



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:33 AM UTC

PDB ID : 5TSH / pdb_00005tsh
Title : PilB from *Geobacter metallireducens* bound to AMP-PNP
Authors : McCallum, M.; Tammam, S.; Khan, A.; Burrows, L.; Howell, P.L.
Deposited on : 2016-10-28
Resolution : 2.30 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

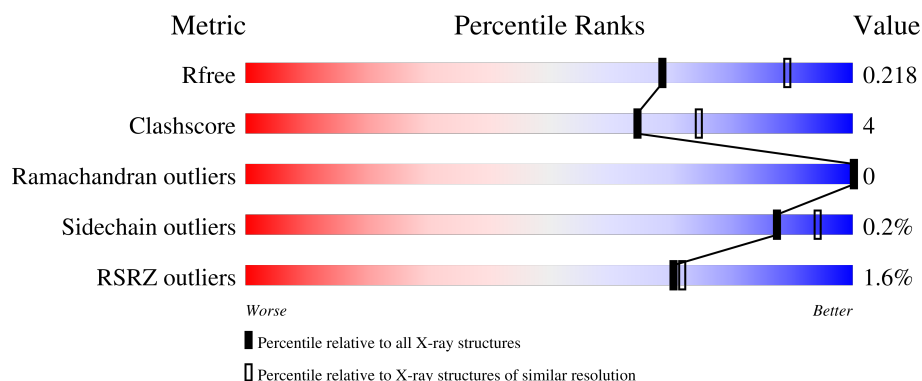
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	588	% 59% 5% 36%
1	B	588	% 58% 6% 36%
1	C	588	% 60% 5% 35%
1	D	588	% 58% 7% 36%
1	E	588	% 59% 7% 34%

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Mol	Chain	Length	Quality of chain
1	F	588	% 59% 6% 35%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17937 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 Type IV pilus biogenesis ATPase PilB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2784	1764	479	525	16			
1	B	376	Total	C	N	O	S	0	0	0
			2844	1807	489	532	16			
1	C	382	Total	C	N	O	S	0	0	0
			2899	1845	499	538	17			
1	D	379	Total	C	N	O	S	0	1	0
			2882	1827	497	541	17			
1	E	387	Total	C	N	O	S	0	0	0
			2920	1855	506	542	17			
1	F	382	Total	C	N	O	S	0	0	0
			2895	1845	498	535	17			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q39VU7
A	-18	GLY	-	expression tag	UNP Q39VU7
A	-17	SER	-	expression tag	UNP Q39VU7
A	-16	SER	-	expression tag	UNP Q39VU7
A	-15	HIS	-	expression tag	UNP Q39VU7
A	-14	HIS	-	expression tag	UNP Q39VU7
A	-13	HIS	-	expression tag	UNP Q39VU7
A	-12	HIS	-	expression tag	UNP Q39VU7
A	-11	HIS	-	expression tag	UNP Q39VU7
A	-10	HIS	-	expression tag	UNP Q39VU7
A	-9	SER	-	expression tag	UNP Q39VU7
A	-8	SER	-	expression tag	UNP Q39VU7
A	-7	GLY	-	expression tag	UNP Q39VU7
A	-6	LEU	-	expression tag	UNP Q39VU7
A	-5	VAL	-	expression tag	UNP Q39VU7
A	-4	PRO	-	expression tag	UNP Q39VU7
A	-3	ARG	-	expression tag	UNP Q39VU7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q39VU7
A	-1	SER	-	expression tag	UNP Q39VU7
A	0	HIS	-	expression tag	UNP Q39VU7
A	482	GLY	ALA	conflict	UNP Q39VU7
B	-19	MET	-	initiating methionine	UNP Q39VU7
B	-18	GLY	-	expression tag	UNP Q39VU7
B	-17	SER	-	expression tag	UNP Q39VU7
B	-16	SER	-	expression tag	UNP Q39VU7
B	-15	HIS	-	expression tag	UNP Q39VU7
B	-14	HIS	-	expression tag	UNP Q39VU7
B	-13	HIS	-	expression tag	UNP Q39VU7
B	-12	HIS	-	expression tag	UNP Q39VU7
B	-11	HIS	-	expression tag	UNP Q39VU7
B	-10	HIS	-	expression tag	UNP Q39VU7
B	-9	SER	-	expression tag	UNP Q39VU7
B	-8	SER	-	expression tag	UNP Q39VU7
B	-7	GLY	-	expression tag	UNP Q39VU7
B	-6	LEU	-	expression tag	UNP Q39VU7
B	-5	VAL	-	expression tag	UNP Q39VU7
B	-4	PRO	-	expression tag	UNP Q39VU7
B	-3	ARG	-	expression tag	UNP Q39VU7
B	-2	GLY	-	expression tag	UNP Q39VU7
B	-1	SER	-	expression tag	UNP Q39VU7
B	0	HIS	-	expression tag	UNP Q39VU7
B	482	GLY	ALA	conflict	UNP Q39VU7
C	-19	MET	-	initiating methionine	UNP Q39VU7
C	-18	GLY	-	expression tag	UNP Q39VU7
C	-17	SER	-	expression tag	UNP Q39VU7
C	-16	SER	-	expression tag	UNP Q39VU7
C	-15	HIS	-	expression tag	UNP Q39VU7
C	-14	HIS	-	expression tag	UNP Q39VU7
C	-13	HIS	-	expression tag	UNP Q39VU7
C	-12	HIS	-	expression tag	UNP Q39VU7
C	-11	HIS	-	expression tag	UNP Q39VU7
C	-10	HIS	-	expression tag	UNP Q39VU7
C	-9	SER	-	expression tag	UNP Q39VU7
C	-8	SER	-	expression tag	UNP Q39VU7
C	-7	GLY	-	expression tag	UNP Q39VU7
C	-6	LEU	-	expression tag	UNP Q39VU7
C	-5	VAL	-	expression tag	UNP Q39VU7
C	-4	PRO	-	expression tag	UNP Q39VU7
C	-3	ARG	-	expression tag	UNP Q39VU7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q39VU7
C	-1	SER	-	expression tag	UNP Q39VU7
C	0	HIS	-	expression tag	UNP Q39VU7
C	482	GLY	ALA	conflict	UNP Q39VU7
D	-19	MET	-	initiating methionine	UNP Q39VU7
D	-18	GLY	-	expression tag	UNP Q39VU7
D	-17	SER	-	expression tag	UNP Q39VU7
D	-16	SER	-	expression tag	UNP Q39VU7
D	-15	HIS	-	expression tag	UNP Q39VU7
D	-14	HIS	-	expression tag	UNP Q39VU7
D	-13	HIS	-	expression tag	UNP Q39VU7
D	-12	HIS	-	expression tag	UNP Q39VU7
D	-11	HIS	-	expression tag	UNP Q39VU7
D	-10	HIS	-	expression tag	UNP Q39VU7
D	-9	SER	-	expression tag	UNP Q39VU7
D	-8	SER	-	expression tag	UNP Q39VU7
D	-7	GLY	-	expression tag	UNP Q39VU7
D	-6	LEU	-	expression tag	UNP Q39VU7
D	-5	VAL	-	expression tag	UNP Q39VU7
D	-4	PRO	-	expression tag	UNP Q39VU7
D	-3	ARG	-	expression tag	UNP Q39VU7
D	-2	GLY	-	expression tag	UNP Q39VU7
D	-1	SER	-	expression tag	UNP Q39VU7
D	0	HIS	-	expression tag	UNP Q39VU7
D	482	GLY	ALA	conflict	UNP Q39VU7
E	-19	MET	-	initiating methionine	UNP Q39VU7
E	-18	GLY	-	expression tag	UNP Q39VU7
E	-17	SER	-	expression tag	UNP Q39VU7
E	-16	SER	-	expression tag	UNP Q39VU7
E	-15	HIS	-	expression tag	UNP Q39VU7
E	-14	HIS	-	expression tag	UNP Q39VU7
E	-13	HIS	-	expression tag	UNP Q39VU7
E	-12	HIS	-	expression tag	UNP Q39VU7
E	-11	HIS	-	expression tag	UNP Q39VU7
E	-10	HIS	-	expression tag	UNP Q39VU7
E	-9	SER	-	expression tag	UNP Q39VU7
E	-8	SER	-	expression tag	UNP Q39VU7
E	-7	GLY	-	expression tag	UNP Q39VU7
E	-6	LEU	-	expression tag	UNP Q39VU7
E	-5	VAL	-	expression tag	UNP Q39VU7
E	-4	PRO	-	expression tag	UNP Q39VU7
E	-3	ARG	-	expression tag	UNP Q39VU7

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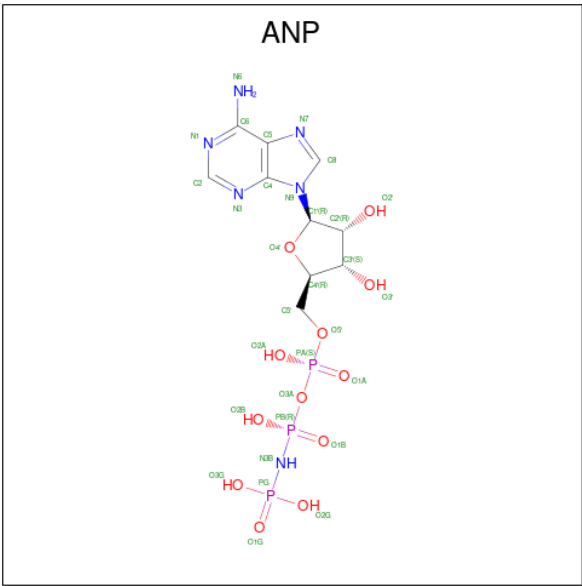
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q39VU7
E	-1	SER	-	expression tag	UNP Q39VU7
E	0	HIS	-	expression tag	UNP Q39VU7
E	482	GLY	ALA	conflict	UNP Q39VU7
F	-19	MET	-	initiating methionine	UNP Q39VU7
F	-18	GLY	-	expression tag	UNP Q39VU7
F	-17	SER	-	expression tag	UNP Q39VU7
F	-16	SER	-	expression tag	UNP Q39VU7
F	-15	HIS	-	expression tag	UNP Q39VU7
F	-14	HIS	-	expression tag	UNP Q39VU7
F	-13	HIS	-	expression tag	UNP Q39VU7
F	-12	HIS	-	expression tag	UNP Q39VU7
F	-11	HIS	-	expression tag	UNP Q39VU7
F	-10	HIS	-	expression tag	UNP Q39VU7
F	-9	SER	-	expression tag	UNP Q39VU7
F	-8	SER	-	expression tag	UNP Q39VU7
F	-7	GLY	-	expression tag	UNP Q39VU7
F	-6	LEU	-	expression tag	UNP Q39VU7
F	-5	VAL	-	expression tag	UNP Q39VU7
F	-4	PRO	-	expression tag	UNP Q39VU7
F	-3	ARG	-	expression tag	UNP Q39VU7
F	-2	GLY	-	expression tag	UNP Q39VU7
F	-1	SER	-	expression tag	UNP Q39VU7
F	0	HIS	-	expression tag	UNP Q39VU7
F	482	GLY	ALA	conflict	UNP Q39VU7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

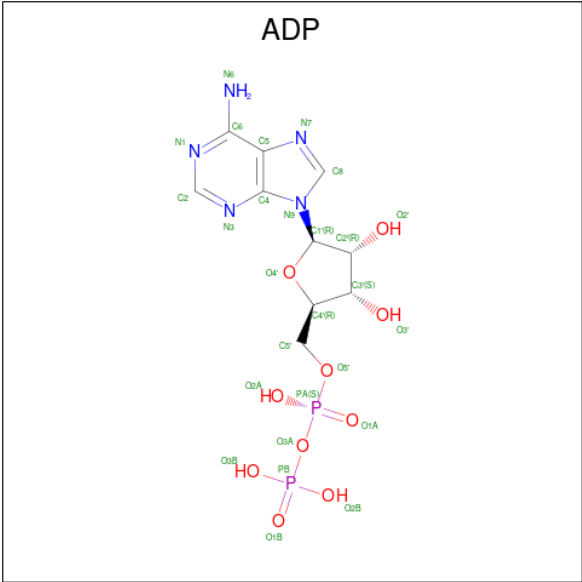


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

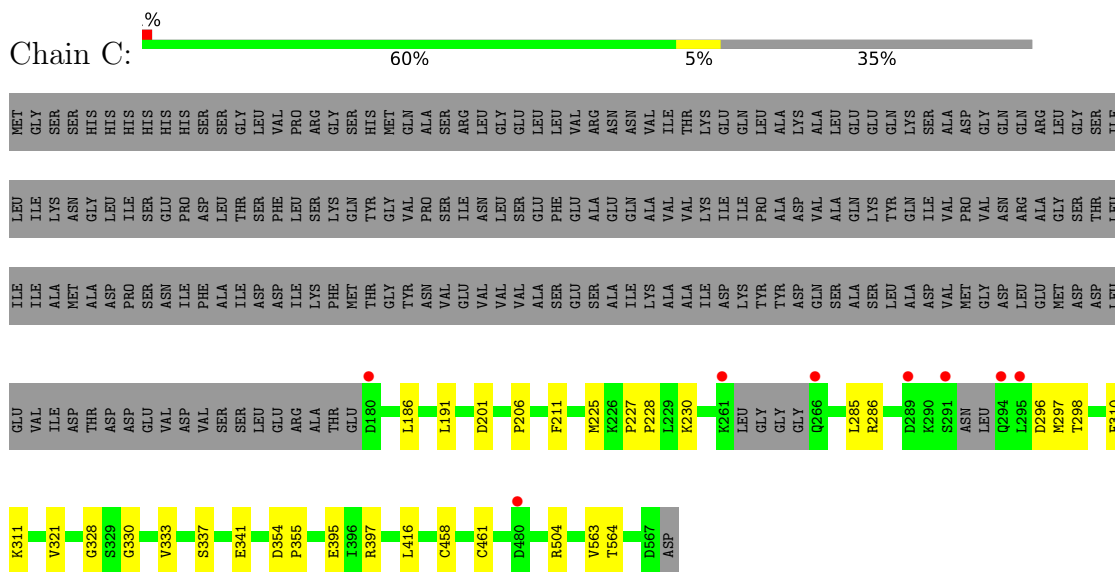
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



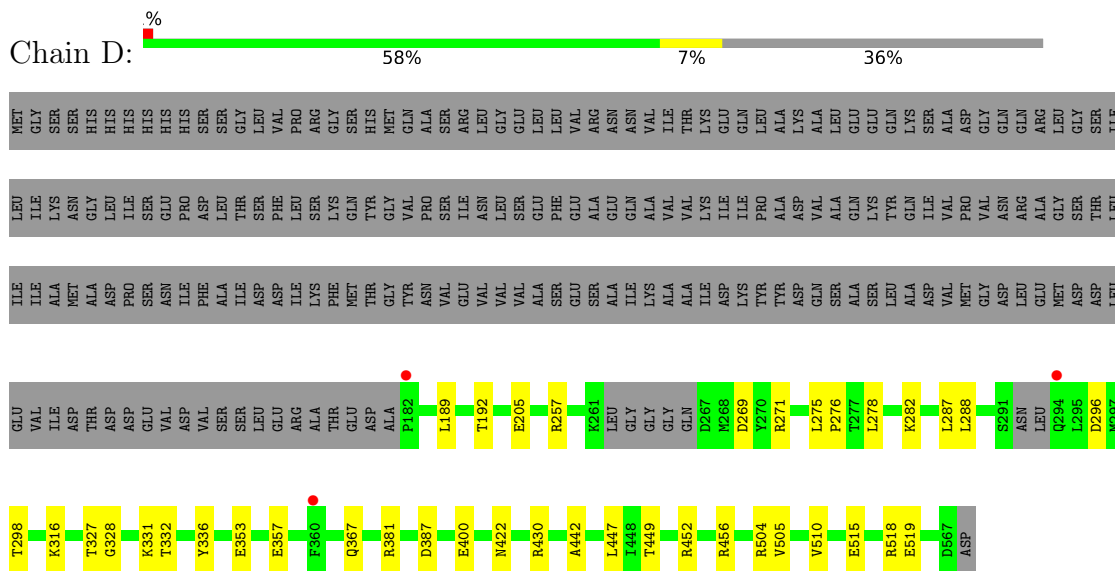
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

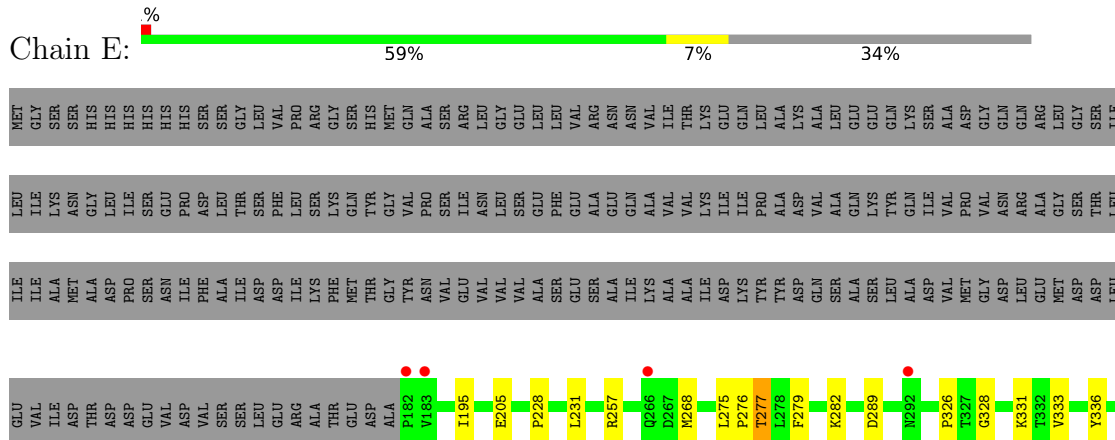
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	82	Total	O	0	0
			82	82		
6	C	75	Total	O	0	0
			75	75		
6	D	76	Total	O	0	0
			76	76		
6	E	96	Total	O	0	0
			96	96		
6	F	101	Total	O	0	0
			101	101		



- Molecule 1: Type IV pilus biogenesis ATPase PilB



- Molecule 1: Type IV pilus biogenesis ATPase PilB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.32Å 99.96Å 109.79Å 112.99° 106.60° 88.91°	Depositor
Resolution (Å)	45.76 – 2.30 45.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.76-2.30) 94.7 (45.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.184 , 0.218 0.185 , 0.218	Depositor DCC
R_{free} test set	2018 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17937	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: ANP, ADP, ZN, 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$
1	A	0.11	0/2826	0.30	0/3831
1	B	0.11	0/2887	0.30	0/3913
1	C	0.11	0/2942	0.30	0/3984
1	D	0.10	0/2927	0.29	0/3964
1	E	0.11	0/2964	0.30	0/4014
1	F	0.10	0/2940	0.30	0/3986
All	All	0.11	0/17486	0.30	0/23692

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2784	0	2688	19	0
1	B	2844	0	2828	25	0
1	C	2899	0	2905	20	0
1	D	2882	0	2860	23	0
1	E	2920	0	2924	27	0
1	F	2895	0	2899	25	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	7	0
3	C	31	0	13	4	0
3	D	31	0	13	4	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	E	27	0	12	2	0
5	F	27	0	12	4	0
6	A	97	0	0	0	0
6	B	82	0	0	0	0
6	C	75	0	0	1	0
6	D	76	0	0	2	0
6	E	96	0	0	3	0
6	F	101	0	0	4	0
All	All	17937	0	17180	135	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 4.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:GLY:H	3:B:602:ANP:HNB1	1.09	0.97
5:F:602:ADP:O2A	6:F:701:HOH:O	1.92	0.87
1:E:515:GLU:OE1	1:E:518:ARG:NH1	2.08	0.86
1:B:562:ARG:HG3	1:E:407:LYS:HD2	1.59	0.82
1:E:328:GLY:N	5:E:602:ADP:O2B	2.11	0.80
1:D:332:THR:HG21	1:D:357:GLU:HG3	1.64	0.79
1:E:442:ALA:HB1	1:E:518:ARG:HG3	1.67	0.75
1:B:425:PRO:HG3	1:B:511:MET:HE1	1.69	0.74
1:C:328:GLY:H	3:C:602:ANP:HNB1	1.36	0.73
1:C:186:LEU:HD11	1:C:225:MET:HE1	1.72	0.72
1:E:257:ARG:NH1	6:E:702:HOH:O	2.15	0.72
1:E:558:GLU:OE2	6:E:701:HOH:O	2.07	0.71
1:D:328:GLY:H	3:D:602:ANP:HNB1	1.39	0.69
1:B:328:GLY:N	3:B:602:ANP:HNB1	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:GLY:N	5:F:602:ADP:O2B	2.20	0.67
1:E:277:THR:HG22	1:E:279:PHE:H	1.61	0.66
1:C:296:ASP:OD1	1:C:298:THR:OG1	2.13	0.65
1:B:321:VAL:HB	1:B:416:LEU:HD23	1.79	0.65
1:F:549:LYS:NZ	6:F:703:HOH:O	2.29	0.64
1:A:216:ARG:NE	1:D:387:ASP:OD2	2.26	0.64
1:E:333:VAL:HG21	5:E:602:ADP:H2'	1.81	0.62
1:F:333:VAL:HG21	5:F:602:ADP:H2'	1.82	0.61
1:D:278:LEU:HD21	1:F:356:VAL:HG21	1.81	0.61
1:D:442:ALA:O	1:D:518:ARG:NE	2.33	0.61
1:D:327:THR:HG23	3:D:602:ANP:O2G	2.02	0.60
1:C:458:CYS:HB3	1:C:461:CYS:HB2	1.84	0.59
1:E:403:GLU:O	1:E:407:LYS:HG2	2.03	0.58
1:F:201:ASP:OD2	1:F:286:ARG:HD3	2.04	0.58
1:D:189:LEU:HA	1:D:192:THR:HG22	1.86	0.57
1:E:531:LYS:HG2	1:E:535:MET:HE2	1.87	0.57
1:E:533:GLU:OE1	1:E:536:ARG:NH2	2.33	0.57
1:A:563:VAL:HG23	1:A:564:THR:HG23	1.87	0.56
1:A:328:GLY:H	3:A:602:ANP:HNB1	1.52	0.55
1:C:333:VAL:HG21	3:C:602:ANP:H2'	1.89	0.55
1:A:225:MET:HE2	1:A:227:PRO:HG3	1.87	0.55
1:E:396:ILE:HG22	1:E:434:MET:HE1	1.89	0.55
1:A:480:ASP:OD1	1:A:480:ASP:N	2.33	0.55
1:D:296:ASP:OD2	1:D:298:THR:HG22	2.06	0.54
1:A:395:GLU:CD	1:A:397:ARG:HE	2.14	0.54
1:C:395:GLU:CD	1:C:397:ARG:HH21	2.16	0.54
1:B:190:ILE:HG12	1:B:225:MET:HE1	1.91	0.53
1:D:430:ARG:NH2	6:D:704:HOH:O	2.42	0.53
1:F:331:LYS:N	5:F:602:ADP:O3B	2.38	0.53
1:C:297:MET:HE1	1:C:310:PHE:HD1	1.74	0.52
1:D:275:LEU:HD22	1:D:276:PRO:HD2	1.91	0.52
1:C:191:LEU:HD21	1:C:285:LEU:HD22	1.91	0.52
1:A:469:ILE:O	1:A:473:ILE:HG12	2.09	0.52
1:A:184:VAL:CB	1:A:238:ARG:HH12	2.22	0.52
1:B:504:ARG:HB2	3:B:602:ANP:C2	2.40	0.52
1:B:533:GLU:OE2	1:B:536:ARG:NH2	2.24	0.52
1:C:297:MET:HE1	1:C:310:PHE:CD1	2.44	0.52
1:E:195:ILE:HD11	1:E:268:MET:HG2	1.93	0.51
1:A:297:MET:HE2	1:A:311:LYS:NZ	2.25	0.51
1:B:442:ALA:O	1:B:518:ARG:NE	2.31	0.51
1:B:330:GLY:HA2	3:B:602:ANP:O2A	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:ARG:HA	1:E:504:ARG:HG2	1.92	0.51
1:B:277:THR:OG1	1:B:280:GLY:O	2.24	0.50
1:C:563:VAL:HG23	1:C:564:THR:HG23	1.94	0.50
1:A:297:MET:HE2	1:A:311:LYS:HZ3	1.77	0.50
1:A:533:GLU:OE1	1:A:536:ARG:NH2	2.40	0.50
1:B:300:LEU:O	3:B:602:ANP:N6	2.40	0.50
1:B:327:THR:HG23	3:B:602:ANP:O1G	2.12	0.49
1:C:211:PHE:CD1	1:C:227:PRO:HG2	2.48	0.49
1:E:228:PRO:HD2	1:E:231:LEU:HD12	1.93	0.49
1:F:442:ALA:HB1	1:F:518:ARG:HG2	1.92	0.49
6:C:706:HOH:O	1:F:282:LYS:HE2	2.13	0.49
1:E:275:LEU:HD12	1:E:276:PRO:HD2	1.95	0.49
1:A:190:ILE:O	1:A:215:TYR:OH	2.30	0.49
1:E:419:LEU:HD12	1:E:427:THR:HG23	1.95	0.49
1:B:504:ARG:HB2	3:B:602:ANP:H2	1.94	0.48
1:A:278:LEU:HD21	1:D:367:GLN:HB2	1.96	0.48
1:C:201:ASP:OD1	1:C:286:ARG:HD3	2.14	0.48
1:E:469:ILE:O	1:E:473:ILE:HG12	2.13	0.48
1:E:533:GLU:OE2	6:E:703:HOH:O	2.20	0.48
1:C:321:VAL:HB	1:C:416:LEU:HD12	1.97	0.47
1:D:504:ARG:HB2	3:D:602:ANP:H2	1.96	0.47
1:B:459:SER:HA	1:B:462:LYS:HD2	1.95	0.47
1:D:336:TYR:OH	1:D:353:GLU:OE1	2.31	0.47
1:E:205:GLU:HG2	1:E:282:LYS:HE3	1.96	0.47
1:D:381:ARG:NH2	1:D:400:GLU:OE2	2.43	0.47
1:B:319:GLY:HA3	1:B:446:ASN:ND2	2.30	0.46
1:C:297:MET:HG2	1:C:337:SER:OG	2.15	0.46
1:E:396:ILE:HB	1:E:419:LEU:HD21	1.96	0.46
1:A:336:TYR:OH	1:A:353:GLU:OE2	2.20	0.46
1:F:213:VAL:HB	1:F:225:MET:HB3	1.96	0.46
1:C:228:PRO:HB2	1:C:230:LYS:HG2	1.98	0.46
1:C:504:ARG:O	3:C:602:ANP:H2	2.16	0.45
1:F:293:LEU:HD11	1:F:333:VAL:HG22	1.98	0.45
1:F:336:TYR:OH	1:F:353:GLU:OE2	2.27	0.45
1:D:271:ARG:HB2	1:D:288:LEU:HD21	1.98	0.45
1:E:268:MET:HE1	1:E:289:ASP:HB2	1.98	0.44
1:A:215:TYR:CD2	1:A:224:VAL:HG11	2.53	0.44
1:F:353:GLU:HB2	1:F:356:VAL:HG22	2.00	0.44
1:F:381:ARG:NH2	6:F:715:HOH:O	2.49	0.44
1:F:370:GLU:HG3	1:F:375:ASN:HB3	2.00	0.43
1:B:516:GLU:OE1	1:B:516:GLU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:ASN:ND2	6:F:716:HOH:O	2.50	0.43
1:F:380:LEU:HB3	1:F:404:ILE:HG21	2.01	0.43
1:B:351:THR:HB	1:B:392:MET:HE3	2.00	0.43
1:A:213:VAL:HB	1:A:225:MET:HB2	2.01	0.43
1:A:306:ALA:HB1	1:A:510:VAL:HG21	2.01	0.43
1:E:336:TYR:OH	1:E:353:GLU:OE1	2.27	0.43
1:C:206:PRO:HA	1:C:211:PHE:HD2	1.83	0.43
1:D:449:THR:HG22	1:D:510:VAL:HG22	2.01	0.43
1:B:286:ARG:NH1	1:E:385:ARG:O	2.52	0.42
1:C:330:GLY:HA2	3:C:602:ANP:O2A	2.19	0.42
1:F:451:GLN:HA	1:F:507:PHE:O	2.19	0.42
1:D:331:LYS:HE2	3:D:602:ANP:O2B	2.20	0.42
1:F:388:PRO:HG2	1:F:413:HIS:CD2	2.54	0.42
1:D:456:ARG:HB2	1:D:505:VAL:HG13	2.00	0.42
1:F:225:MET:HG2	1:F:227:PRO:HD3	2.01	0.42
1:F:240:LYS:NZ	1:F:249:GLU:O	2.52	0.42
1:B:237:SER:O	1:B:241:ILE:HG13	2.20	0.42
1:B:326:PRO:HA	1:B:420:HIS:CD2	2.55	0.42
1:D:257:ARG:HE	1:D:269:ASP:CG	2.27	0.42
1:F:456:ARG:CZ	1:F:505:VAL:HG12	2.50	0.42
1:A:351:THR:HG22	1:A:392:MET:HB3	2.01	0.42
1:B:186:LEU:O	1:B:190:ILE:HG13	2.19	0.42
1:C:354:ASP:HA	1:C:355:PRO:HA	1.84	0.41
1:F:297:MET:HE3	1:F:297:MET:HB2	1.81	0.41
1:B:526:ASN:OD1	1:B:529:GLU:HG3	2.21	0.41
1:D:205:GLU:HG2	1:D:282:LYS:HE3	2.03	0.41
1:E:351:THR:HG21	1:E:353:GLU:OE2	2.20	0.41
1:C:311:LYS:HE3	1:C:341:GLU:OE2	2.20	0.41
1:E:326:PRO:O	1:E:331:LYS:NZ	2.53	0.41
1:F:197:ARG:NH1	1:F:497:ASN:OD1	2.45	0.41
1:F:529:GLU:H	1:F:529:GLU:HG2	1.63	0.41
1:B:456:ARG:HB2	1:B:505:VAL:HG23	2.03	0.41
1:D:316:LYS:NZ	6:D:711:HOH:O	2.54	0.41
1:D:515:GLU:O	1:D:519:GLU:HG2	2.20	0.41
1:F:453:LEU:HD23	1:F:453:LEU:HA	1.89	0.41
1:D:422:ASN:O	1:D:452[A]:ARG:NH2	2.54	0.40
1:B:453:LEU:HD13	1:B:504:ARG:NH1	2.35	0.40
1:A:289:ASP:OD2	1:A:290:LYS:N	2.54	0.40
1:E:380:LEU:HD21	1:E:393:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/588 (63%)	365 (99%)	4 (1%)	0	100	100
1	B	370/588 (63%)	366 (99%)	4 (1%)	0	100	100
1	C	376/588 (64%)	372 (99%)	4 (1%)	0	100	100
1	D	374/588 (64%)	370 (99%)	4 (1%)	0	100	100
1	E	385/588 (66%)	381 (99%)	4 (1%)	0	100	100
1	F	378/588 (64%)	376 (100%)	2 (0%)	0	100	100
All	All	2252/3528 (64%)	2230 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	276/501 (55%)	276 (100%)	0	100	100
1	B	292/501 (58%)	292 (100%)	0	100	100
1	C	300/501 (60%)	300 (100%)	0	100	100
1	D	295/501 (59%)	293 (99%)	2 (1%)	76	87
1	E	301/501 (60%)	300 (100%)	1 (0%)	86	93
1	F	298/501 (60%)	298 (100%)	0	100	100
All	All	1762/3006 (59%)	1759 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	287	LEU
1	D	447	LEU
1	E	277	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	413	HIS
1	A	420	HIS
1	B	451	GLN
1	C	359	ASN
1	C	386	GLN
1	C	429	ASN
1	D	348	ASN
1	D	498	ASN
1	E	364	ASN
1	E	367	GLN
1	E	369	HIS
1	E	386	GLN
1	E	446	ASN
1	E	523	ASN
1	F	386	GLN
1	F	422	ASN

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

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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
5	ADP	E	602	-	28,29,29	1.44	4 (14%)	43,45,45	1.80	8 (18%)
3	ANP	C	602	4	33,33,33	1.95	12 (36%)	45,52,52	2.09	13 (28%)
3	ANP	A	602	4	33,33,33	1.95	11 (33%)	45,52,52	2.03	12 (26%)
3	ANP	D	602	-	33,33,33	2.00	11 (33%)	45,52,52	2.02	12 (26%)
5	ADP	F	602	-	28,29,29	1.43	5 (17%)	43,45,45	1.82	8 (18%)
3	ANP	B	602	-	33,33,33	1.98	11 (33%)	45,52,52	2.06	13 (28%)

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
5	ADP	E	602	-	-	3/16/32/32	0/3/3/3
3	ANP	C	602	4	-	4/18/38/38	0/3/3/3
3	ANP	A	602	4	-	5/18/38/38	0/3/3/3
3	ANP	D	602	-	-	8/18/38/38	0/3/3/3
5	ADP	F	602	-	-	0/16/32/32	0/3/3/3
3	ANP	B	602	-	-	2/18/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	602	ADP	C5-C4	4.80	1.47	1.39
5	F	602	ADP	C5-C4	4.73	1.47	1.39
3	D	602	ANP	C5-C4	4.68	1.47	1.39
3	B	602	ANP	C5-C4	4.68	1.47	1.39
3	D	602	ANP	PG-N3B	4.59	1.75	1.63
3	C	602	ANP	C5-C4	4.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	ANP	PB-N3B	4.55	1.75	1.63
3	B	602	ANP	PB-N3B	4.51	1.75	1.63
3	A	602	ANP	C5-C4	4.51	1.47	1.39
3	B	602	ANP	PG-N3B	4.49	1.75	1.63
3	C	602	ANP	PB-N3B	4.48	1.75	1.63
3	C	602	ANP	PG-N3B	4.35	1.74	1.63
3	A	602	ANP	PB-N3B	4.31	1.74	1.63
3	A	602	ANP	PG-N3B	4.25	1.74	1.63
3	D	602	ANP	PG-O1G	3.38	1.51	1.46
3	B	602	ANP	PG-O1G	3.32	1.51	1.46
3	D	602	ANP	PB-O1B	3.30	1.51	1.46
3	A	602	ANP	PB-O1B	3.20	1.51	1.46
3	B	602	ANP	PB-O1B	3.18	1.51	1.46
3	A	602	ANP	PG-O1G	3.15	1.51	1.46
3	C	602	ANP	PG-O1G	3.13	1.50	1.46
3	C	602	ANP	PB-O1B	2.99	1.50	1.46
5	F	602	ADP	C5-C6	2.77	1.48	1.41
5	E	602	ADP	C5-C6	2.73	1.48	1.41
3	D	602	ANP	C5-C6	2.69	1.48	1.41
3	B	602	ANP	C5-C6	2.66	1.48	1.41
3	C	602	ANP	C5-C6	2.65	1.48	1.41
3	A	602	ANP	C5-C6	2.65	1.48	1.41
3	A	602	ANP	C5-N7	-2.51	1.34	1.39
3	C	602	ANP	C5-N7	-2.41	1.34	1.39
3	B	602	ANP	C5-N7	-2.35	1.34	1.39
5	E	602	ADP	C8-N7	2.34	1.36	1.31
3	A	602	ANP	PB-O2B	-2.34	1.50	1.56
3	D	602	ANP	C5-N7	-2.31	1.34	1.39
5	F	602	ADP	C8-N7	2.31	1.36	1.31
3	C	602	ANP	PG-O3G	-2.28	1.50	1.56
5	F	602	ADP	C5-N7	-2.28	1.34	1.39
3	A	602	ANP	PG-O2G	-2.28	1.50	1.56
3	B	602	ANP	C8-N7	2.27	1.36	1.31
5	E	602	ADP	C5-N7	-2.27	1.34	1.39
3	D	602	ANP	C8-N7	2.25	1.36	1.31
3	A	602	ANP	PG-O3G	-2.21	1.50	1.56
3	C	602	ANP	PG-O2G	-2.21	1.50	1.56
3	D	602	ANP	PB-O2B	-2.16	1.51	1.56
3	C	602	ANP	PB-O2B	-2.15	1.51	1.56
3	A	602	ANP	C8-N7	2.14	1.35	1.31
3	C	602	ANP	C8-N7	2.10	1.35	1.31
3	B	602	ANP	PB-O2B	-2.10	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ANP	PG-O3G	-2.10	1.51	1.56
3	D	602	ANP	PG-O2G	-2.09	1.51	1.56
5	F	602	ADP	PA-O3A	2.07	1.61	1.59
3	B	602	ANP	PG-O2G	-2.06	1.51	1.56
3	C	602	ANP	C4-N9	-2.02	1.33	1.37
3	D	602	ANP	PG-O3G	-2.02	1.51	1.56

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	602	ADP	C5-C4-N3	-5.95	118.53	126.72
3	D	602	ANP	C5-C4-N3	-5.87	118.64	126.72
5	E	602	ADP	C5-C4-N3	-5.85	118.66	126.72
3	B	602	ANP	C5-C4-N3	-5.82	118.70	126.72
3	A	602	ANP	C5-C4-N3	-5.77	118.78	126.72
3	C	602	ANP	C5-C4-N3	-5.73	118.83	126.72
3	C	602	ANP	O1G-PG-N3B	-5.32	103.94	111.77
3	B	602	ANP	O1G-PG-N3B	-4.89	104.57	111.77
3	A	602	ANP	O1G-PG-N3B	-4.74	104.79	111.77
5	F	602	ADP	N3-C4-N9	4.68	135.13	127.17
3	D	602	ANP	O1G-PG-N3B	-4.67	104.89	111.77
3	B	602	ANP	N3-C4-N9	4.65	135.08	127.17
5	E	602	ADP	N3-C4-N9	4.65	135.08	127.17
3	C	602	ANP	N3-C4-N9	4.60	134.99	127.17
3	A	602	ANP	N3-C4-N9	4.59	134.98	127.17
3	D	602	ANP	N3-C4-N9	4.58	134.96	127.17
3	C	602	ANP	O2B-PB-O1B	4.22	118.93	109.87
3	D	602	ANP	O2B-PB-O1B	4.18	118.84	109.87
3	A	602	ANP	O2B-PB-O1B	4.18	118.83	109.87
3	B	602	ANP	O2B-PB-O1B	4.10	118.66	109.87
5	F	602	ADP	C2-N3-C4	3.70	120.87	111.83
3	A	602	ANP	C2-N3-C4	3.68	120.83	111.83
3	B	602	ANP	C2-N3-C4	3.67	120.80	111.83
3	D	602	ANP	C2-N3-C4	3.67	120.80	111.83
3	C	602	ANP	C2-N3-C4	3.66	120.78	111.83
5	E	602	ADP	C2-N3-C4	3.65	120.75	111.83
3	D	602	ANP	C4-C5-N7	-3.56	106.52	110.58
3	A	602	ANP	C4-C5-N7	-3.47	106.62	110.58
5	E	602	ADP	C4-C5-N7	-3.45	106.64	110.58
5	F	602	ADP	C4-C5-N7	-3.43	106.66	110.58
3	B	602	ANP	C4-C5-N7	-3.40	106.69	110.58
3	C	602	ANP	C4-C5-N7	-3.39	106.71	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	ANP	N3-C2-N1	-3.23	123.69	128.58
3	A	602	ANP	N3-C2-N1	-3.22	123.71	128.58
3	B	602	ANP	N3-C2-N1	-3.17	123.79	128.58
5	F	602	ADP	N3-C2-N1	-3.17	123.79	128.58
3	D	602	ANP	N3-C2-N1	-3.15	123.82	128.58
5	E	602	ADP	N3-C2-N1	-3.11	123.87	128.58
3	C	602	ANP	C4-N9-C8	2.70	108.58	105.74
3	A	602	ANP	C4-N9-C8	2.65	108.52	105.74
3	B	602	ANP	C4-N9-C8	2.65	108.52	105.74
3	A	602	ANP	C5-N7-C8	2.57	107.49	103.45
3	D	602	ANP	C5-N7-C8	2.56	107.47	103.45
5	E	602	ADP	C4-N9-C8	2.56	108.42	105.74
5	E	602	ADP	C5-N7-C8	2.51	107.39	103.45
3	B	602	ANP	C5-N7-C8	2.50	107.39	103.45
3	C	602	ANP	C5-N7-C8	2.50	107.38	103.45
5	F	602	ADP	C5-N7-C8	2.50	107.37	103.45
3	D	602	ANP	C4-N9-C8	2.49	108.35	105.74
3	C	602	ANP	O1B-PB-N3B	-2.47	108.14	111.77
5	E	602	ADP	C3'-C2'-C1'	2.46	106.11	101.46
5	F	602	ADP	C4-N9-C8	2.44	108.30	105.74
3	C	602	ANP	O2G-PG-O3G	2.42	114.11	107.59
3	B	602	ANP	O1B-PB-N3B	-2.42	108.20	111.77
5	F	602	ADP	C3'-C2'-C1'	2.39	105.97	101.46
3	B	602	ANP	O2G-PG-O3G	2.36	113.93	107.59
3	B	602	ANP	C3'-C2'-C1'	2.35	105.91	101.46
3	D	602	ANP	O2G-PG-O3G	2.26	113.66	107.59
3	A	602	ANP	O2G-PG-O3G	2.18	113.46	107.59
3	D	602	ANP	O1B-PB-N3B	-2.15	108.60	111.77
3	A	602	ANP	O1B-PB-N3B	-2.10	108.68	111.77
3	A	602	ANP	C6-C5-N7	2.10	136.13	132.09
3	D	602	ANP	C6-C5-N7	2.09	136.12	132.09
3	C	602	ANP	C3'-C2'-C1'	2.09	105.41	101.46
3	C	602	ANP	C6-C5-N7	2.06	136.05	132.09
3	B	602	ANP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ANP	PB-N3B-PG-O1G
3	A	602	ANP	PG-N3B-PB-O1B
3	A	602	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	B	602	ANP	PG-N3B-PB-O1B
3	B	602	ANP	C5'-O5'-PA-O2A
3	C	602	ANP	PG-N3B-PB-O1B
3	C	602	ANP	PA-O3A-PB-O2B
3	D	602	ANP	PB-N3B-PG-O1G
3	D	602	ANP	PG-N3B-PB-O1B
3	D	602	ANP	PA-O3A-PB-O2B
3	D	602	ANP	C5'-O5'-PA-O3A
3	D	602	ANP	O4'-C4'-C5'-O5'
3	D	602	ANP	C3'-C4'-C5'-O5'
3	A	602	ANP	PG-N3B-PB-O3A
3	D	602	ANP	C5'-O5'-PA-O1A
3	C	602	ANP	O4'-C4'-C5'-O5'
5	E	602	ADP	O4'-C4'-C5'-O5'
5	E	602	ADP	C3'-C4'-C5'-O5'
5	E	602	ADP	PA-O3A-PB-O2B
3	A	602	ANP	PA-O3A-PB-O1B
3	C	602	ANP	PA-O3A-PB-O1B
3	D	602	ANP	PA-O3A-PB-O1B

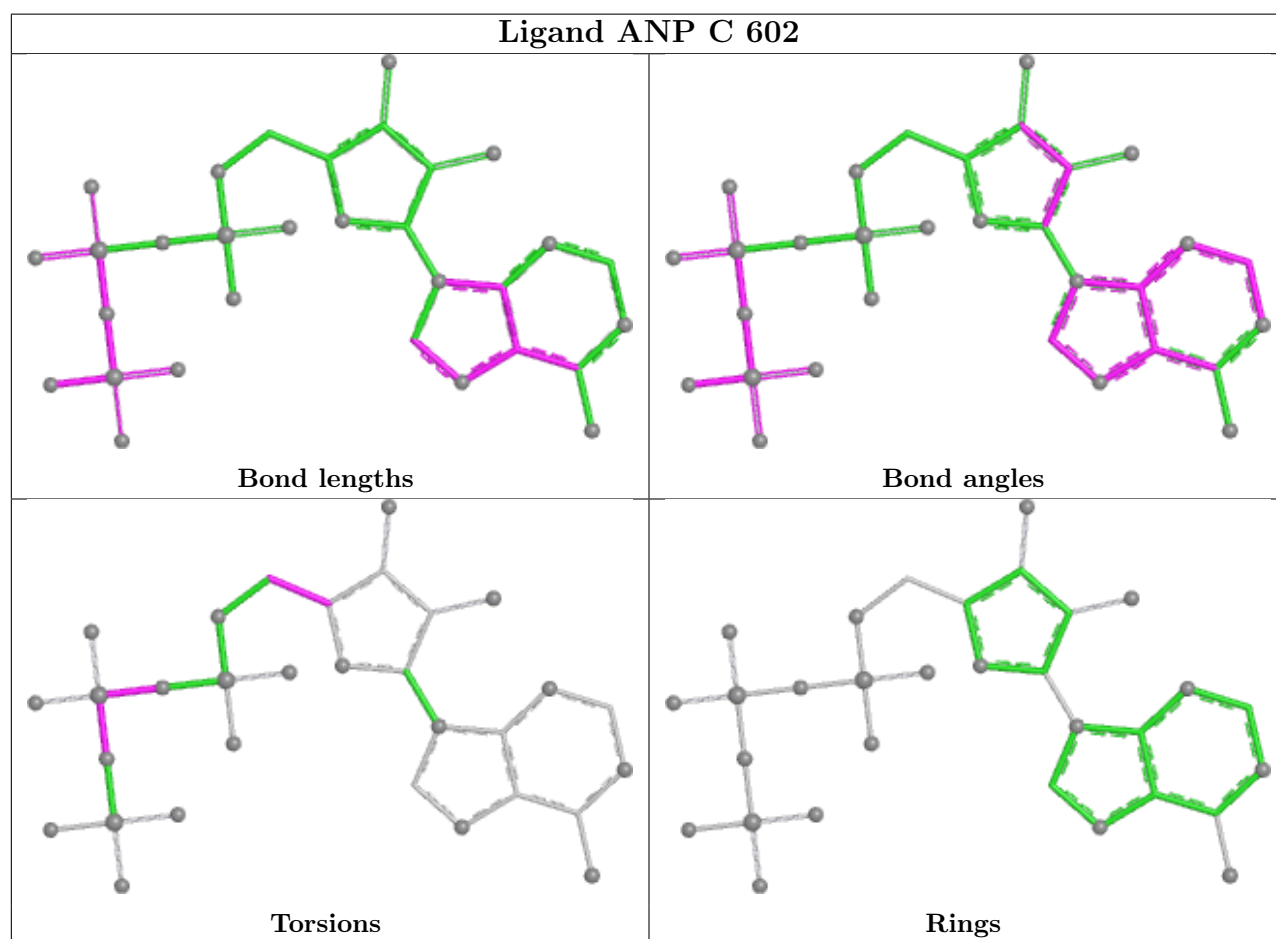
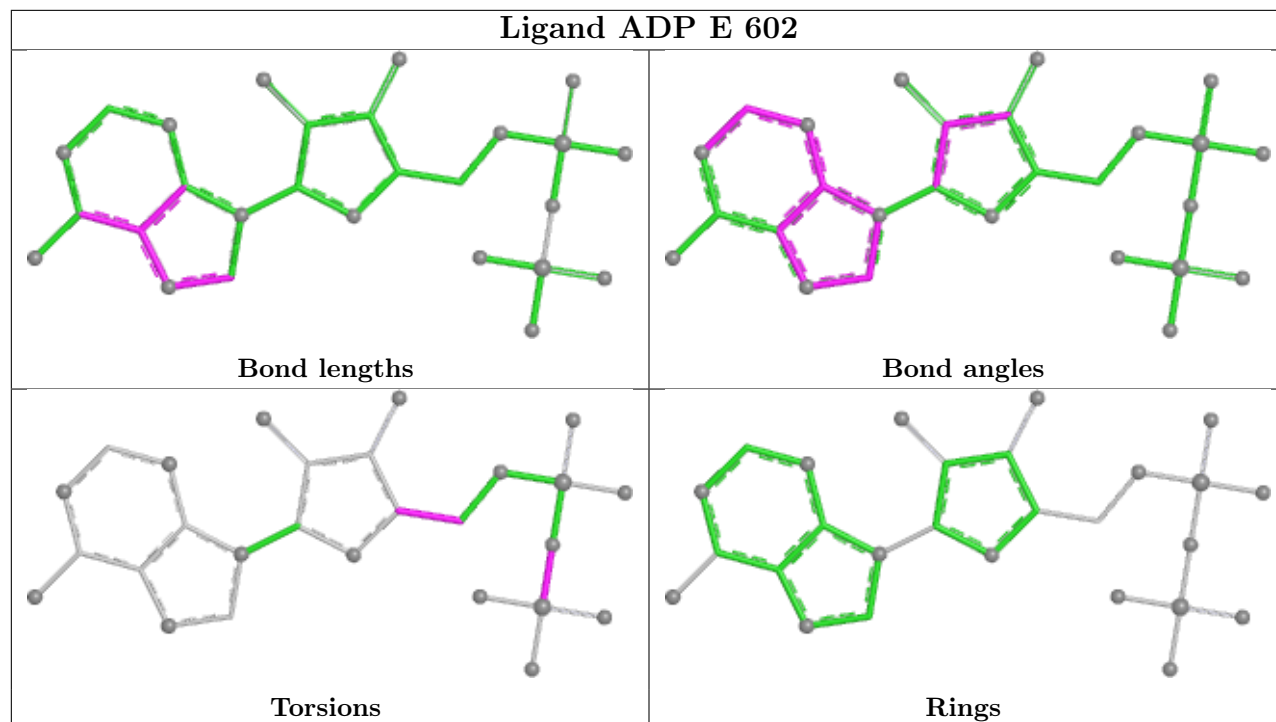
There are no ring outliers.

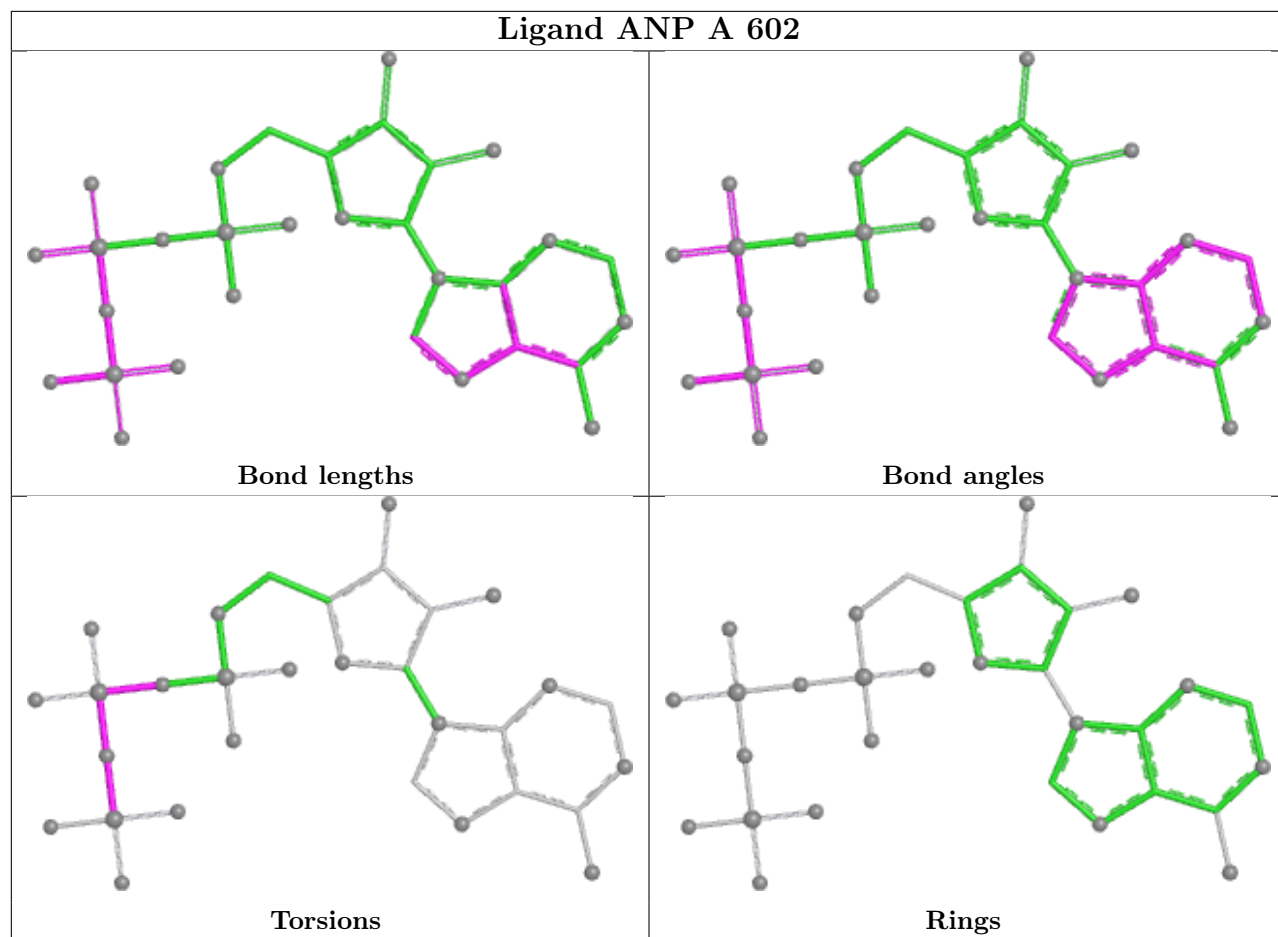
6 monomers are involved in 22 short contacts:

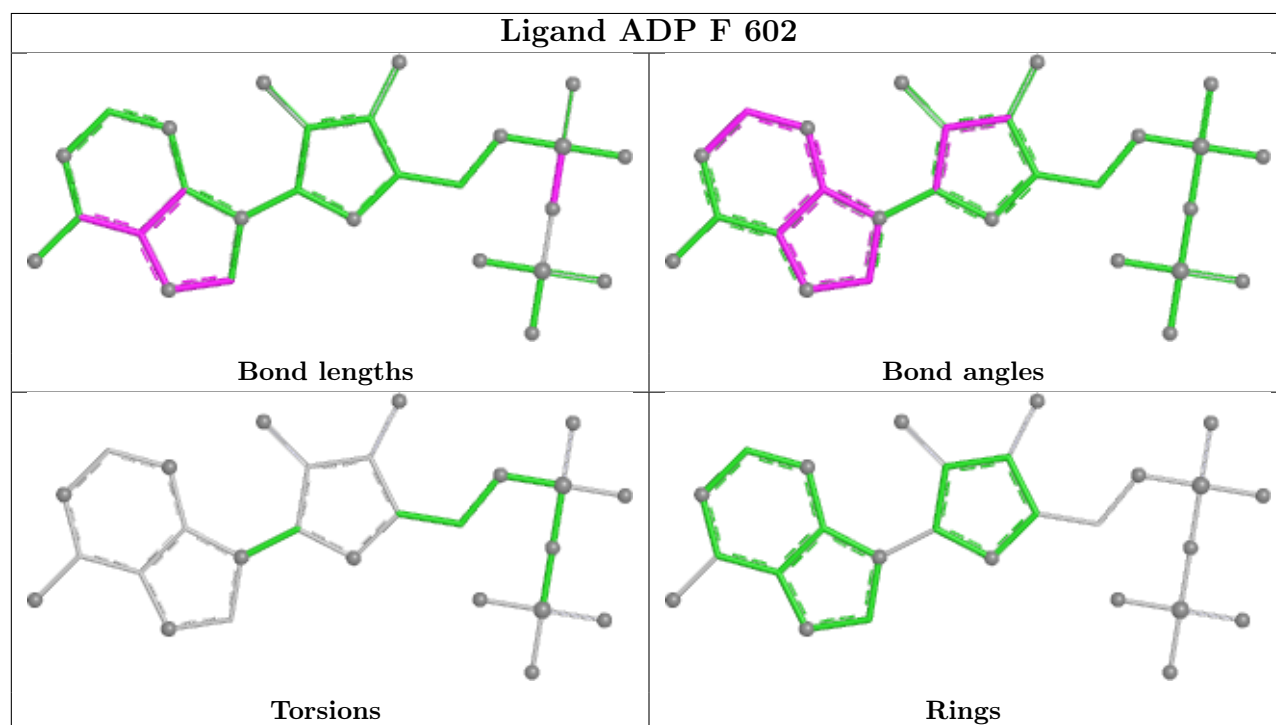
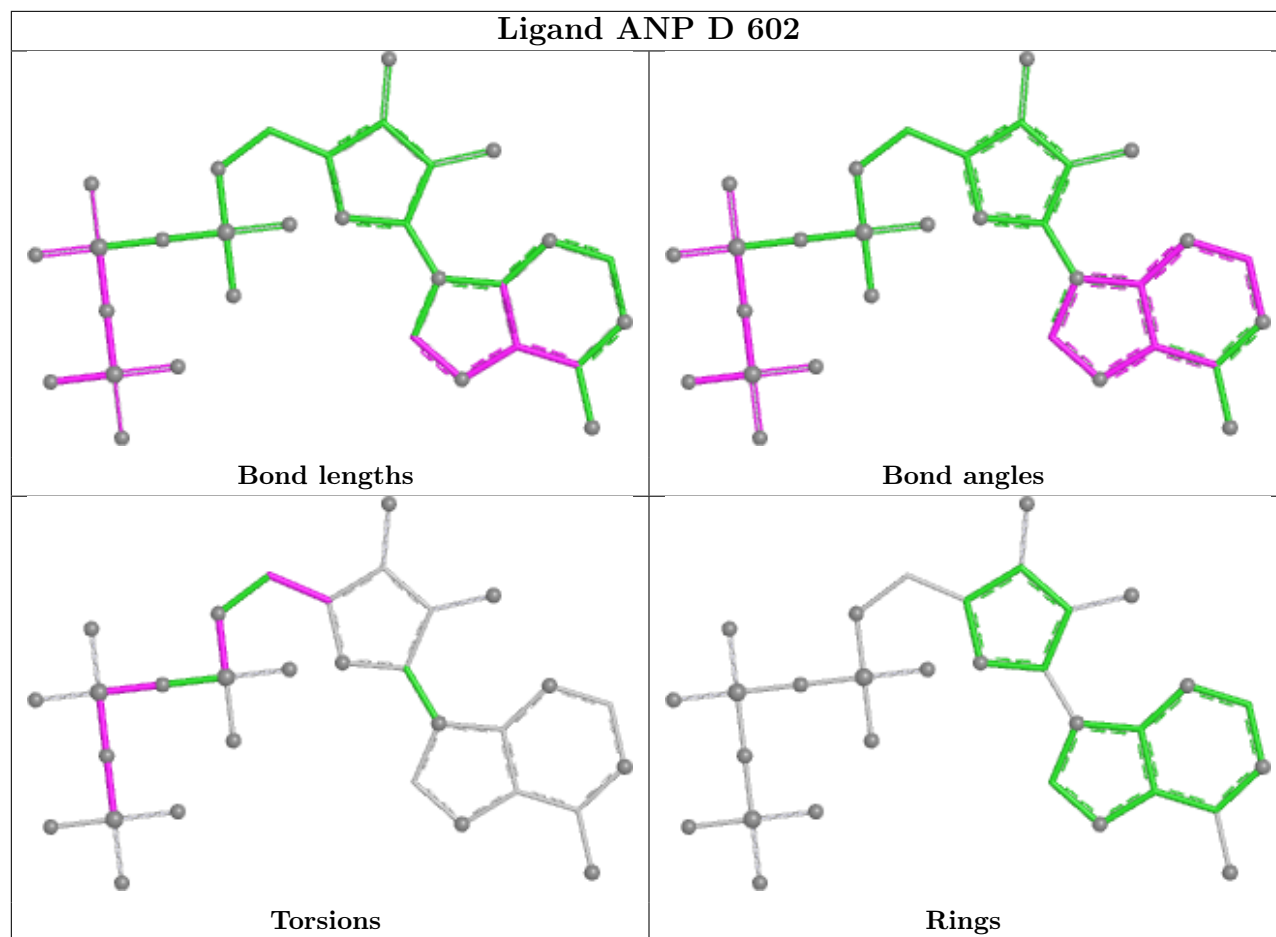
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	602	ADP	2	0
3	C	602	ANP	4	0
3	A	602	ANP	1	0
3	D	602	ANP	4	0
5	F	602	ADP	4	0
3	B	602	ANP	7	0

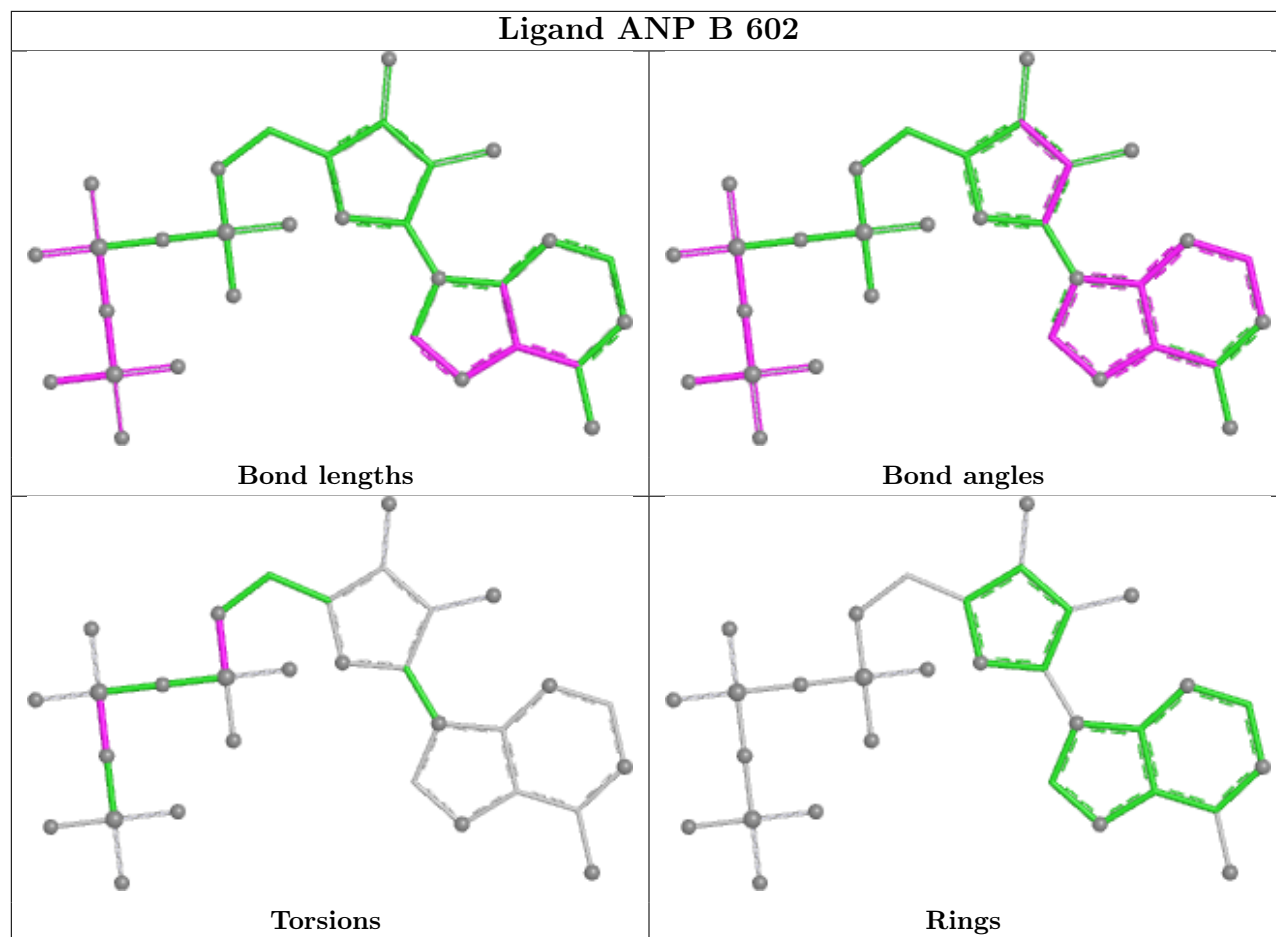
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	375/588 (63%)	0.21	8 (2%) 63 65	26, 47, 82, 90	0
1	B	376/588 (63%)	0.13	8 (2%) 63 65	33, 47, 69, 82	0
1	C	382/588 (64%)	0.16	8 (2%) 63 65	31, 47, 72, 91	0
1	D	379/588 (64%)	0.12	3 (0%) 82 83	20, 47, 70, 80	1 (0%)
1	E	387/588 (65%)	0.08	6 (1%) 70 72	28, 44, 66, 84	0
1	F	382/588 (64%)	0.03	4 (1%) 79 80	27, 43, 66, 78	0
All	All	2281/3528 (64%)	0.12	37 (1%) 70 72	20, 46, 72, 91	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	182	PRO	5.3
1	A	260	ILE	4.3
1	A	295	LEU	3.1
1	C	294	GLN	3.0
1	B	295	LEU	3.0
1	A	241	ILE	2.9
1	B	296	ASP	2.8
1	C	291	SER	2.8
1	C	480	ASP	2.8
1	E	485	TYR	2.8
1	C	295	LEU	2.7
1	D	294	GLN	2.7
1	F	293	LEU	2.5
1	D	182	PRO	2.5
1	E	183	VAL	2.4
1	C	180	ASP	2.4
1	E	266	GLN	2.4
1	C	266	GLN	2.4
1	E	480	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	192	THR	2.4
1	B	293	LEU	2.4
1	B	181	ALA	2.3
1	B	192	THR	2.3
1	B	420	HIS	2.3
1	C	289	ASP	2.2
1	F	295	LEU	2.2
1	F	291	SER	2.2
1	F	180	ASP	2.2
1	A	481	GLU	2.1
1	A	229	LEU	2.1
1	B	269	ASP	2.1
1	E	292	ASN	2.1
1	C	261	LYS	2.1
1	A	233	ASN	2.1
1	B	260	ILE	2.1
1	D	360	PHE	2.1
1	A	360	PHE	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.

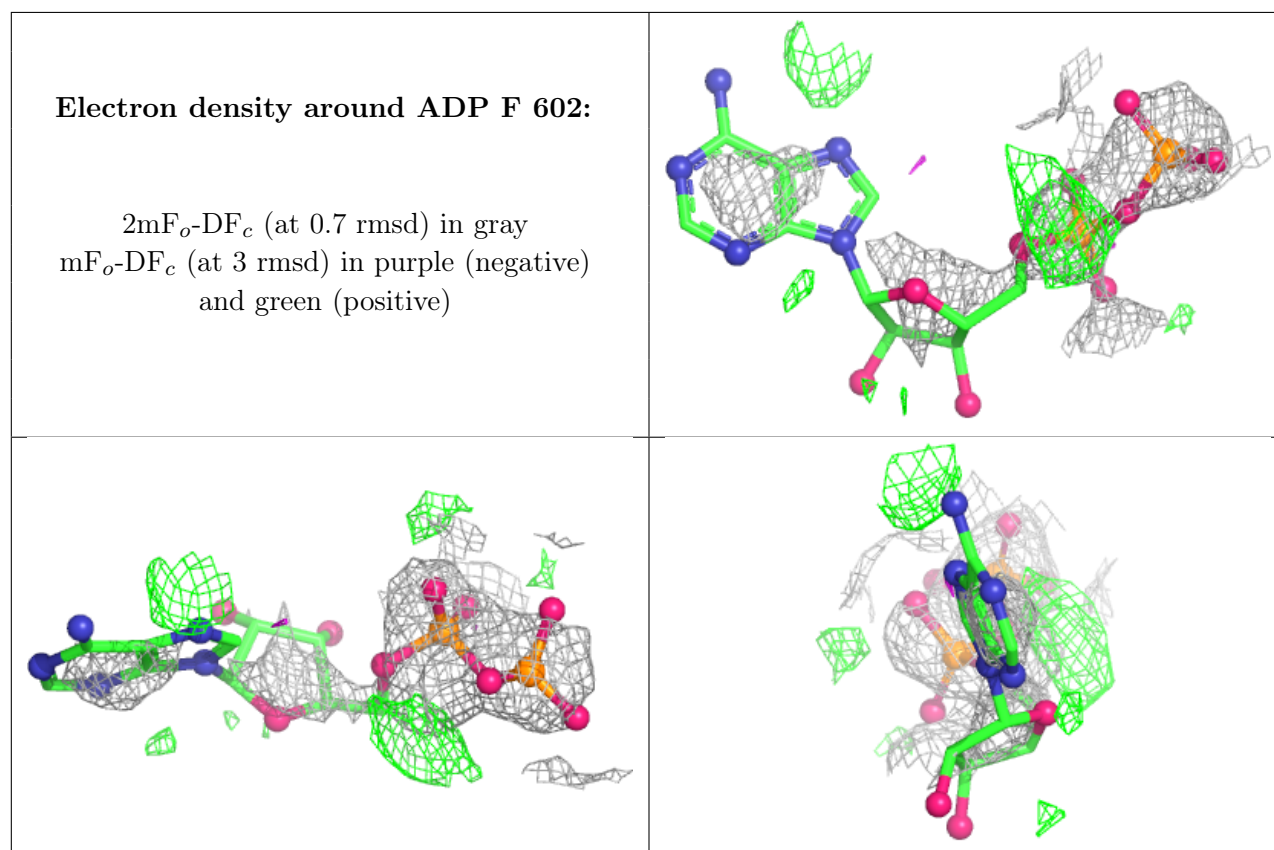
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	F	602	27/27	0.78	0.23	48,56,62,67	27
5	ADP	E	602	27/27	0.81	0.29	44,48,60,63	27
3	ANP	D	602	31/31	0.83	0.19	41,51,61,65	31
3	ANP	B	602	31/31	0.85	0.17	46,50,58,61	31
3	ANP	C	602	31/31	0.96	0.08	32,37,44,51	11

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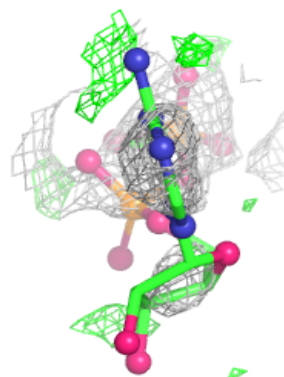
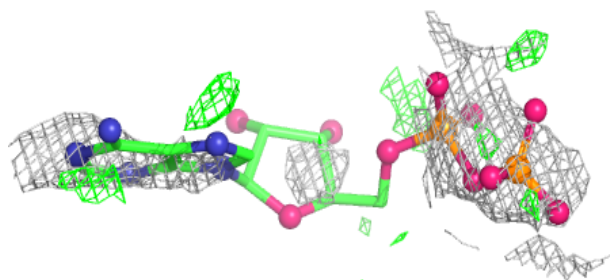
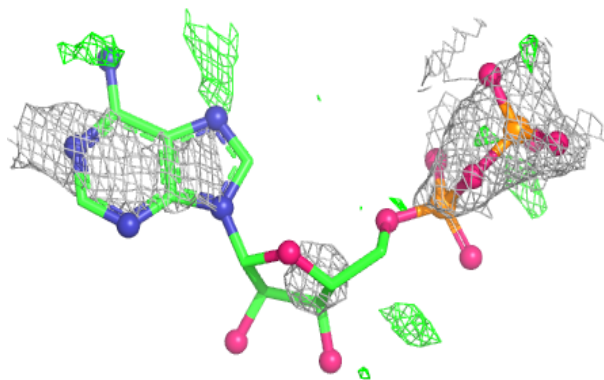
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	A	602	31/31	0.97	0.08	32,33,45,61	0
2	ZN	B	601	1/1	0.98	0.04	41,41,41,41	0
2	ZN	C	601	1/1	0.98	0.12	78,78,78,78	0
2	ZN	E	601	1/1	0.99	0.03	57,57,57,57	0
2	ZN	F	601	1/1	0.99	0.03	40,40,40,40	0
4	MG	A	603	1/1	0.99	0.05	32,32,32,32	0
4	MG	C	603	1/1	0.99	0.02	34,34,34,34	0
2	ZN	A	601	1/1	0.99	0.06	37,37,37,37	0
2	ZN	D	601	1/1	0.99	0.03	48,48,48,48	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.

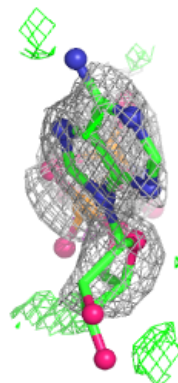
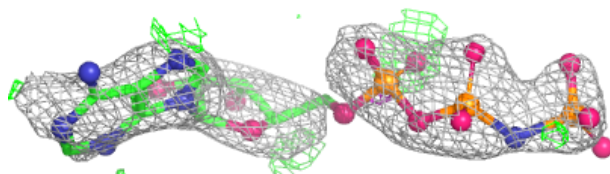
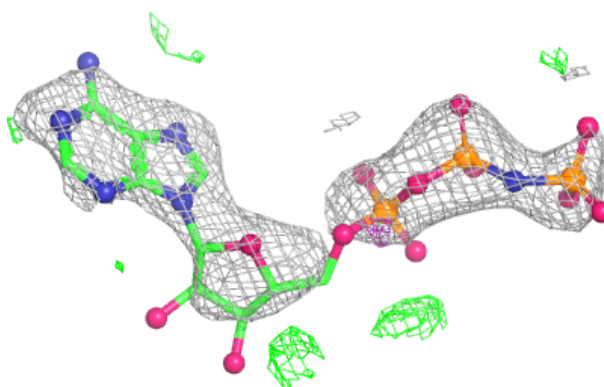


Electron density around ADP E 602:

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

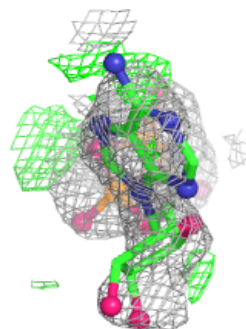
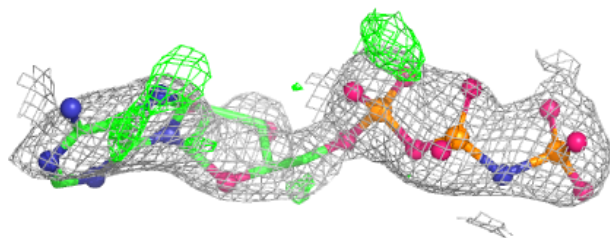
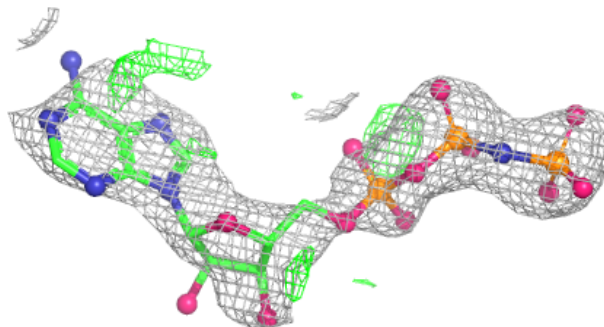
**Electron density around ANP D 602:**

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

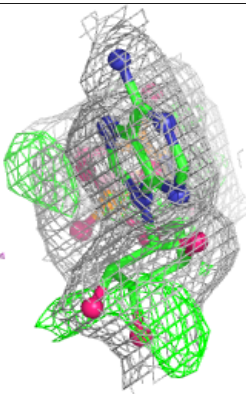
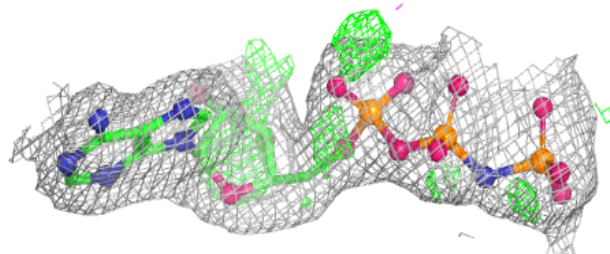
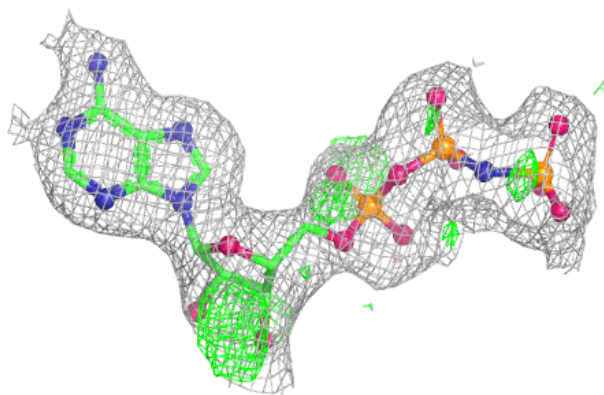


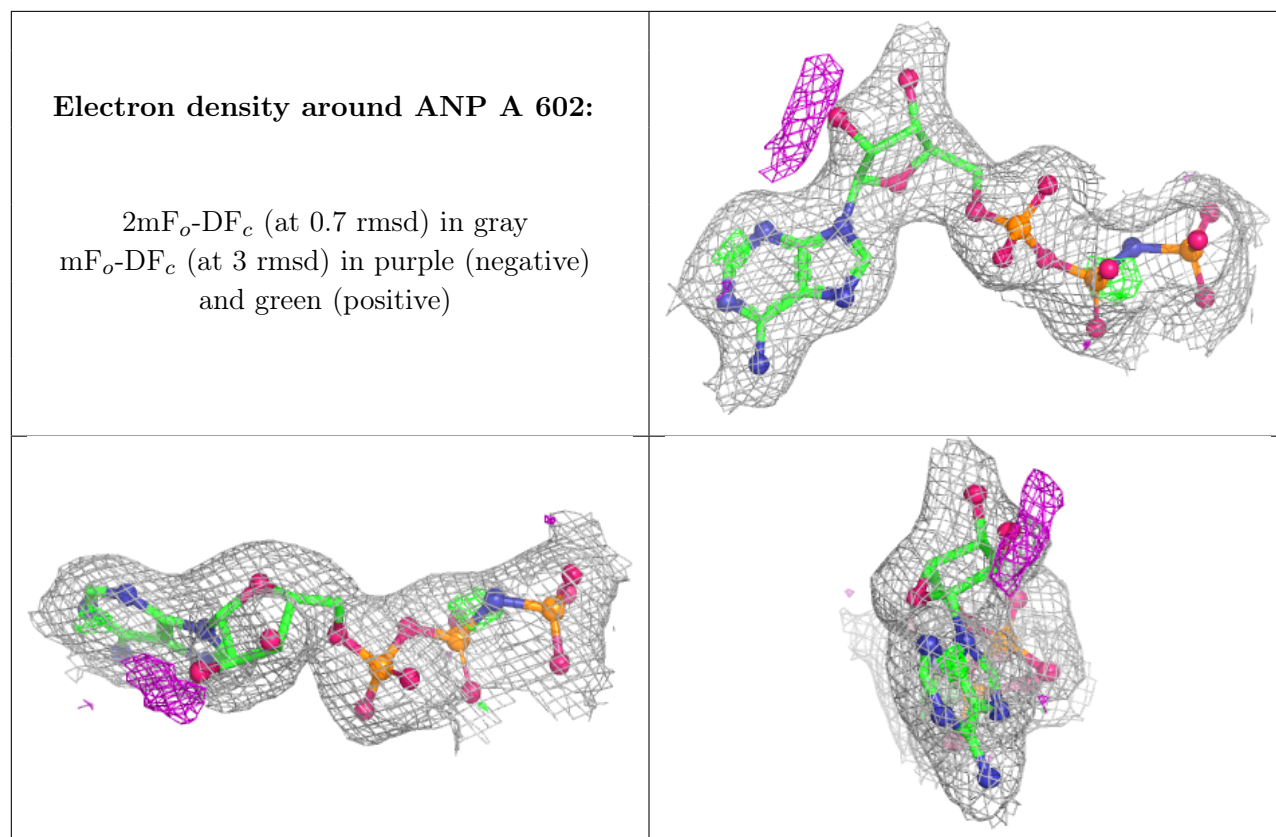
Electron density around ANP B 602:

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

**Electron density around ANP C 602:**

$2mF_o-DF_c$ (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.