



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:16 AM UTC

PDB ID : 6RU8 / pdb_00006ru8
Title : Crystal structure of Casein Kinase I delta (CK1d) in complex with triple phosphorylated p63 PAD3P peptide
Authors : Chaikuad, A.; Tuppi, M.; Gebel, J.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Dotsch, V.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2019-05-27
Resolution : 1.92 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

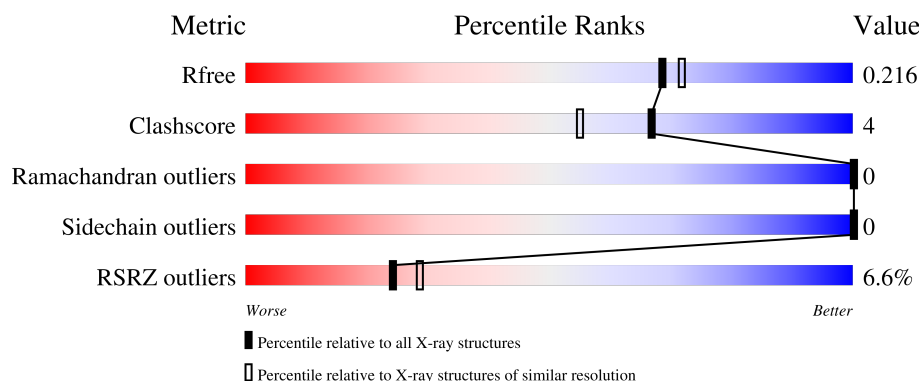
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

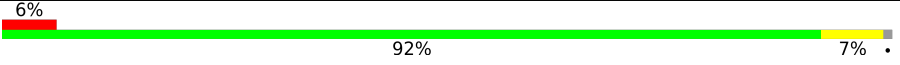
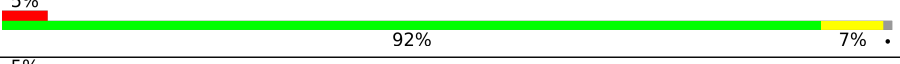
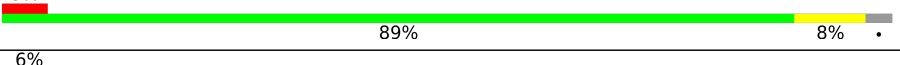
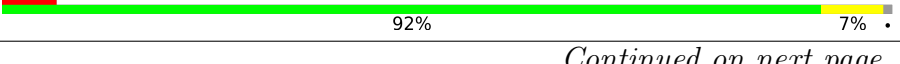
The reported resolution of this entry is 1.92 Å.

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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	296	
1	B	296	
1	C	296	
1	D	296	

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Mol	Chain	Length	Quality of chain
2	E	12	17%50%33%17%
2	F	12	8%50%50%
2	G	12	25%50%25%25%
2	H	12	33%67%8%25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10612 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 Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	2	0
			2395	1537	418	426	14			
1	B	293	Total	C	N	O	S	0	4	0
			2413	1548	425	426	14			
1	C	287	Total	C	N	O	S	0	7	0
			2372	1527	410	418	17			
1	D	293	Total	C	N	O	S	0	6	0
			2415	1551	419	427	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P48730
A	0	MET	-	expression tag	UNP P48730
B	-1	SER	-	expression tag	UNP P48730
B	0	MET	-	expression tag	UNP P48730
C	-1	SER	-	expression tag	UNP P48730
C	0	MET	-	expression tag	UNP P48730
D	-1	SER	-	expression tag	UNP P48730
D	0	MET	-	expression tag	UNP P48730

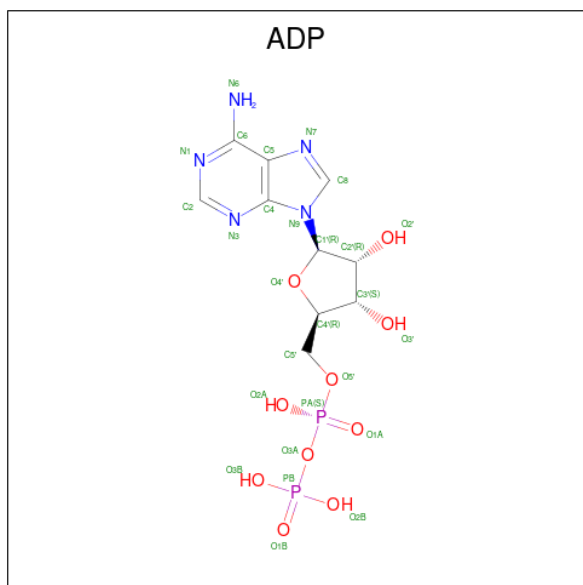
- Molecule 2 is a protein called Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			72	34	10	25	3			
2	F	12	Total	C	N	O	P	0	0	0
			91	46	12	30	3			
2	G	9	Total	C	N	O	P	0	0	0
			66	31	9	23	3			
2	H	9	Total	C	N	O	P	0	0	0
			66	31	9	23	3			

There are 4 discrepancies between the modelled and reference sequences:

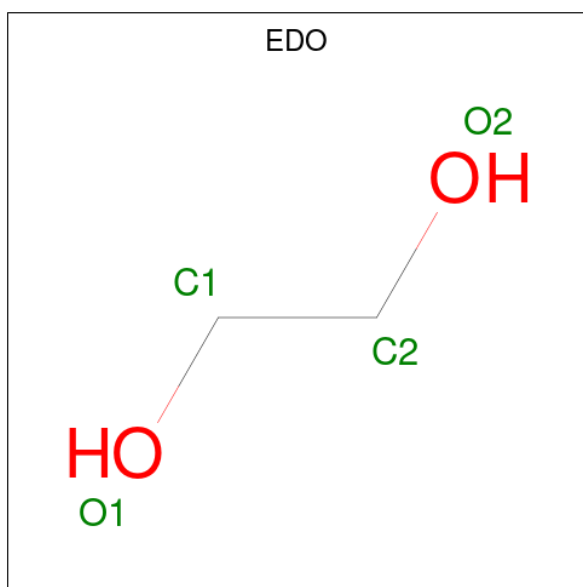
Chain	Residue	Modelled	Actual	Comment	Reference
E	593	TYR	GLU	conflict	UNP Q9H3D4
F	593	TYR	GLU	conflict	UNP Q9H3D4
G	593	TYR	GLU	conflict	UNP Q9H3D4
H	593	TYR	GLU	conflict	UNP Q9H3D4

- 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		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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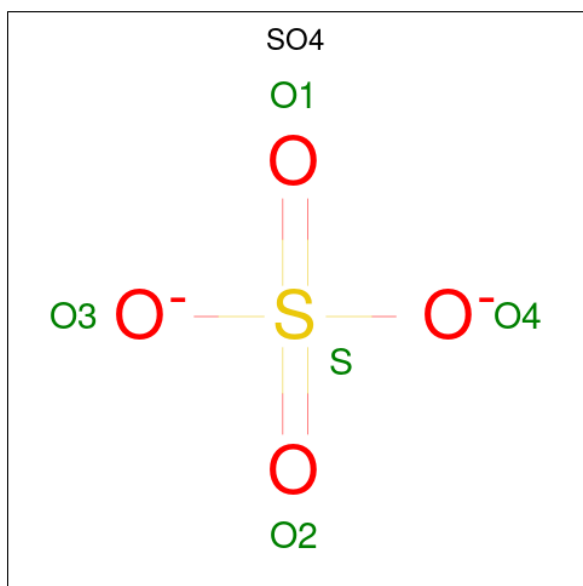
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

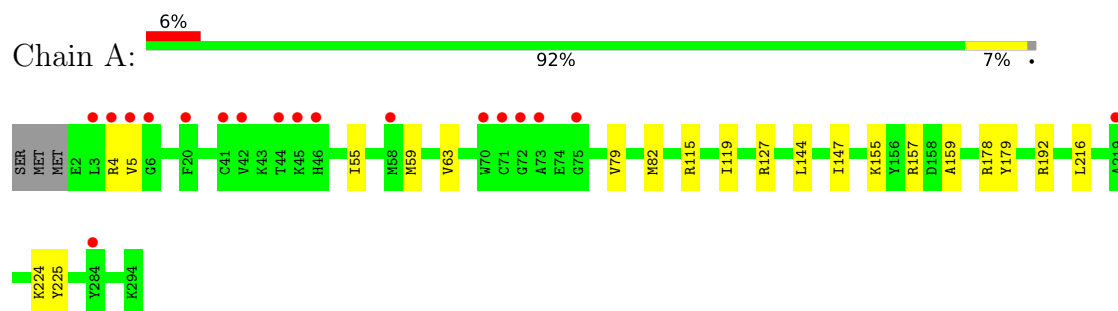
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	132	Total 132	O 132	0	0
7	B	138	Total 138	O 138	0	0
7	C	122	Total 122	O 122	0	0
7	D	112	Total 112	O 112	0	0
7	E	6	Total 6	O 6	0	0
7	F	8	Total 8	O 8	0	0
7	G	3	Total 3	O 3	0	0
7	H	4	Total 4	O 4	0	0

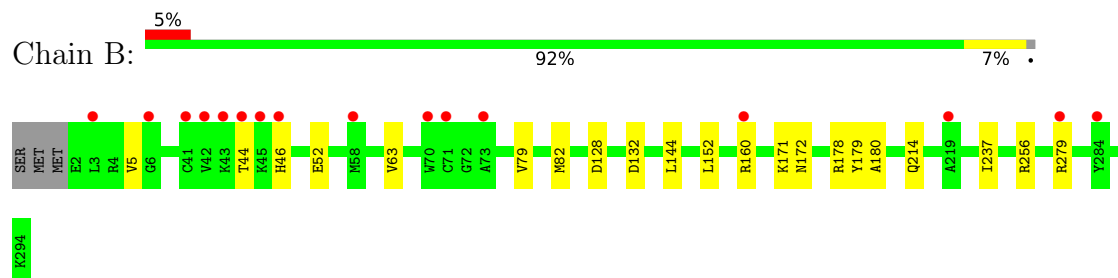
3 Residue-property plots [i](#)

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.

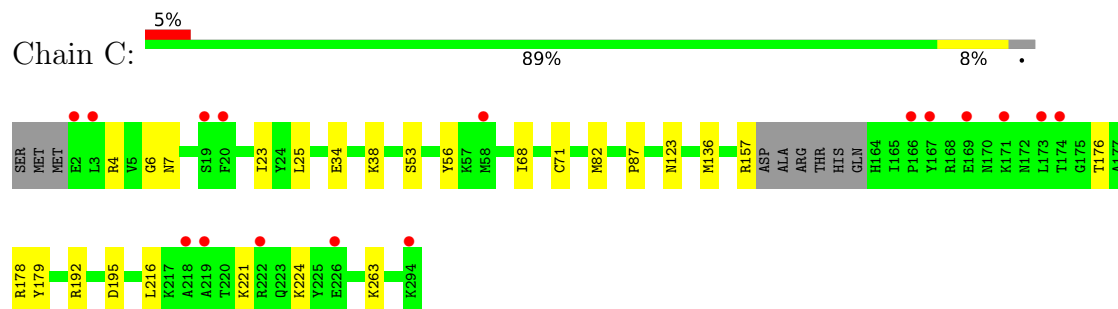
- Molecule 1: Casein kinase I isoform delta



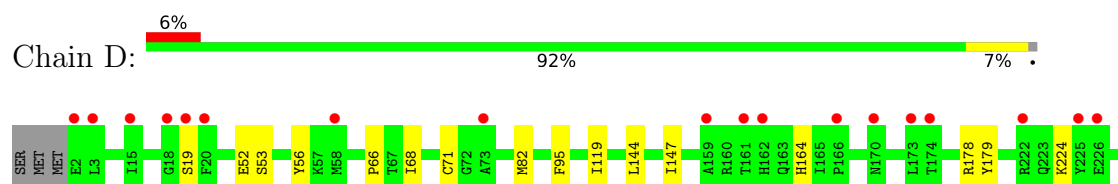
- Molecule 1: Casein kinase I isoform delta



- Molecule 1: Casein kinase I isoform delta

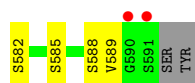


- Molecule 1: Casein kinase I isoform delta

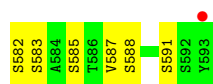




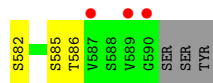
- Molecule 2: Tumor protein 63



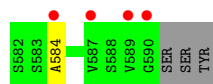
- Molecule 2: Tumor protein 63



- Molecule 2: Tumor protein 63



- Molecule 2: Tumor protein 63



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.73Å 84.13Å 89.29Å 108.60° 105.83° 91.57°	Depositor
Resolution (Å)	48.84 – 1.92 48.84 – 1.92	Depositor EDS
% Data completeness (in resolution range)	92.2 (48.84-1.92) 92.1 (48.84-1.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.172 , 0.211 0.180 , 0.216	Depositor DCC
R_{free} test set	4513 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10612	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: SO4, SEP, EDO, NA, 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	1.07	0/2455	1.21	1/3299 (0.0%)
1	B	1.06	2/2480 (0.1%)	1.20	0/3331
1	C	1.06	0/2446	1.21	1/3283 (0.0%)
1	D	1.03	0/2488	1.23	0/3342
2	E	0.79	0/39	1.13	0/49
2	F	0.72	0/59	1.09	0/75
2	G	0.80	0/33	0.93	0/41
2	H	0.76	0/33	0.98	0/41
All	All	1.05	2/10033 (0.0%)	1.21	2/13461 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ASP	CG-OD2	6.12	1.36	1.25
1	B	180	ALA	C-O	5.25	1.30	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	CG-CD-NE	-5.15	100.67	112.00
1	C	195	ASP	CA-CB-CG	5.01	117.61	112.60

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	2395	0	2400	14	1
1	B	2413	0	2428	17	0
1	C	2372	0	2395	22	0
1	D	2415	0	2429	17	1
2	E	72	0	56	2	0
2	F	91	0	70	5	0
2	G	66	0	50	2	0
2	H	66	0	51	1	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	3	0
3	D	27	0	12	4	0
4	A	20	0	30	3	0
4	B	16	0	24	3	0
4	C	24	0	36	6	0
4	D	12	0	18	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	10	0	0	0	0
7	A	132	0	0	0	0
7	B	138	0	0	2	0
7	C	122	0	0	1	0
7	D	112	0	0	2	0
7	E	6	0	0	0	0
7	F	8	0	0	1	0
7	G	3	0	0	0	0
7	H	4	0	0	1	0
All	All	10612	0	10035	75	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 4.

All (75) 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:D:82[A]:MET:HE2	3:D:301:ADP:HN61	1.34	0.90
1:C:82[A]:MET:HE2	3:C:301:ADP:HN61	1.42	0.84
1:A:192:ARG:HH12	4:A:305:EDO:H12	1.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:HD11	1:B:256[A]:ARG:HD3	1.74	0.68
1:A:82:MET:HE2	3:A:301:ADP:HN61	1.60	0.67
1:C:192:ARG:HH12	1:C:263:LYS:HE3	1.61	0.66
1:D:289:ASP:HA	1:D:292[B]:MET:HE2	1.79	0.65
1:B:171:LYS:HE3	4:B:303:EDO:H11	1.79	0.64
1:B:5:VAL:CG1	1:B:79:VAL:HG11	2.27	0.64
2:F:583:SER:O	2:F:587:VAL:HG23	1.99	0.62
3:D:301:ADP:O1A	7:D:401:HOH:O	2.16	0.60
1:A:5:VAL:CG1	1:A:79:VAL:HG11	2.33	0.58
1:D:238:GLU:OE1	7:D:402:HOH:O	2.17	0.58
1:C:34:GLU:OE2	4:C:303:EDO:H21	2.05	0.56
1:A:155:LYS:NZ	1:A:159:ALA:HB2	2.21	0.56
1:B:172:ASN:HB2	4:B:303:EDO:H21	1.89	0.55
1:B:5:VAL:HG13	1:B:79:VAL:HG11	1.87	0.55
1:C:221:LYS:O	1:C:224:LYS:HB3	2.07	0.54
1:A:63:VAL:CG1	1:A:144[A]:LEU:HD11	2.37	0.54
1:C:87:PRO:HD2	4:C:307:EDO:C1	2.37	0.53
1:B:63:VAL:CG1	1:B:144[A]:LEU:HD11	2.39	0.53
1:D:178:ARG:HD2	1:D:179:TYR:CZ	2.44	0.53
1:C:87:PRO:HD2	4:C:307:EDO:H11	1.90	0.52
1:D:56:TYR:OH	3:D:301:ADP:O2B	2.26	0.51
1:C:178:ARG:HD2	1:C:179:TYR:CZ	2.46	0.51
1:B:178:ARG:HD2	1:B:179:TYR:CZ	2.46	0.50
1:A:63:VAL:HG12	1:A:144[A]:LEU:HD11	1.94	0.50
1:B:171:LYS:CE	4:B:303:EDO:H11	2.42	0.49
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.48	0.49
1:D:238:GLU:HB3	4:D:302:EDO:H22	1.93	0.49
1:C:7:ASN:ND2	7:C:406:HOH:O	2.43	0.48
1:C:56:TYR:OH	3:C:301:ADP:O2B	2.30	0.48
1:D:164:HIS:CG	1:D:261[B]:ASP:OD1	2.66	0.48
1:D:289:ASP:HA	1:D:292[B]:MET:CE	2.43	0.48
1:D:253:ASN:HD21	4:D:302:EDO:H21	1.79	0.48
2:F:588:SEP:O1P	7:F:601:HOH:O	2.19	0.47
1:B:279[B]:ARG:NH2	7:B:404:HOH:O	2.46	0.47
1:D:224:LYS:HD3	2:H:584:ALA:HB3	1.97	0.47
1:C:56:TYR:HB3	1:C:68[A]:ILE:CG1	2.45	0.47
1:D:19:SER:HB3	7:H:601:HOH:O	2.15	0.46
1:B:128:ASP:OD2	2:F:588:SEP:O3P	2.35	0.45
1:A:155:LYS:HZ3	1:A:159:ALA:HB2	1.82	0.45
1:C:53:SER:HB2	1:C:71[A]:CYS:SG	2.57	0.45
1:A:225:TYR:OH	2:E:589:VAL:HG11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:O	1:A:224:LYS:NZ	2.44	0.44
1:B:152:LEU:CD2	2:F:591:SER:HA	2.47	0.44
1:B:160:ARG:NH1	7:B:410:HOH:O	2.51	0.44
1:C:82[A]:MET:HE2	3:C:301:ADP:N6	2.23	0.44
1:C:192:ARG:HH12	1:C:263:LYS:CE	2.28	0.44
1:C:216:LEU:O	1:C:224:LYS:NZ	2.44	0.44
1:C:123:ASN:OD1	1:C:157:ARG:NE	2.43	0.43
2:G:582:SEP:O1P	2:G:585:SEP:O3P	2.36	0.43
1:D:56:TYR:HB3	1:D:68[A]:ILE:CG1	2.48	0.43
1:C:136:MET:HB2	4:C:307:EDO:H12	2.00	0.43
1:D:56:TYR:CE1	1:D:66:PRO:HG2	2.54	0.42
1:A:55:ILE:O	1:A:59:MET:HG2	2.19	0.42
1:B:44:THR:HG22	1:B:46:HIS:H	1.85	0.42
1:D:53:SER:HB2	1:D:71[A]:CYS:SG	2.59	0.42
1:C:25:LEU:HD23	4:C:302:EDO:H22	2.00	0.42
1:A:119:ILE:HD11	1:A:147:ILE:HG21	2.02	0.42
1:B:52:GLU:OE2	3:B:301:ADP:O3B	2.37	0.42
1:C:176:THR:HG23	2:G:586:THR:HA	2.01	0.42
1:A:157:ARG:NH1	4:A:305:EDO:C1	2.83	0.42
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.94	0.42
1:C:82[B]:MET:HE3	1:C:82[B]:MET:HB3	1.87	0.42
1:C:23:ILE:HD11	1:C:38:LYS:HD2	2.02	0.41
2:E:582:SEP:O1P	2:E:585:SEP:O1P	2.38	0.41
1:C:34:GLU:CD	4:C:303:EDO:H21	2.46	0.41
1:A:127:ARG:HH22	4:A:306:EDO:H22	1.86	0.41
1:B:82:MET:HE2	3:B:301:ADP:HN61	1.86	0.41
1:D:52:GLU:OE2	3:D:301:ADP:O3B	2.39	0.41
1:D:119:ILE:CD1	1:D:147:ILE:HD13	2.50	0.41
1:B:63:VAL:HG12	1:B:144[A]:LEU:HD11	2.02	0.41
1:B:214:GLN:HG2	2:F:585:SEP:O2P	2.21	0.41
1:C:4:ARG:HD2	1:C:6:GLY:O	2.21	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:4:ARG:NH1	1:D:95:PHE:O[1_656]	2.18	0.02

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	293/296 (99%)	290 (99%)	3 (1%)	0	100	100
1	B	295/296 (100%)	292 (99%)	3 (1%)	0	100	100
1	C	290/296 (98%)	286 (99%)	4 (1%)	0	100	100
1	D	297/296 (100%)	292 (98%)	5 (2%)	0	100	100
2	E	6/12 (50%)	6 (100%)	0	0	100	100
2	F	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
2	G	5/12 (42%)	5 (100%)	0	0	100	100
2	H	5/12 (42%)	5 (100%)	0	0	100	100
All	All	1199/1232 (97%)	1183 (99%)	16 (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	256/260 (98%)	256 (100%)	0	100	100
1	B	259/260 (100%)	259 (100%)	0	100	100
1	C	257/260 (99%)	257 (100%)	0	100	100
1	D	261/260 (100%)	261 (100%)	0	100	100
2	E	5/7 (71%)	5 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	4/7 (57%)	4 (100%)	0	100	100
2	H	4/7 (57%)	4 (100%)	0	100	100
All	All	1053/1068 (99%)	1053 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	223	GLN
1	A	271	GLN
1	B	78	ASN
1	B	183	ASN
1	D	253	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	SEP	E	582	2	8,9,10	0.64	0	7,12,14	0.85	0
2	SEP	F	582	2	8,9,10	0.86	0	7,12,14	1.18	1 (14%)
2	SEP	G	585	2	8,9,10	0.81	0	7,12,14	0.82	0
2	SEP	E	588	2	8,9,10	1.09	0	7,12,14	1.70	2 (28%)
2	SEP	H	582	2	8,9,10	0.64	0	7,12,14	0.63	0
2	SEP	F	588	2	8,9,10	1.08	0	7,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	F	585	2	8,9,10	0.68	0	7,12,14	0.77	0
2	SEP	G	582	2	8,9,10	0.62	0	7,12,14	0.72	0
2	SEP	H	588	2	8,9,10	0.77	0	7,12,14	0.72	0
2	SEP	E	585	2	8,9,10	0.69	0	7,12,14	1.16	0
2	SEP	H	585	2	8,9,10	0.59	0	7,12,14	0.66	0
2	SEP	G	588	2	8,9,10	0.61	0	7,12,14	0.76	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	SEP	E	582	2	-	5/6/8/10	-
2	SEP	F	582	2	-	0/6/8/10	-
2	SEP	G	585	2	-	0/6/8/10	-
2	SEP	E	588	2	-	2/6/8/10	-
2	SEP	H	582	2	-	1/6/8/10	-
2	SEP	F	588	2	-	1/6/8/10	-
2	SEP	F	585	2	-	0/6/8/10	-
2	SEP	G	582	2	-	0/6/8/10	-
2	SEP	H	588	2	-	1/6/8/10	-
2	SEP	E	585	2	-	0/6/8/10	-
2	SEP	H	585	2	-	0/6/8/10	-
2	SEP	G	588	2	-	4/6/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	588	SEP	O3P-P-O2P	2.69	117.89	107.80
2	E	588	SEP	OG-P-O1P	2.38	112.87	106.44
2	F	582	SEP	OG-CB-CA	-2.22	105.98	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	582	SEP	N-CA-CB-OG
2	E	582	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
2	E	582	SEP	CB-OG-P-O1P
2	E	582	SEP	CB-OG-P-O3P
2	E	588	SEP	CB-OG-P-O3P
2	G	588	SEP	CB-OG-P-O1P
2	G	588	SEP	CB-OG-P-O2P
2	G	588	SEP	CB-OG-P-O3P
2	H	588	SEP	CA-CB-OG-P
2	E	582	SEP	CB-OG-P-O2P
2	E	588	SEP	CA-CB-OG-P
2	F	588	SEP	CA-CB-OG-P
2	G	588	SEP	CA-CB-OG-P
2	H	582	SEP	CB-OG-P-O3P

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	582	SEP	1	0
2	G	585	SEP	1	0
2	F	588	SEP	2	0
2	F	585	SEP	1	0
2	G	582	SEP	1	0
2	E	585	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	303	-	3,3,3	0.12	0	2,2,2	0.11	0
4	EDO	B	305	-	3,3,3	0.11	0	2,2,2	0.14	0
6	SO4	B	307	-	4,4,4	0.32	0	6,6,6	0.10	0
4	EDO	C	306	-	3,3,3	0.17	0	2,2,2	0.05	0
4	EDO	B	304	-	3,3,3	0.10	0	2,2,2	0.07	0
4	EDO	B	302	-	3,3,3	0.28	0	2,2,2	0.16	0
4	EDO	B	303	-	3,3,3	0.08	0	2,2,2	0.16	0
3	ADP	A	301	-	28,29,29	0.52	0	43,45,45	0.49	0
6	SO4	B	308	-	4,4,4	0.29	0	6,6,6	0.07	0
4	EDO	C	302	-	3,3,3	0.10	0	2,2,2	0.13	0
3	ADP	C	301	-	28,29,29	0.50	0	43,45,45	0.53	0
4	EDO	C	304	-	3,3,3	0.02	0	2,2,2	0.24	0
4	EDO	A	304	-	3,3,3	0.32	0	2,2,2	0.26	0
3	ADP	B	301	-	28,29,29	0.62	0	43,45,45	0.45	0
6	SO4	A	308	-	4,4,4	0.39	0	6,6,6	0.07	0
4	EDO	D	303	-	3,3,3	0.06	0	2,2,2	0.08	0
4	EDO	C	305	-	3,3,3	0.10	0	2,2,2	0.17	0
4	EDO	A	306	-	3,3,3	0.17	0	2,2,2	0.08	0
3	ADP	D	301	-	28,29,29	0.59	1 (3%)	43,45,45	0.52	0
4	EDO	D	304	-	3,3,3	0.17	0	2,2,2	0.05	0
4	EDO	D	302	-	3,3,3	0.33	0	2,2,2	0.04	0
4	EDO	A	305	-	3,3,3	0.22	0	2,2,2	0.08	0
4	EDO	A	302	-	3,3,3	0.24	0	2,2,2	0.06	0
4	EDO	C	307	-	3,3,3	0.26	0	2,2,2	0.23	0
4	EDO	A	303	-	3,3,3	0.04	0	2,2,2	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	303	-	-	1/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
3	ADP	A	301	-	-	2/16/32/32	0/3/3/3
4	EDO	C	302	-	-	1/1/1/1	-
3	ADP	C	301	-	-	2/16/32/32	0/3/3/3
4	EDO	C	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	304	-	-	1/1/1/1	-
3	ADP	B	301	-	-	1/16/32/32	0/3/3/3
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	C	305	-	-	1/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
3	ADP	D	301	-	-	3/16/32/32	0/3/3/3
4	EDO	D	304	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	C	307	-	-	1/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	ADP	PB-O2B	-2.08	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	ADP	C5'-O5'-PA-O1A
3	D	301	ADP	C5'-O5'-PA-O1A
4	A	303	EDO	O1-C1-C2-O2
4	C	302	EDO	O1-C1-C2-O2
4	C	306	EDO	O1-C1-C2-O2
4	C	307	EDO	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
3	C	301	ADP	PB-O3A-PA-O1A
3	D	301	ADP	PB-O3A-PA-O1A
3	C	301	ADP	PB-O3A-PA-O2A
4	A	304	EDO	O1-C1-C2-O2
3	A	301	ADP	PB-O3A-PA-O1A
3	A	301	ADP	PB-O3A-PA-O2A
4	A	305	EDO	O1-C1-C2-O2
4	C	305	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	B	304	EDO	O1-C1-C2-O2
4	C	303	EDO	O1-C1-C2-O2

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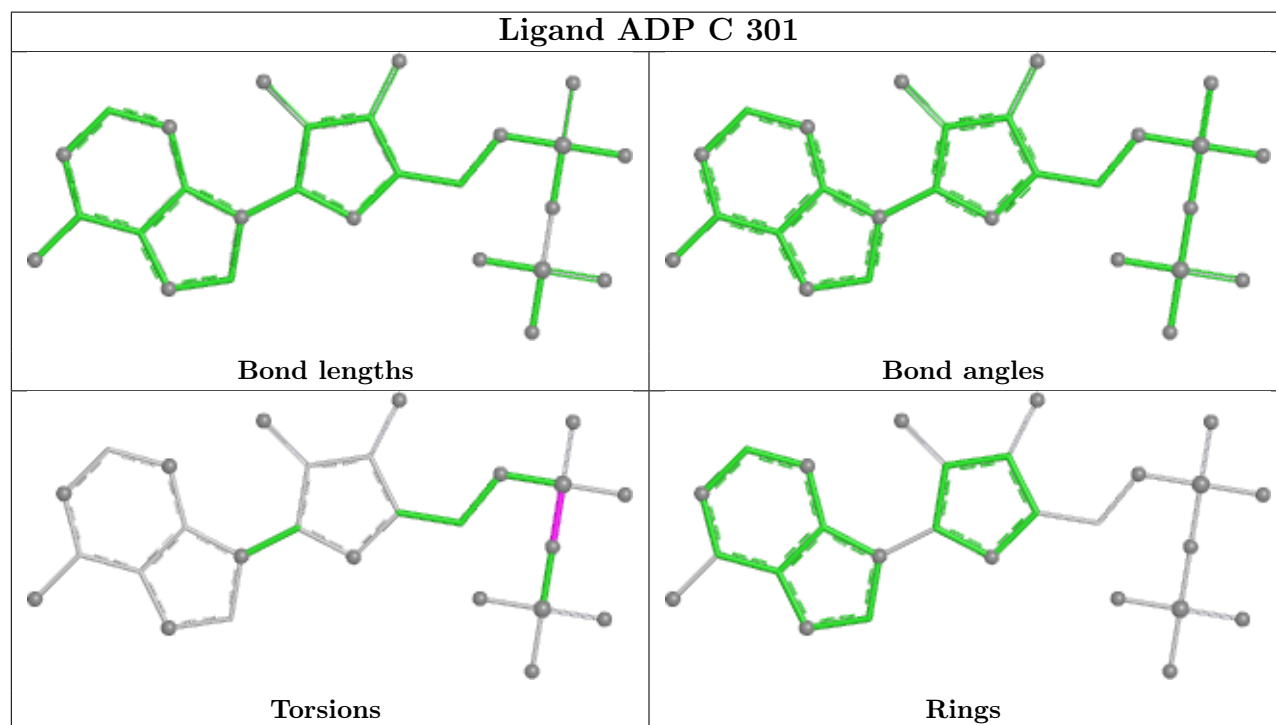
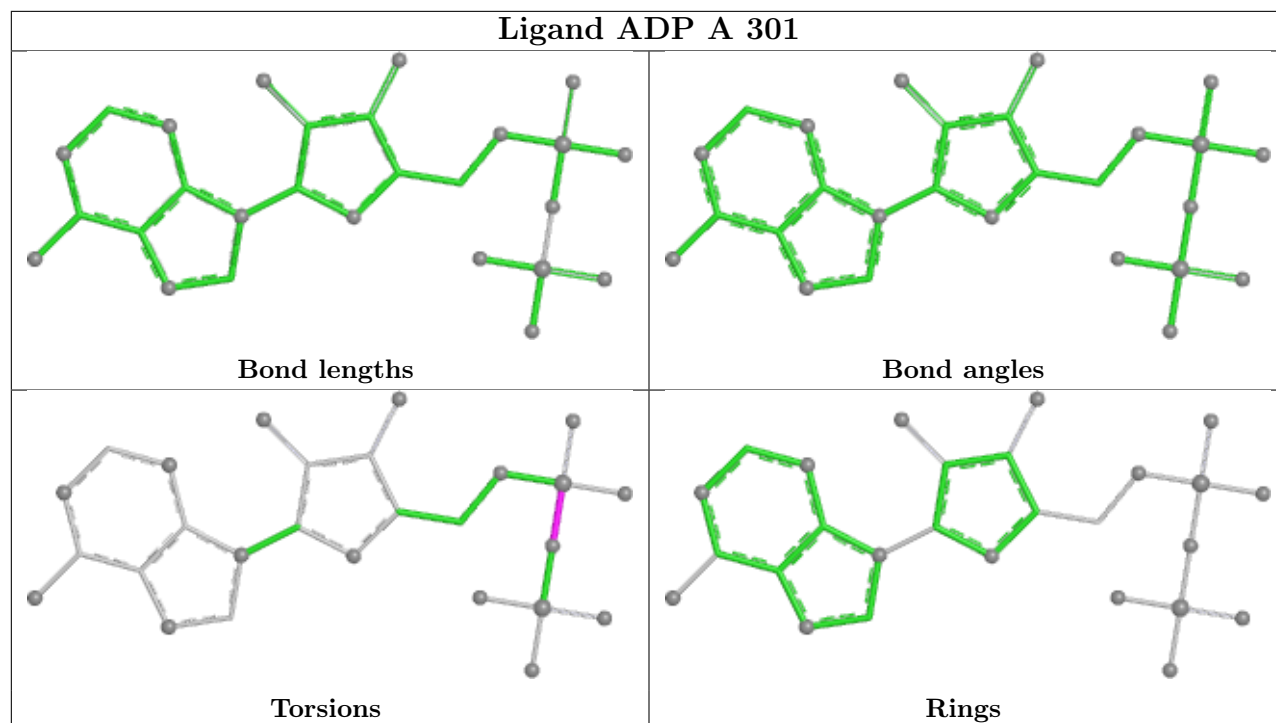
Mol	Chain	Res	Type	Atoms
4	D	304	EDO	O1-C1-C2-O2
3	D	301	ADP	PB-O3A-PA-O2A
4	A	306	EDO	O1-C1-C2-O2

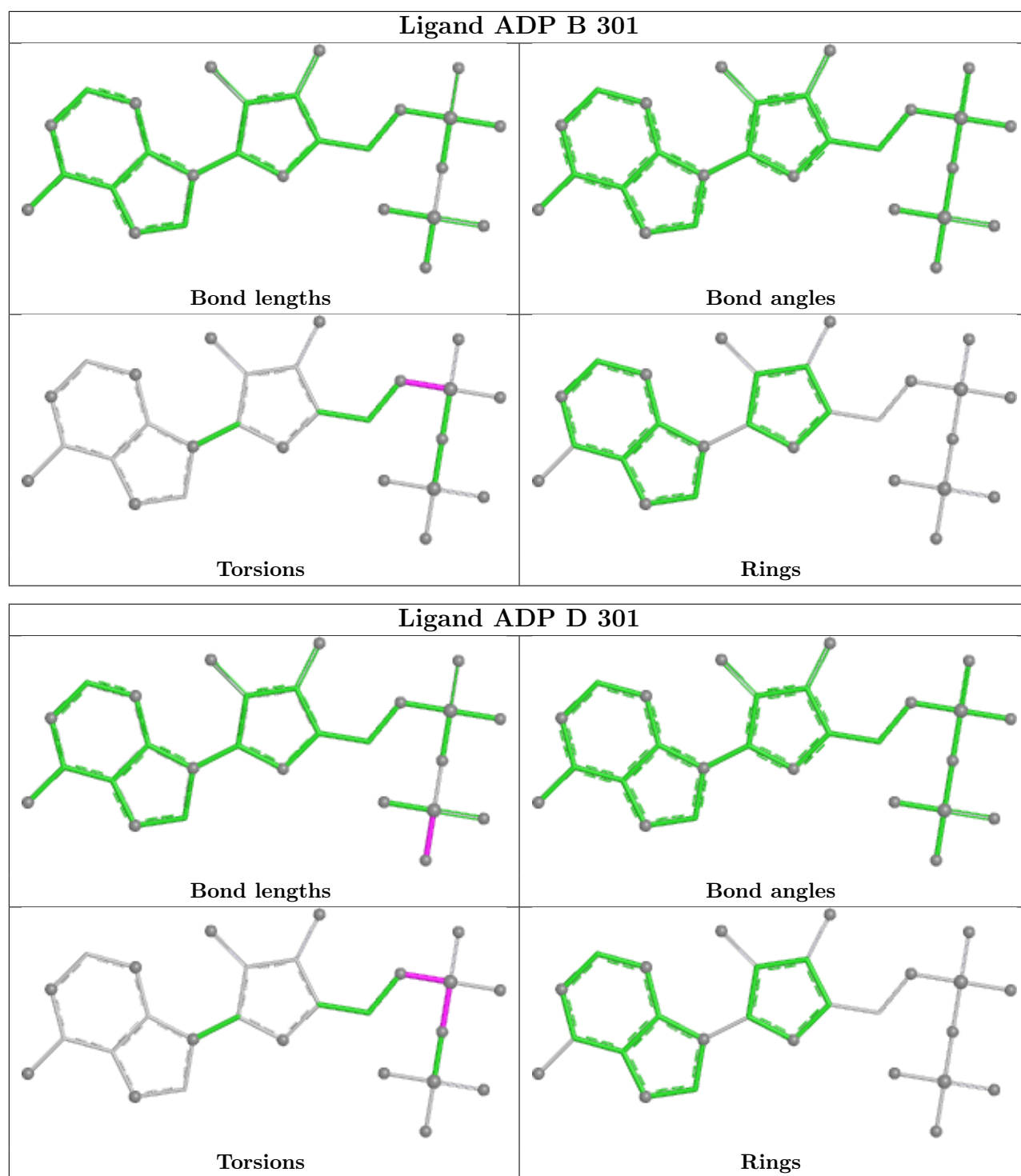
There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	EDO	2	0
4	B	303	EDO	3	0
3	A	301	ADP	1	0
4	C	302	EDO	1	0
3	C	301	ADP	3	0
3	B	301	ADP	2	0
4	A	306	EDO	1	0
3	D	301	ADP	4	0
4	D	302	EDO	2	0
4	A	305	EDO	2	0
4	C	307	EDO	3	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	293/296 (98%)	0.19	18 (6%) 27 31	18, 32, 64, 94	2 (0%)
1	B	293/296 (98%)	0.16	16 (5%) 30 35	18, 32, 58, 81	4 (1%)
1	C	287/296 (96%)	0.27	16 (5%) 30 35	16, 32, 64, 84	7 (2%)
1	D	293/296 (98%)	0.28	19 (6%) 25 29	19, 34, 69, 103	6 (2%)
2	E	7/12 (58%)	1.13	2 (28%) 1 1	36, 40, 54, 73	0
2	F	9/12 (75%)	1.06	1 (11%) 10 13	38, 44, 58, 64	0
2	G	6/12 (50%)	2.41	3 (50%) 0 0	58, 65, 73, 74	0
2	H	6/12 (50%)	2.30	4 (66%) 0 0	56, 65, 71, 73	0
All	All	1194/1232 (96%)	0.26	79 (6%) 24 29	16, 33, 67, 103	19 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	LYS	4.6
1	B	6	GLY	4.4
1	D	161	THR	4.3
1	A	3	LEU	4.0
1	D	159	ALA	4.0
1	A	44	THR	3.8
2	G	589	VAL	3.8
1	C	3	LEU	3.7
1	D	170	ASN	3.5
1	D	58	MET	3.5
1	B	42	VAL	3.4
1	C	58	MET	3.4
2	G	587	VAL	3.4
1	D	174	THR	3.4
1	C	167	TYR	3.3
1	C	19	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	591	SER	3.3
1	A	6	GLY	3.3
1	B	219	ALA	3.2
2	H	589	VAL	3.0
1	A	72	GLY	3.0
1	A	219	ALA	3.0
1	D	294	LYS	2.9
1	D	162	HIS	2.9
1	D	3	LEU	2.9
1	B	44	THR	2.9
1	C	173	LEU	2.9
1	A	46	HIS	2.8
1	B	70	TRP	2.8
1	C	219	ALA	2.7
1	D	20	PHE	2.7
1	B	3	LEU	2.7
1	D	166	PRO	2.7
2	H	590	GLY	2.6
1	C	20	PHE	2.6
1	D	226	GLU	2.6
1	D	19	SER	2.6
1	B	284	TYR	2.6
1	C	174	THR	2.6
1	B	46	HIS	2.6
1	B	58	MET	2.6
1	B	71	CYS	2.5
1	C	2	GLU	2.5
1	C	226	GLU	2.5
2	H	584	ALA	2.5
1	A	41	CYS	2.5
1	B	41	CYS	2.5
2	F	593	TYR	2.5
1	A	5	VAL	2.5
2	H	587	VAL	2.5
1	D	2	GLU	2.4
1	B	73	ALA	2.4
1	A	45	LYS	2.4
1	D	225	TYR	2.3
1	A	71	CYS	2.3
1	D	173	LEU	2.3
1	B	279[A]	ARG	2.2
1	A	20	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	590	GLY	2.2
1	C	222	ARG	2.2
2	G	590	GLY	2.2
1	C	169	GLU	2.2
1	D	18	GLY	2.2
1	B	43	LYS	2.2
1	C	294	LYS	2.2
1	D	73	ALA	2.2
1	A	4	ARG	2.2
1	A	58	MET	2.1
1	D	15	ILE	2.1
1	B	45	LYS	2.1
1	A	73	ALA	2.1
1	C	218	ALA	2.1
1	A	284	TYR	2.1
1	C	166	PRO	2.1
1	A	70	TRP	2.0
1	A	75	GLY	2.0
1	A	42	VAL	2.0
1	B	160	ARG	2.0
1	D	222	ARG	2.0

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

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
2	SEP	H	582	10/11	0.78	0.13	68,76,85,87	0
2	SEP	G	588	10/11	0.80	0.12	60,64,68,73	0
2	SEP	G	582	10/11	0.81	0.12	76,81,82,84	0
2	SEP	H	588	10/11	0.83	0.12	58,62,68,75	0
2	SEP	F	582	10/11	0.88	0.11	49,53,57,59	0
2	SEP	E	582	10/11	0.90	0.11	46,50,56,60	0
2	SEP	H	585	10/11	0.95	0.09	38,43,48,51	0
2	SEP	E	588	10/11	0.95	0.07	34,36,41,43	0
2	SEP	F	588	10/11	0.96	0.07	38,40,42,42	0
2	SEP	G	585	10/11	0.97	0.06	37,43,49,50	0
2	SEP	F	585	10/11	0.99	0.04	30,32,34,36	0
2	SEP	E	585	10/11	0.99	0.04	29,31,34,34	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

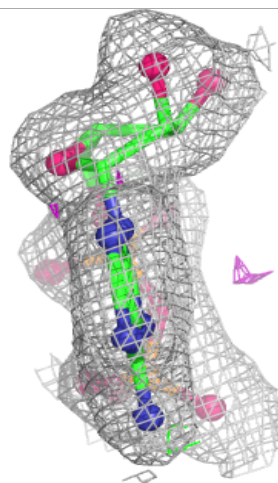
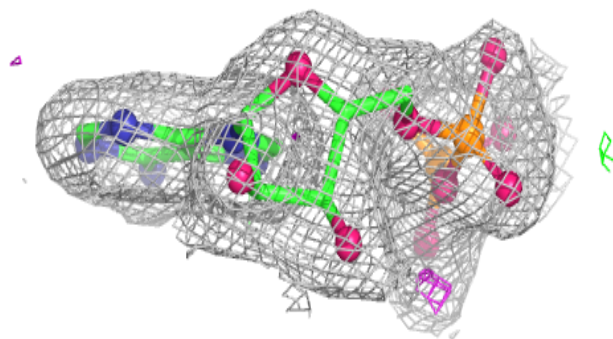
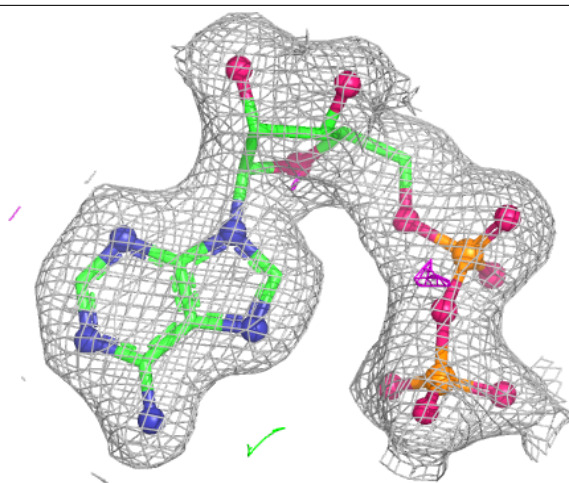
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	308	5/5	0.71	0.14	73,74,81,82	0
4	EDO	A	305	4/4	0.74	0.16	45,45,50,55	0
4	EDO	B	303	4/4	0.79	0.14	61,61,64,66	0
4	EDO	A	306	4/4	0.83	0.17	54,56,57,58	0
4	EDO	C	306	4/4	0.84	0.19	43,44,44,48	0
4	EDO	D	302	4/4	0.86	0.16	34,40,41,44	0
4	EDO	B	305	4/4	0.87	0.12	52,52,53,54	0
4	EDO	B	304	4/4	0.87	0.13	53,54,57,60	0
4	EDO	D	304	4/4	0.88	0.13	53,53,57,58	0
4	EDO	B	302	4/4	0.89	0.15	35,37,38,44	0
5	NA	A	307	1/1	0.89	0.20	47,47,47,47	0
4	EDO	C	305	4/4	0.89	0.12	50,50,50,51	0
4	EDO	A	302	4/4	0.90	0.11	39,45,47,47	0
4	EDO	D	303	4/4	0.91	0.12	57,57,58,59	0
4	EDO	C	303	4/4	0.91	0.12	42,43,44,44	0
4	EDO	C	302	4/4	0.92	0.11	48,50,52,53	0
4	EDO	A	303	4/4	0.92	0.12	43,45,47,50	0
4	EDO	A	304	4/4	0.92	0.12	43,46,46,47	0
6	SO4	B	307	5/5	0.93	0.08	54,55,58,61	0
6	SO4	A	308	5/5	0.93	0.09	52,52,59,62	0
4	EDO	C	307	4/4	0.94	0.11	49,50,50,53	0
4	EDO	C	304	4/4	0.94	0.09	53,57,58,65	0
5	NA	B	306	1/1	0.95	0.07	42,42,42,42	0
3	ADP	D	301	27/27	0.97	0.06	27,35,40,43	0
3	ADP	A	301	27/27	0.97	0.06	26,32,37,39	0
3	ADP	B	301	27/27	0.97	0.05	22,31,36,38	0
3	ADP	C	301	27/27	0.97	0.06	26,32,37,41	0

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

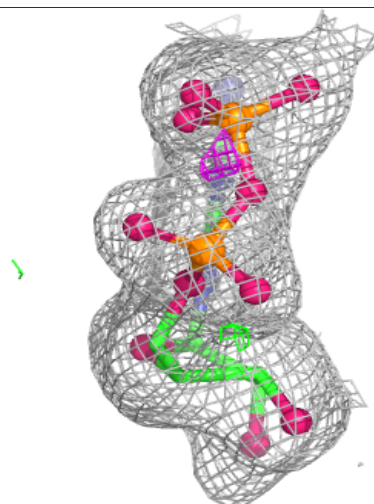
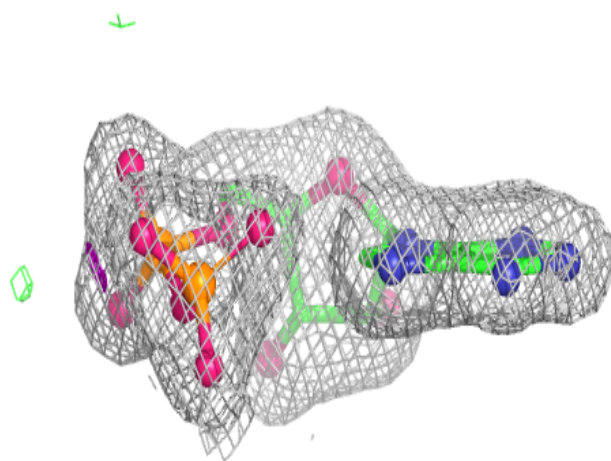
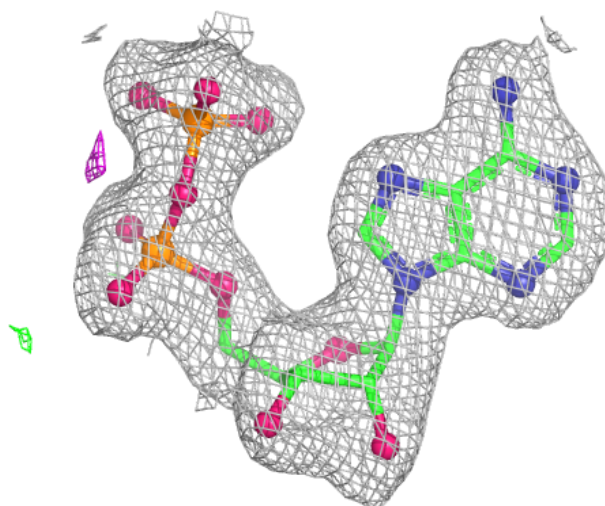
Electron density around ADP D 301:

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



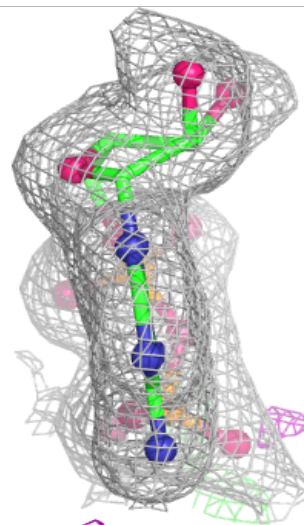
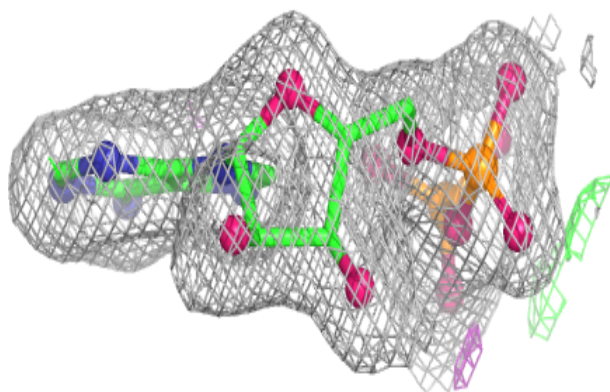
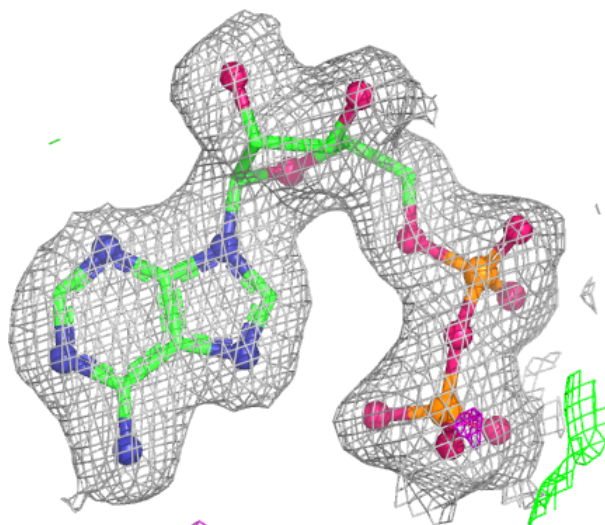
Electron density around ADP A 301:

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



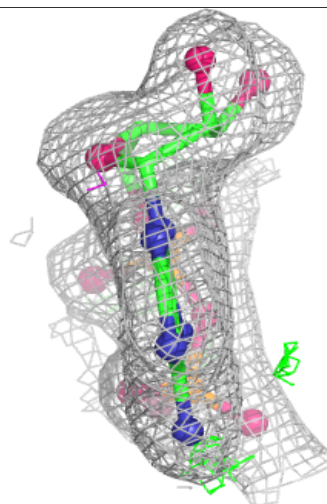
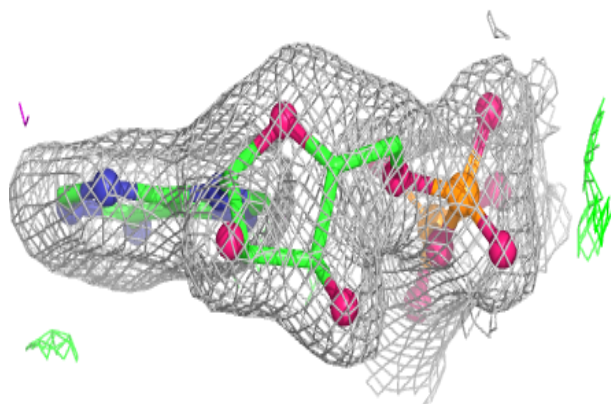
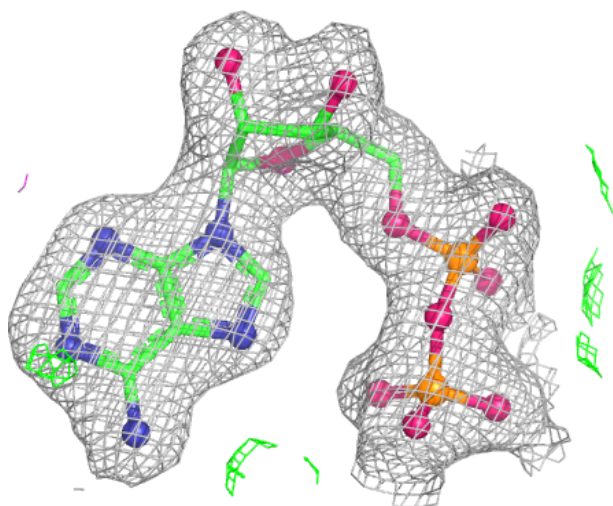
Electron density around ADP B 301:

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



Electron density around ADP C 301:

$2mF_o-DF_c$ (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.