



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:00 PM UTC

PDB ID : 4IHQ / pdb_00004ihq
Title : Archaeum Assembly ATPase FlaI bound to ADP
Authors : Reindl, S.; Williams, G.J.; Tainer, J.A.
Deposited on : 2012-12-19
Resolution : 2.00 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

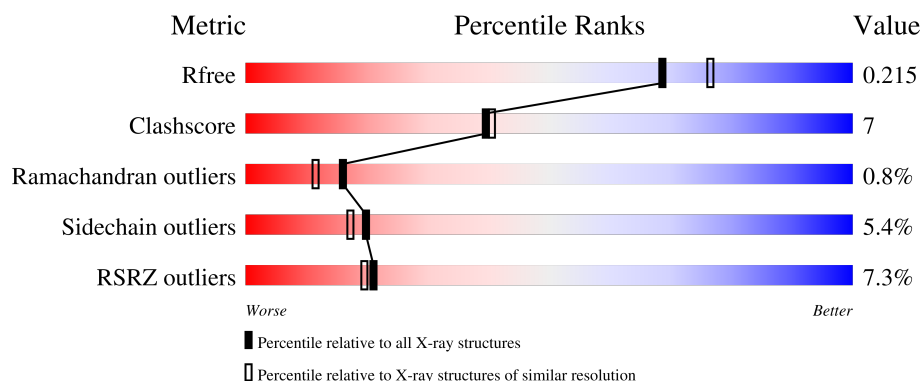
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	513	6% 81% 17% .
1	B	513	9% 78% 20% .
1	C	513	6% 83% 15% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13401 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.

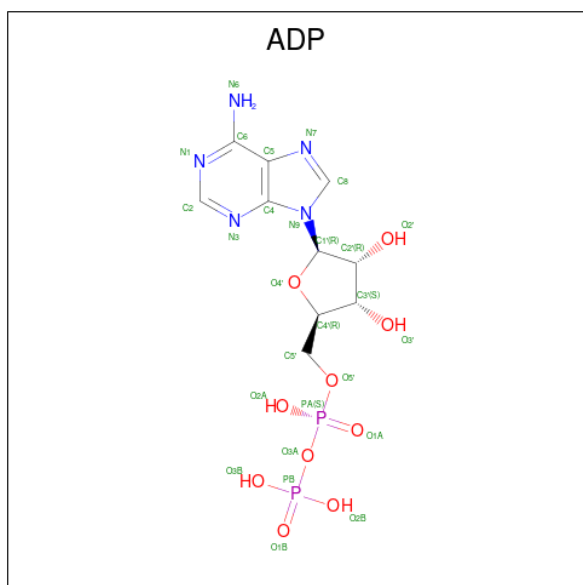
- Molecule 1 is a protein called FlaI ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	113	7	0
			4176	2680	700	781	15			
1	B	512	Total	C	N	O	S	109	10	0
			4189	2690	704	781	14			
1	C	511	Total	C	N	O	S	149	7	0
			4169	2676	702	776	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	ALA	GLU	engineered mutation	UNP Q4J9L0
B	336	ALA	GLU	engineered mutation	UNP Q4J9L0
C	336	ALA	GLU	engineered mutation	UNP Q4J9L0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

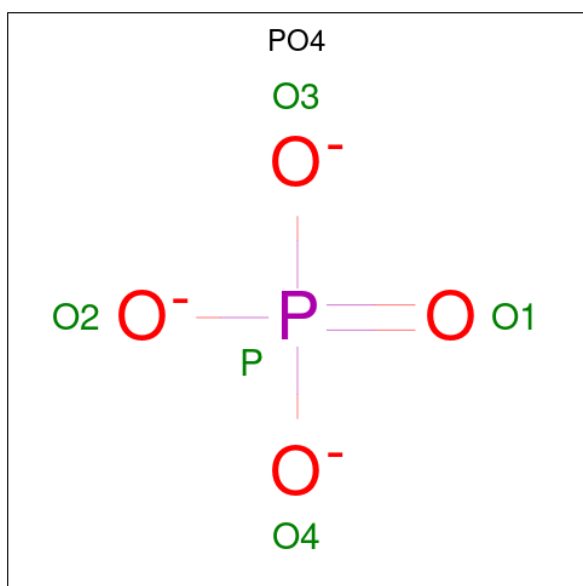


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

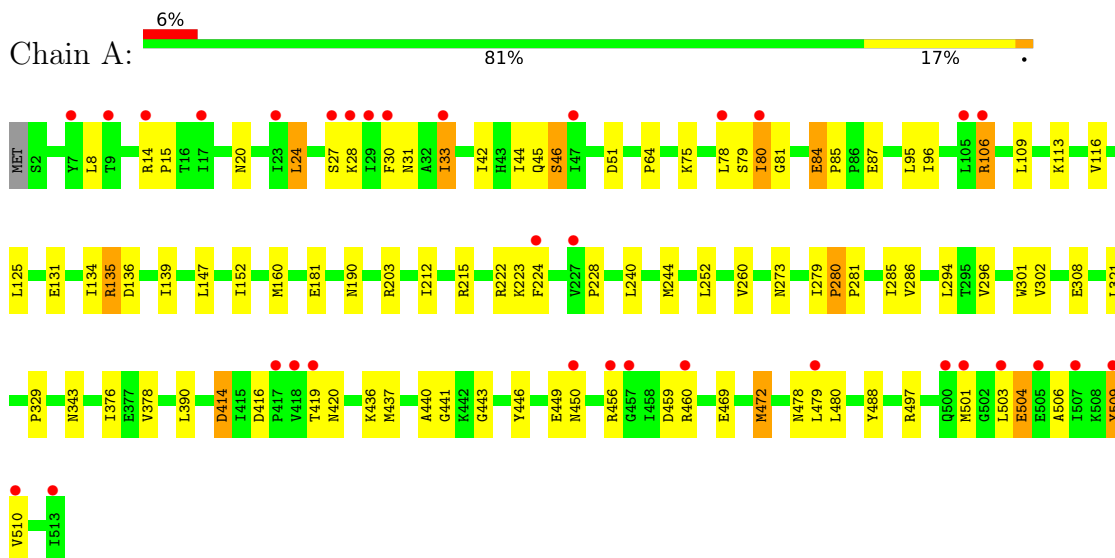
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	257	Total	O	0	0
			257	257		
6	B	241	Total	O	0	0
			241	241		
6	C	268	Total	O	0	0
			268	268		

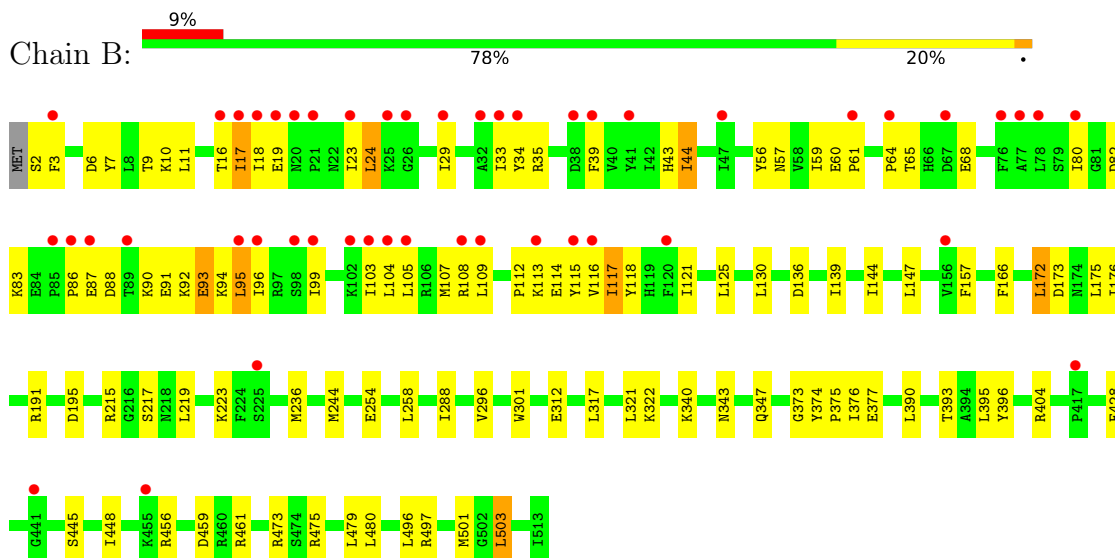
3 Residue-property plots [i](#)

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

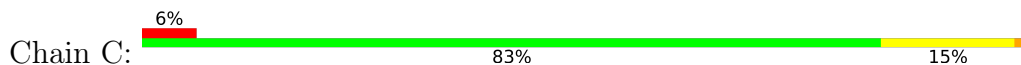
• Molecule 1: FlaI ATPase

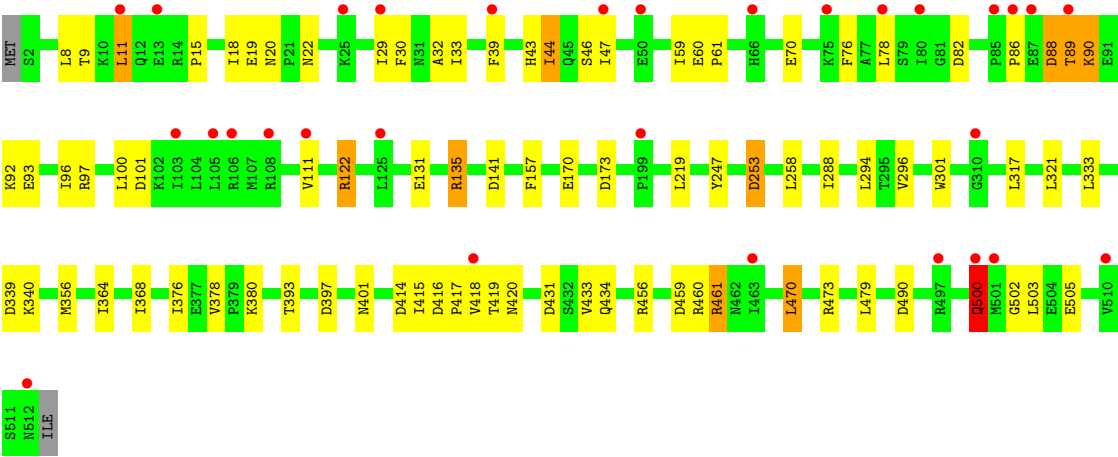


• Molecule 1: FlaI ATPase



• Molecule 1: FlaI ATPase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.46Å 148.08Å 123.63Å 90.00° 131.60° 90.00°	Depositor
Resolution (Å)	45.99 – 2.00 45.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.99-2.00) 99.8 (45.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.214 0.188 , 0.215	Depositor DCC
R_{free} test set	12884 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13401	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, EDO, MG, PO4

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	0.44	0/4279	0.83	6/5798 (0.1%)
1	B	0.47	0/4304	0.83	3/5830 (0.1%)
1	C	0.48	0/4272	0.80	1/5787 (0.0%)
All	All	0.46	0/12855	0.82	10/17415 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ARG	N-CA-C	11.66	125.35	111.82
1	A	440	ALA	N-CA-C	7.65	119.26	111.07
1	B	60	GLU	CA-C-N	6.63	127.21	120.38
1	B	60	GLU	C-N-CA	6.63	127.21	120.38
1	A	280	PRO	CA-C-N	5.84	125.38	119.19
1	A	280	PRO	C-N-CA	5.84	125.38	119.19
1	A	20	ASN	N-CA-C	5.54	113.21	108.22
1	A	212	ILE	CB-CA-C	-5.37	106.14	111.30
1	C	500	GLN	N-CA-C	-5.16	103.68	110.33
1	B	93	GLU	N-CA-C	-5.10	104.66	111.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4176	0	4237	53	1
1	B	4189	0	4268	64	1
1	C	4169	0	4238	50	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
5	A	8	0	12	1	0
5	B	4	0	6	0	0
6	A	257	0	0	6	2
6	B	241	0	0	6	0
6	C	268	0	0	13	2
All	All	13401	0	12797	164	3

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 7.

All (164) 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:61:PRO:HB3	1:B:115:TYR:HD2	1.23	1.03
1:B:34:TYR:OH	6:B:912:HOH:O	1.94	0.85
1:C:490:ASP:OD1	6:C:796:HOH:O	1.95	0.83
1:B:373:GLY:HA3	6:C:931:HOH:O	1.77	0.82
1:C:141:ASP:OD2	6:C:934:HOH:O	1.99	0.81
1:A:44:ILE:HD12	1:A:160:MET:HE1	1.63	0.81
1:B:61:PRO:HB3	1:B:115:TYR:CD2	2.13	0.78
1:C:461:ARG:HH11	1:C:461:ARG:HB3	1.48	0.78
1:C:473:ARG:HG3	1:C:503:LEU:HD11	1.67	0.76
1:A:479:LEU:HD23	1:A:510:VAL:HG13	1.70	0.71
1:C:173:ASP:OD1	6:C:932:HOH:O	2.08	0.71
1:B:195:ASP:OD1	6:B:933:HOH:O	2.09	0.70
1:C:97:ARG:O	6:C:795:HOH:O	2.09	0.69
1:A:443:GLY:HA2	1:A:449:GLU:OE2	1.93	0.68
1:B:2:SER:OG	6:B:904:HOH:O	2.12	0.68
1:C:170:GLU:OE2	6:C:935:HOH:O	2.11	0.67
1:B:35:ARG:O	6:B:937:HOH:O	2.11	0.67
1:B:112:PRO:HB2	1:B:115:TYR:HD1	1.58	0.67
1:A:24:LEU:O	1:A:27:SER:OG	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:O	6:C:942:HOH:O	2.13	0.66
1:A:75:LYS:NZ	6:A:916:HOH:O	2.23	0.66
1:A:414:ASP:OD1	6:A:799:HOH:O	2.14	0.65
1:C:419:THR:O	6:C:959:HOH:O	2.15	0.64
1:C:500:GLN:O	1:C:502:GLY:N	2.28	0.64
1:C:461:ARG:HB3	1:C:461:ARG:NH1	2.12	0.64
1:B:64:PRO:HG3	1:B:116:VAL:HG22	1.80	0.64
1:A:478:ASN:OD1	6:A:919:HOH:O	2.15	0.64
1:A:136:ASP:HB3	1:A:139:ILE:HG12	1.79	0.63
1:A:30:PHE:O	1:A:46:SER:OG	2.16	0.63
1:A:414:ASP:CG	6:A:799:HOH:O	2.42	0.62
1:A:416:ASP:O	1:A:420:ASN:N	2.33	0.61
1:A:64:PRO:HG3	1:A:116:VAL:HG22	1.82	0.61
1:A:343:ASN:HD21	5:A:605:EDO:H11	1.68	0.58
1:B:23:ILE:HG23	1:B:24:LEU:HD22	1.86	0.57
1:C:101:ASP:O	6:C:938:HOH:O	2.17	0.57
1:A:419:THR:N	6:A:838:HOH:O	2.38	0.57
1:C:76:PHE:HZ	1:C:96:ILE:HG13	1.68	0.57
1:C:93:GLU:OE1	6:C:907:HOH:O	2.17	0.57
1:C:20:ASN:OD1	1:C:22:ASN:ND2	2.37	0.56
1:B:65:THR:N	1:B:68:GLU:OE1	2.36	0.56
1:B:88:ASP:HB3	1:B:92:LYS:HD2	1.86	0.56
1:A:228:PRO:HG2	1:A:488:TYR:CD1	2.40	0.56
1:B:80:ILE:HG22	1:B:83:LYS:NZ	2.21	0.56
1:B:16:THR:OG1	1:B:17:ILE:N	2.39	0.56
1:B:88:ASP:O	1:B:92:LYS:HB2	2.06	0.55
1:A:79:SER:O	1:A:80:ILE:HG13	2.07	0.55
1:B:130:LEU:HD21	1:B:144:ILE:HD11	1.88	0.55
1:C:131:GLU:OE1	1:C:135:ARG:NH2	2.40	0.54
1:C:18:ILE:HG12	1:C:32:ALA:HB1	1.89	0.54
1:A:244[B]:MET:HE1	1:A:437:MET:SD	2.48	0.53
1:A:223:LYS:O	1:A:224:PHE:HB3	2.07	0.53
1:C:420:ASN:HA	6:C:937:HOH:O	2.08	0.53
1:B:112:PRO:HB2	1:B:115:TYR:CD1	2.39	0.53
1:C:88:ASP:OD1	1:C:89:THR:N	2.40	0.53
1:B:459:ASP:OD2	1:B:461:ARG:NH1	2.42	0.52
1:A:260:VAL:HG13	1:A:390:LEU:HD11	1.90	0.52
1:B:64:PRO:HG2	1:B:116:VAL:HG13	1.91	0.52
1:C:253:ASP:OD2	1:C:473:ARG:NH2	2.43	0.52
1:C:416:ASP:OD2	1:C:418:VAL:HG23	2.09	0.51
1:A:139:ILE:HD12	1:A:152:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:OE2	6:A:827:HOH:O	2.20	0.50
1:A:136:ASP:O	1:A:223:LYS:NZ	2.45	0.50
1:A:506:ALA:O	1:A:510:VAL:HG12	2.11	0.49
1:C:60:GLU:CD	1:C:122:ARG:HH21	2.21	0.49
1:C:39:PHE:O	1:C:61:PRO:HD3	2.12	0.49
1:A:228:PRO:HG2	1:A:488:TYR:CG	2.48	0.49
1:B:475[B]:ARG:NH2	6:B:905:HOH:O	2.43	0.49
1:B:88:ASP:OD1	1:B:90:LYS:N	2.46	0.49
1:C:333:LEU:HD22	1:C:356:MET:HB2	1.95	0.48
1:B:93:GLU:O	1:B:95:LEU:N	2.45	0.48
1:B:296:VAL:HB	1:B:301:TRP:CD2	2.49	0.48
1:B:104:LEU:HB3	1:B:113:LYS:HE3	1.95	0.48
1:B:254:GLU:OE2	1:B:456:ARG:HD2	2.14	0.48
1:B:173:ASP:OD1	1:B:217:SER:OG	2.27	0.48
1:C:459:ASP:OD1	1:C:460:ARG:N	2.46	0.48
1:C:247:TYR:HA	1:C:470:LEU:HD11	1.95	0.48
1:C:376:ILE:HG22	1:C:378:VAL:HG23	1.95	0.48
1:A:203:ARG:HG2	1:A:224:PHE:CE2	2.49	0.48
1:A:79:SER:O	1:A:81:GLY:N	2.47	0.47
1:A:84:GLU:HG2	1:A:85:PRO:HD2	1.96	0.47
1:B:43:HIS:HB2	1:B:59:ILE:HD11	1.95	0.47
1:B:117:ILE:O	1:B:121:ILE:HG12	2.14	0.47
1:B:497:ARG:HH11	1:B:501:MET:HE1	1.78	0.47
1:C:8:LEU:O	1:C:11:LEU:HB2	2.14	0.47
1:B:86:PRO:HB2	1:B:92:LYS:CD	2.44	0.47
1:B:343:ASN:OD1	1:B:347[B]:GLN:NE2	2.48	0.47
1:C:76:PHE:CZ	1:C:96:ILE:HG13	2.50	0.47
1:B:343:ASN:ND2	1:B:377:GLU:O	2.47	0.47
1:C:288:ILE:HG22	1:C:317:LEU:HD22	1.96	0.47
1:C:460:ARG:HG2	1:C:461:ARG:HG2	1.97	0.47
1:B:3:PHE:N	6:B:904:HOH:O	2.48	0.47
1:B:82:ASP:OD1	1:B:83:LYS:N	2.48	0.46
1:C:414[A]:ASP:OD1	1:C:415:ILE:N	2.33	0.46
1:A:190:ASN:OD1	1:B:312:GLU:HG3	2.16	0.46
1:A:446:TYR:O	1:A:450:ASN:HB2	2.15	0.46
1:C:364:ILE:O	1:C:368:ILE:HG12	2.16	0.46
1:C:418:VAL:HG23	1:C:419:THR:HG23	1.96	0.46
1:B:44:ILE:HD12	1:B:157:PHE:CZ	2.50	0.46
1:A:286:VAL:HG23	1:A:329:PRO:HB3	1.98	0.46
1:B:114:GLU:H	1:B:114:GLU:CD	2.24	0.46
1:C:296:VAL:HB	1:C:301:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:MET:HG2	1:A:503:LEU:HB3	1.98	0.45
1:B:86:PRO:HB2	1:B:92:LYS:HD3	1.98	0.45
1:B:136:ASP:O	1:B:223:LYS:NZ	2.50	0.45
1:A:106:ARG:CG	1:A:106:ARG:HH11	2.30	0.45
1:A:240:LEU:HB2	1:A:244[B]:MET:SD	2.55	0.45
1:C:416:ASP:HA	1:C:417:PRO:HD3	1.80	0.45
1:C:397:ASP:OD2	1:C:401:ASN:HB2	2.16	0.45
1:B:43:HIS:HB3	1:B:57:ASN:HB2	1.97	0.45
1:A:509:TYR:CD2	1:A:509:TYR:C	2.94	0.45
1:C:30:PHE:CE2	1:C:46:SER:HB3	2.52	0.45
1:B:56:TYR:CZ	1:B:139:ILE:HD11	2.52	0.44
1:B:172:LEU:HG	1:B:217:SER:O	2.17	0.44
1:A:51:ASP:HA	1:B:496:LEU:HD13	2.00	0.44
1:C:15:PRO:HB2	1:C:33:ILE:HG13	2.00	0.44
1:C:431:ASP:OD1	1:C:433:VAL:HG22	2.17	0.44
1:A:14:ARG:HA	1:A:15:PRO:HD3	1.69	0.44
1:A:131:GLU:OE1	1:A:135:ARG:NE	2.46	0.44
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.83	0.44
1:B:343:ASN:HB2	1:B:376:ILE:O	2.18	0.44
1:C:11:LEU:HD12	1:C:11:LEU:HA	1.85	0.43
1:A:96:ILE:HD12	1:A:125:LEU:HD21	2.01	0.43
1:A:147:LEU:O	1:A:215:ARG:NH2	2.51	0.43
1:B:288:ILE:HG22	1:B:317:LEU:HD22	2.00	0.43
1:B:95:LEU:O	1:B:99:ILE:HG13	2.19	0.43
1:B:147:LEU:O	1:B:215:ARG:NH2	2.52	0.43
1:B:99:ILE:O	1:B:103:ILE:HG23	2.19	0.43
1:B:497:ARG:HH11	1:B:501:MET:CE	2.32	0.43
1:A:33:ILE:HA	1:A:42:ILE:O	2.19	0.42
1:C:8:LEU:HD21	1:C:33:ILE:HD12	2.00	0.42
1:A:279:ILE:HG21	1:A:285:ILE:HD11	2.00	0.42
1:C:473:ARG:NH1	6:C:818:HOH:O	2.44	0.42
1:A:8:LEU:HD21	1:A:33:ILE:HD12	2.01	0.42
1:B:244:MET:HA	1:B:428:PHE:CZ	2.55	0.42
1:A:296:VAL:HB	1:A:301:TRP:CD2	2.54	0.42
1:A:376:ILE:HG22	1:A:378:VAL:HG23	2.01	0.42
1:C:43:HIS:HB2	1:C:59:ILE:HD11	2.02	0.42
1:B:393:THR:HG23	1:B:395:LEU:HG	2.01	0.42
1:B:497:ARG:NH1	1:B:501:MET:HE1	2.35	0.42
1:B:7:TYR:O	1:B:10:LYS:HG2	2.20	0.42
1:B:374:TYR:CG	1:B:375:PRO:HA	2.55	0.42
1:C:380:LYS:NZ	1:C:420:ASN:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:CD2	1:C:456[B]:ARG:HD3	2.56	0.41
1:C:44:ILE:H	1:C:44:ILE:HG13	1.73	0.41
1:C:44:ILE:HD13	1:C:157:PHE:CZ	2.55	0.41
1:B:39:PHE:O	1:B:61:PRO:HD2	2.21	0.41
1:B:107:MET:O	1:B:113:LYS:NZ	2.54	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.83	0.41
1:A:480:LEU:HD23	1:A:510:VAL:HG21	2.03	0.41
1:A:134:ILE:HA	1:A:223:LYS:HE2	2.03	0.41
1:B:473:ARG:HG3	1:B:503:LEU:HD21	2.03	0.41
1:C:100:LEU:HB3	6:C:795:HOH:O	2.20	0.41
1:A:469:GLU:O	1:A:472:MET:HB3	2.21	0.41
1:B:44:ILE:H	1:B:44:ILE:HG12	1.71	0.41
1:B:80:ILE:HG22	1:B:83:LYS:HZ2	1.85	0.41
1:B:445:SER:HB3	1:B:448:ILE:HB	2.02	0.41
1:B:61:PRO:HG2	1:B:118:TYR:CD2	2.56	0.40
1:B:166:PHE:CZ	1:B:175:LEU:HD22	2.56	0.40
1:A:286:VAL:HG22	1:A:302:VAL:HB	2.03	0.40
1:C:339:ASP:OD2	1:C:340:LYS:HG3	2.21	0.40
1:A:459:ASP:OD2	1:A:460:ARG:N	2.53	0.40
1:A:497:ARG:O	1:A:501:MET:HG2	2.21	0.40
1:A:497:ARG:HG2	1:A:501:MET:HE2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:OE2	1:B:108:ARG:NH1[3_455]	1.68	0.52
6:A:823:HOH:O	6:C:952:HOH:O[2_657]	1.72	0.48
6:A:856:HOH:O	6:C:952:HOH:O[2_657]	1.76	0.44

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	517/513 (101%)	493 (95%)	20 (4%)	4 (1%)	16	11
1	B	520/513 (101%)	492 (95%)	22 (4%)	6 (1%)	10	6
1	C	516/513 (101%)	490 (95%)	23 (4%)	3 (1%)	21	17
All	All	1553/1539 (101%)	1475 (95%)	65 (4%)	13 (1%)	16	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	C	82	ASP
1	C	88	ASP
1	B	94	LYS
1	A	441	GLY
1	B	95	LEU
1	A	28	LYS
1	A	31	ASN
1	B	87[A]	GLU
1	B	87[B]	GLU
1	C	86	PRO
1	B	19	GLU
1	B	18	ILE

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	468/462 (101%)	444 (95%)	24 (5%)	21	19
1	B	471/462 (102%)	443 (94%)	28 (6%)	18	14
1	C	467/462 (101%)	440 (94%)	27 (6%)	18	15
All	All	1406/1386 (101%)	1327 (94%)	79 (6%)	20	16

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	33	ILE
1	A	45	GLN
1	A	46	SER
1	A	78	LEU
1	A	84	GLU
1	A	87[A]	GLU
1	A	87[B]	GLU
1	A	95	LEU
1	A	106	ARG
1	A	109	LEU
1	A	113	LYS
1	A	135	ARG
1	A	252	LEU
1	A	273	ASN
1	A	294	LEU
1	A	308[A]	GLU
1	A	308[B]	GLU
1	A	321	LEU
1	A	414	ASP
1	A	436	LYS
1	A	472	MET
1	A	504	GLU
1	A	509	TYR
1	B	6	ASP
1	B	9	THR
1	B	11	LEU
1	B	17	ILE
1	B	24	LEU
1	B	29	ILE
1	B	33	ILE
1	B	44	ILE
1	B	91	GLU
1	B	96	ILE
1	B	105	LEU
1	B	109	LEU
1	B	117	ILE
1	B	125	LEU
1	B	172	LEU
1	B	176	ILE
1	B	191	ARG
1	B	219	LEU
1	B	236	MET

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Mol	Chain	Res	Type
1	B	258	LEU
1	B	321	LEU
1	B	322	LYS
1	B	340[A]	LYS
1	B	340[B]	LYS
1	B	390	LEU
1	B	404	ARG
1	B	480	LEU
1	B	503	LEU
1	C	9	THR
1	C	11	LEU
1	C	19	GLU
1	C	29	ILE
1	C	44	ILE
1	C	47	ILE
1	C	70	GLU
1	C	78	LEU
1	C	89	THR
1	C	90	LYS
1	C	92	LYS
1	C	111	VAL
1	C	122	ARG
1	C	135	ARG
1	C	219	LEU
1	C	253	ASP
1	C	258[A]	LEU
1	C	258[B]	LEU
1	C	294	LEU
1	C	321	LEU
1	C	393	THR
1	C	434	GLN
1	C	461	ARG
1	C	470	LEU
1	C	479	LEU
1	C	500	GLN
1	C	505	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	450	ASN

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Mol	Chain	Res	Type
1	B	205	ASN
1	B	300	ASN
1	B	384	ASN
1	B	392	GLN
1	C	205	ASN
1	C	218	ASN
1	C	420	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 [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	601	3	28,29,29	1.43	4 (14%)	43,45,45	1.85	11 (25%)
2	ADP	B	601	3	28,29,29	1.54	6 (21%)	43,45,45	1.94	10 (23%)
5	EDO	B	603	-	3,3,3	0.48	0	2,2,2	0.33	0
4	PO4	A	603	-	4,4,4	0.88	0	6,6,6	0.56	0
5	EDO	A	605	-	3,3,3	0.44	0	2,2,2	0.33	0
2	ADP	A	601	3	28,29,29	1.51	5 (17%)	43,45,45	1.85	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	601	3	-	1/16/32/32	0/3/3/3
2	ADP	B	601	3	-	0/16/32/32	0/3/3/3
5	EDO	B	603	-	-	1/1/1/1	-
5	EDO	A	605	-	-	0/1/1/1	-
2	ADP	A	601	3	-	0/16/32/32	0/3/3/3
5	EDO	A	604	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C5-C4	4.90	1.47	1.39
2	C	601	ADP	C5-C4	4.61	1.47	1.39
2	B	601	ADP	PA-O3A	4.33	1.64	1.59
2	B	601	ADP	C5-C4	4.10	1.46	1.39
2	A	601	ADP	C5-C6	2.74	1.48	1.41
2	C	601	ADP	C5-C6	2.70	1.48	1.41
2	A	601	ADP	C8-N7	2.59	1.36	1.31
2	A	601	ADP	C5-N7	-2.56	1.34	1.39
2	C	601	ADP	PA-O3A	2.48	1.62	1.59
2	B	601	ADP	PB-O3B	-2.41	1.45	1.54
2	C	601	ADP	C8-N7	2.23	1.36	1.31
2	A	601	ADP	PA-O3A	2.22	1.61	1.59
2	B	601	ADP	C8-N7	2.12	1.35	1.31
2	B	601	ADP	C5-C6	2.10	1.46	1.41
2	B	601	ADP	C5-N7	-2.02	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-5.61	118.99	126.72
2	A	601	ADP	C5-C4-N3	-5.57	119.05	126.72
2	C	601	ADP	C5-C4-N3	-5.34	119.36	126.72
2	B	601	ADP	N3-C4-N9	5.17	135.96	127.17
2	C	601	ADP	N3-C4-N9	4.44	134.72	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	N3-C4-N9	4.30	134.47	127.17
2	A	601	ADP	C4-C5-N7	-4.04	105.96	110.58
2	B	601	ADP	C4-N9-C8	3.69	109.61	105.74
2	C	601	ADP	N3-C2-N1	-3.62	123.10	128.58
2	C	601	ADP	C2-N3-C4	3.58	120.58	111.83
2	A	601	ADP	C2-N3-C4	3.54	120.48	111.83
2	B	601	ADP	C2-N3-C4	3.54	120.47	111.83
2	B	601	ADP	N3-C2-N1	-3.43	123.39	128.58
2	C	601	ADP	C4-C5-N7	-3.35	106.76	110.58
2	C	601	ADP	C4-N9-C8	3.25	109.15	105.74
2	A	601	ADP	N3-C2-N1	-3.23	123.70	128.58
2	A	601	ADP	C5-N7-C8	3.14	108.39	103.45
2	B	601	ADP	O2A-PA-O3A	2.89	115.09	107.27
2	A	601	ADP	C4-N9-C8	2.89	108.77	105.74
2	C	601	ADP	O3B-PB-O2B	2.64	117.71	107.80
2	B	601	ADP	C4-C5-N7	-2.61	107.59	110.58
2	C	601	ADP	C5-N7-C8	2.58	107.50	103.45
2	B	601	ADP	N9-C8-N7	-2.56	110.31	113.94
2	B	601	ADP	C5-N7-C8	2.54	107.44	103.45
2	A	601	ADP	N9-C8-N7	-2.49	110.40	113.94
2	A	601	ADP	C6-C5-N7	2.36	136.64	132.09
2	C	601	ADP	N9-C8-N7	-2.30	110.67	113.94
2	C	601	ADP	C2-N1-C6	2.29	122.49	118.73
2	B	601	ADP	N6-C6-N1	2.23	123.34	118.38
2	C	601	ADP	C6-C5-N7	2.20	136.33	132.09
2	A	601	ADP	C2-N1-C6	2.09	122.17	118.73
2	A	601	ADP	O4'-C1'-N9	-2.08	104.09	108.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

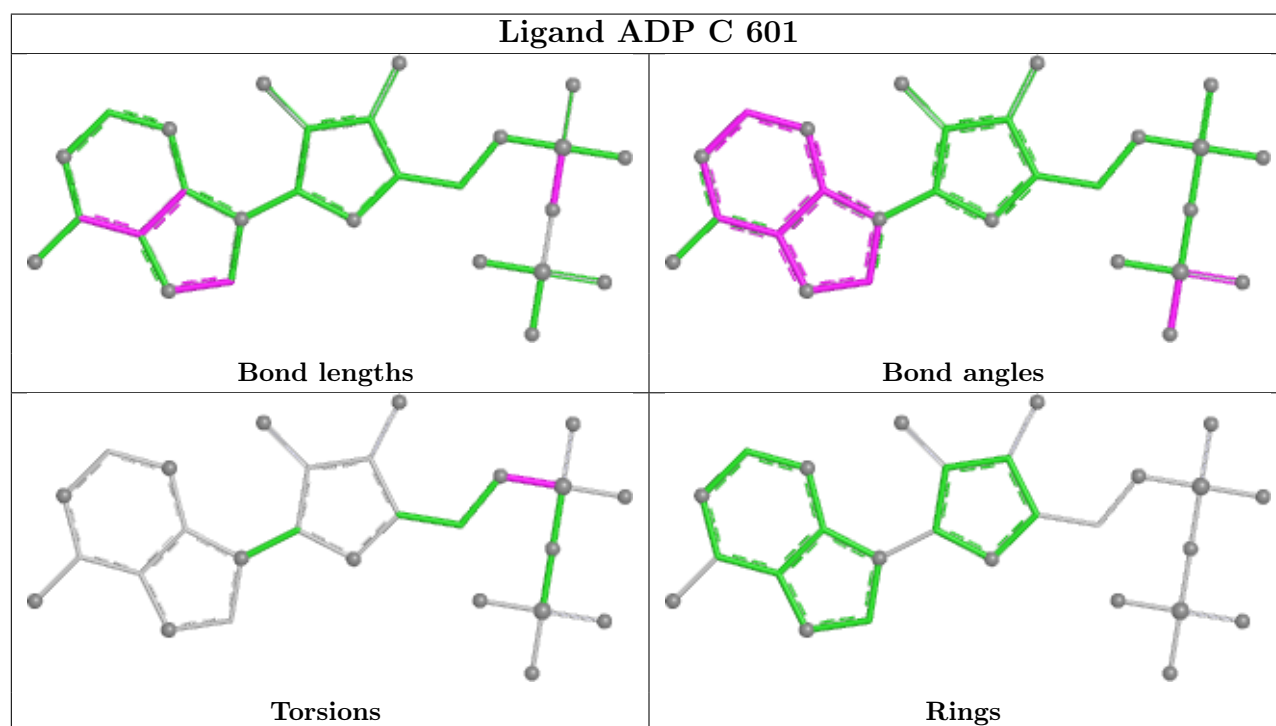
Mol	Chain	Res	Type	Atoms
5	B	603	EDO	O1-C1-C2-O2
2	C	601	ADP	C5'-O5'-PA-O1A

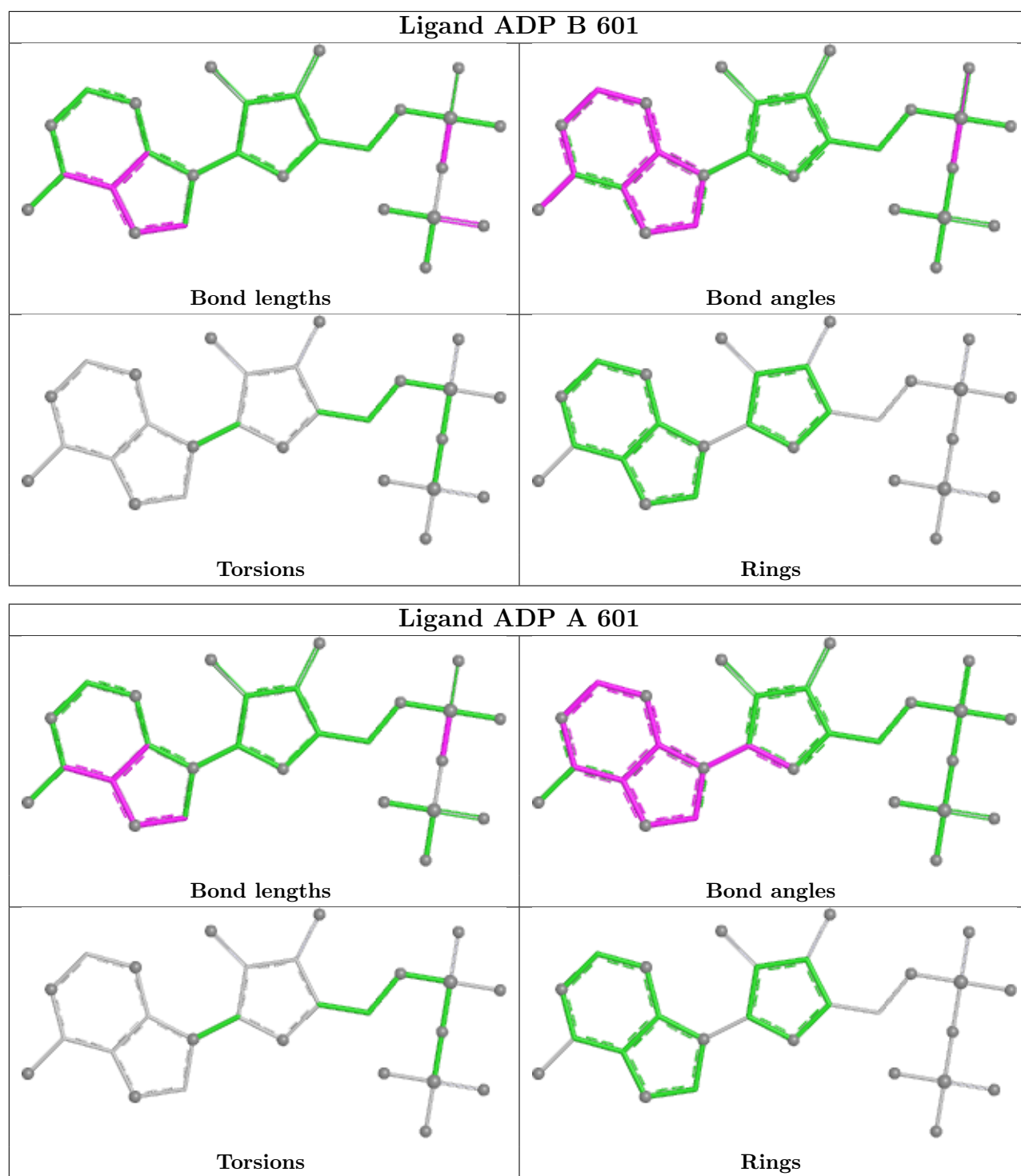
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	512/513 (99%)	0.34	33 (6%)	25	24	13, 49, 95, 126	33 (6%)
1	B	511/513 (99%)	0.44	48 (9%)	14	13	14, 47, 120, 147	32 (6%)
1	C	506/513 (98%)	0.37	30 (5%)	28	27	20, 51, 96, 123	35 (6%)
All	All	1529/1539 (99%)	0.38	111 (7%)	21	19	13, 49, 104, 147	100 (6%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	501[A]	MET	9.3
1	B	29	ILE	5.6
1	A	27	SER	4.5
1	B	115	TYR	4.4
1	B	80	ILE	4.2
1	A	80	ILE	4.1
1	B	116	VAL	3.9
1	A	224	PHE	3.9
1	A	503	LEU	3.8
1	B	34	TYR	3.7
1	C	80	ILE	3.7
1	B	109	LEU	3.7
1	C	86	PRO	3.7
1	B	23	ILE	3.7
1	B	78	LEU	3.6
1	A	513	ILE	3.6
1	C	50	GLU	3.5
1	A	106	ARG	3.5
1	B	105	LEU	3.4
1	C	106	ARG	3.4
1	C	47	ILE	3.4
1	B	39	PHE	3.3
1	A	29	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	419	THR	3.2
1	B	108	ARG	3.2
1	B	17	ILE	3.2
1	B	18	ILE	3.2
1	A	510	VAL	3.2
1	C	85	PRO	3.1
1	C	66	HIS	3.1
1	B	86	PRO	3.1
1	B	76	PHE	3.0
1	A	78	LEU	3.0
1	B	33	ILE	3.0
1	B	21	PRO	2.9
1	B	95	LEU	2.9
1	A	17	ILE	2.9
1	C	103	ILE	2.8
1	B	32	ALA	2.8
1	C	418	VAL	2.8
1	A	457	GLY	2.8
1	B	89	THR	2.8
1	A	30	PHE	2.8
1	B	20	ASN	2.7
1	B	3	PHE	2.6
1	B	120	PHE	2.6
1	B	85	PRO	2.6
1	B	25	LYS	2.6
1	A	23	ILE	2.6
1	A	500	GLN	2.6
1	B	99	ILE	2.6
1	A	507	ILE	2.5
1	B	96	ILE	2.5
1	B	103	ILE	2.5
1	B	19	GLU	2.5
1	C	89	THR	2.5
1	B	61	PRO	2.5
1	B	77	ALA	2.5
1	C	500	GLN	2.5
1	A	479	LEU	2.5
1	B	113	LYS	2.5
1	A	28	LYS	2.4
1	B	441	GLY	2.4
1	C	310	GLY	2.4
1	C	87	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	2.4
1	A	509	TYR	2.4
1	C	463	ILE	2.4
1	B	41	TYR	2.4
1	A	105	LEU	2.4
1	C	512	ASN	2.4
1	A	418	VAL	2.4
1	B	98	SER	2.4
1	B	16	THR	2.4
1	B	87[A]	GLU	2.3
1	C	11	LEU	2.3
1	A	47	ILE	2.3
1	C	199	PRO	2.3
1	A	7	TYR	2.3
1	A	456	ARG	2.3
1	B	455	LYS	2.3
1	C	105	LEU	2.3
1	C	25	LYS	2.3
1	B	47	ILE	2.3
1	A	460	ARG	2.3
1	C	108	ARG	2.3
1	B	67	ASP	2.3
1	B	102	LYS	2.3
1	A	9	THR	2.2
1	C	29	ILE	2.2
1	B	38	ASP	2.2
1	B	26	GLY	2.2
1	C	125	LEU	2.2
1	C	510	VAL	2.2
1	C	13	GLU	2.2
1	A	14	ARG	2.2
1	A	450	ASN	2.2
1	A	505	GLU	2.1
1	B	104	LEU	2.1
1	B	417	PRO	2.1
1	C	111	VAL	2.1
1	B	225	SER	2.1
1	C	497[A]	ARG	2.1
1	A	33	ILE	2.1
1	A	417	PRO	2.0
1	B	64	PRO	2.0
1	B	156	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	39	PHE	2.0
1	A	501	MET	2.0
1	C	78	LEU	2.0
1	C	75	LYS	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](#)

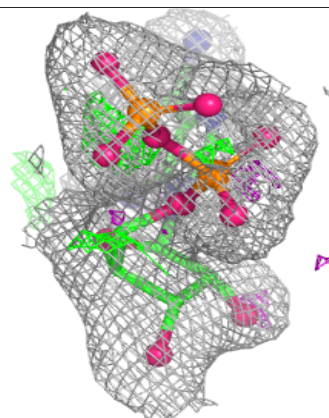
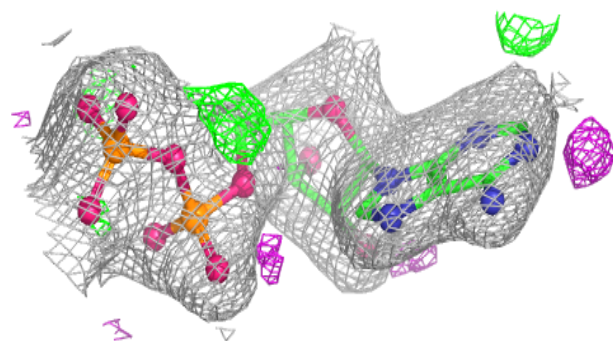
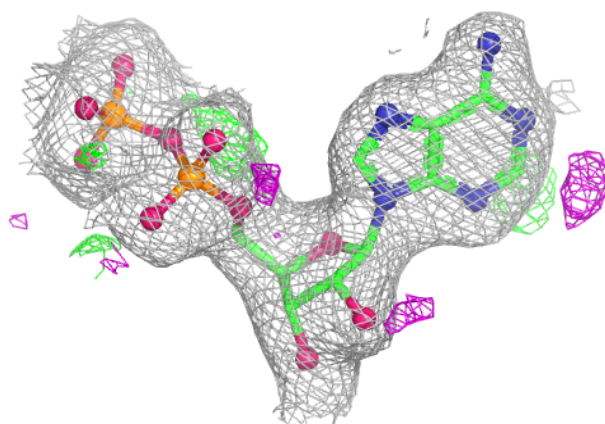
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	B	602	1/1	0.79	0.13	35,35,35,35	0
5	EDO	A	605	4/4	0.79	0.20	61,69,72,74	0
4	PO4	A	603	5/5	0.81	0.17	40,52,61,66	5
5	EDO	A	604	4/4	0.92	0.12	41,48,51,54	0
5	EDO	B	603	4/4	0.92	0.15	58,62,67,73	0
2	ADP	C	601	27/27	0.97	0.07	29,45,51,53	0
2	ADP	A	601	27/27	0.98	0.05	30,34,41,43	0
2	ADP	B	601	27/27	0.98	0.05	20,30,36,36	0
3	MG	C	602	1/1	0.99	0.02	31,31,31,31	0
3	MG	A	602	1/1	1.00	0.02	32,32,32,32	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.

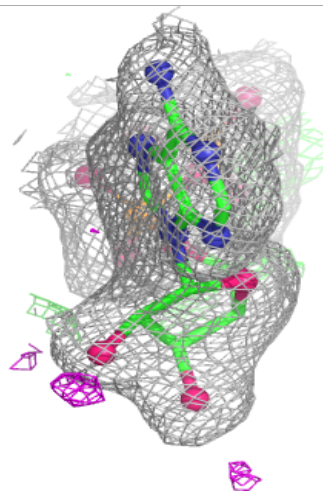
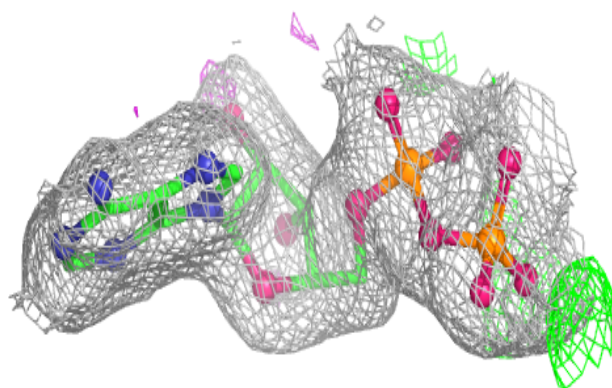
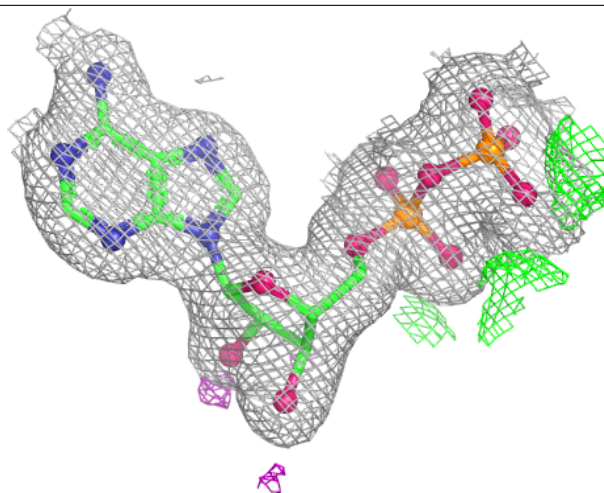
Electron density around ADP C 601:

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



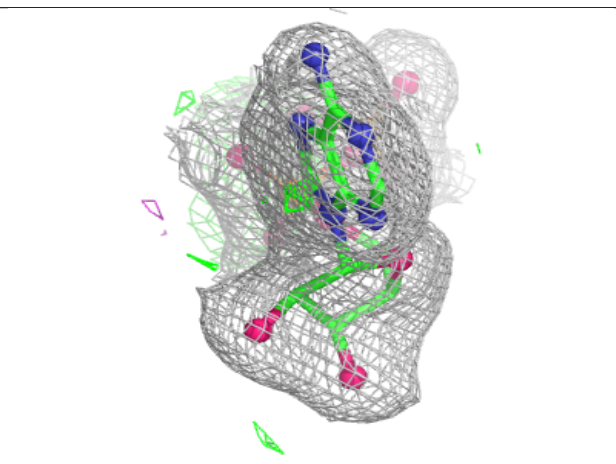
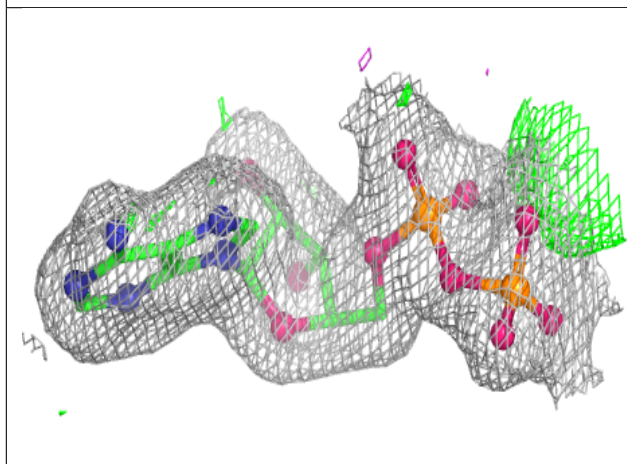
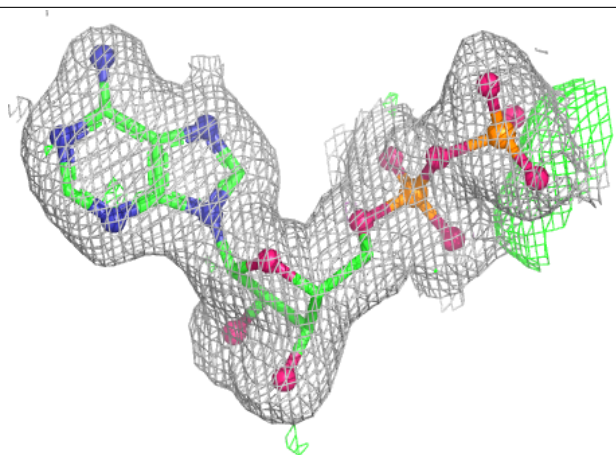
Electron density around ADP A 601:

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



Electron density around ADP B 601:

$2mF_o-DF_c$ (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.