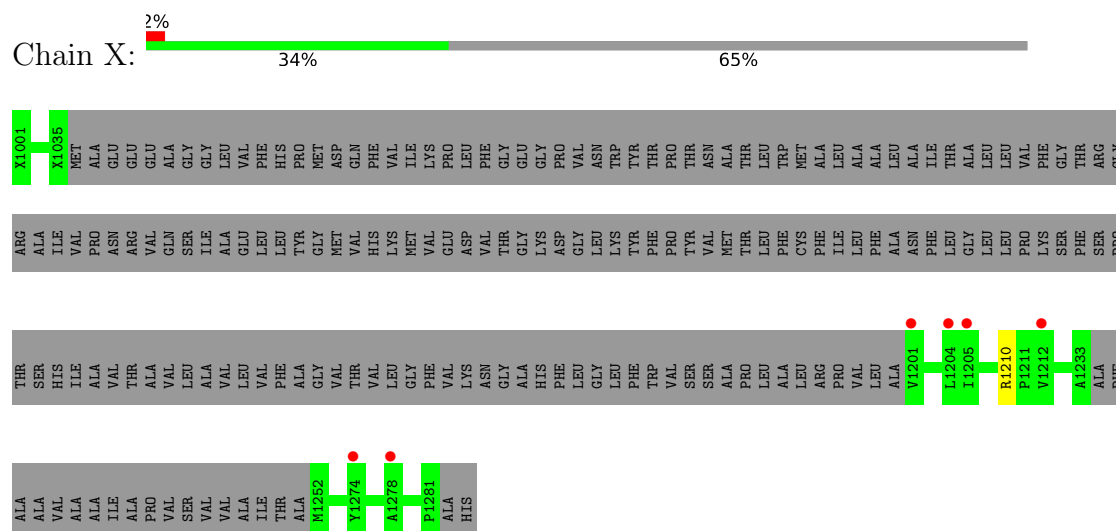
There are no outlier residues recorded for this chain.

- Molecule 11: Chain W

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a,ATP synthase subunit a

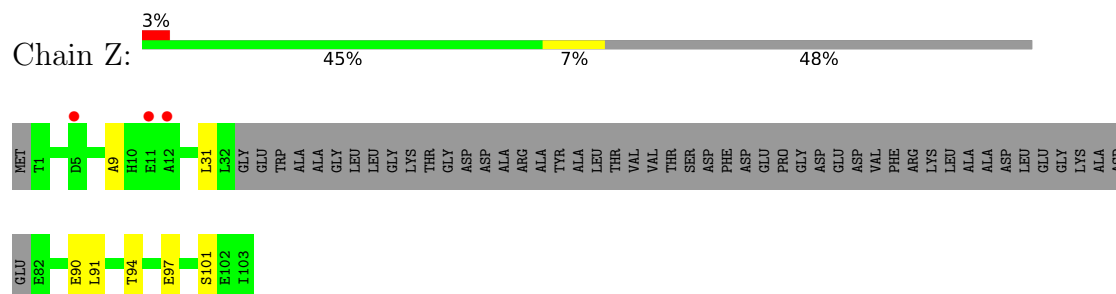


- Molecule 13: Chain Y

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: Zeta inhibitor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.00Å 187.94Å 164.72Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	36.84 – 3.98 36.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.84-3.98) 98.7 (36.84-3.98)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.295 , 0.324 0.292 , 0.315	Depositor DCC
R_{free} test set	2791 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	119.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	31527	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: ATP, ADP, MG

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$
4	A	0.55	1/3864 (0.0%)	0.86	0/5227
4	B	0.53	0/3805	0.86	3/5146 (0.1%)
4	C	0.52	0/3705	0.88	4/5015 (0.1%)
5	D	0.51	0/3562	0.82	2/4840 (0.0%)
5	E	0.51	2/3544 (0.1%)	0.81	3/4815 (0.1%)
5	F	0.49	0/3543	0.80	1/4814 (0.0%)
6	G	0.57	0/1990	0.88	2/2674 (0.1%)
7	H	0.63	0/543	0.97	3/755 (0.4%)
8	I	0.52	0/365	0.86	2/504 (0.4%)
9	J	0.63	0/357	1.15	0/491
9	K	0.64	0/357	1.15	0/491
9	L	0.64	0/357	1.15	0/491
9	M	0.64	0/357	1.15	0/491
9	N	0.64	0/357	1.15	0/491
9	O	0.64	0/357	1.15	0/491
9	P	0.64	0/357	1.15	0/491
9	Q	0.64	0/357	1.15	0/491
9	R	0.63	0/357	1.15	0/491
9	S	0.63	0/357	1.15	0/491
9	T	0.63	0/357	1.14	0/491
9	U	0.63	0/357	1.15	0/491
12	X	0.53	0/309	1.30	2/428 (0.5%)
14	Z	0.67	0/450	0.93	0/599
All	All	0.54	3/29964 (0.0%)	0.90	22/40709 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	40	ARG	CZ-NH1	6.76	1.42	1.32
5	E	259	GLN	CD-OE1	6.51	1.35	1.23
5	E	326	ASP	CG-OD1	5.29	1.35	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	307	LEU	N-CA-C	-8.60	98.94	110.55
4	C	314	ASN	N-CA-CB	-7.62	99.20	110.17
7	H	49	ASP	N-CA-C	6.38	117.90	111.07
7	H	49	ASP	CB-CA-C	6.36	120.86	110.88
4	C	106	ARG	NE-CZ-NH2	6.32	124.89	119.20
7	H	49	ASP	N-CA-CB	6.29	119.14	110.01
4	B	139	ARG	NE-CZ-NH2	6.05	124.65	119.20
5	E	402	ARG	NE-CZ-NH2	5.76	124.39	119.20
12	X	1210	ARG	CA-C-N	5.72	125.08	118.85
12	X	1210	ARG	C-N-CA	5.72	125.08	118.85
6	G	180	PHE	CB-CA-C	-5.63	100.03	109.65
5	E	92	VAL	N-CA-C	5.58	116.22	110.36
5	F	134	VAL	CB-CA-C	-5.54	104.87	111.97
5	D	54	ARG	CG-CD-NE	-5.52	99.86	112.00
4	B	402	ALA	N-CA-C	5.39	122.27	110.80
5	D	271	ILE	N-CA-C	-5.33	104.05	108.63
5	E	92	VAL	CB-CA-C	-5.30	105.09	111.88
4	B	476	GLN	OE1-CD-NE2	5.19	127.79	122.60
6	G	143	LEU	N-CA-C	5.17	116.61	110.97
4	C	374	ARG	CG-CD-NE	5.15	123.33	112.00
8	I	10	SER	CA-C-N	5.00	125.27	119.47
8	I	10	SER	C-N-CA	5.00	125.27	119.47

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	1	100	0	23	0	0
2	2	75	0	17	0	0
3	3	95	0	21	0	0
4	A	3811	0	3875	35	0
4	B	3754	0	3822	42	0
4	C	3652	0	3709	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	3508	0	3532	36	0
5	E	3490	0	3513	38	0
5	F	3489	0	3517	48	0
6	G	1978	0	2035	26	0
7	H	544	0	277	4	0
8	I	366	0	176	0	0
9	J	358	0	209	1	0
9	K	358	0	209	1	0
9	L	358	0	209	0	0
9	M	358	0	209	0	0
9	N	358	0	209	0	0
9	O	358	0	209	0	0
9	P	358	0	209	0	0
9	Q	358	0	209	0	0
9	R	358	0	209	0	0
9	S	358	0	209	0	0
9	T	358	0	209	1	0
9	U	358	0	209	1	0
10	V	390	0	80	0	0
11	W	620	0	127	0	0
12	X	486	0	181	0	0
13	Y	270	0	58	0	0
14	Z	447	0	449	4	0
15	A	31	0	12	0	0
15	C	31	0	12	0	0
15	D	31	0	12	0	0
15	F	31	0	12	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	F	1	0	0	0	0
17	B	27	0	12	0	0
All	All	31527	0	27980	273	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 5.

All (273) 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)
5:F:191:LEU:HD11	5:F:195:MET:HE3	1.59	0.84
5:F:278:GLN:H	5:F:278:GLN:HE21	1.24	0.83
5:D:386:ILE:HD11	6:G:17:THR:HG22	1.59	0.82
5:E:176:SER:HB2	5:E:211:VAL:HG12	1.62	0.80
14:Z:31:LEU:HD23	14:Z:91:LEU:HD22	1.64	0.80
4:A:146:MET:HE1	4:A:182:THR:HG21	1.65	0.79
5:D:48:LEU:HD21	5:D:54:ARG:HG3	1.67	0.77
4:A:433:GLN:HG2	4:A:434:TYR:CE2	2.21	0.76
6:G:180:PHE:CE1	6:G:240:ALA:HB3	2.21	0.75
6:G:98:ILE:HD11	6:G:177:TYR:HA	1.68	0.74
5:F:91:ASN:HD21	5:F:95:GLU:HB2	1.52	0.73
7:H:73:GLU:O	7:H:75:MET:N	2.22	0.72
4:C:146:MET:HE3	4:C:266:LEU:HD13	1.71	0.72
4:B:218:VAL:HG13	4:B:227:MET:HE3	1.71	0.71
4:C:146:MET:HE1	4:C:266:LEU:HD22	1.71	0.71
4:B:146:MET:C	4:B:146:MET:HE2	2.15	0.70
4:C:206:ALA:HB1	4:C:209:GLN:OE1	1.93	0.68
4:C:76:PHE:HE2	4:C:246:LEU:HD22	1.58	0.67
4:C:137:MET:HE1	5:D:192:TYR:CD2	2.30	0.67
5:F:278:GLN:HE21	5:F:278:GLN:N	1.92	0.67
6:G:106:LEU:HD13	6:G:116:VAL:HG11	1.78	0.66
6:G:24:MET:CE	6:G:250:MET:HE2	2.27	0.65
4:B:411:LEU:HD23	4:B:415:THR:HB	1.78	0.65
4:A:5:ALA:HB1	4:A:32:LEU:HD13	1.79	0.64
5:D:48:LEU:HD11	5:D:54:ARG:HG2	1.79	0.64
5:F:56:ILE:HD13	5:F:226:MET:HE1	1.78	0.64
5:E:165:ILE:HD13	5:E:211:VAL:HG11	1.79	0.64
5:F:170:LYS:O	5:F:171:VAL:HG22	1.98	0.62
5:F:92:VAL:HB	5:F:228:VAL:HG13	1.82	0.61
6:G:24:MET:HE3	6:G:250:MET:HE2	1.82	0.61
4:B:247:ALA:HB3	4:B:248:PRO:HD3	1.80	0.61
4:A:391:VAL:HG21	4:A:446:ILE:HG23	1.83	0.61
4:A:179:ALA:HB1	4:A:268:ILE:HD13	1.82	0.61
5:F:32:GLU:OE2	5:F:39:ARG:NH1	2.34	0.60
4:C:404:PHE:HA	14:Z:9:ALA:HB1	1.84	0.60
5:D:162:MET:SD	5:D:191:LEU:HD13	2.42	0.60
4:C:301:TYR:CE1	4:C:305:ARG:HG3	2.37	0.59
4:A:384:MET:HE2	4:A:388:ALA:HB2	1.84	0.59
5:D:386:ILE:HD11	6:G:17:THR:CG2	2.31	0.59
5:D:176:SER:HB2	5:D:211:VAL:HG22	1.84	0.59
5:F:46:GLN:HG2	5:F:54:ARG:HB2	1.83	0.59
4:B:428:LEU:HD22	4:B:445:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:36:GLN:HE21	6:G:36:GLN:HA	1.68	0.58
5:D:181:VAL:HG13	5:D:228:VAL:HG13	1.84	0.58
4:B:51:GLU:OE2	4:B:90:ARG:HB2	2.03	0.58
5:E:146:LYS:HG2	5:E:324:HIS:O	2.04	0.58
5:F:48:LEU:HD21	5:F:54:ARG:HG3	1.85	0.58
6:G:118:ILE:HD13	6:G:129:LEU:HD23	1.84	0.58
5:E:404:ARG:O	5:E:408:ARG:HG2	2.03	0.58
6:G:180:PHE:HE1	6:G:240:ALA:HB3	1.63	0.58
4:B:384:MET:HE1	4:B:442:ILE:CG2	2.34	0.57
4:C:64:LEU:HD12	4:C:286:LEU:HD11	1.86	0.57
4:A:247:ALA:HB3	4:A:248:PRO:HD3	1.86	0.57
4:A:391:VAL:HG21	4:A:446:ILE:CG2	2.35	0.56
4:C:179:ALA:HB1	4:C:268:ILE:HD13	1.86	0.56
4:B:465:TRP:CH2	4:B:469:LEU:HD13	2.41	0.56
5:F:363:HIS:CD2	5:F:430:LEU:HD11	2.41	0.56
4:B:391:VAL:HG21	4:B:446:ILE:CG2	2.35	0.56
4:A:102:GLU:O	4:A:106:ARG:NH1	2.37	0.56
5:F:60:ALA:HB1	5:F:62:GLU:OE1	2.06	0.56
5:E:384:ILE:HG12	5:E:392:LEU:HD11	1.88	0.55
4:A:137:MET:HE1	5:E:192:TYR:CD2	2.42	0.55
5:D:254:ILE:HD11	5:D:288:MET:SD	2.46	0.55
6:G:4:LEU:HD23	6:G:8:LYS:HD2	1.88	0.55
4:C:384:MET:HE1	4:C:442:ILE:CG2	2.36	0.55
4:A:161:ARG:NH1	4:A:198:LYS:O	2.33	0.55
5:E:233:LEU:HD21	5:E:291:ARG:HB2	1.88	0.55
5:F:134:VAL:HG13	5:F:410:LEU:HD22	1.88	0.55
4:B:295:TYR:CZ	4:B:339:ILE:HD11	2.42	0.55
5:F:48:LEU:HD11	5:F:54:ARG:HG2	1.88	0.54
6:G:57:THR:HG21	6:G:198:ILE:HG23	1.90	0.54
4:B:97:VAL:HB	4:B:98:PRO:HD2	1.90	0.54
5:E:89:ILE:HD11	5:E:192:TYR:CD1	2.42	0.54
5:D:317:ALA:HB3	5:D:318:PRO:CD	2.37	0.54
4:C:444:ILE:HG21	4:C:473:LEU:HD11	1.90	0.54
5:F:317:ALA:HB3	5:F:318:PRO:CD	2.38	0.54
5:E:147:ILE:HD13	5:E:303:ILE:CD1	2.38	0.54
14:Z:90:GLU:O	14:Z:94:THR:OG1	2.23	0.53
5:E:28:LEU:HD13	5:E:112:HIS:CD2	2.43	0.53
4:A:41:VAL:HB	4:A:71:VAL:HG12	1.90	0.53
4:B:383:ALA:HB2	4:B:489:ARG:O	2.08	0.53
4:B:151:LYS:HG2	4:B:442:ILE:HG23	1.90	0.53
4:B:391:VAL:HG21	4:B:446:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:15:VAL:HG21	5:D:267:LEU:HB2	1.91	0.53
4:B:144:GLU:OE1	4:B:312:LYS:NZ	2.39	0.53
4:A:363:ARG:HA	4:A:364:PRO:C	2.34	0.53
5:E:171:VAL:HG23	5:E:172:HIS:CD2	2.44	0.53
5:F:136:ASP:HB3	5:F:430:LEU:HD13	1.91	0.52
5:F:426:VAL:HG11	5:F:457:GLY:HA3	1.91	0.52
4:C:183:ILE:HD11	4:C:268:ILE:HD12	1.92	0.52
5:D:201:ILE:CD1	5:D:213:LEU:HD11	2.40	0.51
6:G:148:ARG:NH1	6:G:236:LEU:HD22	2.26	0.51
4:A:439:ASN:O	4:A:443:VAL:HG23	2.11	0.51
4:C:196:GLY:O	4:C:198:LYS:N	2.43	0.51
4:C:284:LEU:HD21	4:C:290:PRO:HB3	1.92	0.51
4:C:307:LEU:O	4:C:308:GLU:CB	2.57	0.51
4:A:148:THR:HA	4:A:182:THR:HG23	1.93	0.51
4:A:55:PHE:HB3	4:A:56:PRO:HD2	1.92	0.51
4:C:465:TRP:CH2	4:C:469:LEU:HD22	2.46	0.51
5:D:261:GLY:HA3	5:D:278:GLN:HE22	1.76	0.50
5:D:387:LEU:HD13	5:D:391:GLU:HG2	1.94	0.50
5:F:65:VAL:HB	5:F:68:LEU:HD13	1.92	0.50
4:C:421:ARG:NH2	4:C:450:THR:O	2.45	0.50
5:E:180:GLY:HA3	5:E:183:GLU:HG2	1.94	0.50
4:B:168:ILE:HD11	4:B:330:THR:CG2	2.42	0.50
5:E:167:ASN:O	5:E:171:VAL:HG22	2.11	0.50
6:G:98:ILE:CD1	6:G:177:TYR:HA	2.40	0.49
4:B:363:ARG:HA	4:B:364:PRO:C	2.37	0.49
5:F:419:VAL:HG23	5:F:420:PHE:CE1	2.48	0.49
5:D:134:VAL:HG22	5:D:410:LEU:HB3	1.93	0.49
4:C:454:LEU:HD21	4:C:465:TRP:CH2	2.46	0.49
5:D:317:ALA:HB3	5:D:318:PRO:HD3	1.94	0.49
6:G:274:ALA:HA	6:G:277:THR:OG1	2.13	0.49
4:C:138:PRO:O	4:C:314:ASN:HB2	2.13	0.49
5:D:201:ILE:HD11	5:D:213:LEU:HD11	1.93	0.49
5:E:162:MET:HE3	5:E:416:VAL:CG1	2.43	0.49
4:C:363:ARG:HA	4:C:364:PRO:C	2.38	0.49
5:F:27:ILE:HD12	5:F:46:GLN:HA	1.94	0.49
5:F:440:VAL:HG23	5:F:459:ILE:HD11	1.94	0.48
6:G:180:PHE:CZ	6:G:240:ALA:HB3	2.48	0.48
4:B:63:VAL:HG13	4:B:71:VAL:CG1	2.43	0.48
5:F:317:ALA:HB3	5:F:318:PRO:HD3	1.95	0.48
5:D:92:VAL:HG13	5:D:93:VAL:HG13	1.95	0.48
4:A:428:LEU:HD12	4:A:466:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:38:ILE:HD11	4:B:74:VAL:HG13	1.95	0.48
5:F:363:HIS:CD2	5:F:434:ILE:HD11	2.49	0.48
4:B:411:LEU:HD23	4:B:415:THR:CB	2.42	0.48
4:B:387:VAL:O	4:B:391:VAL:HG23	2.14	0.48
5:F:143:LYS:O	5:F:301:THR:OG1	2.27	0.48
4:B:55:PHE:CD2	4:B:82:ILE:HD11	2.48	0.47
5:E:385:ALA:HB3	5:E:386:ILE:HD12	1.96	0.47
4:B:354:GLU:CD	4:B:367:ASN:HD22	2.22	0.47
4:B:310:SER:OG	4:B:324:ALA:HB2	2.14	0.47
4:B:142:VAL:HG11	4:B:160:GLY:HA3	1.96	0.47
4:A:169:GLY:O	4:A:175:LYS:HE2	2.15	0.47
4:C:227:MET:HE1	4:C:232:VAL:HG23	1.97	0.47
4:A:183:ILE:HD11	4:A:268:ILE:HD12	1.97	0.47
4:A:384:MET:HE3	4:A:387:VAL:HG23	1.97	0.47
4:A:433:GLN:CG	4:A:434:TYR:CE2	2.96	0.47
4:C:55:PHE:HB3	4:C:56:PRO:HD2	1.97	0.47
5:F:288:MET:CE	5:F:292:ILE:HD11	2.45	0.47
4:C:146:MET:CE	4:C:266:LEU:HD13	2.42	0.47
5:E:386:ILE:HG21	6:G:29:ALA:HB3	1.97	0.47
4:C:301:TYR:CZ	5:D:221:PRO:HA	2.50	0.46
5:D:386:ILE:HG22	6:G:90:LEU:HD11	1.96	0.46
5:E:150:PHE:HD2	5:E:330:VAL:HG22	1.81	0.46
5:F:58:MET:CE	5:F:224:ALA:HA	2.46	0.46
5:F:143:LYS:O	5:F:301:THR:HG23	2.15	0.46
5:F:341:TYR:HA	5:F:342:PRO:C	2.40	0.46
4:C:448:ALA:HB2	4:C:503:LEU:HD21	1.97	0.46
5:D:130:THR:HA	5:D:168:ILE:HD11	1.97	0.46
5:E:162:MET:HE3	5:E:416:VAL:HG11	1.98	0.46
5:E:398:LEU:HD21	5:E:402:ARG:NH2	2.30	0.46
5:F:396:ASP:O	5:F:400:VAL:HG23	2.16	0.46
7:H:73:GLU:O	7:H:76:GLY:N	2.49	0.46
4:C:442:ILE:O	4:C:446:ILE:HG12	2.15	0.46
5:F:130:THR:HA	5:F:168:ILE:HD11	1.97	0.46
4:A:454:LEU:HD21	4:A:465:TRP:CE3	2.51	0.46
4:B:205:VAL:CG2	4:B:251:ALA:CB	2.94	0.46
5:E:91:ASN:OD1	5:E:95:GLU:N	2.49	0.46
4:C:328:ILE:HD11	4:C:343:VAL:HG21	1.97	0.46
5:D:277:TYR:HE2	5:D:317:ALA:HB2	1.81	0.46
5:F:436:SER:CA	5:F:459:ILE:HD12	2.46	0.46
4:B:401:MET:HA	4:B:401:MET:HE2	1.98	0.45
4:C:28:VAL:HG13	4:C:88:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:137:MET:HA	4:C:137:MET:HE2	1.98	0.45
5:E:147:ILE:HD13	5:E:303:ILE:HD13	1.98	0.45
4:C:194:ALA:C	4:C:196:GLY:N	2.73	0.45
5:E:226:MET:HE3	5:E:227:ARG:CZ	2.46	0.45
4:A:167:ILE:HG22	4:A:175:LYS:HB2	1.99	0.45
4:B:102:GLU:HG3	4:B:123:ALA:HA	1.97	0.45
4:C:216:GLN:HE22	5:F:123:THR:HA	1.81	0.45
4:C:247:ALA:HB3	4:C:248:PRO:HD3	1.99	0.45
4:C:79:ASP:HA	4:C:82:ILE:HD12	1.98	0.45
5:D:233:LEU:HD11	5:D:291:ARG:NE	2.31	0.45
4:B:146:MET:HE2	4:B:147:ALA:N	2.32	0.45
4:B:273:SER:O	4:B:277:VAL:HG13	2.16	0.45
5:E:377:TYR:CE1	5:E:400:VAL:HG13	2.51	0.45
4:A:444:ILE:HG21	4:A:473:LEU:HD11	1.99	0.45
4:B:428:LEU:HD22	4:B:445:VAL:HG22	2.00	0.45
5:E:137:LEU:HD22	5:E:437:PHE:CD2	2.52	0.45
5:D:277:TYR:CE1	5:D:316:PRO:HG2	2.52	0.44
5:E:272:PRO:HD2	6:G:284:ILE:HD13	1.99	0.44
4:A:391:VAL:HG22	4:A:450:THR:CG2	2.47	0.44
4:A:260:ASP:C	4:A:261:ASN:HD22	2.26	0.44
4:C:384:MET:HE1	4:C:442:ILE:HG21	1.99	0.44
5:D:341:TYR:HA	5:D:342:PRO:C	2.42	0.44
6:G:176:PHE:CE1	6:G:190:ALA:HB2	2.52	0.44
5:F:11:VAL:O	5:F:12:ILE:HD13	2.17	0.44
5:F:40:LEU:HD23	5:F:64:LEU:HD21	1.99	0.44
6:G:36:GLN:HA	6:G:36:GLN:NE2	2.32	0.44
4:C:97:VAL:HB	4:C:98:PRO:HD2	1.99	0.44
4:C:398:TYR:CD1	4:C:422:GLY:HA3	2.53	0.44
4:C:404:PHE:CA	14:Z:9:ALA:HB1	2.47	0.44
5:F:229:ALA:HB1	5:F:288:MET:HE3	2.00	0.44
4:B:65:ASN:N	4:B:65:ASN:HD22	2.15	0.44
4:C:339:ILE:HB	4:C:340:PRO:HD3	1.99	0.44
5:D:58:MET:HE3	5:D:224:ALA:HA	1.99	0.44
5:F:274:ALA:O	5:F:275:VAL:HG12	2.17	0.44
4:B:304:SER:HB3	5:F:218:MET:HB2	1.98	0.44
4:B:158:PRO:HG2	4:B:377:SER:HA	2.00	0.43
4:C:63:VAL:HG13	4:C:71:VAL:HG13	2.00	0.43
4:C:331:GLN:HB3	5:F:314:THR:HG22	2.00	0.43
5:E:254:ILE:HG21	5:E:321:THR:HG21	2.00	0.43
4:C:315:GLU:HA	4:C:319:ALA:HB2	2.00	0.43
5:E:384:ILE:CG1	5:E:392:LEU:HD11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:99:VAL:HG13	6:G:129:LEU:HD11	2.00	0.43
4:B:63:VAL:HG13	4:B:71:VAL:HG13	2.00	0.43
5:E:341:TYR:HA	5:E:342:PRO:C	2.43	0.43
9:T:23:ALA:HA	9:U:24:ALA:CB	2.48	0.43
4:A:205:VAL:HG22	4:A:251:ALA:CB	2.48	0.43
4:C:63:VAL:HG13	4:C:71:VAL:CG1	2.48	0.43
5:F:48:LEU:HD21	5:F:54:ARG:CG	2.49	0.43
4:A:271:ASP:HB2	4:A:327:ILE:O	2.19	0.43
4:C:138:PRO:C	4:C:314:ASN:HB2	2.43	0.43
5:F:89:ILE:HD11	5:F:192:TYR:CD1	2.53	0.43
4:A:146:MET:HE1	4:A:182:THR:CG2	2.44	0.43
4:B:401:MET:O	4:B:403:ALA:N	2.51	0.43
4:B:444:ILE:HG21	4:B:473:LEU:HD11	2.01	0.43
6:G:193:VAL:CG2	6:G:227:VAL:HG13	2.49	0.43
4:A:310:SER:OG	4:A:324:ALA:HB2	2.18	0.43
5:F:386:ILE:HD11	6:G:260:MET:HE1	2.00	0.43
4:B:340:PRO:O	4:B:344:ILE:HG13	2.19	0.43
5:E:317:ALA:HB3	5:E:318:PRO:CD	2.49	0.43
5:D:370:VAL:HG13	5:D:406:ILE:HG21	2.01	0.43
4:A:454:LEU:HD21	4:A:465:TRP:CZ3	2.53	0.42
4:B:339:ILE:HD12	4:B:339:ILE:H	1.83	0.42
5:E:317:ALA:HB3	5:E:318:PRO:HD3	2.01	0.42
7:H:29:GLY:O	7:H:30:ILE:C	2.62	0.42
5:D:436:SER:HB3	5:D:459:ILE:HB	2.00	0.42
5:E:165:ILE:HG21	5:E:211:VAL:HG13	2.01	0.42
9:J:23:ALA:HA	9:K:24:ALA:CB	2.48	0.42
5:E:389:MET:C	5:E:391:GLU:H	2.28	0.42
5:F:137:LEU:HD22	5:F:437:PHE:CD2	2.53	0.42
4:C:411:LEU:O	4:C:416:GLN:NE2	2.51	0.42
6:G:21:THR:HG22	6:G:250:MET:HE3	2.01	0.42
5:D:8:ILE:HD12	5:D:68:LEU:HB2	2.02	0.42
5:E:426:VAL:HG21	5:E:457:GLY:HA3	2.00	0.42
4:A:284:LEU:HD11	4:A:294:ALA:O	2.20	0.42
4:B:30:GLN:O	4:B:31:VAL:HB	2.19	0.42
4:C:146:MET:HE2	4:C:200:LEU:HD21	2.01	0.42
5:D:58:MET:CE	5:D:224:ALA:HA	2.50	0.42
4:B:350:GLN:HG3	4:B:352:PHE:CZ	2.54	0.41
4:C:241:ALA:HB3	4:C:242:PRO:HD3	2.01	0.41
5:E:162:MET:HA	5:E:165:ILE:HD12	2.02	0.41
5:E:275:VAL:O	5:E:275:VAL:HG12	2.20	0.41
4:B:156:MET:CE	4:B:368:THR:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:277:TYR:HD2	5:D:281:LEU:HD12	1.85	0.41
5:F:356:PRO:HD3	5:F:364:TYR:CE1	2.55	0.41
4:C:136:ILE:HD13	5:D:185:THR:HG23	2.02	0.41
4:C:233:VAL:HG21	4:C:251:ALA:HB2	2.02	0.41
5:D:233:LEU:HD11	5:D:291:ARG:CZ	2.51	0.41
5:E:252:ASP:HA	5:E:253:ASN:HA	1.93	0.41
5:F:92:VAL:HG21	5:F:227:ARG:HB2	2.03	0.41
5:F:436:SER:HB3	5:F:459:ILE:HD12	2.03	0.41
4:A:63:VAL:HG13	4:A:71:VAL:CG2	2.50	0.41
4:A:63:VAL:HG13	4:A:71:VAL:HG22	2.01	0.41
4:C:301:TYR:CE1	4:C:305:ARG:CG	3.04	0.41
4:C:491:VAL:O	4:C:492:ALA:HB2	2.21	0.41
5:D:183:GLU:H	5:D:217:GLN:NE2	2.19	0.41
5:E:370:VAL:HG13	5:E:406:ILE:HG21	2.02	0.41
4:C:428:LEU:HD11	4:C:454:LEU:HD11	2.03	0.41
5:D:281:LEU:C	5:D:281:LEU:HD23	2.46	0.41
6:G:106:LEU:CD1	6:G:116:VAL:HG11	2.49	0.41
5:E:165:ILE:CD1	5:E:211:VAL:HG11	2.48	0.40
7:H:44:TYR:O	7:H:50:LEU:CB	2.69	0.40
5:D:15:VAL:CG2	5:D:264:VAL:HG23	2.51	0.40
5:F:253:ASN:OD1	5:F:255:PHE:HB3	2.21	0.40
4:C:206:ALA:CB	4:C:209:GLN:OE1	2.66	0.40
4:C:489:ARG:HG3	4:C:495:LEU:HD22	2.02	0.40
4:A:339:ILE:N	4:A:340:PRO:CD	2.85	0.40
4:C:33:SER:HB2	5:F:47:HIS:O	2.22	0.40
5:F:356:PRO:HD3	5:F:364:TYR:CD1	2.56	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	
4	A	501/511 (98%)	470 (94%)	24 (5%)	7 (1%)	9	39
4	B	490/511 (96%)	459 (94%)	26 (5%)	5 (1%)	12	45
4	C	482/511 (94%)	463 (96%)	15 (3%)	4 (1%)	16	51
5	D	468/474 (99%)	448 (96%)	19 (4%)	1 (0%)	43	75
5	E	464/474 (98%)	439 (95%)	22 (5%)	3 (1%)	21	57
5	F	464/474 (98%)	439 (95%)	23 (5%)	2 (0%)	30	65
6	G	246/290 (85%)	233 (95%)	8 (3%)	5 (2%)	6	33
7	H	108/188 (57%)	90 (83%)	12 (11%)	6 (6%)	1	18
8	I	73/148 (49%)	66 (90%)	5 (7%)	2 (3%)	4	28
9	J	72/77 (94%)	72 (100%)	0	0	100	100
9	K	72/77 (94%)	72 (100%)	0	0	100	100
9	L	72/77 (94%)	72 (100%)	0	0	100	100
9	M	72/77 (94%)	72 (100%)	0	0	100	100
9	N	72/77 (94%)	72 (100%)	0	0	100	100
9	O	72/77 (94%)	72 (100%)	0	0	100	100
9	P	72/77 (94%)	72 (100%)	0	0	100	100
9	Q	72/77 (94%)	72 (100%)	0	0	100	100
9	R	72/77 (94%)	72 (100%)	0	0	100	100
9	S	72/77 (94%)	72 (100%)	0	0	100	100
9	T	72/77 (94%)	72 (100%)	0	0	100	100
9	U	72/77 (94%)	72 (100%)	0	0	100	100
12	X	59/283 (21%)	58 (98%)	1 (2%)	0	100	100
14	Z	50/104 (48%)	47 (94%)	2 (4%)	1 (2%)	6	33
All	All	4269/4892 (87%)	4076 (96%)	157 (4%)	36 (1%)	16	51

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	23	ALA
4	A	199	THR
4	B	402	ALA
4	C	197	MET
4	C	492	ALA
5	E	274	ALA
5	F	143	LYS

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Mol	Chain	Res	Type
6	G	67	PRO
6	G	133	TYR
7	H	73	GLU
7	H	74	ARG
7	H	75	MET
14	Z	101	SER
4	A	24	GLU
4	A	171	ARG
4	B	80	ARG
4	B	237	ALA
4	B	412	ASP
5	F	171	VAL
6	G	61	ALA
7	H	30	ILE
7	H	112	LYS
8	I	55	GLY
8	I	73	ASN
4	A	21	GLN
4	A	121	LEU
4	A	409	SER
6	G	134	GLY
4	C	195	ASP
6	G	66	ALA
4	B	31	VAL
4	C	408	GLY
5	D	23	GLN
5	E	390	ASP
7	H	29	GLY
5	E	275	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	
4	A	396/401 (99%)	371 (94%)	25 (6%)	16	40
4	B	391/401 (98%)	370 (95%)	21 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	379/401 (94%)	361 (95%)	18 (5%)	23	46
5	D	371/375 (99%)	354 (95%)	17 (5%)	24	47
5	E	372/375 (99%)	362 (97%)	10 (3%)	39	60
5	F	372/375 (99%)	354 (95%)	18 (5%)	23	46
6	G	203/227 (89%)	195 (96%)	8 (4%)	28	50
14	Z	45/81 (56%)	44 (98%)	1 (2%)	45	64
All	All	2529/2636 (96%)	2411 (95%)	118 (5%)	23	46

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	33	SER
4	A	71	VAL
4	A	103	LEU
4	A	113	ASN
4	A	127	ARG
4	A	146	MET
4	A	167	ILE
4	A	168	ILE
4	A	198	LYS
4	A	209	GLN
4	A	246	LEU
4	A	282	MET
4	A	304	SER
4	A	314	ASN
4	A	323	THR
4	A	356	GLU
4	A	372	VAL
4	A	393	LEU
4	A	410	ASP
4	A	415	THR
4	A	417	LYS
4	A	443	VAL
4	A	445	VAL
4	A	446	ILE
4	A	508	LYS
4	B	30	GLN
4	B	65	ASN
4	B	74	VAL
4	B	89	LYS

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Mol	Chain	Res	Type
4	B	102	GLU
4	B	146	MET
4	B	210	LYS
4	B	227	MET
4	B	277	VAL
4	B	304	SER
4	B	345	SER
4	B	346	ILE
4	B	350	GLN
4	B	377	SER
4	B	393	LEU
4	B	400	GLU
4	B	417	LYS
4	B	421	ARG
4	B	460	ARG
4	B	463	THR
4	B	494	GLU
4	C	28	VAL
4	C	52	MET
4	C	74	VAL
4	C	103	LEU
4	C	111	LEU
4	C	127	ARG
4	C	146	MET
4	C	157	ILE
4	C	217	LEU
4	C	277	VAL
4	C	335	VAL
4	C	372	VAL
4	C	409	SER
4	C	410	ASP
4	C	415	THR
4	C	433	GLN
4	C	435	SER
4	C	445	VAL
5	D	39	ARG
5	D	54	ARG
5	D	56	ILE
5	D	121	GLN
5	D	126	GLU
5	D	162	MET
5	D	181	VAL

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Mol	Chain	Res	Type
5	D	210	GLN
5	D	228	VAL
5	D	233	LEU
5	D	262	SER
5	D	264	VAL
5	D	267	LEU
5	D	278	GLN
5	D	292	ILE
5	D	331	LEU
5	D	389	MET
5	E	46	GLN
5	E	56	ILE
5	E	62	GLU
5	E	92	VAL
5	E	107	GLN
5	E	146	LYS
5	E	219	ASN
5	E	228	VAL
5	E	248	LEU
5	E	268	LEU
5	F	24	LEU
5	F	36	ASN
5	F	39	ARG
5	F	46	GLN
5	F	54	ARG
5	F	107	GLN
5	F	134	VAL
5	F	171	VAL
5	F	219	ASN
5	F	228	VAL
5	F	233	LEU
5	F	245	THR
5	F	275	VAL
5	F	278	GLN
5	F	353	ILE
5	F	420	PHE
5	F	459	ILE
5	F	469	LEU
6	G	36	GLN
6	G	79	HIS
6	G	101	LEU
6	G	153	ASN

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Mol	Chain	Res	Type
6	G	157	ILE
6	G	159	ASP
6	G	215	GLU
6	G	277	THR
14	Z	97	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	113	ASN
4	A	186	GLN
4	A	261	ASN
4	A	314	ASN
4	A	380	GLN
4	A	406	GLN
4	A	439	ASN
4	A	475	ASN
4	B	18	ASN
4	B	48	GLN
4	B	65	ASN
4	B	186	GLN
4	B	331	GLN
4	B	439	ASN
4	B	467	HIS
4	C	65	ASN
4	C	122	ASN
4	C	216	GLN
4	C	261	ASN
4	C	439	ASN
5	D	19	GLN
5	D	35	ASN
5	D	189	ASN
5	D	210	GLN
5	D	217	GLN
5	D	278	GLN
5	D	375	GLN
5	E	36	ASN
5	E	107	GLN
5	E	189	ASN
5	E	219	ASN
5	E	289	GLN
5	E	304	GLN

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Mol	Chain	Res	Type
5	E	407	GLN
5	F	10	GLN
5	F	35	ASN
5	F	36	ASN
5	F	46	GLN
5	F	51	ASN
5	F	91	ASN
5	F	121	GLN
5	F	189	ASN
5	F	217	GLN
5	F	278	GLN
5	F	350	ASN
5	F	363	HIS
5	F	365	GLN
5	F	375	GLN
5	F	467	GLN
6	G	9	ASN
6	G	36	GLN
6	G	79	HIS
6	G	139	ASN
14	Z	10	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
15	ATP	C	600	16	32,33,33	1.51	6 (18%)	48,52,52	1.77	11 (22%)
17	ADP	B	600	16	28,29,29	1.49	5 (17%)	43,45,45	1.88	10 (23%)
15	ATP	D	600	16	32,33,33	1.44	5 (15%)	48,52,52	1.83	12 (25%)
15	ATP	A	600	16	32,33,33	1.50	4 (12%)	48,52,52	1.77	8 (16%)
15	ATP	F	600	16	32,33,33	1.51	5 (15%)	48,52,52	1.75	9 (18%)

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
15	ATP	C	600	16	-	2/22/38/38	0/3/3/3
17	ADP	B	600	16	-	0/16/32/32	0/3/3/3
15	ATP	D	600	16	-	0/22/38/38	0/3/3/3
15	ATP	A	600	16	-	0/22/38/38	0/3/3/3
15	ATP	F	600	16	-	7/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	600	ATP	C5-C4	5.12	1.48	1.39
15	F	600	ATP	C5-C4	4.92	1.47	1.39
17	B	600	ADP	C5-C4	4.88	1.47	1.39
15	C	600	ATP	C5-C4	4.83	1.47	1.39
15	D	600	ATP	C5-C4	4.74	1.47	1.39
17	B	600	ADP	C5-C6	2.97	1.49	1.41
15	D	600	ATP	C5-C6	2.83	1.48	1.41
15	F	600	ATP	C5-C6	2.79	1.48	1.41
15	A	600	ATP	C5-C6	2.75	1.48	1.41
15	C	600	ATP	C5-C6	2.75	1.48	1.41
15	F	600	ATP	C5-N7	-2.62	1.34	1.39
15	A	600	ATP	C5-N7	-2.60	1.34	1.39
15	F	600	ATP	PB-O3B	2.56	1.62	1.59
15	C	600	ATP	PB-O3B	2.55	1.62	1.59
17	B	600	ADP	C8-N7	2.43	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	600	ATP	C5-N7	-2.42	1.34	1.39
15	D	600	ATP	C8-N7	2.41	1.36	1.31
15	C	600	ATP	PA-O3A	2.39	1.62	1.59
15	C	600	ATP	C5-N7	-2.36	1.34	1.39
15	C	600	ATP	C8-N7	2.36	1.36	1.31
15	A	600	ATP	C8-N7	2.33	1.36	1.31
15	F	600	ATP	C8-N7	2.32	1.36	1.31
17	B	600	ADP	C5-N7	-2.24	1.35	1.39
15	D	600	ATP	PB-O3B	2.10	1.61	1.59
17	B	600	ADP	PA-O3A	2.08	1.61	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	600	ATP	C5-C4-N3	-5.97	118.50	126.72
15	F	600	ATP	C5-C4-N3	-5.95	118.52	126.72
17	B	600	ADP	C5-C4-N3	-5.82	118.71	126.72
15	D	600	ATP	C5-C4-N3	-5.62	118.98	126.72
15	C	600	ATP	C5-C4-N3	-5.57	119.05	126.72
15	A	600	ATP	N3-C4-N9	4.75	135.25	127.17
17	B	600	ADP	N3-C4-N9	4.71	135.18	127.17
15	F	600	ATP	N3-C4-N9	4.65	135.07	127.17
15	C	600	ATP	N3-C4-N9	4.55	134.91	127.17
15	D	600	ATP	N3-C4-N9	4.39	134.64	127.17
17	B	600	ADP	C2-N3-C4	3.99	121.57	111.83
17	B	600	ADP	N3-C2-N1	-3.93	122.63	128.58
15	D	600	ATP	N3-C2-N1	-3.89	122.70	128.58
15	D	600	ATP	C2-N3-C4	3.88	121.30	111.83
15	F	600	ATP	C2-N3-C4	3.86	121.26	111.83
15	A	600	ATP	C2-N3-C4	3.76	121.02	111.83
15	C	600	ATP	C2-N3-C4	3.74	120.97	111.83
15	C	600	ATP	N3-C2-N1	-3.71	122.96	128.58
15	A	600	ATP	N3-C2-N1	-3.58	123.17	128.58
15	F	600	ATP	N3-C2-N1	-3.48	123.31	128.58
15	F	600	ATP	C4-C5-N7	-3.47	106.61	110.58
15	D	600	ATP	C4-C5-N7	-3.46	106.63	110.58
17	B	600	ADP	C4-C5-N7	-3.42	106.67	110.58
15	C	600	ATP	C4-C5-N7	-3.40	106.69	110.58
15	A	600	ATP	C4-C5-N7	-3.37	106.73	110.58
15	C	600	ATP	C4-N9-C8	3.01	108.90	105.74
17	B	600	ADP	C4-N9-C8	2.86	108.74	105.74
17	B	600	ADP	C5-N7-C8	2.69	107.67	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	600	ATP	O4'-C1'-N9	2.67	113.22	108.09
15	D	600	ATP	C4-N9-C8	2.62	108.49	105.74
15	D	600	ATP	C5-N7-C8	2.58	107.50	103.45
15	C	600	ATP	C5-N7-C8	2.57	107.49	103.45
15	D	600	ATP	C3'-C2'-C1'	2.56	106.30	101.46
15	A	600	ATP	C5-N7-C8	2.49	107.36	103.45
15	F	600	ATP	C5-N7-C8	2.49	107.36	103.45
15	F	600	ATP	C3'-C2'-C1'	2.43	106.06	101.46
15	F	600	ATP	C4-N9-C8	2.30	108.15	105.74
15	D	600	ATP	C6-C5-N7	2.23	136.38	132.09
15	A	600	ATP	C4-N9-C8	2.22	108.07	105.74
17	B	600	ADP	N9-C8-N7	-2.21	110.80	113.94
17	B	600	ADP	C6-C5-N7	2.20	136.34	132.09
15	C	600	ATP	C2-N1-C6	2.17	122.30	118.73
15	A	600	ATP	C2-N1-C6	2.17	122.29	118.73
15	C	600	ATP	N9-C8-N7	-2.15	110.88	113.94
15	D	600	ATP	C2-N1-C6	2.12	122.22	118.73
15	C	600	ATP	C6-C5-N7	2.09	136.12	132.09
17	B	600	ADP	C2-N1-C6	2.09	122.16	118.73
15	D	600	ATP	N9-C8-N7	-2.07	111.00	113.94
15	F	600	ATP	C6-C5-N7	2.04	136.02	132.09
15	C	600	ATP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

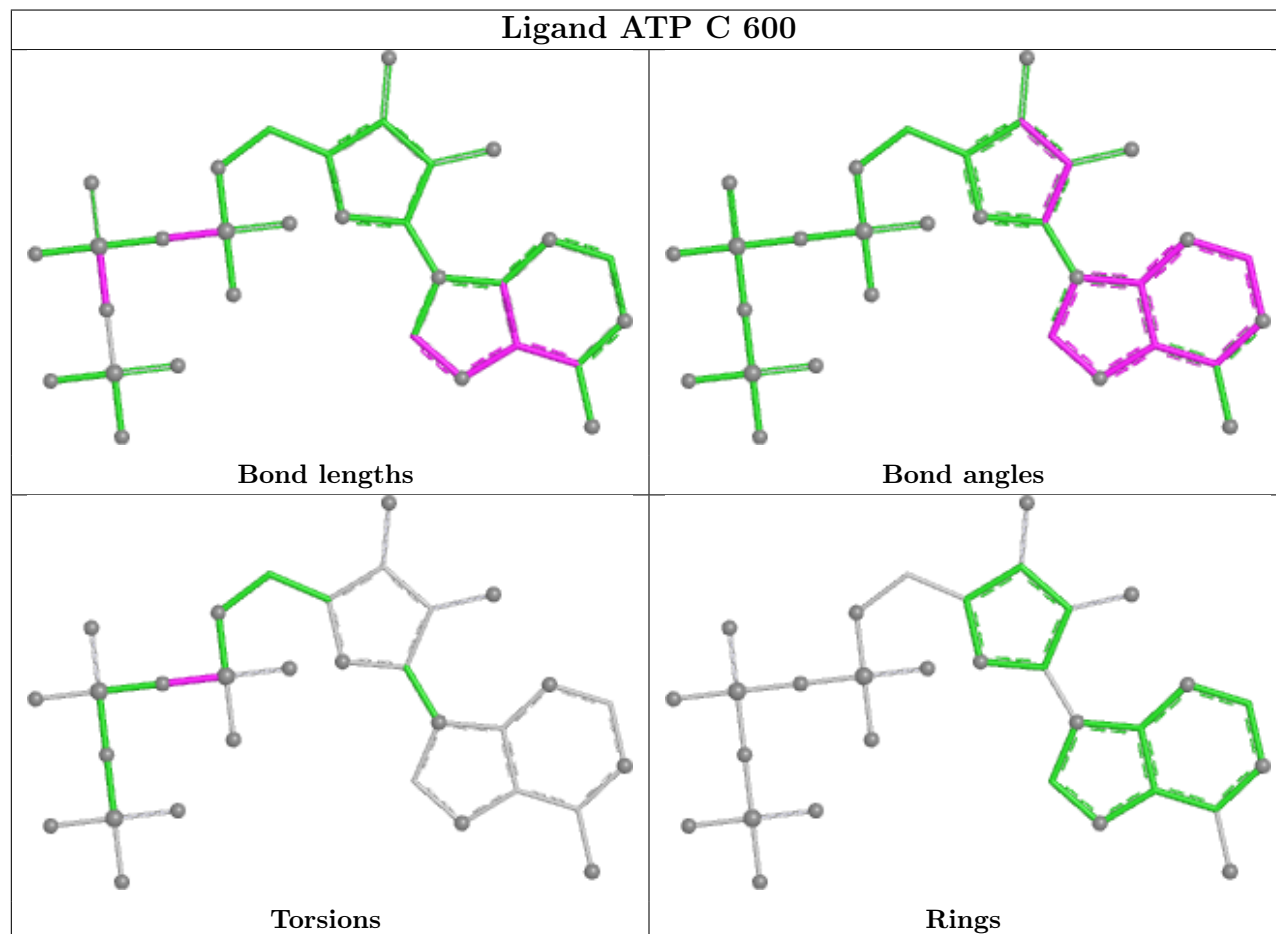
Mol	Chain	Res	Type	Atoms
15	F	600	ATP	C5'-O5'-PA-O2A
15	F	600	ATP	C5'-O5'-PA-O3A
15	F	600	ATP	O4'-C4'-C5'-O5'
15	F	600	ATP	C3'-C4'-C5'-O5'
15	C	600	ATP	PB-O3A-PA-O1A
15	F	600	ATP	C5'-O5'-PA-O1A
15	F	600	ATP	PA-O3A-PB-O1B
15	F	600	ATP	PA-O3A-PB-O2B
15	C	600	ATP	PB-O3A-PA-O2A

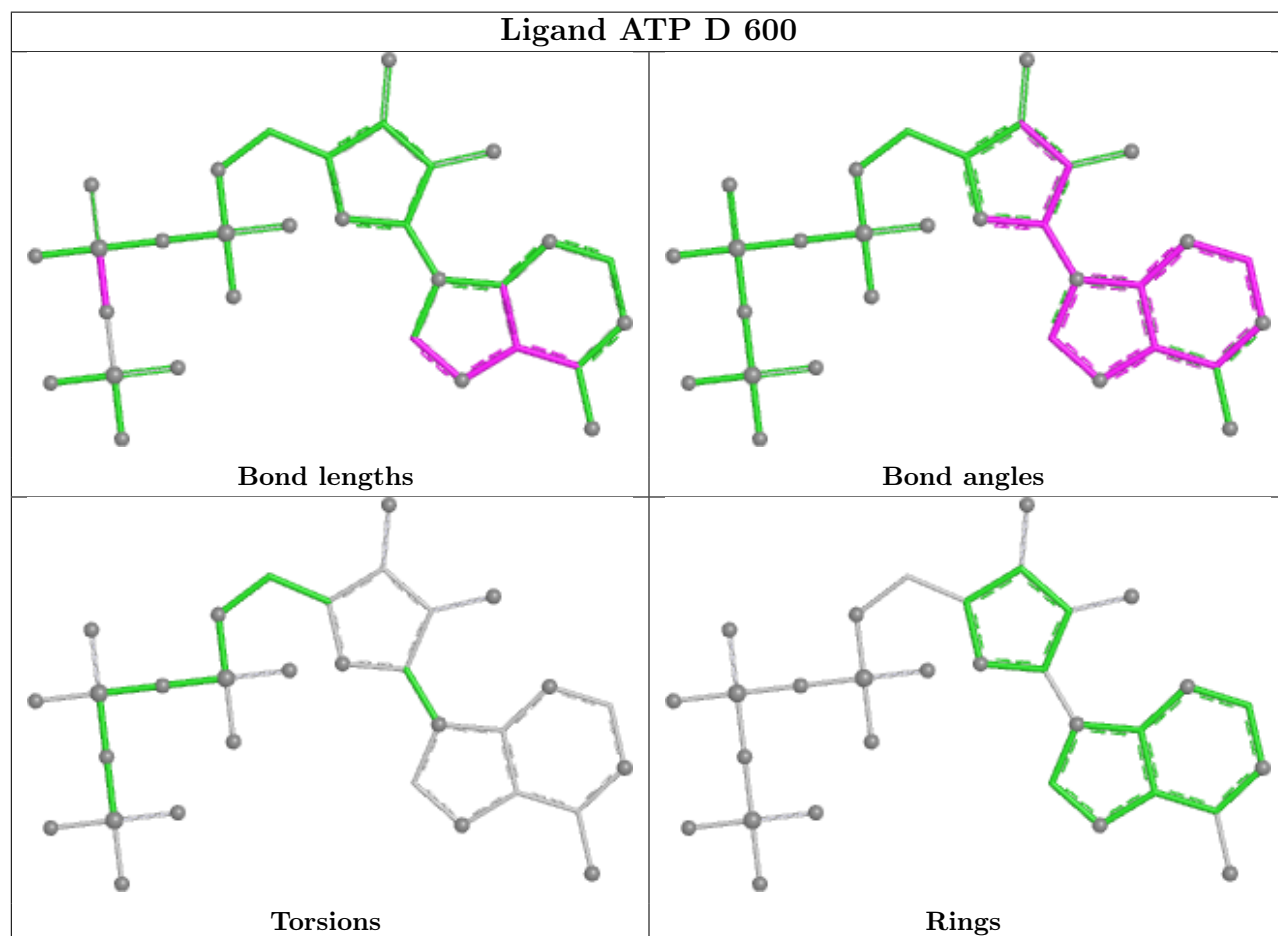
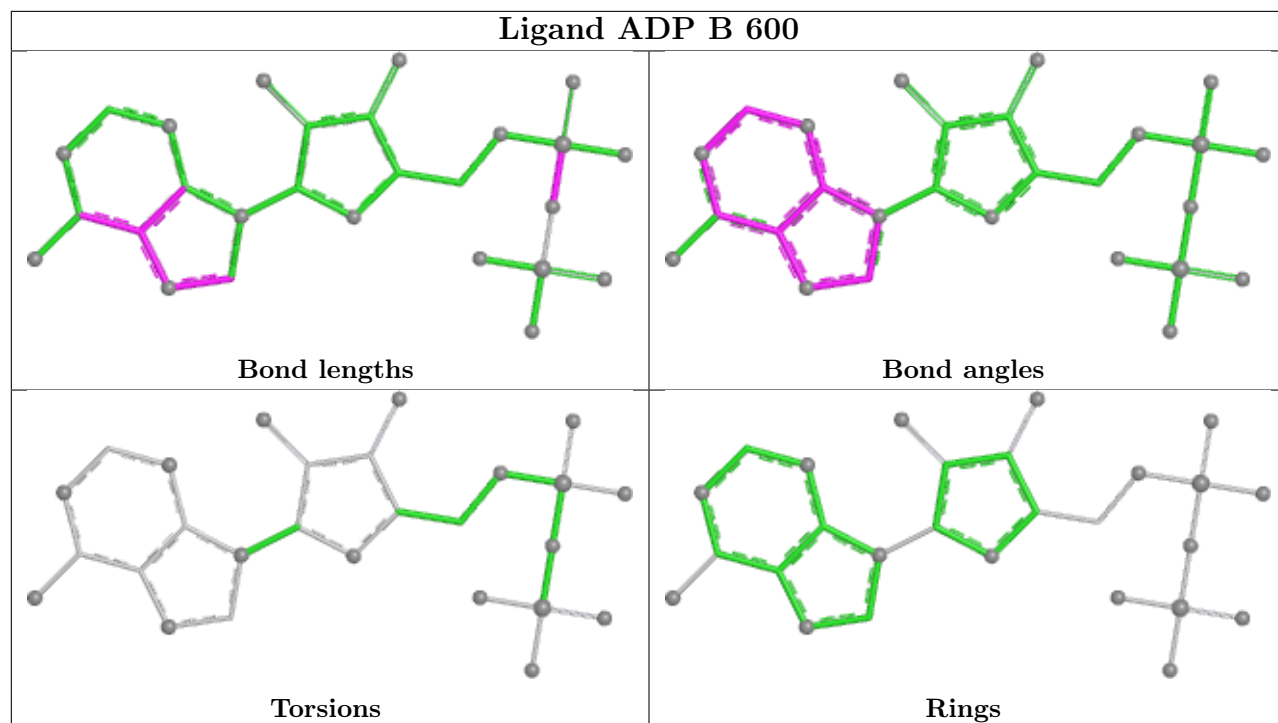
There are no ring outliers.

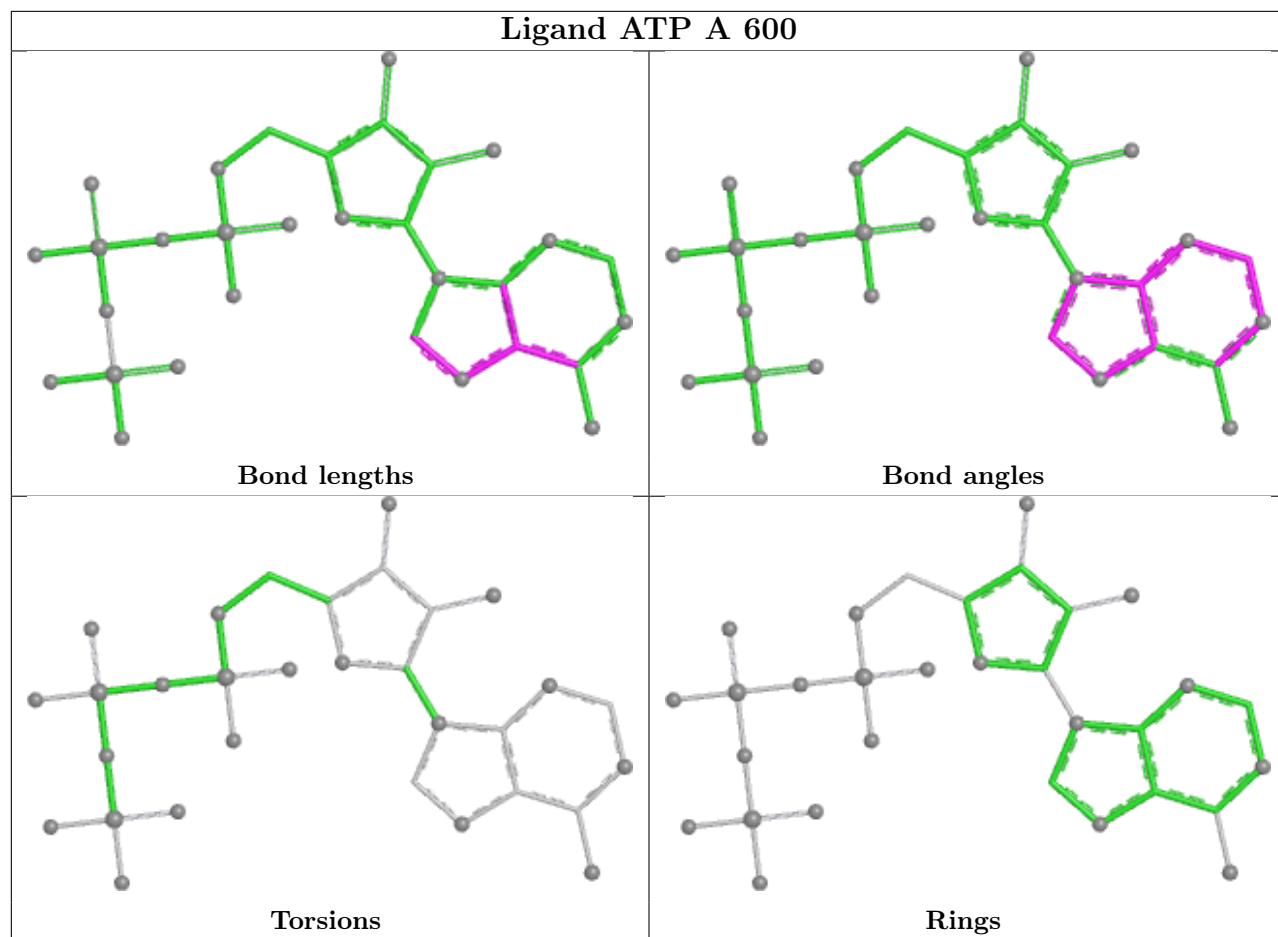
No monomer is involved in short contacts.

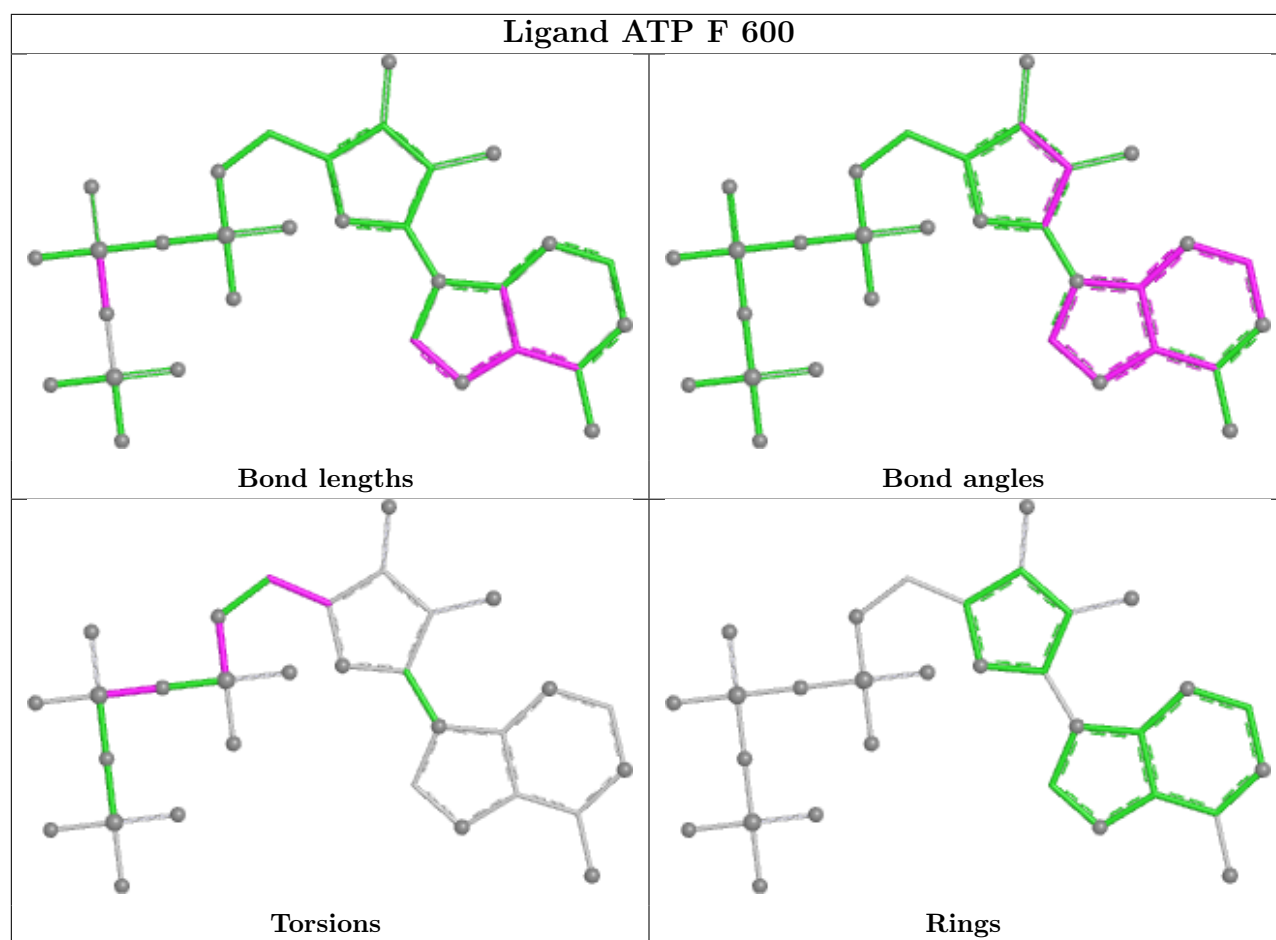
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 [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	1	0/20	-	-	-	-
2	2	0/15	-	-	-	-
3	3	0/19	-	-	-	-
4	A	505/511 (98%)	0.70	53 (10%) 11 14	73, 123, 205, 249	0
4	B	496/511 (97%)	0.54	42 (8%) 16 18	59, 112, 185, 216	0
4	C	484/511 (94%)	0.58	36 (7%) 20 20	67, 107, 159, 206	0
5	D	470/474 (99%)	0.58	38 (8%) 18 18	73, 107, 156, 186	0
5	E	466/474 (98%)	0.53	38 (8%) 17 18	72, 131, 203, 247	0
5	F	466/474 (98%)	0.48	26 (5%) 30 25	58, 100, 153, 189	0
6	G	260/290 (89%)	0.66	28 (10%) 11 13	80, 143, 203, 224	0
7	H	110/188 (58%)	0.54	9 (8%) 17 18	110, 152, 185, 215	0
8	I	75/148 (50%)	0.58	3 (4%) 42 32	167, 207, 238, 241	0
9	J	74/77 (96%)	1.78	19 (25%) 1 4	217, 279, 383, 417	0
9	K	74/77 (96%)	2.05	15 (20%) 3 5	182, 295, 402, 415	0
9	L	74/77 (96%)	1.25	14 (18%) 3 6	224, 296, 463, 488	0
9	M	74/77 (96%)	0.88	7 (9%) 14 16	209, 279, 409, 418	0
9	N	74/77 (96%)	1.20	17 (22%) 2 4	214, 273, 401, 421	0
9	O	74/77 (96%)	1.21	13 (17%) 4 7	220, 287, 352, 363	0
9	P	74/77 (96%)	1.46	18 (24%) 2 4	222, 304, 397, 443	0
9	Q	74/77 (96%)	1.78	21 (28%) 1 3	266, 349, 427, 451	0
9	R	74/77 (96%)	1.64	24 (32%) 1 2	200, 315, 439, 449	0
9	S	74/77 (96%)	1.09	9 (12%) 8 12	239, 320, 445, 471	0
9	T	74/77 (96%)	0.79	8 (10%) 11 13	260, 317, 430, 437	0
9	U	74/77 (96%)	1.34	12 (16%) 4 8	231, 279, 431, 447	0
10	V	0/78	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
11	W	0/124	-	-	-	-
12	X	63/283 (22%)	0.68	6 (9%) 14 16	147, 201, 252, 268	0
13	Y	0/54	-	-	-	-
14	Z	54/104 (51%)	0.43	3 (5%) 30 25	135, 172, 218, 248	0
All	All	4337/5202 (83%)	0.74	459 (10%) 11 13	58, 131, 361, 488	0

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	K	61	ALA	24.4
9	K	64	ILE	20.9
9	Q	61	ALA	14.5
12	X	1205	ILE	13.0
9	K	68	LEU	11.6
9	K	60	GLU	11.2
9	J	57	ALA	11.0
9	J	61	ALA	11.0
9	N	18	VAL	10.9
9	U	54	ILE	9.8
9	K	65	PHE	9.7
9	O	68	LEU	8.7
9	U	53	PHE	8.4
9	Q	57	ALA	8.3
9	U	57	ALA	7.7
9	Q	30	VAL	7.3
9	R	57	ALA	7.0
9	Q	27	VAL	6.9
5	D	212	ALA	6.7
5	F	260	ALA	6.7
4	B	225	GLY	6.6
9	J	53	PHE	6.6
4	C	389	GLY	6.5
9	R	50	ALA	6.5
9	J	71	LEU	6.5
9	P	71	LEU	6.4
9	U	76	ALA	6.4
9	L	38	ALA	6.4
4	C	335	VAL	6.3
9	S	43	SER	6.2
9	R	53	PHE	6.2
9	U	31	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
9	J	68	LEU	6.0
9	R	27	VAL	6.0
9	J	74	LEU	5.9
9	L	18	VAL	5.9
9	O	18	VAL	5.8
4	A	181	ASP	5.8
4	B	378	ALA	5.7
4	A	491	VAL	5.7
9	Q	31	ALA	5.7
4	A	378	ALA	5.6
5	E	150	PHE	5.6
4	B	332	ALA	5.6
9	P	75	PHE	5.4
9	N	48	GLN	5.4
4	B	488	ASP	5.3
9	S	57	ALA	5.2
7	H	87	LEU	5.2
9	L	35	LEU	5.2
9	U	68	LEU	5.2
9	O	72	LEU	5.1
4	B	228	ALA	5.1
5	D	430	LEU	5.1
9	J	54	ILE	5.0
4	A	95	VAL	4.9
9	K	67	PHE	4.9
6	G	43	ARG	4.9
6	G	193	VAL	4.9
4	A	379	ALA	4.8
5	E	325	LEU	4.8
5	F	263	GLU	4.8
9	M	34	TYR	4.7
4	B	393	LEU	4.6
4	C	128	ILE	4.6
9	N	21	ALA	4.6
5	E	80	PRO	4.6
9	M	31	ALA	4.5
6	G	142	ASP	4.5
9	Q	55	GLY	4.5
5	D	390	ASP	4.5
9	R	31	ALA	4.5
4	C	148	THR	4.4
5	D	21	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
4	A	145	PRO	4.4
5	F	102	PRO	4.4
4	A	150	LEU	4.4
6	G	196	ALA	4.3
9	T	31	ALA	4.3
4	B	67	GLU	4.3
5	E	141	TYR	4.3
4	C	155	ALA	4.2
5	D	363	HIS	4.2
4	B	55	PHE	4.2
9	J	21	ALA	4.2
5	D	433	THR	4.2
9	R	61	ALA	4.2
5	E	160	LEU	4.1
4	B	271	ASP	4.1
9	U	72	LEU	4.1
9	R	60	GLU	4.1
4	A	180	LEU	4.1
4	B	65	ASN	4.0
9	L	53	PHE	4.0
4	A	132	LYS	4.0
5	D	85	THR	4.0
9	M	18	VAL	3.9
9	O	76	ALA	3.9
5	E	148	GLY	3.9
4	C	94	ILE	3.9
5	D	434	ILE	3.9
4	C	388	ALA	3.9
9	O	44	ALA	3.9
9	L	43	SER	3.9
9	Q	64	ILE	3.8
4	A	159	VAL	3.8
4	C	182	THR	3.8
5	F	204	ASP	3.8
4	B	187	ALA	3.7
4	A	202	CYS	3.7
4	B	226	ALA	3.7
5	E	38	LYS	3.7
4	B	376	GLY	3.7
9	L	48	GLN	3.7
5	F	164	LEU	3.7
4	A	196	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
4	B	136	ILE	3.6
9	N	68	LEU	3.6
4	A	146	MET	3.6
4	A	426	THR	3.6
5	E	420	PHE	3.6
4	C	340	PRO	3.6
4	A	121	LEU	3.6
9	U	64	ILE	3.6
4	C	147	ALA	3.6
6	G	143	LEU	3.6
5	D	211	VAL	3.5
9	P	42	PRO	3.5
4	C	406	GLN	3.5
4	B	209	GLN	3.5
9	P	38	ALA	3.5
4	A	434	TYR	3.5
9	R	51	THR	3.5
9	N	38	ALA	3.4
6	G	109	LEU	3.4
5	D	62	GLU	3.4
9	Q	47	SER	3.4
9	O	75	PHE	3.4
4	B	364	PRO	3.4
9	L	36	ALA	3.4
4	A	144	GLU	3.4
4	B	189	TYR	3.3
6	G	195	PRO	3.3
4	C	46	LYS	3.3
9	P	53	PHE	3.3
5	F	100	GLY	3.3
9	Q	28	GLY	3.3
4	A	103	LEU	3.3
4	B	388	ALA	3.3
9	U	61	ALA	3.3
7	H	75	MET	3.3
5	D	213	LEU	3.2
9	S	31	ALA	3.2
9	J	29	ASN	3.2
9	P	72	LEU	3.2
4	A	492	ALA	3.2
5	E	217	GLN	3.2
4	B	331	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
4	A	57	GLY	3.2
9	N	64	ILE	3.2
9	R	54	ILE	3.2
5	D	407	GLN	3.2
9	O	21	ALA	3.2
4	B	491	VAL	3.1
7	H	71	LEU	3.1
5	E	147	ILE	3.1
9	T	54	ILE	3.1
9	R	20	MET	3.1
9	J	58	PHE	3.1
9	Q	11	LEU	3.1
9	T	68	LEU	3.1
4	B	375	VAL	3.1
5	D	251	VAL	3.1
9	J	31	ALA	3.1
5	E	371	GLN	3.1
5	E	257	PHE	3.1
12	X	1204	LEU	3.1
9	K	43	SER	3.1
9	N	61	ALA	3.1
9	O	3	ASN	3.1
4	C	49	ALA	3.0
9	N	45	ALA	3.0
4	A	245	TYR	3.0
5	F	103	VAL	3.0
9	T	30	VAL	3.0
5	F	88	ARG	3.0
6	G	88	ARG	3.0
9	M	36	ALA	3.0
4	B	171	ARG	3.0
9	P	11	LEU	3.0
4	B	210	LYS	3.0
4	B	61	GLY	3.0
4	B	124	SER	3.0
6	G	42	ALA	3.0
9	P	43	SER	3.0
6	G	46	ALA	3.0
9	J	49	THR	2.9
4	A	177	ALA	2.9
4	C	390	PRO	2.9
9	J	60	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
9	R	11	LEU	2.9
4	A	431	GLN	2.9
4	B	377	SER	2.9
7	H	5	SER	2.9
9	S	61	ALA	2.9
4	A	430	LYS	2.9
5	E	254	ILE	2.9
4	C	185	ASN	2.9
9	J	65	PHE	2.9
9	N	41	ASN	2.9
9	R	3	ASN	2.9
9	N	42	PRO	2.9
9	R	42	PRO	2.9
9	P	18	VAL	2.8
6	G	213	PRO	2.8
9	R	17	CYS	2.8
4	B	380	GLN	2.8
5	D	122	ALA	2.8
4	A	266	LEU	2.8
9	K	31	ALA	2.8
9	N	44	ALA	2.8
5	D	275	VAL	2.8
4	C	50	GLY	2.8
12	X	1278	ALA	2.8
5	E	344	VAL	2.8
9	J	75	PHE	2.8
6	G	173	ALA	2.8
5	F	168	ILE	2.7
14	Z	12	ALA	2.7
5	F	165	ILE	2.7
9	R	30	VAL	2.7
5	E	164	LEU	2.7
5	F	101	GLY	2.7
9	P	10	TYR	2.7
9	P	17	CYS	2.7
9	T	55	GLY	2.7
4	B	499	ILE	2.7
9	P	3	ASN	2.7
9	P	44	ALA	2.7
4	B	327	ILE	2.7
6	G	181	GLU	2.7
4	A	153	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
4	A	133	ALA	2.7
6	G	190	ALA	2.7
9	O	36	ALA	2.7
9	O	46	ALA	2.7
9	L	41	ASN	2.7
6	G	140	HIS	2.6
12	X	1201	VAL	2.6
4	A	262	GLY	2.6
5	D	22	GLY	2.6
5	E	390	ASP	2.6
5	E	146	LYS	2.6
9	M	68	LEU	2.6
9	S	53	PHE	2.6
5	D	252	ASP	2.6
9	P	68	LEU	2.6
6	G	154	ALA	2.6
5	E	329	THR	2.6
9	S	56	MET	2.6
5	E	326	ASP	2.6
4	C	394	GLU	2.6
4	C	178	ILE	2.6
4	B	172	GLN	2.6
9	Q	59	ALA	2.6
4	A	100	GLY	2.6
4	A	473	LEU	2.6
4	B	173	THR	2.6
9	M	43	SER	2.6
4	C	131	VAL	2.6
5	E	352	ARG	2.6
5	F	114	GLN	2.6
8	I	60	THR	2.6
9	R	64	ILE	2.6
9	T	43	SER	2.6
4	A	392	LYS	2.6
4	C	387	VAL	2.6
5	D	129	VAL	2.6
5	F	36	ASN	2.6
9	N	3	ASN	2.6
9	U	71	LEU	2.6
9	T	76	ALA	2.6
5	D	87	GLY	2.6
4	A	374	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
9	J	47	SER	2.5
5	E	330	VAL	2.5
9	R	18	VAL	2.5
4	C	78	ASP	2.5
5	E	430	LEU	2.5
9	P	15	LEU	2.5
4	C	179	ALA	2.5
4	C	187	ALA	2.5
9	L	37	GLY	2.5
4	A	220	LYS	2.5
5	D	102	PRO	2.5
6	G	125	GLY	2.5
9	R	43	SER	2.5
9	J	25	MET	2.5
4	A	129	ALA	2.5
9	L	31	ALA	2.5
4	A	290	PRO	2.5
4	C	167	ILE	2.5
5	E	226	MET	2.5
9	K	25	MET	2.5
9	Q	21	ALA	2.5
4	B	374	ARG	2.5
9	U	30	VAL	2.5
9	O	48	GLN	2.5
5	E	103	VAL	2.5
9	Q	54	ILE	2.4
6	G	16	ASN	2.4
9	K	55	GLY	2.4
5	E	421	THR	2.4
4	C	391	VAL	2.4
9	Q	76	ALA	2.4
5	F	432	ASP	2.4
4	B	366	VAL	2.4
8	I	52	VAL	2.4
6	G	192	GLN	2.4
9	L	49	THR	2.4
5	E	59	ASP	2.4
14	Z	5	ASP	2.4
5	E	40	LEU	2.4
6	G	69	LEU	2.4
4	C	125	GLU	2.4
4	C	110	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	436	PRO	2.4
9	N	19	GLY	2.4
9	K	58	PHE	2.4
5	E	303	ILE	2.4
9	K	59	ALA	2.4
9	N	65	PHE	2.4
4	A	178	ILE	2.4
4	B	125	GLU	2.4
9	S	60	GLU	2.4
9	O	6	GLN	2.3
5	D	48	LEU	2.3
9	N	30	VAL	2.3
9	P	40	ARG	2.3
5	F	141	TYR	2.3
4	B	400	GLU	2.3
5	D	327	ALA	2.3
9	R	38	ALA	2.3
5	D	250	PHE	2.3
5	E	387	LEU	2.3
5	D	350	ASN	2.3
5	F	145	GLY	2.3
9	Q	66	SER	2.3
4	A	106	ARG	2.3
5	D	215	TYR	2.3
5	F	259	GLN	2.3
9	R	39	LEU	2.3
4	A	143	HIS	2.3
5	D	328	THR	2.3
9	R	49	THR	2.3
7	H	12	ILE	2.3
7	H	65	GLU	2.3
9	S	47	SER	2.3
4	C	153	VAL	2.3
5	E	219	ASN	2.3
5	D	368	ARG	2.3
6	G	148	ARG	2.3
4	B	75	ILE	2.3
9	L	47	SER	2.3
4	C	130	ASP	2.3
7	H	49	ASP	2.3
5	E	33	THR	2.3
9	K	41	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
9	N	46	ALA	2.3
9	P	36	ALA	2.3
5	D	316	PRO	2.3
6	G	48	ARG	2.3
9	N	49	THR	2.2
9	O	71	LEU	2.2
9	R	15	LEU	2.2
5	E	322	PHE	2.2
9	Q	19	GLY	2.2
4	C	154	ASP	2.2
9	K	71	LEU	2.2
5	D	229	ALA	2.2
6	G	124	LYS	2.2
4	A	188	ASN	2.2
9	J	33	ASN	2.2
4	A	429	MET	2.2
9	L	68	LEU	2.2
5	F	460	GLU	2.2
5	D	83	ASP	2.2
5	D	137	LEU	2.2
4	A	7	GLU	2.2
6	G	44	PRO	2.2
4	C	261	ASN	2.2
8	I	82	ARG	2.2
4	A	494	GLU	2.2
5	F	222	PRO	2.2
9	R	58	PHE	2.2
4	A	17	LYS	2.2
5	F	267	LEU	2.2
7	H	66	ALA	2.1
9	Q	70	ALA	2.1
9	R	76	ALA	2.1
5	E	177	VAL	2.1
5	D	178	PHE	2.1
9	K	63	GLY	2.1
5	F	169	ALA	2.1
4	C	139	ARG	2.1
4	A	160	GLY	2.1
4	B	145	PRO	2.1
9	M	15	LEU	2.1
9	Q	15	LEU	2.1
9	T	62	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	99	ALA	2.1
9	Q	29	ASN	2.1
12	X	1212	VAL	2.1
12	X	1274	TYR	2.1
9	Q	17	CYS	2.1
9	S	17	CYS	2.1
5	D	301	THR	2.1
5	F	185	THR	2.1
4	B	23	ALA	2.1
9	L	57	ALA	2.1
5	F	208	LYS	2.1
5	D	437	PHE	2.1
4	A	393	LEU	2.1
4	C	384	MET	2.1
5	D	389	MET	2.1
5	F	104	GLU	2.1
14	Z	11	GLU	2.1
4	A	120	PRO	2.1
4	A	364	PRO	2.1
4	B	270	ASP	2.1
4	A	496	GLU	2.1
5	F	87	GLY	2.0
4	B	485	THR	2.0
5	E	62	GLU	2.0
6	G	174	THR	2.0
5	D	179	ALA	2.0
5	F	282	ALA	2.0
9	P	21	ALA	2.0
9	U	67	PHE	2.0
9	Q	20	MET	2.0
6	G	79	HIS	2.0
5	E	320	THR	2.0
4	C	81	ASP	2.0
6	G	135	ASP	2.0
4	B	147	ALA	2.0
4	C	404	PHE	2.0
5	E	331	LEU	2.0
6	G	144	SER	2.0
5	D	180	GLY	2.0
7	H	57	PRO	2.0
4	C	199	THR	2.0
5	D	421	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	130	ASP	2.0
4	A	386	SER	2.0
5	E	246	ASP	2.0
9	J	62	LEU	2.0
5	E	265	SER	2.0
4	A	142	VAL	2.0
4	A	372	VAL	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](#)

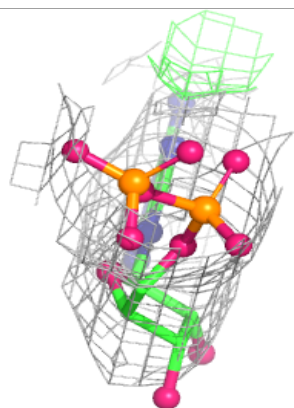
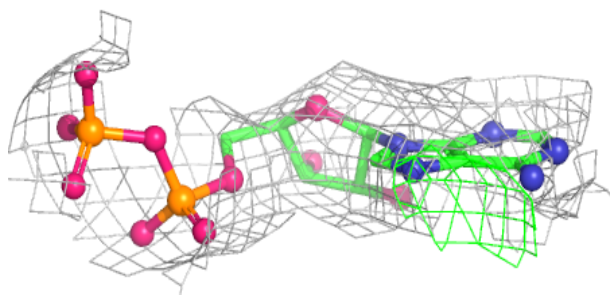
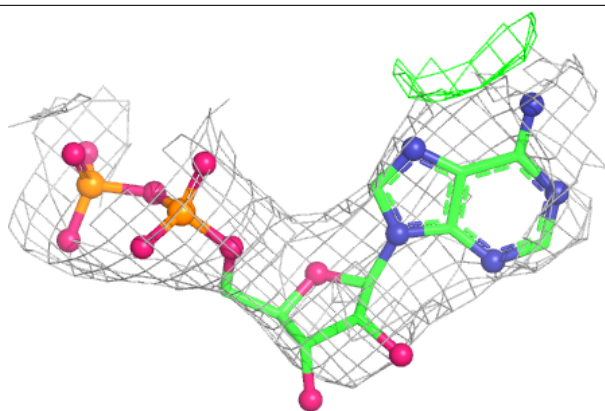
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	ADP	B	600	27/27	0.72	0.13	155,165,171,173	0
16	MG	A	601	1/1	0.92	0.16	78,78,78,78	0
15	ATP	A	600	31/31	0.93	0.11	96,98,105,106	0
15	ATP	D	600	31/31	0.93	0.10	90,96,152,153	0
15	ATP	C	600	31/31	0.94	0.08	103,110,115,118	0
15	ATP	F	600	31/31	0.95	0.10	69,74,109,110	0
16	MG	C	601	1/1	0.96	0.10	48,48,48,48	0
16	MG	B	601	1/1	0.96	0.15	72,72,72,72	0
16	MG	F	601	1/1	0.99	0.07	35,35,35,35	0
16	MG	D	601	1/1	0.99	0.04	41,41,41,41	0

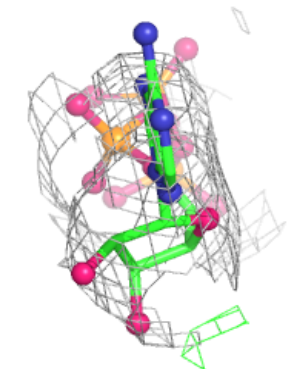
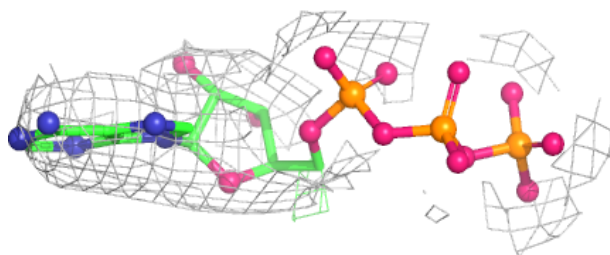
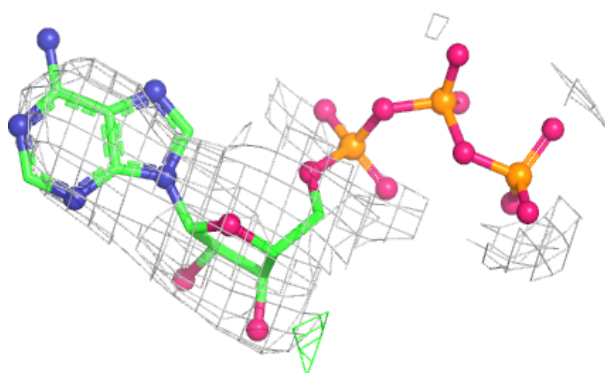
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

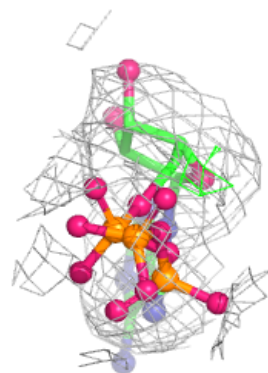
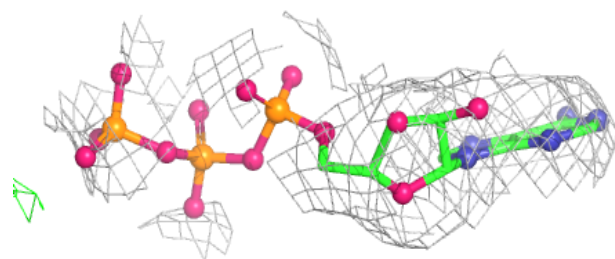
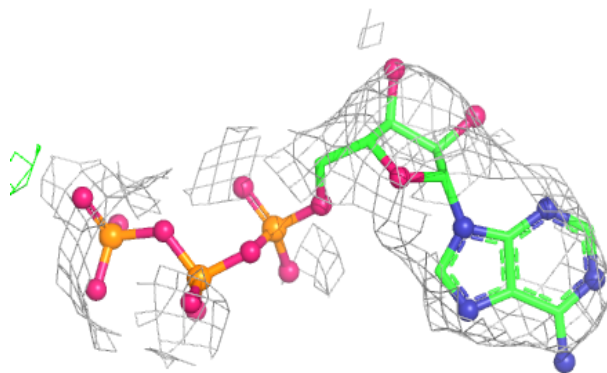
**Electron density around ATP A 600:**

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

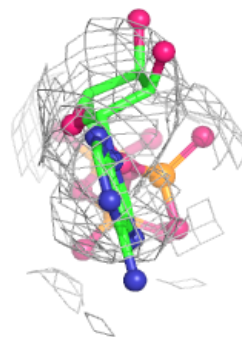
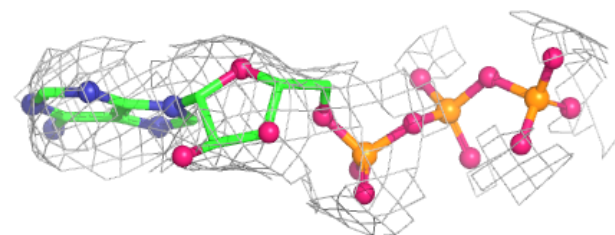
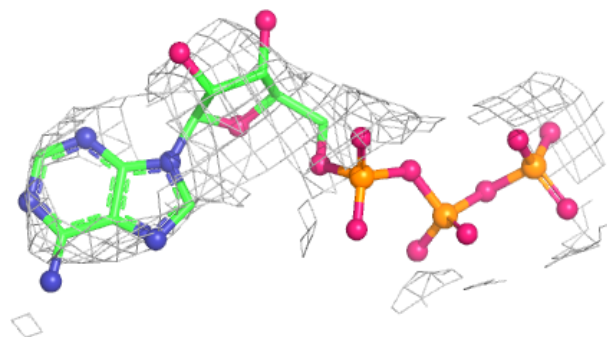


Electron density around ATP D 600:

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

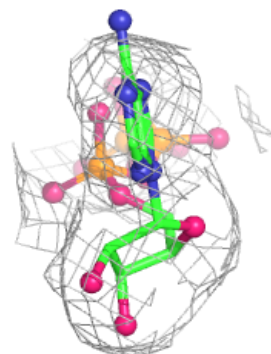
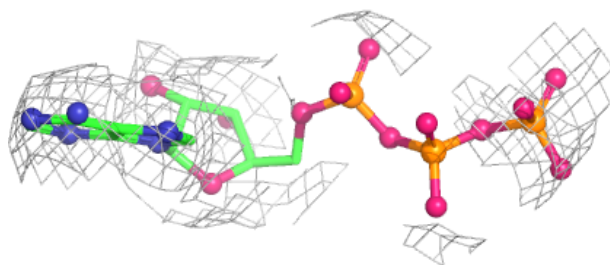
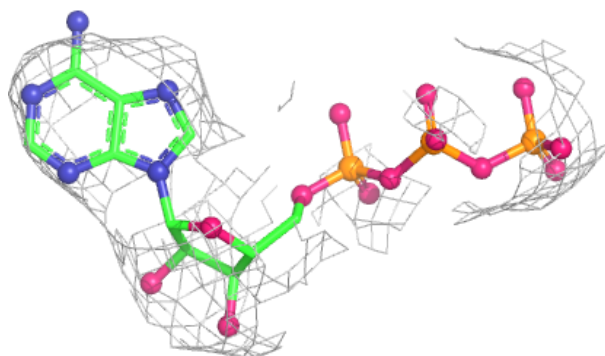
**Electron density around ATP C 600:**

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



Electron density around ATP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.