



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:28 PM UTC

PDB ID : 5YA2 / pdb_00005ya2
Title : Crystal structure of LsrK-HPr complex with ADP
Authors : Ryu, K.S.; Ha, J.H.
Deposited on : 2017-08-30
Resolution : 2.70 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

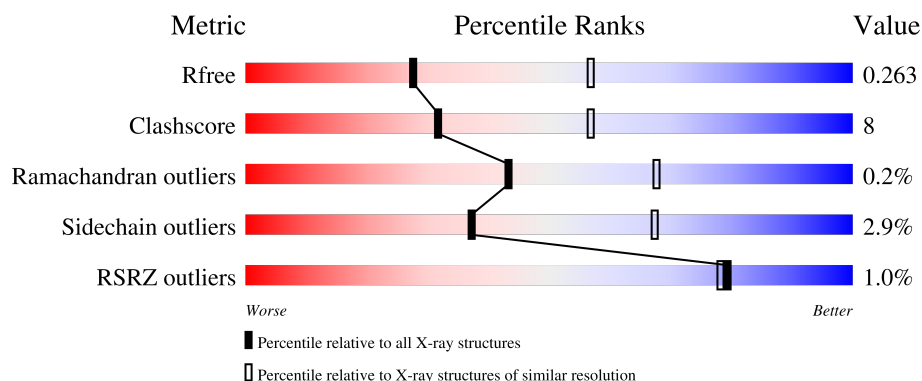
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	540	 70% 17% 11%
1	B	540	 72% 15% 11%
2	C	85	 87% 13%
2	D	85	 84% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8686 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 Autoinducer-2 kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3623	2287	628	685	23			
1	B	478	Total	C	N	O	S	0	0	0
			3623	2287	628	685	23			

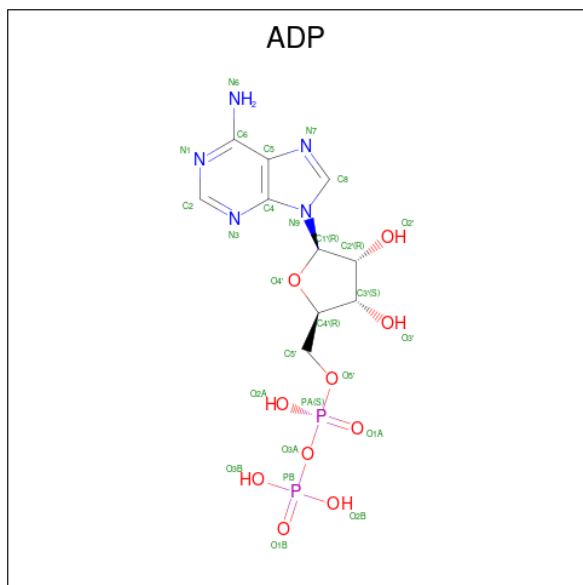
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP P77432
A	-8	HIS	-	expression tag	UNP P77432
A	-7	HIS	-	expression tag	UNP P77432
A	-6	HIS	-	expression tag	UNP P77432
A	-5	HIS	-	expression tag	UNP P77432
A	-4	HIS	-	expression tag	UNP P77432
A	-3	SER	-	expression tag	UNP P77432
A	-2	GLU	-	expression tag	UNP P77432
A	-1	ASP	-	expression tag	UNP P77432
A	0	PRO	-	expression tag	UNP P77432
B	-9	HIS	-	expression tag	UNP P77432
B	-8	HIS	-	expression tag	UNP P77432
B	-7	HIS	-	expression tag	UNP P77432
B	-6	HIS	-	expression tag	UNP P77432
B	-5	HIS	-	expression tag	UNP P77432
B	-4	HIS	-	expression tag	UNP P77432
B	-3	SER	-	expression tag	UNP P77432
B	-2	GLU	-	expression tag	UNP P77432
B	-1	ASP	-	expression tag	UNP P77432
B	0	PRO	-	expression tag	UNP P77432

- Molecule 2 is a protein called Phosphocarrier protein HPr.

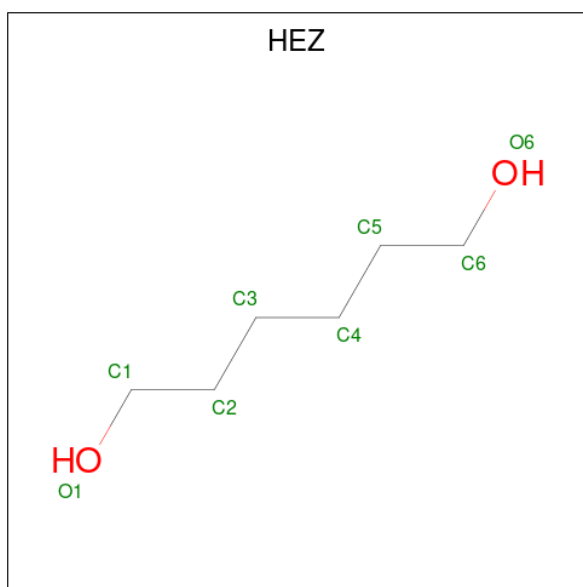
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	85	Total	C	N	O	S	0	0	0
			640	401	107	130	2			
2	D	85	Total	C	N	O	S	0	0	0
			640	401	107	130	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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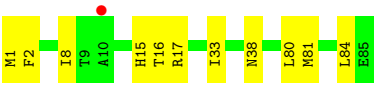
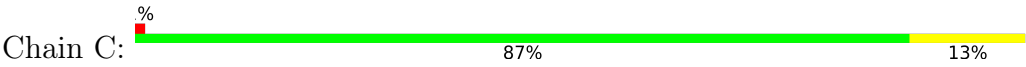
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

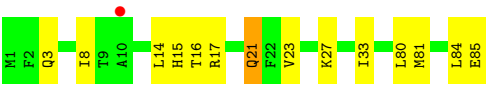
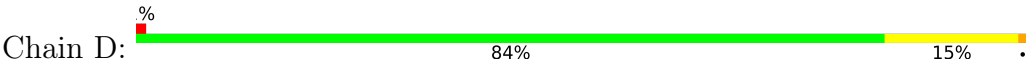
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	28	Total	O	0	0
			28	28		
6	C	5	Total	O	0	0
			5	5		
6	D	5	Total	O	0	0
			5	5		

- Molecule 1: Autoinducer-2 kinase





● Molecule 2: Phosphocarrier protein HPr



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.25Å 101.25Å 344.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.32 – 2.70 46.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (46.32-2.70) 96.9 (46.32-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.255 0.221 , 0.263	Depositor DCC
R_{free} test set	1991 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.488 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8686	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: PO4, HEZ, ADP

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	0.35	0/3697	0.84	7/5029 (0.1%)
1	B	0.38	0/3697	0.89	9/5029 (0.2%)
2	C	0.33	0/647	0.73	0/871
2	D	0.37	0/647	0.78	0/871
All	All	0.36	0/8688	0.85	16/11800 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	TRP	N-CA-C	13.96	120.23	108.78
1	A	43	TRP	N-CA-C	7.75	115.13	108.78
1	B	474	MET	N-CA-C	7.04	118.61	111.07
1	A	313	PHE	CB-CA-C	-7.02	108.49	116.63
1	B	43	TRP	CA-C-O	6.39	121.65	117.94
1	B	452	VAL	CA-C-N	6.25	132.94	121.70
1	B	452	VAL	C-N-CA	6.25	132.94	121.70
1	A	452	VAL	CA-C-N	6.22	132.91	121.70
1	A	452	VAL	C-N-CA	6.22	132.91	121.70
1	B	43	TRP	CB-CA-C	-5.85	108.65	117.07
1	A	43	TRP	CA-C-O	5.61	121.19	117.94
1	B	373	HIS	N-CA-C	-5.45	95.75	111.00
1	A	502	ARG	N-CA-C	5.42	117.19	111.28
1	A	56	GLU	CB-CA-C	-5.39	108.67	116.54
1	B	56	GLU	CB-CA-C	-5.35	108.73	116.54
1	B	313	PHE	CB-CA-C	-5.07	110.34	117.23

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	3623	0	3583	68	1
1	B	3623	0	3583	53	0
2	C	640	0	653	6	0
2	D	640	0	653	11	1
3	A	27	0	12	2	0
3	B	27	0	12	0	0
4	A	8	0	14	0	0
4	B	8	0	14	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
6	A	22	0	0	1	0
6	B	28	0	0	0	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
All	All	8686	0	8524	138	1

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 8.

All (138) 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:452:VAL:HA	1:B:453:LYS:HB2	1.43	1.01
1:A:452:VAL:HA	1:A:453:LYS:HB2	1.44	0.98
2:D:21:GLN:HE21	2:D:21:GLN:HA	1.39	0.84
2:D:21:GLN:HA	2:D:21:GLN:NE2	1.94	0.80
1:B:101:ASN:OD1	1:B:214:ARG:NH1	2.23	0.71
1:B:118:ARG:NH1	1:B:122:GLU:OE1	2.27	0.68
1:A:101:ASN:OD1	1:A:214:ARG:NH1	2.27	0.68
1:A:15:MET:HE2	1:A:26:ALA:HB1	1.77	0.67
2:D:15:HIS:CD2	2:D:16:THR:H	2.13	0.66
1:A:322:ARG:NH2	3:A:601:ADP:O1B	2.28	0.66
1:A:118:ARG:NH1	1:A:122:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:CYS:SG	1:A:502:ARG:NH1	2.69	0.65
2:C:15:HIS:CD2	2:C:16:THR:H	2.15	0.65
2:D:21:GLN:HE21	2:D:21:GLN:CA	2.10	0.65
1:B:15:MET:HE2	1:B:26:ALA:HB1	1.79	0.63
1:A:318:MET:HE1	1:A:398:GLU:HG3	1.79	0.62
1:B:339:ASP:O	1:B:342:THR:OG1	2.16	0.62
1:A:72:GLN:NE2	1:A:76:ASN:OD1	2.32	0.61
1:B:325:PHE:HB3	1:B:390:LYS:HE3	1.83	0.60
1:B:451:VAL:HG12	1:B:485:GLU:HG3	1.85	0.59
1:A:113:ASP:OD1	1:A:115:ARG:HG2	2.01	0.59
1:A:322:ARG:NH1	1:A:323:ASP:OD1	2.36	0.59
1:A:441:ASP:O	1:A:495:HIS:HB2	2.03	0.59
1:A:319:ARG:NH2	3:A:601:ADP:O3B	2.33	0.58
1:B:498:TYR:O	1:B:502:ARG:HG3	2.05	0.57
1:B:433:LYS:HD3	1:B:486:ARG:HD3	1.87	0.56
1:A:433:LYS:HD3	1:A:486:ARG:HD3	1.87	0.56
2:C:17:ARG:NH1	6:C:201:HOH:O	2.39	0.55
1:A:233:SER:O	1:A:237:GLU:HG3	2.07	0.55
1:A:348:ALA:HB1	1:A:395:ARG:HB2	1.89	0.54
1:B:398:GLU:HA	1:B:435:TRP:CZ2	2.43	0.54
1:B:452:VAL:CA	1:B:453:LYS:HB2	2.30	0.54
1:A:277:TRP:CG	1:A:314:THR:HG21	2.43	0.53
1:A:107:TRP:CZ3	1:A:154:LEU:HD11	2.44	0.53
1:A:318:MET:HE1	1:A:398:GLU:CG	2.39	0.53
1:B:436:SER:HB2	1:B:488:HIS:CE1	2.45	0.52
1:A:452:VAL:CA	1:A:453:LYS:HB2	2.30	0.52
1:A:86:ALA:HB2	1:A:468:ALA:HB2	1.92	0.52
1:A:398:GLU:HG2	1:A:435:TRP:CE2	2.44	0.51
1:A:398:GLU:HA	1:A:435:TRP:CZ2	2.46	0.51
1:B:86:ALA:HB2	1:B:468:ALA:HB2	1.93	0.51
1:A:66:ALA:O	1:A:70:MET:HG3	2.11	0.51
1:A:314:THR:O	1:A:317:THR:OG1	2.25	0.51
1:B:43:TRP:HZ3	1:B:62:ASN:HB3	1.75	0.50
1:B:503:ASP:OD1	1:B:504:LYS:N	2.45	0.50
1:A:436:SER:HB2	1:A:488:HIS:CE1	2.46	0.50
1:A:15:MET:HE1	1:A:70:MET:HA	1.93	0.50
2:C:38:ASN:ND2	5:C:101:PO4:O4	2.41	0.50
1:B:107:TRP:CZ3	1:B:154:LEU:HD11	2.46	0.50
1:A:499:GLN:HA	1:A:502:ARG:HG3	1.93	0.50
1:B:158:ARG:HB3	1:B:161:ILE:HD13	1.93	0.50
2:C:80:LEU:O	2:C:84:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:O	1:A:416:SER:OG	2.23	0.49
2:D:8:ILE:HG12	2:D:81:MET:HE1	1.93	0.49
1:A:355:SER:OG	1:A:395:ARG:HG2	2.13	0.49
1:B:398:GLU:HG2	1:B:435:TRP:CE2	2.47	0.49
1:A:174:TRP:HE1	1:A:178:MET:HE2	1.77	0.48
1:B:66:ALA:O	1:B:70:MET:HG3	2.12	0.48
1:A:158:ARG:HB3	1:A:161:ILE:HD13	1.94	0.48
1:A:356:TRP:CE2	1:A:387:LYS:HE2	2.49	0.48
1:B:96:ILE:HD12	1:B:168:ILE:HD11	1.94	0.48
1:A:43:TRP:HZ3	1:A:62:ASN:HB3	1.79	0.48
1:A:113:ASP:OD1	1:A:113:ASP:C	2.57	0.48
1:A:336:LEU:HB3	1:A:338:ILE:HG13	1.96	0.47
1:A:356:TRP:CD2	1:A:387:LYS:HE2	2.49	0.47
1:B:412:ILE:O	1:B:416:SER:OG	2.23	0.47
1:A:503:ASP:OD1	1:A:504:LYS:HG3	2.14	0.47
1:B:37:ALA:HB3	1:B:77:ALA:HB2	1.97	0.47
1:B:355:SER:OG	1:B:395:ARG:HG2	2.15	0.47
1:B:453:LYS:HB3	1:B:454:GLU:H	1.56	0.47
1:A:389:ASN:N	1:A:389:ASN:OD1	2.48	0.47
1:A:476:GLU:OE1	1:A:476:GLU:N	2.39	0.47
1:B:318:MET:HE3	1:B:394:PHE:CE2	2.50	0.47
1:B:436:SER:HB3	1:B:449:ILE:HD11	1.96	0.47
2:C:8:ILE:HG12	2:C:81:MET:HE1	1.96	0.47
1:A:466:VAL:HG21	1:A:474:MET:HG3	1.98	0.46
1:B:60:ASN:O	1:B:64:GLN:HG2	2.15	0.46
1:B:401:ALA:HB3	1:B:435:TRP:CZ2	2.51	0.46
1:A:96:ILE:HD12	1:A:168:ILE:HD11	1.96	0.46
1:B:206:ALA:HB1	4:B:702:HEZ:H61	1.97	0.46
1:A:317:THR:O	1:A:320:TRP:HB3	2.16	0.46
1:B:277:TRP:CG	1:B:314:THR:HG21	2.51	0.46
1:B:389:ASN:OD1	1:B:389:ASN:N	2.49	0.45
1:B:15:MET:HE1	1:B:70:MET:HA	1.98	0.45
1:B:119:GLU:HG3	1:B:153:TRP:HB2	1.99	0.45
1:A:453:LYS:HB3	1:A:454:GLU:H	1.56	0.45
2:D:23:VAL:HG12	2:D:27:LYS:HE2	1.98	0.45
1:A:43:TRP:HB3	1:A:44:ARG:H	1.53	0.45
1:A:451:VAL:HG22	1:A:485:GLU:HG3	1.99	0.45
2:D:80:LEU:O	2:D:84:LEU:HB2	2.17	0.45
1:A:436:SER:HB3	1:A:449:ILE:HD11	1.99	0.45
1:B:476:GLU:H	1:B:476:GLU:CD	2.18	0.44
1:B:263:VAL:HA	1:B:268:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:HB3	1:B:44:ARG:H	1.44	0.44
1:B:398:GLU:HA	1:B:435:TRP:HZ2	1.81	0.44
1:B:440:ALA:O	1:B:490:PRO:HB3	2.18	0.44
2:D:15:HIS:CG	2:D:16:THR:H	2.36	0.44
1:A:277:TRP:CD1	1:A:314:THR:HG21	2.53	0.43
1:B:64:GLN:O	1:B:68:GLU:HG3	2.18	0.43
1:A:30:ASP:HB3	1:A:36:ILE:HD11	1.99	0.43
1:A:263:VAL:HA	1:A:268:GLN:NE2	2.33	0.43
1:A:353:PRO:HG3	1:A:494:LYS:HD3	1.99	0.43
1:B:295:ARG:HH11	1:B:310:ILE:HD12	1.83	0.43
2:D:81:MET:HE3	2:D:81:MET:HB3	1.86	0.43
1:A:362:PHE:CE2	1:A:376:PRO:HB3	2.54	0.42
1:B:403:ILE:HA	1:B:442:VAL:HG11	2.01	0.42
1:A:192:THR:HG22	1:A:297:ASN:HD21	1.84	0.42
1:A:356:TRP:CD1	1:A:387:LYS:HG2	2.54	0.42
1:A:398:GLU:HA	1:A:435:TRP:HZ2	1.83	0.42
1:A:120:VAL:HG12	1:A:124:LYS:HE3	2.02	0.42
1:A:10:SER:OG	1:A:11:LYS:N	2.52	0.42
1:A:58:ASP:O	1:A:62:ASN:ND2	2.53	0.42
1:A:491:ASP:HA	1:A:492:PRO:HD3	1.90	0.41
1:B:10:SER:OG	1:B:11:LYS:N	2.53	0.41
1:B:398:GLU:C	1:B:435:TRP:HE1	2.28	0.41
1:A:435:TRP:HD1	1:A:435:TRP:HA	1.73	0.41
1:A:498:TYR:O	1:A:501:SER:OG	2.29	0.41
1:A:100:ASN:HB2	6:A:708:HOH:O	2.20	0.41
1:B:96:ILE:HD13	1:B:96:ILE:HA	1.92	0.41
1:A:119:GLU:HG3	1:A:153:TRP:HB2	2.03	0.41
1:A:131:PHE:CZ	1:A:210:MET:HE1	2.55	0.41
1:B:55:MET:HE2	1:B:55:MET:HA	2.02	0.41
1:B:89:ALA:O	1:B:250:GLY:HA3	2.21	0.41
1:B:61:LYS:O	1:B:65:LEU:HG	2.20	0.41
1:B:115:ARG:HE	1:B:115:ARG:HB2	1.63	0.41
1:B:174:TRP:HE1	1:B:178:MET:HE2	1.86	0.41
1:B:192:THR:HG22	1:B:297:ASN:HD21	1.85	0.41
2:C:1:MET:HG2	2:C:2:PHE:N	2.36	0.41
2:D:17:ARG:HH22	2:D:85:GLU:HG2	1.86	0.41
1:A:60:ASN:O	1:A:64:GLN:HG2	2.21	0.40
1:B:342:THR:O	1:B:346:GLU:HG2	2.22	0.40
1:B:353:PRO:HG3	1:B:494:LYS:HD3	2.03	0.40
1:A:44:ARG:O	1:A:61:LYS:HD3	2.22	0.40
1:A:491:ASP:CG	1:A:494:LYS:HG3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.90	0.40
2:D:84:LEU:HD12	2:D:84:LEU:HA	1.94	0.40
1:A:503:ASP:OD1	1:A:504:LYS:N	2.54	0.40
1:A:24:ILE:HD13	1:A:24:ILE:HA	1.98	0.40

All (1) 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:177:TYR:OH	2:D:3:GLN:OE1[5_555]	2.10	0.10

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	472/540 (87%)	449 (95%)	22 (5%)	1 (0%)	43	68
1	B	472/540 (87%)	450 (95%)	21 (4%)	1 (0%)	43	68
2	C	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
2	D	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
All	All	1110/1250 (89%)	1063 (96%)	45 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	LYS
1	B	453	LYS

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	381/435 (88%)	372 (98%)	9 (2%)	43	72
1	B	381/435 (88%)	368 (97%)	13 (3%)	32	62
2	C	70/70 (100%)	69 (99%)	1 (1%)	59	82
2	D	70/70 (100%)	67 (96%)	3 (4%)	26	54
All	All	902/1010 (89%)	876 (97%)	26 (3%)	37	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	64	GLN
1	A	82	GLU
1	A	113	ASP
1	A	164	GLN
1	A	216	ASP
1	A	297	ASN
1	A	435	TRP
1	A	452	VAL
1	B	38	VAL
1	B	44	ARG
1	B	82	GLU
1	B	112	VAL
1	B	216	ASP
1	B	297	ASN
1	B	336	LEU
1	B	342	THR
1	B	346	GLU
1	B	435	TRP
1	B	451	VAL
1	B	452	VAL
1	B	476	GLU
2	C	33	ILE
2	D	14	LEU

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Mol	Chain	Res	Type
2	D	21	GLN
2	D	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	141	GLN
1	A	189	ASN
1	A	297	ASN
1	B	141	GLN
1	B	189	ASN
1	B	279	GLN
1	B	297	ASN
1	B	411	GLN
2	C	4	GLN
2	C	51	GLN
2	D	21	GLN

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](#)

10 ligands are modelled in this entry.

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	$\# Z > 2$
3	ADP	A	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.86	8 (18%)
5	PO4	A	605	-	4,4,4	0.95	0	6,6,6	0.45	0
4	HEZ	A	602	-	7,7,7	0.38	0	6,6,6	0.70	0
5	PO4	B	703	-	4,4,4	0.95	0	6,6,6	0.46	0
5	PO4	D	101	-	4,4,4	0.95	0	6,6,6	0.47	0
4	HEZ	B	702	-	7,7,7	0.39	0	6,6,6	0.70	0
5	PO4	A	603	-	4,4,4	0.96	0	6,6,6	0.51	0
5	PO4	C	101	-	4,4,4	0.95	0	6,6,6	0.46	0
5	PO4	A	604	-	4,4,4	0.95	0	6,6,6	0.46	0
3	ADP	B	701	-	28,29,29	1.46	5 (17%)	43,45,45	1.86	8 (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
3	ADP	A	601	-	-	2/16/32/32	0/3/3/3
4	HEZ	B	702	-	-	3/5/5/5	-
4	HEZ	A	602	-	-	1/5/5/5	-
3	ADP	B	701	-	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ADP	C5-C4	4.90	1.47	1.39
3	A	601	ADP	C5-C4	4.83	1.47	1.39
3	B	701	ADP	C5-C6	2.83	1.48	1.41
3	A	601	ADP	C5-C6	2.74	1.48	1.41
3	B	701	ADP	C8-N7	2.41	1.36	1.31
3	A	601	ADP	C8-N7	2.33	1.36	1.31
3	B	701	ADP	PA-O3A	2.28	1.62	1.59
3	A	601	ADP	C5-N7	-2.27	1.34	1.39
3	B	701	ADP	C5-N7	-2.19	1.35	1.39
3	A	601	ADP	PA-O3A	2.09	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ADP	C5-C4-N3	-6.21	118.17	126.72
3	A	601	ADP	C5-C4-N3	-6.05	118.38	126.72
3	A	601	ADP	N3-C4-N9	4.79	135.31	127.17
3	B	701	ADP	N3-C4-N9	4.79	135.31	127.17
3	B	701	ADP	C2-N3-C4	3.82	121.17	111.83
3	A	601	ADP	C2-N3-C4	3.72	120.92	111.83
3	B	701	ADP	C4-C5-N7	-3.53	106.54	110.58
3	A	601	ADP	C4-C5-N7	-3.41	106.69	110.58
3	B	701	ADP	N3-C2-N1	-3.21	123.73	128.58
3	A	601	ADP	N3-C2-N1	-3.15	123.82	128.58
3	A	601	ADP	C3'-C2'-C1'	2.69	106.55	101.46
3	B	701	ADP	C3'-C2'-C1'	2.55	106.29	101.46
3	B	701	ADP	C5-N7-C8	2.53	107.42	103.45
3	A	601	ADP	C5-N7-C8	2.49	107.36	103.45
3	A	601	ADP	C4-N9-C8	2.35	108.20	105.74
3	B	701	ADP	C4-N9-C8	2.11	107.95	105.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	HEZ	C3-C4-C5-C6
3	A	601	ADP	O4'-C4'-C5'-O5'
4	A	602	HEZ	C1-C2-C3-C4
3	A	601	ADP	C5'-O5'-PA-O1A
4	B	702	HEZ	C4-C5-C6-O6
4	B	702	HEZ	C2-C3-C4-C5

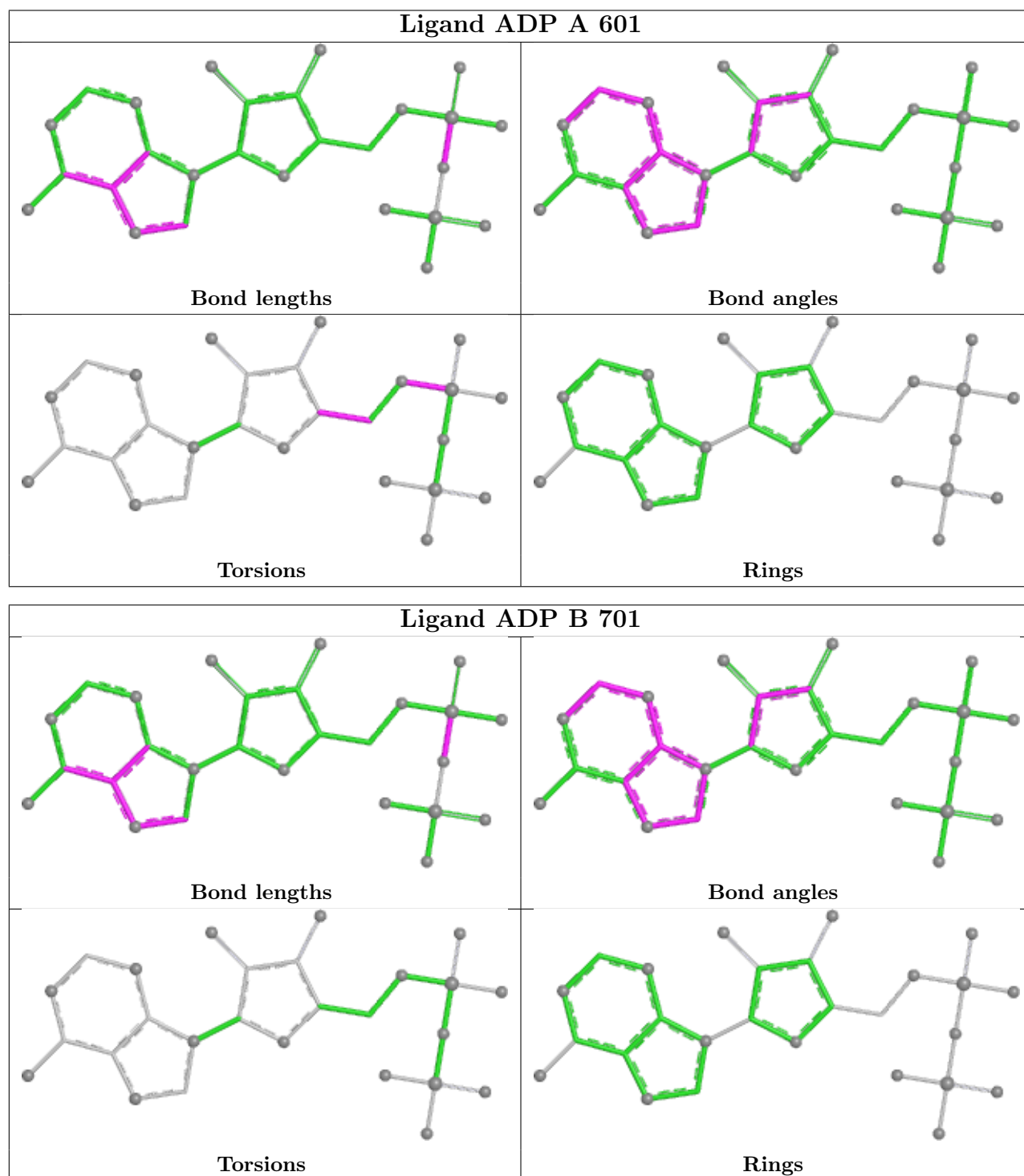
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	2	0
4	B	702	HEZ	1	0
5	C	101	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	478/540 (88%)	-0.19	4 (0%) 82 81	40, 79, 126, 171	0
1	B	478/540 (88%)	-0.23	5 (1%) 79 78	42, 79, 125, 162	0
2	C	85/85 (100%)	-0.42	1 (1%) 76 75	44, 81, 120, 155	0
2	D	85/85 (100%)	-0.50	1 (1%) 76 75	45, 80, 126, 157	0
All	All	1126/1250 (90%)	-0.25	11 (0%) 79 78	40, 80, 126, 171	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	10	ALA	3.1
1	B	112	VAL	2.5
1	B	353	PRO	2.4
1	B	43	TRP	2.4
1	A	71	ARG	2.3
1	B	498	TYR	2.3
2	C	10	ALA	2.2
1	A	364	ASP	2.2
1	B	373	HIS	2.1
1	A	496	GLU	2.1
1	A	498	TYR	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](#)

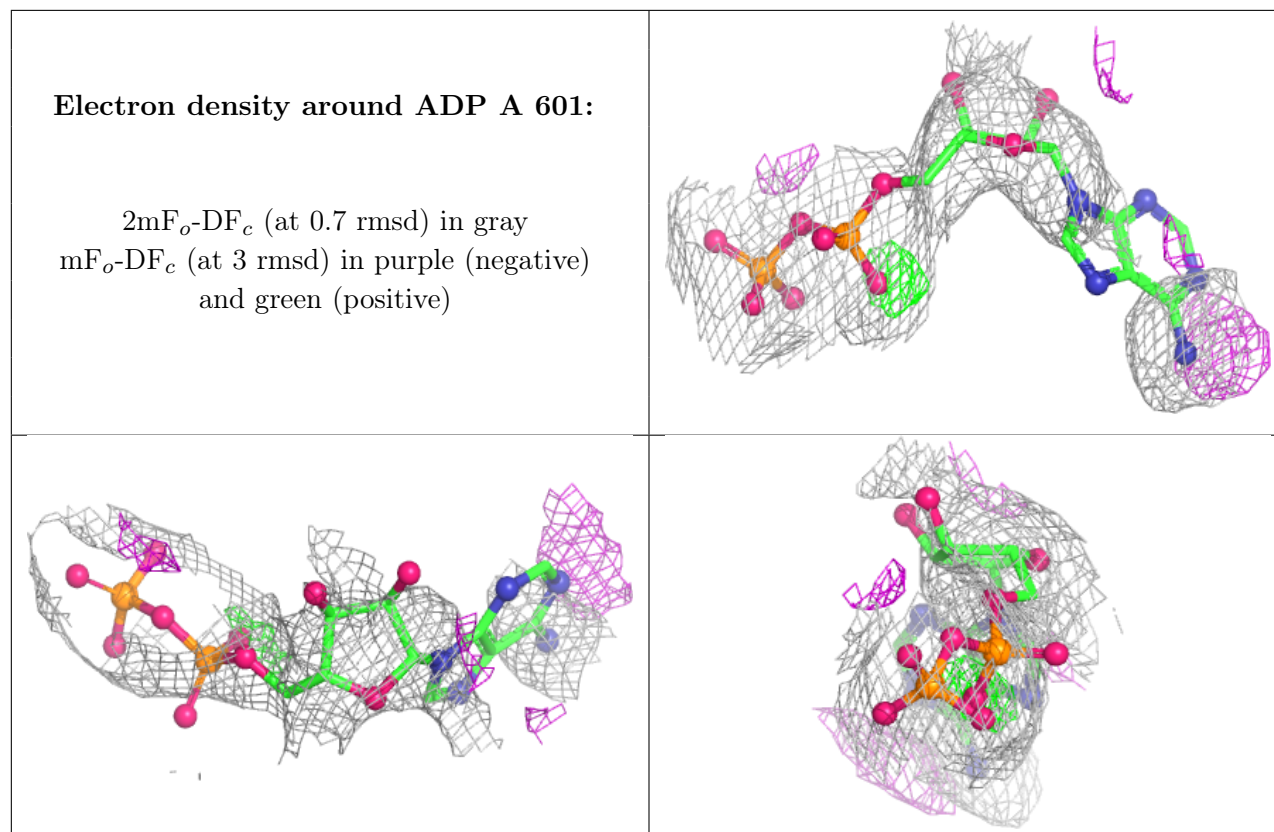
There are no oligosaccharides in this entry.

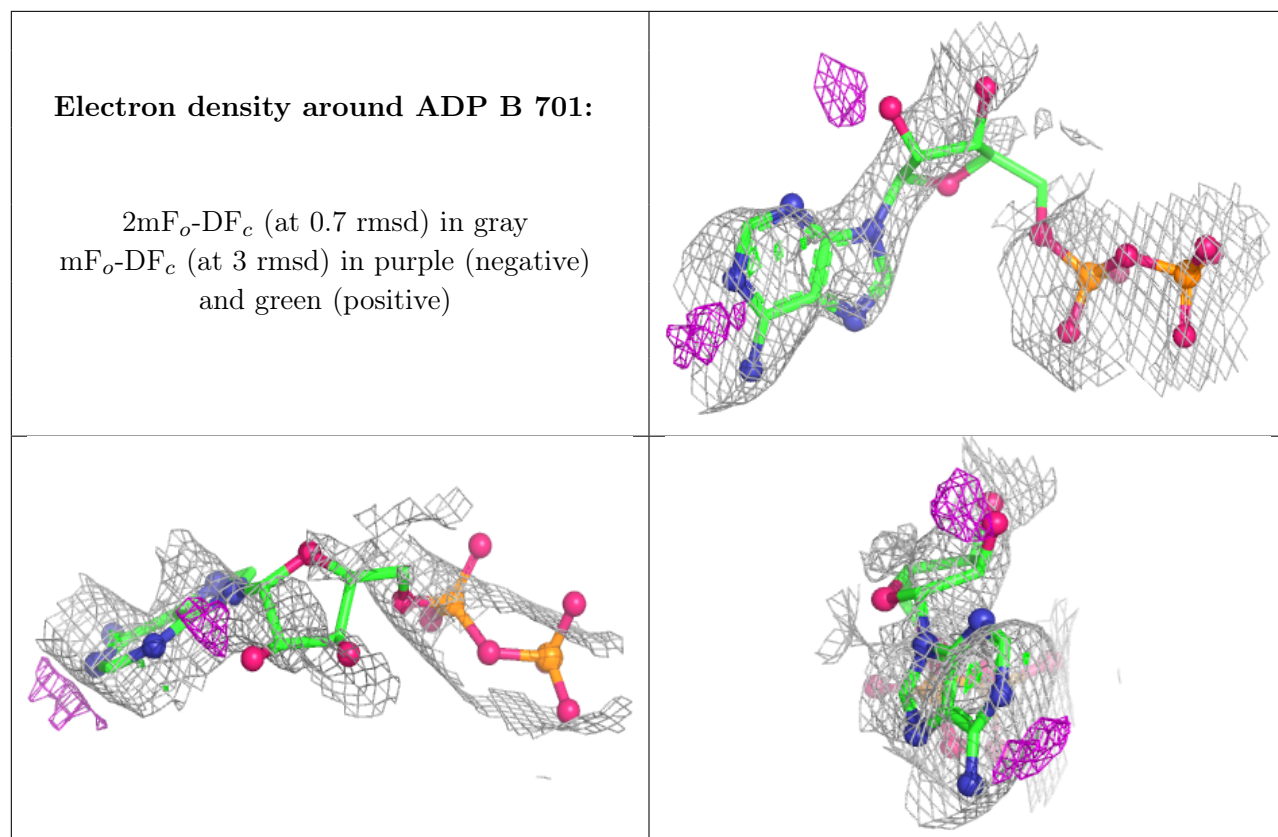
6.4 Ligands ⓘ

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
5	PO4	C	101	5/5	0.95	0.08	127,130,137,139	0
3	ADP	A	601	27/27	0.96	0.14	122,160,225,262	0
5	PO4	D	101	5/5	0.96	0.07	122,132,132,139	0
3	ADP	B	701	27/27	0.97	0.12	119,153,197,211	0
5	PO4	A	603	5/5	0.98	0.09	86,89,131,131	0
5	PO4	A	604	5/5	0.98	0.10	106,115,121,123	0
5	PO4	A	605	5/5	0.98	0.06	77,82,102,102	0
5	PO4	B	703	5/5	0.98	0.08	115,116,122,130	0
4	HEZ	A	602	8/8	0.98	0.09	53,72,83,84	0
4	HEZ	B	702	8/8	0.98	0.11	49,67,84,91	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.