Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2022 – 12:59 am BST

PDB ID	:	8AR8
Title	:	Bovine glutamate dehydrogenase in complex with ADP at 2.4 A resolution
Authors	:	Aleshin, V.A.; Bellinzoni, M.
Deposited on	:	2022-08-15
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

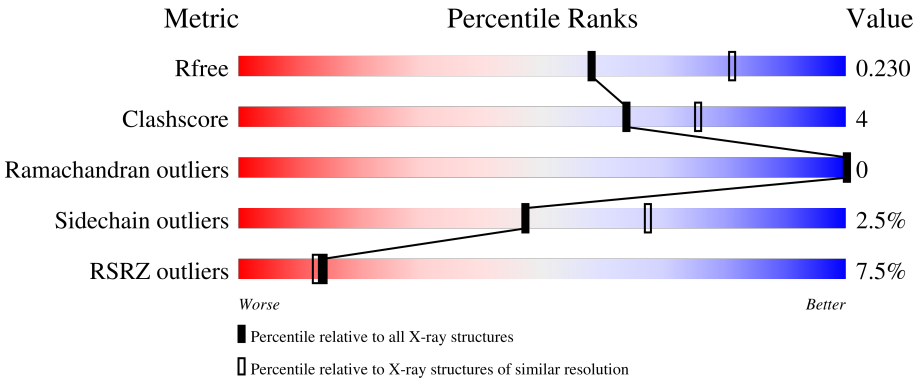
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	561	10% 76% 11% 13%
1	B	561	5% 78% 10% 11%
1	C	561	3% 78% 10% 12%
1	D	561	6% 79% 9% 12%
1	E	561	9% 78% 9% 13%

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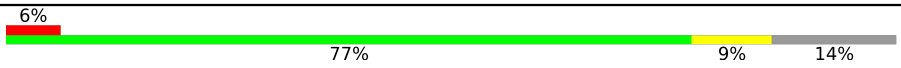
Mol	Chain	Length	Quality of chain
1	F	561	

2 Entry composition

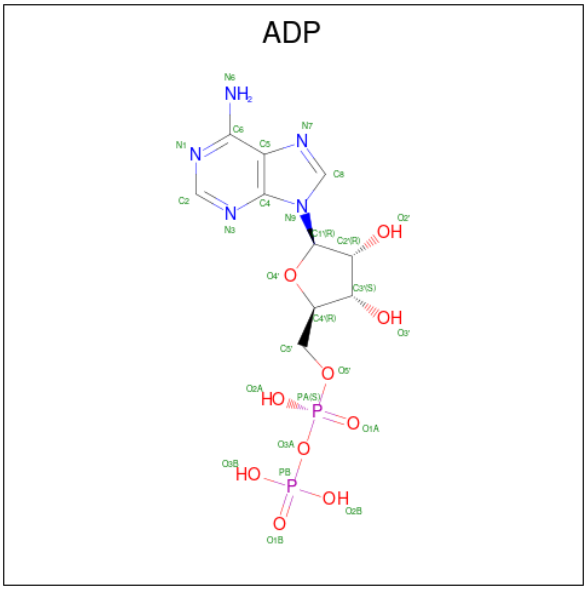
There are 3 unique types of molecules in this entry. The entry contains 24118 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase (NAD(P)(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3770	2385	659	707	19			
1	B	497	Total	C	N	O	S	0	0	0
			3860	2440	677	724	19			
1	C	494	Total	C	N	O	S	0	0	0
			3865	2441	678	727	19			
1	D	495	Total	C	N	O	S	0	0	0
			3863	2444	677	723	19			
1	E	489	Total	C	N	O	S	0	0	0
			3812	2410	669	714	19			
1	F	483	Total	C	N	O	S	0	0	0
			3767	2384	659	705	19			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

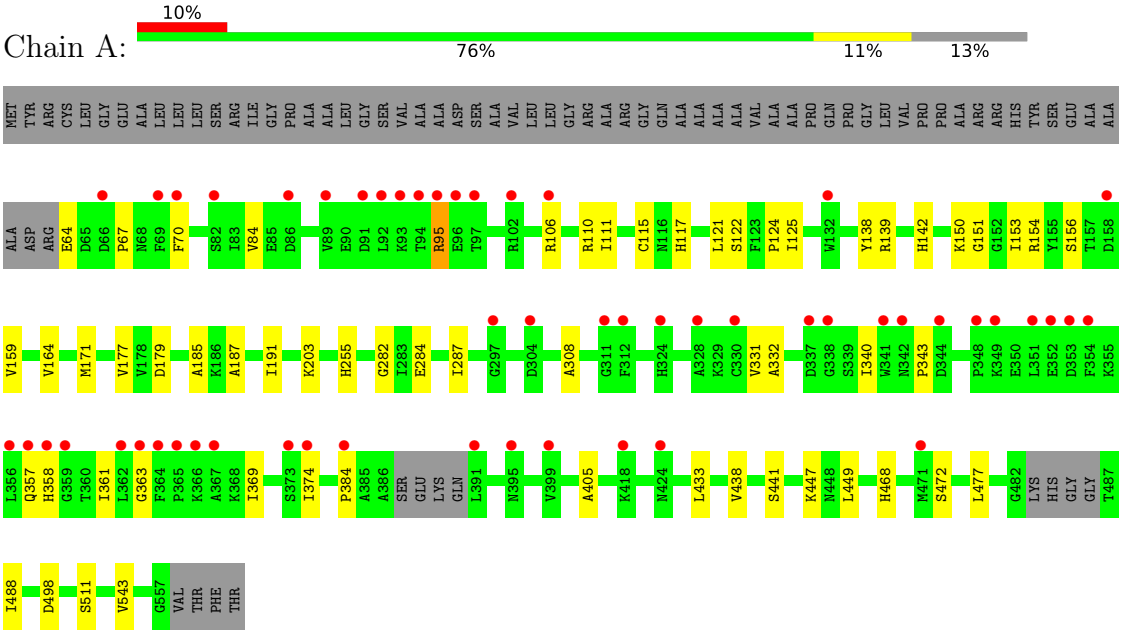
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		
3	B	174	Total	O	0	0
			174	174		
3	C	191	Total	O	0	0
			191	191		
3	D	179	Total	O	0	0
			179	179		
3	E	146	Total	O	0	0
			146	146		
3	F	168	Total	O	0	0
			168	168		

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.

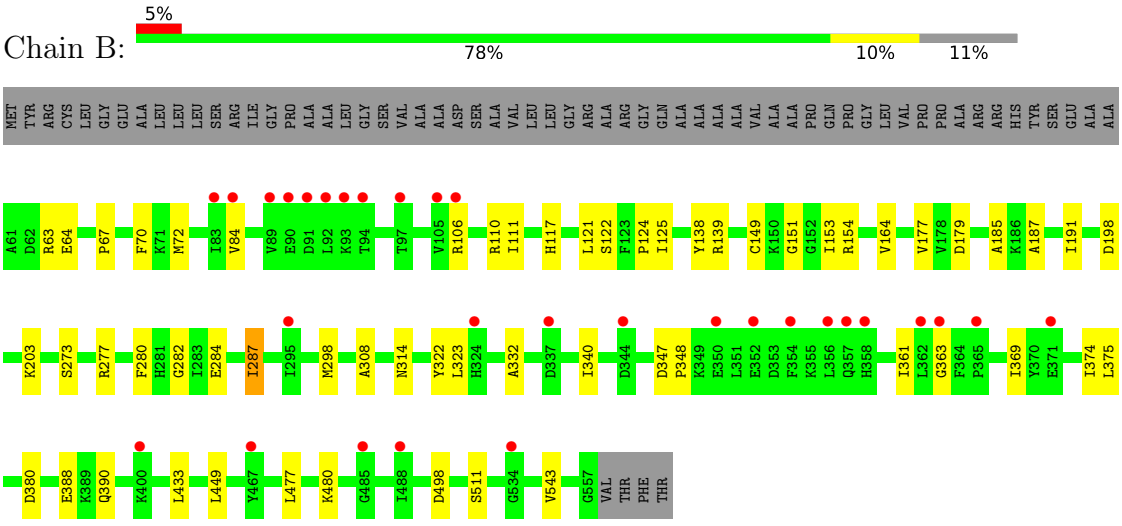
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain A:



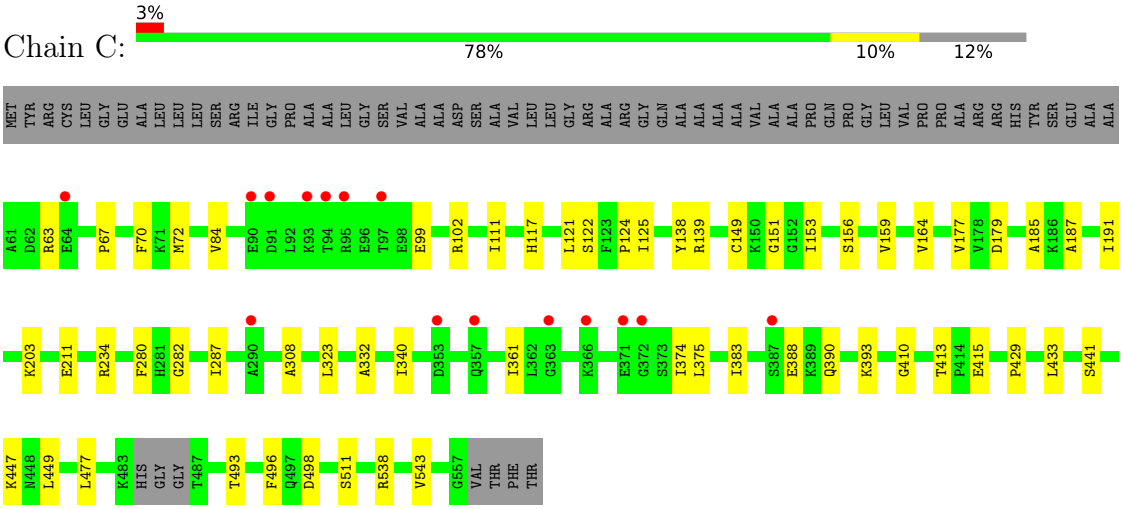
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain B:



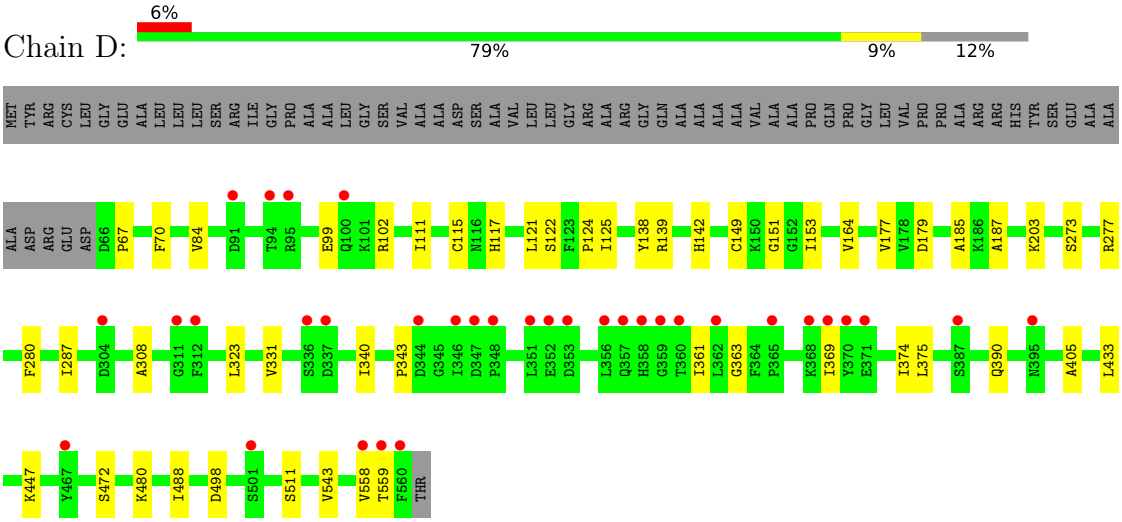
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain C:



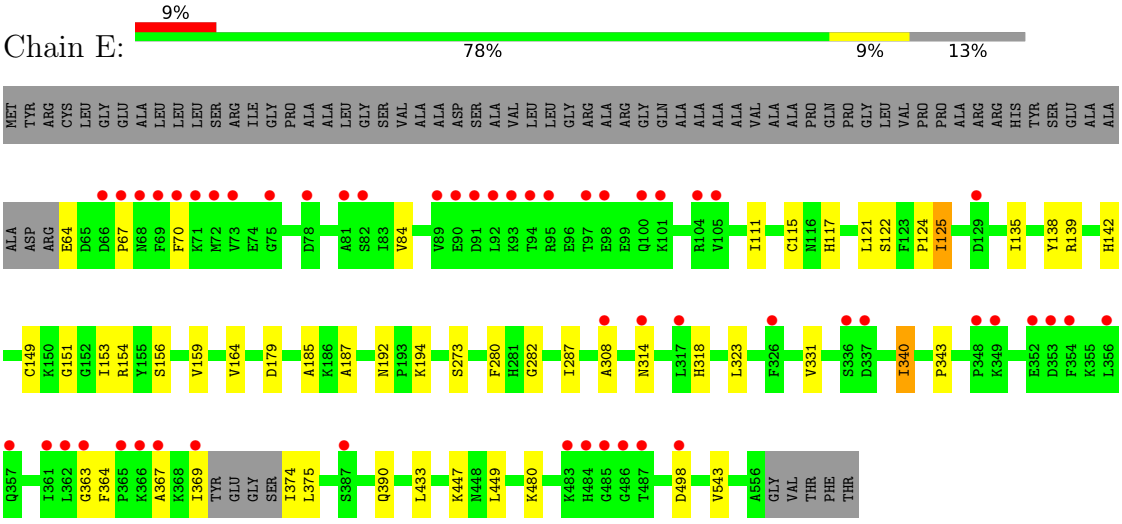
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain D:



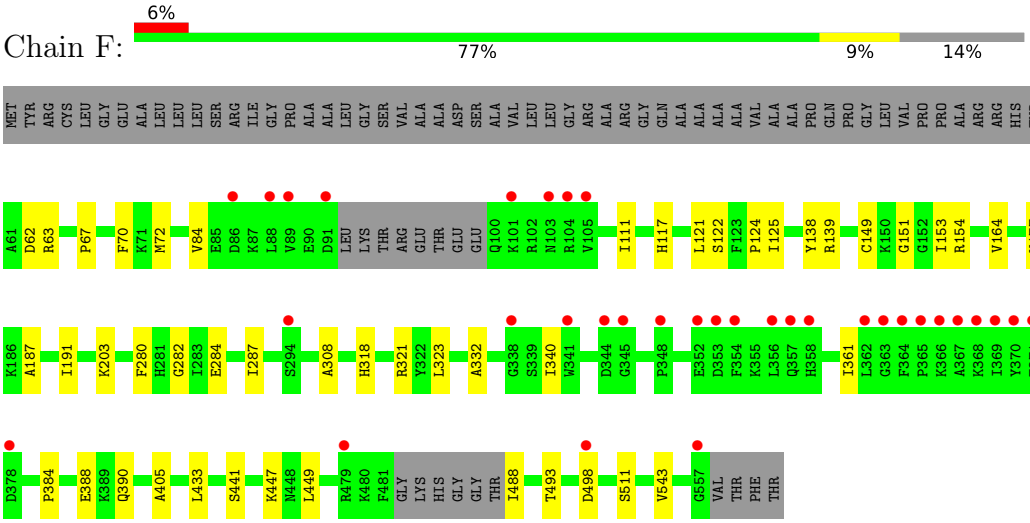
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain E:



• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

Chain F:


6%
77%
9%
14%
MET TYR ARG CYS LEU GLY GLU ALA LEU LEU LEU SER ARG ILE GLY PRO ALA ALA LEU GLY SER VAL ALA ALA ASP SER ALA VAL LEU LEU GLY ARG ALA ARG GLY GLN ALA ALA ALA VAL ALA ALA PRO GLN PRO GLY LEU VAL PRO PRO ALA ARG ARG HIS TYR SER GLU ALA ALA
A61 D62 R63 P67 F70 K71 M72 V84 E85 D86 K87 L88 V89 E90 D91 LEU LYS THR ARG GLU THR GLU GLU Q100 K101 R102 N103 R104 V105 I111 H117 L121 S122 F123 P124 I125 Y138 R139 C149 K150 G151 G152 I153 R154 V164 V177 V178 D179 A185
K186 A187 I191 K203 F280 H281 G282 I283 E284 I287 S294 A308 H318 R321 Y322 L323 A332 G338 S339 I340 W341 D344 G345 P348 E352 D353 F354 K355 L356 Q357 H358 I361 L362 G363 F364 P365 K366 A367 K368 I369 Y370 E371 I374 L375
D378 P384 E388 K389 Q390 A405 L433 S441 K447 N448 L449 R479 K480 F481 GLY LYS HIS GLY GLY THR I488 T493 D498 S511 V543 G557 VAL THR PHE THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.51Å 92.03Å 119.57Å 99.35° 106.73° 109.73°	Depositor
Resolution (Å)	47.46 – 2.40 47.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	76.3 (47.46-2.40) 76.3 (47.46-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.204 , 0.236 0.198 , 0.230	Depositor DCC
R_{free} test set	4664 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24118	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.30	0/3848	0.47	0/5196
1	B	0.31	0/3942	0.48	0/5322
1	C	0.31	0/3945	0.48	0/5322
1	D	0.31	0/3946	0.49	0/5327
1	E	0.32	0/3891	0.48	0/5251
1	F	0.31	0/3846	0.47	0/5190
All	All	0.31	0/23418	0.48	0/31608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3770	0	3720	41	0
1	B	3860	0	3813	41	0
1	C	3865	0	3831	39	0
1	D	3863	0	3827	30	0
1	E	3812	0	3778	36	0
1	F	3767	0	3725	34	0
2	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	2	0
2	C	27	0	12	3	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	2	0
3	A	161	0	0	2	0
3	B	174	0	0	1	0
3	C	191	0	0	0	0
3	D	179	0	0	0	0
3	E	146	0	0	0	0
3	F	168	0	0	0	0
All	All	24118	0	22766	193	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (193) 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:C:393:LYS:HB2	1:C:415:GLU:HG3	1.54	0.87
1:E:125:ILE:HD13	1:E:135:ILE:HG13	1.58	0.83
1:B:106:ARG:HH21	1:B:110:ARG:HH22	1.43	0.67
1:C:111:ILE:HG12	1:F:124:PRO:HB3	1.77	0.67
1:B:106:ARG:NH2	1:B:110:ARG:HH22	1.93	0.66
1:A:95:ARG:NH1	1:B:198:ASP:H	1.95	0.64
1:B:273:SER:O	1:B:277:ARG:HG3	1.98	0.64
1:B:124:PRO:HB3	1:D:111:ILE:HG12	1.81	0.63
1:B:179:ASP:HB3	2:B:601:ADP:O3B	2.01	0.61
1:B:363:GLY:H	1:B:369:ILE:HD11	1.66	0.60
1:E:273:SER:HB2	1:E:318:HIS:HD2	1.66	0.60
1:C:179:ASP:HB3	2:C:601:ADP:O2B	2.01	0.59
1:E:340:ILE:HD13	1:E:364:PHE:HB3	1.84	0.59
1:A:363:GLY:H	1:A:369:ILE:HD11	1.67	0.59
1:D:273:SER:O	1:D:277:ARG:HG3	2.03	0.59
1:C:280:PHE:HD1	1:C:323:LEU:HD23	1.67	0.59
1:D:179:ASP:HB3	2:D:601:ADP:O1B	2.03	0.59
1:D:488:ILE:HG23	1:E:480:LYS:HG2	1.85	0.59
1:F:179:ASP:HB3	2:F:601:ADP:O1B	2.03	0.59
1:D:363:GLY:H	1:D:369:ILE:HD11	1.65	0.59
1:E:179:ASP:HB3	2:E:601:ADP:O1B	2.03	0.59
1:A:282:GLY:HA3	1:A:433:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASP:HB3	2:A:601:ADP:O3B	2.03	0.57
1:E:363:GLY:H	1:E:369:ILE:HD11	1.68	0.57
1:E:340:ILE:HG12	1:E:367:ALA:HB1	1.87	0.57
1:C:124:PRO:HB3	1:F:111:ILE:HG12	1.88	0.55
1:B:111:ILE:HG12	1:D:124:PRO:HB3	1.88	0.55
1:E:308:ALA:HB1	1:E:374:ILE:HD13	1.89	0.55
1:D:308:ALA:HB1	1:D:374:ILE:HD13	1.89	0.55
1:F:308:ALA:HB1	1:F:374:ILE:HD13	1.88	0.55
1:A:151:GLY:HA3	1:A:185:ALA:O	2.08	0.54
1:B:308:ALA:HB1	1:B:374:ILE:HD13	1.90	0.54
1:B:106:ARG:NH2	1:B:110:ARG:NH2	2.56	0.54
1:A:121:LEU:CD2	1:E:117:HIS:CD2	2.91	0.54
1:C:308:ALA:HB1	1:C:374:ILE:HD13	1.88	0.54
1:C:117:HIS:CD2	1:F:121:LEU:CD2	2.91	0.54
1:E:340:ILE:HG12	1:E:367:ALA:CB	2.38	0.54
1:D:151:GLY:HA3	1:D:185:ALA:O	2.08	0.53
1:A:308:ALA:HB1	1:A:374:ILE:HD13	1.89	0.53
1:F:151:GLY:HA3	1:F:185:ALA:O	2.08	0.53
1:B:151:GLY:HA3	1:B:185:ALA:O	2.09	0.52
1:C:151:GLY:HA3	1:C:185:ALA:O	2.09	0.52
1:E:151:GLY:HA3	1:E:185:ALA:O	2.09	0.52
1:C:63:ARG:NH1	1:C:410:GLY:O	2.44	0.51
1:A:121:LEU:CD2	1:E:117:HIS:HD2	2.24	0.51
1:A:111:ILE:HG12	1:E:124:PRO:HB3	1.93	0.51
1:F:63:ARG:NH2	1:F:72:MET:SD	2.84	0.51
1:A:117:HIS:CD2	1:E:121:LEU:CD2	2.94	0.51
1:B:121:LEU:CD2	1:D:117:HIS:CD2	2.95	0.50
1:F:62:ASP:HB2	1:F:154:ARG:HH12	1.76	0.50
1:F:280:PHE:HD1	1:F:323:LEU:HD23	1.75	0.50
1:B:63:ARG:NH2	1:B:72:MET:SD	2.85	0.49
1:C:139:ARG:HD2	1:C:187:ALA:HB2	1.94	0.49
1:D:480:LYS:HG2	1:F:488:ILE:HG23	1.93	0.49
1:B:117:HIS:CD2	1:D:121:LEU:CD2	2.96	0.49
1:E:125:ILE:HD13	1:E:135:ILE:CG1	2.37	0.49
1:C:117:HIS:HD2	1:F:121:LEU:CD2	2.25	0.49
1:C:282:GLY:HA3	1:C:433:LEU:CD1	2.43	0.48
1:D:280:PHE:HD1	1:D:323:LEU:HD23	1.77	0.48
1:F:139:ARG:HD2	1:F:187:ALA:HB2	1.95	0.48
1:A:340:ILE:HG22	1:A:369:ILE:HD13	1.96	0.48
1:A:117:HIS:HD2	1:E:121:LEU:CD2	2.25	0.48
1:C:63:ARG:NH2	1:C:72:MET:SD	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ARG:HB2	1:F:388:GLU:HA	1.96	0.48
1:B:139:ARG:HD2	1:B:187:ALA:HB2	1.96	0.48
1:D:139:ARG:HD2	1:D:187:ALA:HB2	1.96	0.48
1:F:67:PRO:HA	1:F:70:PHE:CD2	2.49	0.48
1:A:447:LYS:NZ	2:C:601:ADP:O2A	2.44	0.47
1:E:84:VAL:CG1	1:E:543:VAL:HG13	2.44	0.47
1:F:125:ILE:HD12	1:F:203:LYS:HB3	1.96	0.47
1:B:280:PHE:HD1	1:B:323:LEU:HD23	1.78	0.47
1:A:125:ILE:HD12	1:A:203:LYS:HB3	1.96	0.47
1:A:139:ARG:HD2	1:A:187:ALA:HB2	1.96	0.47
1:B:121:LEU:CD2	1:D:117:HIS:HD2	2.28	0.47
1:D:139:ARG:HH11	1:D:187:ALA:HB2	1.79	0.47
1:E:273:SER:HB2	1:E:318:HIS:CD2	2.48	0.47
1:A:106:ARG:NH2	1:A:110:ARG:HH12	2.12	0.47
1:A:124:PRO:HB3	1:E:111:ILE:HG12	1.96	0.47
1:B:149:CYS:HB3	1:B:185:ALA:HB2	1.97	0.47
1:B:340:ILE:HG22	1:B:369:ILE:HD13	1.97	0.47
1:C:121:LEU:CD2	1:F:117:HIS:CD2	2.97	0.47
1:A:153:ILE:HG12	1:A:187:ALA:HB3	1.97	0.47
1:F:375:LEU:HD11	1:F:390:GLN:HB3	1.97	0.47
1:B:106:ARG:HH21	1:B:110:ARG:NH2	2.12	0.47
1:E:139:ARG:HH11	1:E:187:ALA:HB2	1.80	0.47
1:A:67:PRO:HA	1:A:70:PHE:CD2	2.51	0.46
1:B:125:ILE:HD12	1:B:203:LYS:HB3	1.97	0.46
1:E:192:ASN:OD1	1:E:194:LYS:HG2	2.16	0.46
1:E:280:PHE:HD1	1:E:323:LEU:HD12	1.79	0.46
1:C:153:ILE:HG12	1:C:187:ALA:HB3	1.97	0.46
1:A:357:GLN:HG3	1:A:358:HIS:CE1	2.51	0.46
1:D:125:ILE:HD12	1:D:203:LYS:HB3	1.97	0.46
1:E:153:ILE:HG12	1:E:187:ALA:HB3	1.97	0.46
1:F:284:GLU:HA	1:F:287:ILE:HG22	1.98	0.46
1:A:472:SER:HA	1:C:493:THR:HG23	1.97	0.46
1:B:67:PRO:HA	1:B:70:PHE:CD2	2.50	0.46
1:C:67:PRO:HA	1:C:70:PHE:CD2	2.51	0.46
1:C:125:ILE:HD12	1:C:203:LYS:HB3	1.96	0.46
1:C:139:ARG:HH11	1:C:187:ALA:HB2	1.81	0.46
1:D:340:ILE:HG22	1:D:369:ILE:HD13	1.98	0.46
2:D:601:ADP:O1A	1:E:447:LYS:NZ	2.42	0.46
1:E:282:GLY:HA3	1:E:433:LEU:HD12	1.98	0.46
1:A:488:ILE:HG23	1:B:480:LYS:HG2	1.97	0.46
1:B:282:GLY:HA3	1:B:433:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASN:HB3	3:B:703:HOH:O	2.15	0.46
1:C:149:CYS:HB3	1:C:185:ALA:HB2	1.98	0.46
1:C:121:LEU:CD2	1:F:117:HIS:HD2	2.29	0.45
1:A:255:HIS:HD2	3:A:719:HOH:O	1.99	0.45
1:C:282:GLY:HA3	1:C:433:LEU:HD12	1.97	0.45
1:F:139:ARG:HH11	1:F:187:ALA:HB2	1.81	0.45
1:D:84:VAL:CG1	1:D:543:VAL:HG13	2.47	0.45
1:E:375:LEU:HD11	1:E:390:GLN:HB3	1.98	0.45
1:F:153:ILE:HG12	1:F:187:ALA:HB3	1.98	0.45
1:F:318:HIS:HD2	1:F:321:ARG:NH1	2.15	0.45
1:E:139:ARG:HD2	1:E:187:ALA:HB2	1.97	0.45
1:B:153:ILE:HG12	1:B:187:ALA:HB3	1.99	0.45
1:C:340:ILE:HG12	1:C:361:ILE:HD12	1.99	0.45
1:D:375:LEU:HD11	1:D:390:GLN:HB3	1.98	0.45
1:E:84:VAL:HG12	1:E:543:VAL:HG13	1.98	0.45
1:F:149:CYS:HB3	1:F:185:ALA:HB2	1.99	0.45
1:B:84:VAL:CG1	1:B:543:VAL:HG13	2.47	0.45
1:B:117:HIS:HD2	1:D:121:LEU:CD2	2.30	0.45
1:D:153:ILE:HG12	1:D:187:ALA:HB3	1.97	0.45
1:D:447:LYS:NZ	2:F:601:ADP:O1A	2.44	0.44
1:A:340:ILE:HG12	1:A:361:ILE:HD12	2.00	0.44
1:A:84:VAL:HG12	1:A:543:VAL:HG13	2.00	0.44
1:F:125:ILE:HD13	1:F:125:ILE:HA	1.88	0.44
1:A:139:ARG:HH11	1:A:187:ALA:HB2	1.81	0.44
1:B:84:VAL:HG12	1:B:543:VAL:HG13	2.00	0.44
1:B:125:ILE:HD13	1:B:125:ILE:HA	1.86	0.44
1:C:63:ARG:HB2	1:C:388:GLU:HA	1.98	0.44
1:D:149:CYS:HB3	1:D:185:ALA:HB2	1.99	0.44
1:B:139:ARG:HH11	1:B:187:ALA:HB2	1.81	0.44
1:A:84:VAL:CG1	1:A:543:VAL:HG13	2.48	0.44
1:C:125:ILE:HD13	1:C:125:ILE:HA	1.89	0.44
1:C:375:LEU:HD11	1:C:390:GLN:HB3	1.98	0.44
1:F:340:ILE:HG12	1:F:361:ILE:HD12	2.00	0.44
1:D:67:PRO:HA	1:D:70:PHE:CD2	2.52	0.43
1:D:340:ILE:HG12	1:D:361:ILE:HD12	2.00	0.43
1:B:63:ARG:HB2	1:B:388:GLU:HA	2.01	0.43
1:B:340:ILE:HG12	1:B:361:ILE:HD12	1.99	0.43
1:B:375:LEU:HD11	1:B:390:GLN:HB3	2.00	0.43
1:F:282:GLY:HA3	1:F:433:LEU:HD12	2.01	0.43
1:F:84:VAL:CG1	1:F:543:VAL:HG13	2.48	0.43
1:D:84:VAL:HG12	1:D:543:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.90	0.43
1:E:67:PRO:HA	1:E:70:PHE:CD2	2.53	0.43
2:E:601:ADP:PA	1:F:447:LYS:HZ1	2.42	0.43
1:A:438:VAL:O	1:A:441:SER:HB2	2.19	0.43
1:C:84:VAL:CG1	1:C:543:VAL:HG13	2.48	0.43
1:C:429:PRO:HG3	1:C:538:ARG:HA	2.01	0.43
1:A:468:HIS:HB3	1:C:496:PHE:CD1	2.54	0.43
1:C:84:VAL:HG12	1:C:543:VAL:HG13	2.00	0.43
1:E:115:CYS:HA	1:E:142:HIS:HA	2.02	0.42
1:A:255:HIS:CD2	3:A:719:HOH:O	2.71	0.42
1:C:323:LEU:HD11	1:C:383:ILE:HD11	2.02	0.42
1:A:115:CYS:HA	1:A:142:HIS:HA	2.02	0.42
1:B:477:LEU:HD13	1:C:477:LEU:HD21	2.01	0.42
1:E:331:VAL:HG22	1:E:343:PRO:HA	2.01	0.42
1:C:393:LYS:CB	1:C:415:GLU:HG3	2.39	0.42
1:F:84:VAL:HG12	1:F:543:VAL:HG13	2.01	0.42
1:A:64:GLU:HB2	1:A:154:ARG:HH12	1.85	0.42
1:F:332:ALA:HB1	1:F:374:ILE:HG21	2.02	0.42
1:F:318:HIS:CD2	1:F:321:ARG:NH1	2.88	0.41
1:D:405:ALA:HB1	1:D:433:LEU:HD21	2.03	0.41
1:B:277:ARG:HG2	1:B:322:TYR:CE2	2.55	0.41
1:C:332:ALA:HB1	1:C:374:ILE:HG21	2.02	0.41
1:E:192:ASN:HD21	1:E:194:LYS:HE3	1.86	0.41
1:A:447:LYS:HZ1	2:C:601:ADP:PA	2.42	0.41
1:B:64:GLU:HB2	1:B:154:ARG:HH12	1.86	0.41
1:E:64:GLU:HB2	1:E:154:ARG:HH12	1.85	0.41
1:A:331:VAL:HG22	1:A:343:PRO:HA	2.03	0.41
1:B:298:MET:HE1	1:B:380:ASP:HB3	2.03	0.41
1:D:472:SER:HA	1:F:493:THR:HG23	2.03	0.41
1:A:106:ARG:HH21	1:A:110:ARG:HH12	1.69	0.41
1:A:477:LEU:HD21	1:C:477:LEU:HD13	2.03	0.41
1:B:332:ALA:HB1	1:B:374:ILE:HG21	2.03	0.41
1:C:156:SER:HB3	1:C:159:VAL:HG13	2.02	0.41
1:C:211:GLU:OE1	1:F:117:HIS:NE2	2.53	0.41
1:D:115:CYS:HA	1:D:142:HIS:HA	2.03	0.41
1:E:149:CYS:HB3	1:E:185:ALA:HB2	2.02	0.41
1:E:192:ASN:ND2	1:E:194:LYS:HE3	2.35	0.41
1:E:156:SER:HB3	1:E:159:VAL:HG13	2.03	0.41
1:C:413:THR:OG1	1:C:415:GLU:HG2	2.21	0.40
1:A:384:PRO:HD2	1:A:405:ALA:O	2.22	0.40
1:B:347:ASP:HA	1:B:348:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ADP:O2A	1:C:447:LYS:NZ	2.45	0.40
1:A:150:LYS:O	1:A:171:MET:HG2	2.21	0.40
1:A:156:SER:HB3	1:A:159:VAL:HG13	2.03	0.40
1:A:332:ALA:HB1	1:A:374:ILE:HG21	2.03	0.40
1:D:331:VAL:HG22	1:D:343:PRO:HA	2.02	0.40
1:F:384:PRO:HD2	1:F:405:ALA:O	2.22	0.40
1:B:284:GLU:HA	1:B:287:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/561 (86%)	473 (98%)	7 (2%)	0	100	100
1	B	495/561 (88%)	490 (99%)	5 (1%)	0	100	100
1	C	490/561 (87%)	481 (98%)	9 (2%)	0	100	100
1	D	493/561 (88%)	487 (99%)	6 (1%)	0	100	100
1	E	485/561 (86%)	477 (98%)	8 (2%)	0	100	100
1	F	477/561 (85%)	471 (99%)	6 (1%)	0	100	100
All	All	2920/3366 (87%)	2879 (99%)	41 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	399/455 (88%)	388 (97%)	11 (3%)	43	63
1	B	408/455 (90%)	399 (98%)	9 (2%)	52	71
1	C	412/455 (90%)	399 (97%)	13 (3%)	39	59
1	D	411/455 (90%)	400 (97%)	11 (3%)	44	65
1	E	405/455 (89%)	396 (98%)	9 (2%)	52	71
1	F	400/455 (88%)	391 (98%)	9 (2%)	50	70
All	All	2435/2730 (89%)	2373 (98%)	62 (2%)	47	67

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	122	SER
1	A	138	TYR
1	A	164	VAL
1	A	177	VAL
1	A	191	ILE
1	A	284	GLU
1	A	287	ILE
1	A	449	LEU
1	A	498	ASP
1	A	511	SER
1	B	122	SER
1	B	138	TYR
1	B	164	VAL
1	B	177	VAL
1	B	191	ILE
1	B	287	ILE
1	B	449	LEU
1	B	498	ASP
1	B	511	SER
1	C	99	GLU
1	C	102	ARG
1	C	122	SER
1	C	138	TYR
1	C	164	VAL
1	C	177	VAL
1	C	191	ILE
1	C	234	ARG

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Mol	Chain	Res	Type
1	C	287	ILE
1	C	441	SER
1	C	449	LEU
1	C	498	ASP
1	C	511	SER
1	D	99	GLU
1	D	102	ARG
1	D	122	SER
1	D	138	TYR
1	D	164	VAL
1	D	177	VAL
1	D	287	ILE
1	D	498	ASP
1	D	511	SER
1	D	558	VAL
1	D	559	THR
1	E	122	SER
1	E	125	ILE
1	E	138	TYR
1	E	164	VAL
1	E	287	ILE
1	E	314	ASN
1	E	340	ILE
1	E	449	LEU
1	E	498	ASP
1	F	122	SER
1	F	138	TYR
1	F	164	VAL
1	F	177	VAL
1	F	191	ILE
1	F	441	SER
1	F	449	LEU
1	F	498	ASP
1	F	511	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	532	ASN
1	D	497	GLN
1	E	314	ASN

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Mol	Chain	Res	Type
1	E	318	HIS
1	E	409	ASN
1	E	434	ASN
1	F	544	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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	$\#\|Z\| > 2$
2	ADP	C	601	-	24,29,29	0.70	0	29,45,45	0.75	1 (3%)
2	ADP	A	601	-	24,29,29	0.70	0	29,45,45	0.82	1 (3%)
2	ADP	B	601	-	24,29,29	0.68	0	29,45,45	0.81	1 (3%)
2	ADP	E	601	-	24,29,29	0.69	0	29,45,45	0.75	1 (3%)
2	ADP	D	601	-	24,29,29	0.69	0	29,45,45	0.78	1 (3%)
2	ADP	F	601	-	24,29,29	0.69	0	29,45,45	0.78	1 (3%)

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	-	-	4/12/32/32	0/3/3/3
2	ADP	A	601	-	-	3/12/32/32	0/3/3/3
2	ADP	B	601	-	-	3/12/32/32	0/3/3/3
2	ADP	E	601	-	-	3/12/32/32	0/3/3/3
2	ADP	D	601	-	-	3/12/32/32	0/3/3/3
2	ADP	F	601	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	ADP	C5-C6-N6	2.48	124.12	120.35
2	C	601	ADP	C5-C6-N6	2.46	124.09	120.35
2	A	601	ADP	C5-C6-N6	2.45	124.07	120.35
2	B	601	ADP	C5-C6-N6	2.43	124.05	120.35
2	F	601	ADP	C5-C6-N6	2.41	124.02	120.35
2	E	601	ADP	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	ADP	PA-O3A-PB-O3B
2	D	601	ADP	PA-O3A-PB-O3B
2	E	601	ADP	PA-O3A-PB-O3B
2	F	601	ADP	PA-O3A-PB-O3B
2	E	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	O4'-C4'-C5'-O5'
2	D	601	ADP	O4'-C4'-C5'-O5'
2	F	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	PA-O3A-PB-O1B
2	B	601	ADP	PA-O3A-PB-O1B
2	C	601	ADP	PA-O3A-PB-O1B
2	D	601	ADP	PA-O3A-PB-O1B
2	E	601	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	PA-O3A-PB-O3B
2	C	601	ADP	PA-O3A-PB-O2B

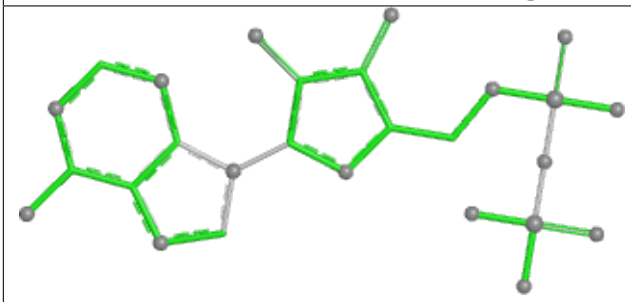
There are no ring outliers.

6 monomers are involved in 12 short contacts:

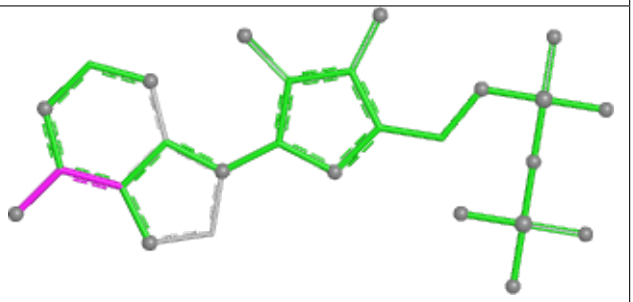
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	ADP	3	0
2	A	601	ADP	1	0
2	B	601	ADP	2	0
2	E	601	ADP	2	0
2	D	601	ADP	2	0
2	F	601	ADP	2	0

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 then 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.

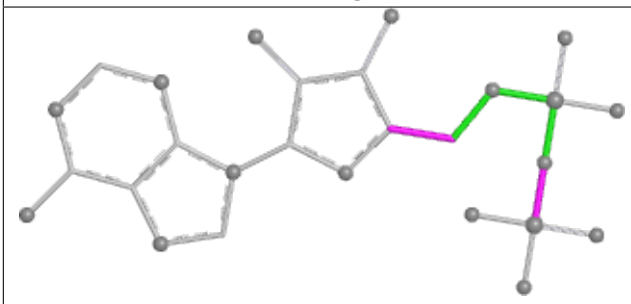
Ligand ADP C 601



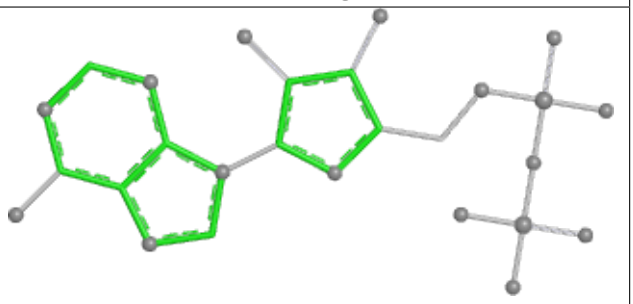
Bond lengths



Bond angles

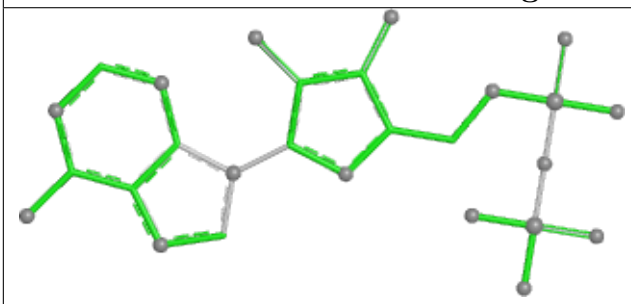


Torsions

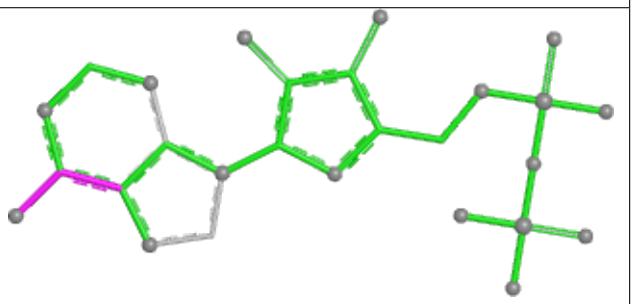


Rings

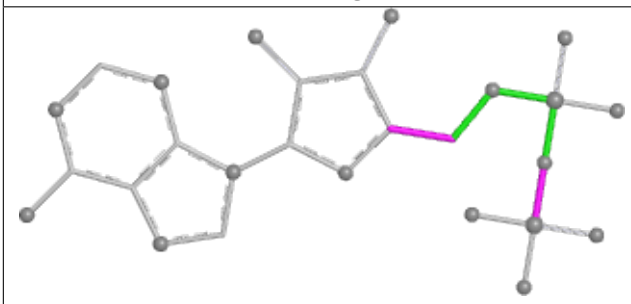
Ligand ADP A 601



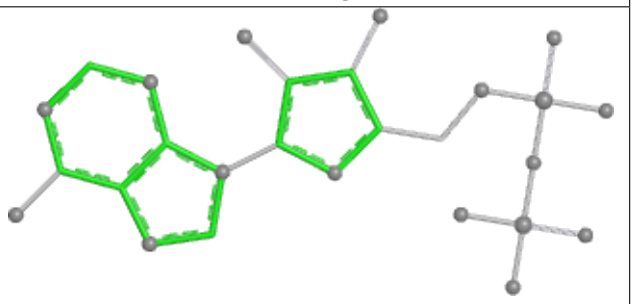
Bond lengths



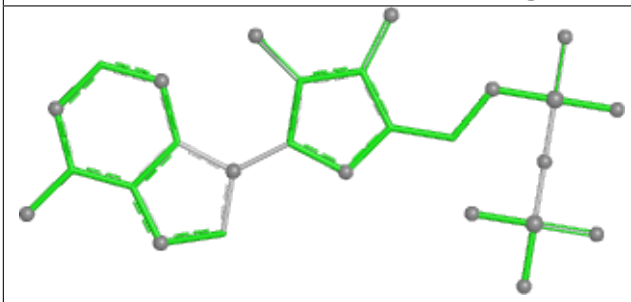
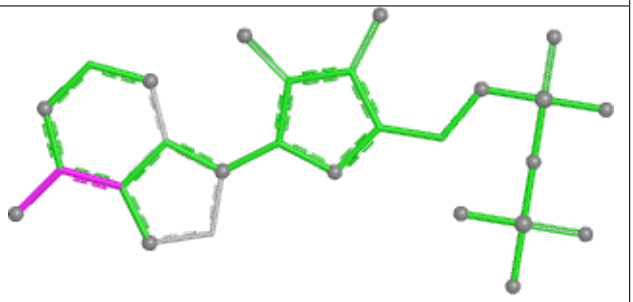
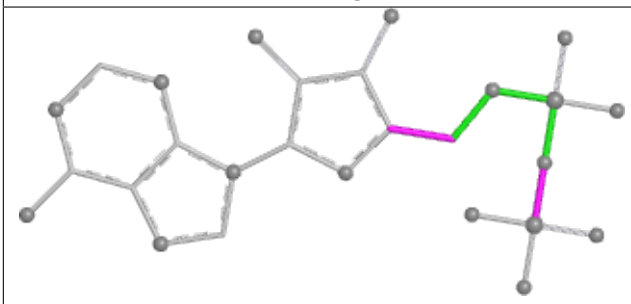
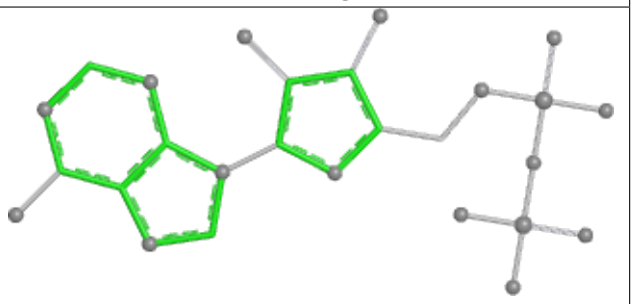
Bond angles

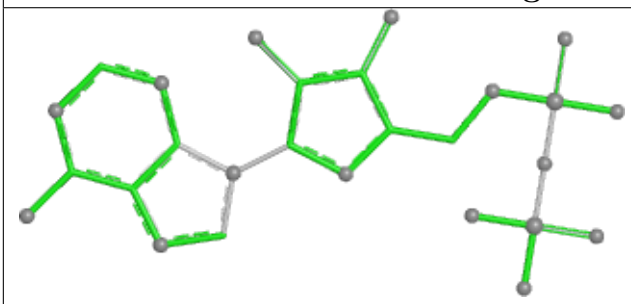
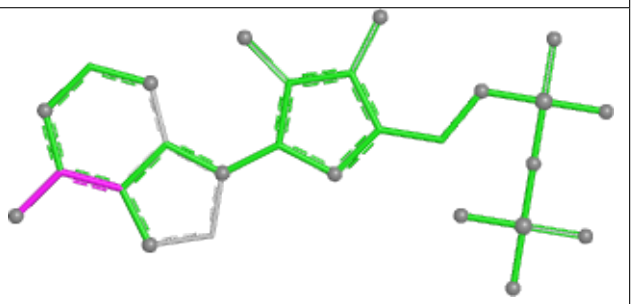
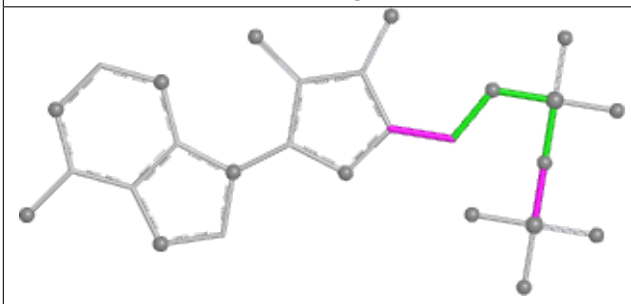
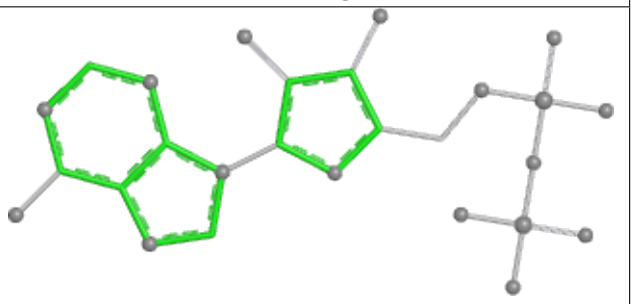


Torsions

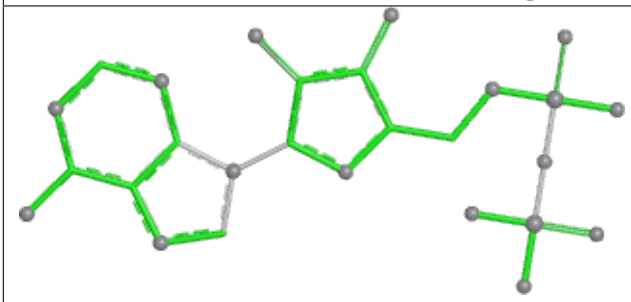


Rings

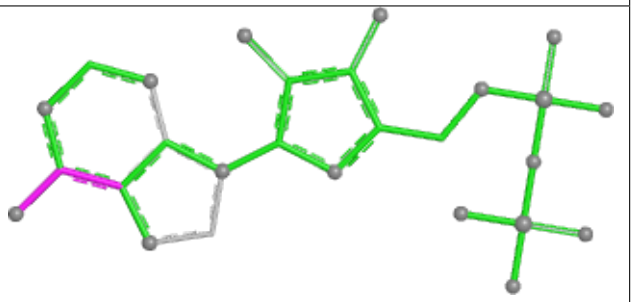
Ligand ADP B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

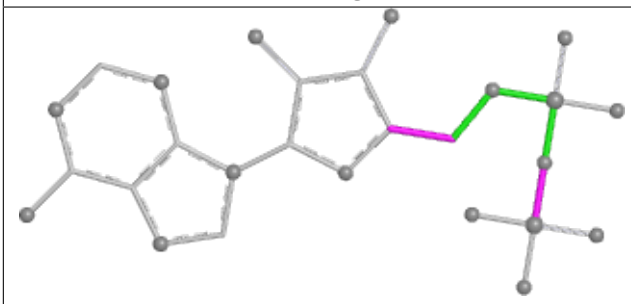
Ligand ADP D 601



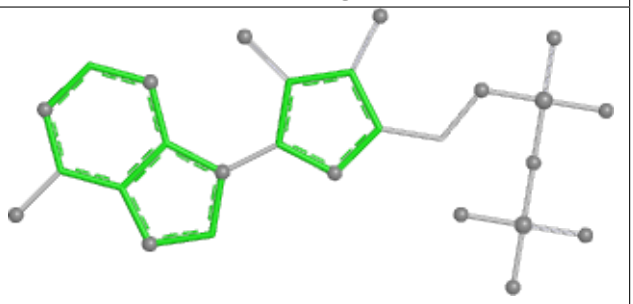
Bond lengths



Bond angles

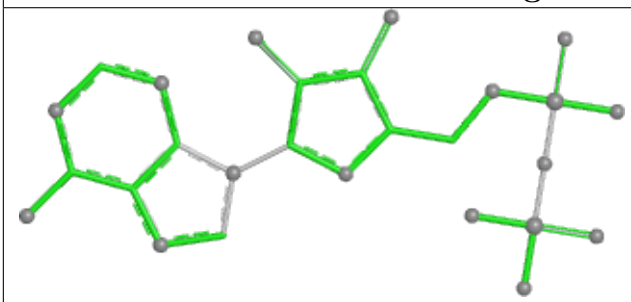


Torsions

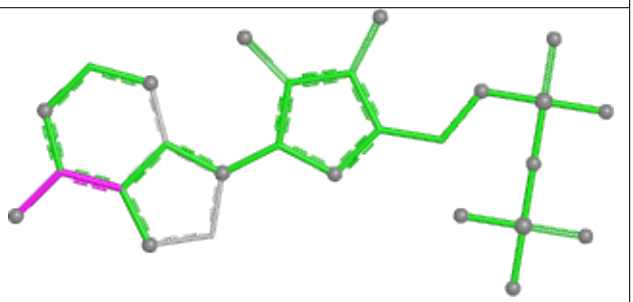


Rings

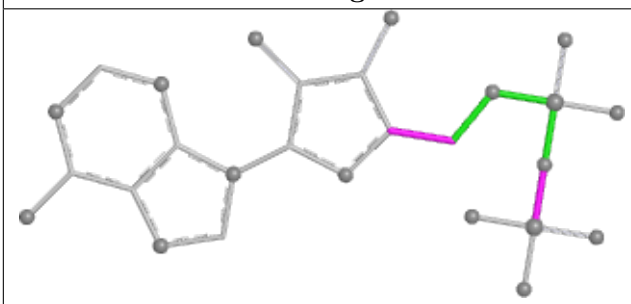
Ligand ADP F 601



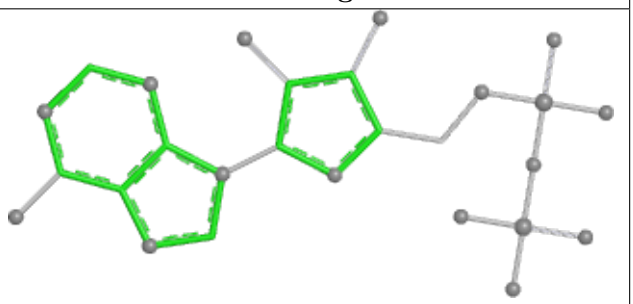
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	486/561 (86%)	0.59	54 (11%) 5 4	21, 42, 94, 106	0
1	B	497/561 (88%)	0.25	30 (6%) 21 20	15, 35, 73, 89	0
1	C	494/561 (88%)	0.06	15 (3%) 50 49	19, 33, 63, 77	0
1	D	495/561 (88%)	0.29	34 (6%) 16 15	17, 36, 75, 91	0
1	E	489/561 (87%)	0.49	53 (10%) 5 5	19, 40, 84, 104	0
1	F	483/561 (86%)	0.32	34 (7%) 16 15	17, 36, 76, 89	0
All	All	2944/3366 (87%)	0.33	220 (7%) 14 13	15, 37, 80, 106	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	67	PRO	12.1
1	A	338	GLY	11.1
1	E	91	ASP	8.6
1	E	485	GLY	8.3
1	A	367	ALA	7.2
1	D	337	ASP	7.2
1	F	356	LEU	7.0
1	D	357	GLN	6.9
1	A	365	PRO	6.5
1	A	91	ASP	6.5
1	D	365	PRO	6.4
1	A	94	THR	6.1
1	E	348	PRO	6.0
1	E	363	GLY	6.0
1	C	387	SER	5.9
1	A	97	THR	5.8
1	A	357	GLN	5.7
1	F	89	VAL	5.5
1	D	370	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	68	ASN	5.5
1	E	357	GLN	5.4
1	A	93	LYS	5.4
1	A	337	ASP	5.3
1	B	91	ASP	5.2
1	B	357	GLN	5.2
1	E	369	ILE	5.1
1	E	101	LYS	5.1
1	A	95	ARG	5.0
1	D	356	LEU	5.0
1	D	371	GLU	4.9
1	E	486	GLY	4.7
1	A	366	LYS	4.7
1	F	357	GLN	4.6
1	E	95	ARG	4.6
1	D	558	VAL	4.5
1	B	89	VAL	4.5
1	A	358	HIS	4.5
1	A	92	LEU	4.4
1	A	424	ASN	4.4
1	B	467	TYR	4.4
1	B	344	ASP	4.4
1	D	467	TYR	4.2
1	F	364	PHE	4.2
1	F	354	PHE	4.1
1	B	83	ILE	4.0
1	B	97	THR	4.0
1	C	90	GLU	4.0
1	D	358	HIS	3.9
1	A	89	VAL	3.9
1	B	363	GLY	3.9
1	A	304	ASP	3.9
1	E	337	ASP	3.9
1	F	378	ASP	3.9
1	A	341	TRP	3.9
1	A	102	ARG	3.8
1	D	359	GLY	3.8
1	E	94	THR	3.7
1	E	336	SER	3.7
1	F	365	PRO	3.7
1	E	69	PHE	3.7
1	C	371	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLU	3.7
1	B	534	GLY	3.7
1	B	94	THR	3.7
1	E	66	ASP	3.6
1	F	344	ASP	3.6
1	E	352	GLU	3.6
1	D	560	PHE	3.6
1	A	363	GLY	3.6
1	F	352	GLU	3.5
1	F	91	ASP	3.5
1	D	369	ILE	3.5
1	E	89	VAL	3.5
1	F	368	LYS	3.5
1	D	387	SER	3.4
1	C	363	GLY	3.4
1	B	488	ILE	3.4
1	C	93	LYS	3.4
1	A	86	ASP	3.4
1	F	88	LEU	3.4
1	C	290	ALA	3.4
1	E	354	PHE	3.4
1	A	359	GLY	3.4
1	B	92	LEU	3.4
1	A	311	GLY	3.3
1	E	70	PHE	3.3
1	D	352	GLU	3.3
1	A	297	GLY	3.3
1	A	351	LEU	3.3
1	E	366	LYS	3.2
1	B	400	LYS	3.2
1	C	353	ASP	3.2
1	E	97	THR	3.2
1	E	387	SER	3.2
1	B	358	HIS	3.2
1	F	367	ALA	3.1
1	C	97	THR	3.1
1	B	295	ILE	3.1
1	E	100	GLN	3.1
1	E	71	LYS	3.1
1	F	341	TRP	3.1
1	F	86	ASP	3.1
1	F	353	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	357	GLN	3.0
1	A	158	ASP	3.0
1	E	362	LEU	3.0
1	E	498	ASP	3.0
1	A	418	LYS	3.0
1	F	369	ILE	3.0
1	A	312	PHE	3.0
1	C	91	ASP	2.9
1	C	366	LYS	2.9
1	F	363	GLY	2.9
1	D	311	GLY	2.9
1	F	104	ARG	2.9
1	A	395	ASN	2.9
1	A	391	LEU	2.9
1	D	304	ASP	2.8
1	F	362	LEU	2.8
1	A	373	SER	2.8
1	B	93	LYS	2.8
1	F	358	HIS	2.8
1	D	368	LYS	2.8
1	A	356	LEU	2.7
1	F	371	GLU	2.7
1	D	94	THR	2.7
1	D	91	ASP	2.7
1	E	92	LEU	2.7
1	B	371	GLU	2.7
1	F	370	TYR	2.7
1	F	345	GLY	2.7
1	D	100	GLN	2.7
1	F	103	ASN	2.6
1	E	72	MET	2.6
1	D	395	ASN	2.6
1	E	483	LYS	2.6
1	A	362	LEU	2.6
1	D	347	ASP	2.6
1	E	365	PRO	2.6
1	A	352	GLU	2.6
1	D	351	LEU	2.5
1	E	356	LEU	2.5
1	A	66	ASP	2.5
1	D	501	SER	2.5
1	F	479	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	346	ILE	2.5
1	E	93	LYS	2.5
1	D	344	ASP	2.5
1	A	354	PHE	2.5
1	E	104	ARG	2.5
1	E	90	GLU	2.5
1	E	308	ALA	2.5
1	E	367	ALA	2.5
1	A	348	PRO	2.4
1	A	106	ARG	2.4
1	A	374	ILE	2.4
1	E	129	ASP	2.4
1	B	354	PHE	2.4
1	B	105	VAL	2.4
1	A	344	ASP	2.4
1	E	317	LEU	2.4
1	E	105	VAL	2.4
1	E	314	ASN	2.4
1	C	94	THR	2.4
1	E	73	VAL	2.4
1	F	557	GLY	2.4
1	A	328	ALA	2.4
1	D	353	ASP	2.4
1	B	362	LEU	2.4
1	D	362	LEU	2.4
1	F	338	GLY	2.4
1	A	69	PHE	2.4
1	A	82	SER	2.4
1	B	485	GLY	2.3
1	C	95	ARG	2.3
1	A	132	TRP	2.3
1	A	342	ASN	2.3
1	E	81	ALA	2.3
1	D	95	ARG	2.3
1	E	353	ASP	2.3
1	E	484	HIS	2.3
1	A	471	MET	2.3
1	E	487	THR	2.3
1	F	294	SER	2.3
1	A	330	CYS	2.3
1	E	78	ASP	2.3
1	C	64	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	350	GLU	2.3
1	E	98	GLU	2.3
1	B	365	PRO	2.2
1	A	399	VAL	2.2
1	E	326	PHE	2.2
1	A	384	PRO	2.2
1	B	106	ARG	2.2
1	B	337	ASP	2.2
1	A	324	HIS	2.2
1	D	360	THR	2.2
1	F	366	LYS	2.2
1	D	348	PRO	2.2
1	A	96	GLU	2.2
1	A	353	ASP	2.1
1	A	70	PHE	2.1
1	F	105	VAL	2.1
1	F	498	ASP	2.1
1	E	75	GLY	2.1
1	E	361	ILE	2.1
1	A	364	PHE	2.1
1	A	349	LYS	2.1
1	B	324	HIS	2.1
1	E	82	SER	2.1
1	B	352	GLU	2.1
1	F	101	LYS	2.1
1	B	356	LEU	2.1
1	D	312	PHE	2.1
1	C	372	GLY	2.1
1	B	84	VAL	2.0
1	D	336	SER	2.0
1	E	349	LYS	2.0
1	D	559	THR	2.0
1	F	348	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

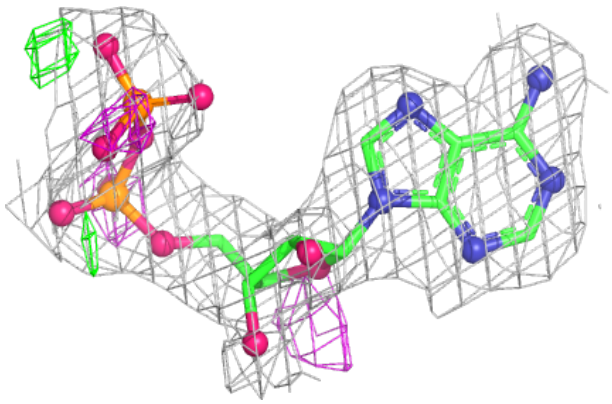
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

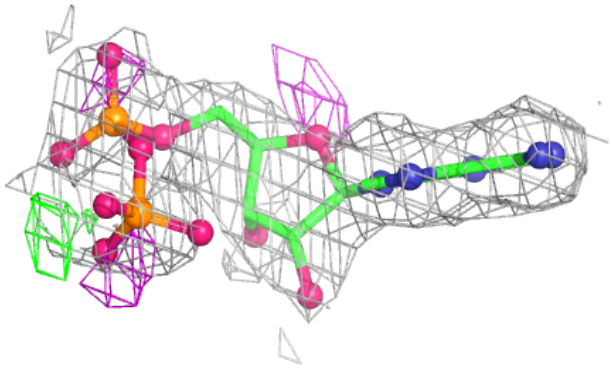
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	601	27/27	0.88	0.20	44,51,59,59	0
2	ADP	E	601	27/27	0.88	0.16	50,52,59,60	0
2	ADP	D	601	27/27	0.91	0.15	53,56,63,63	0
2	ADP	C	601	27/27	0.91	0.16	53,56,63,63	0
2	ADP	F	601	27/27	0.92	0.16	43,47,53,53	0
2	ADP	A	601	27/27	0.93	0.14	45,47,50,51	0

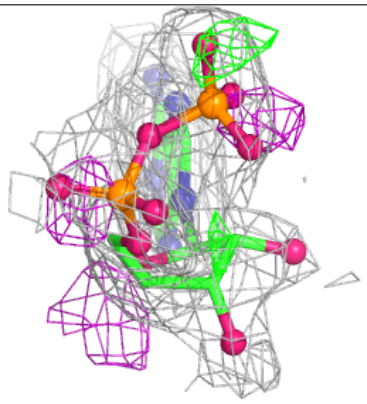
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 601:

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

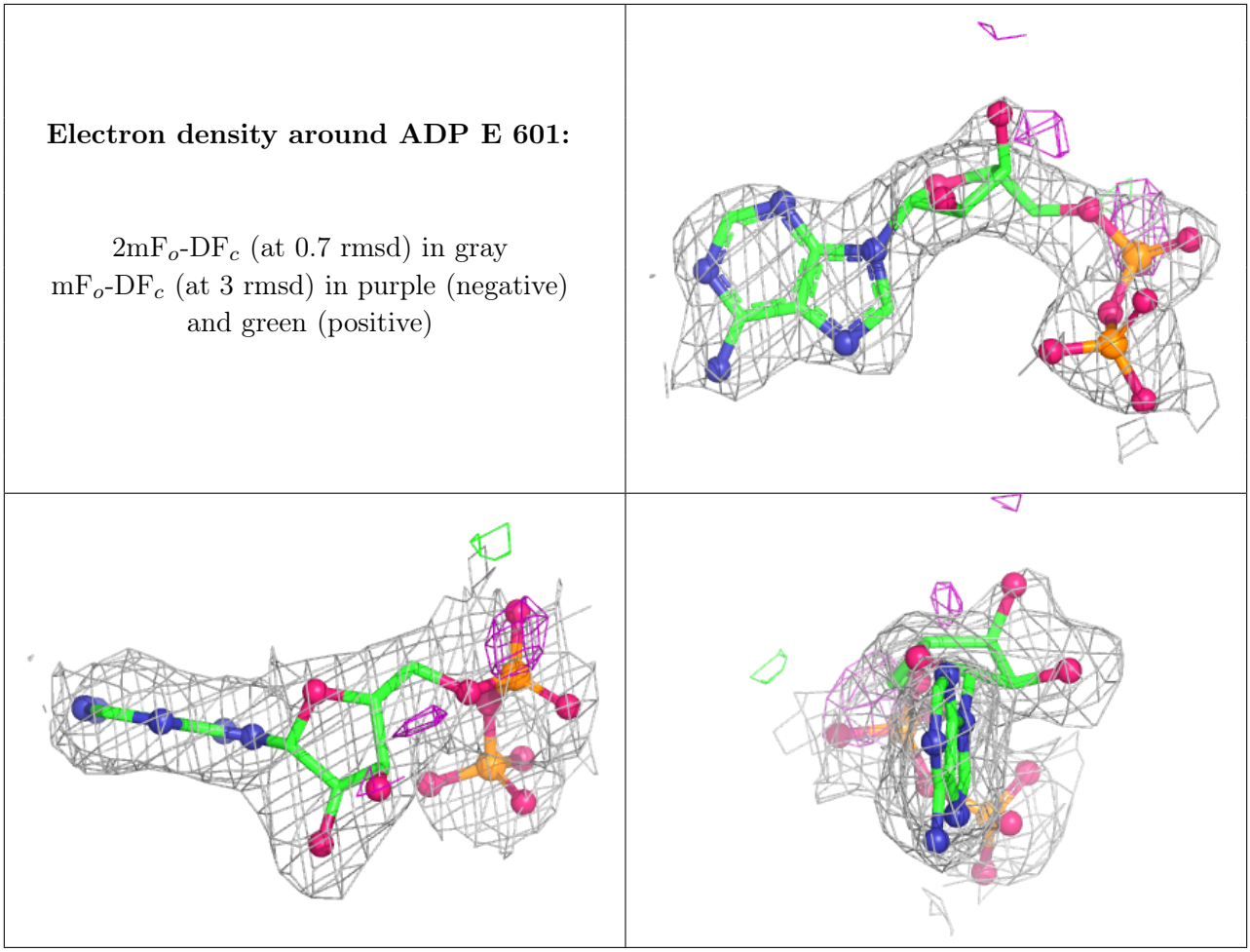






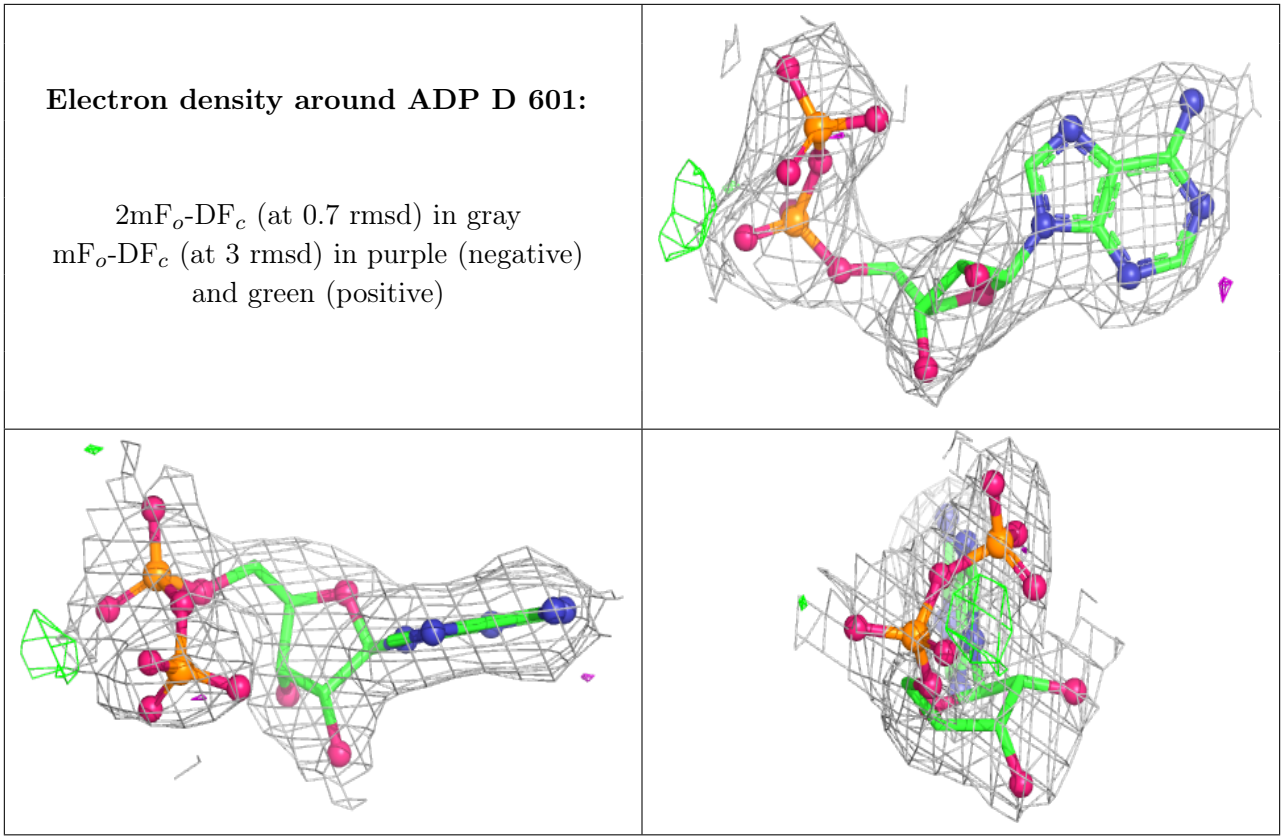
Electron density around ADP E 601:

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



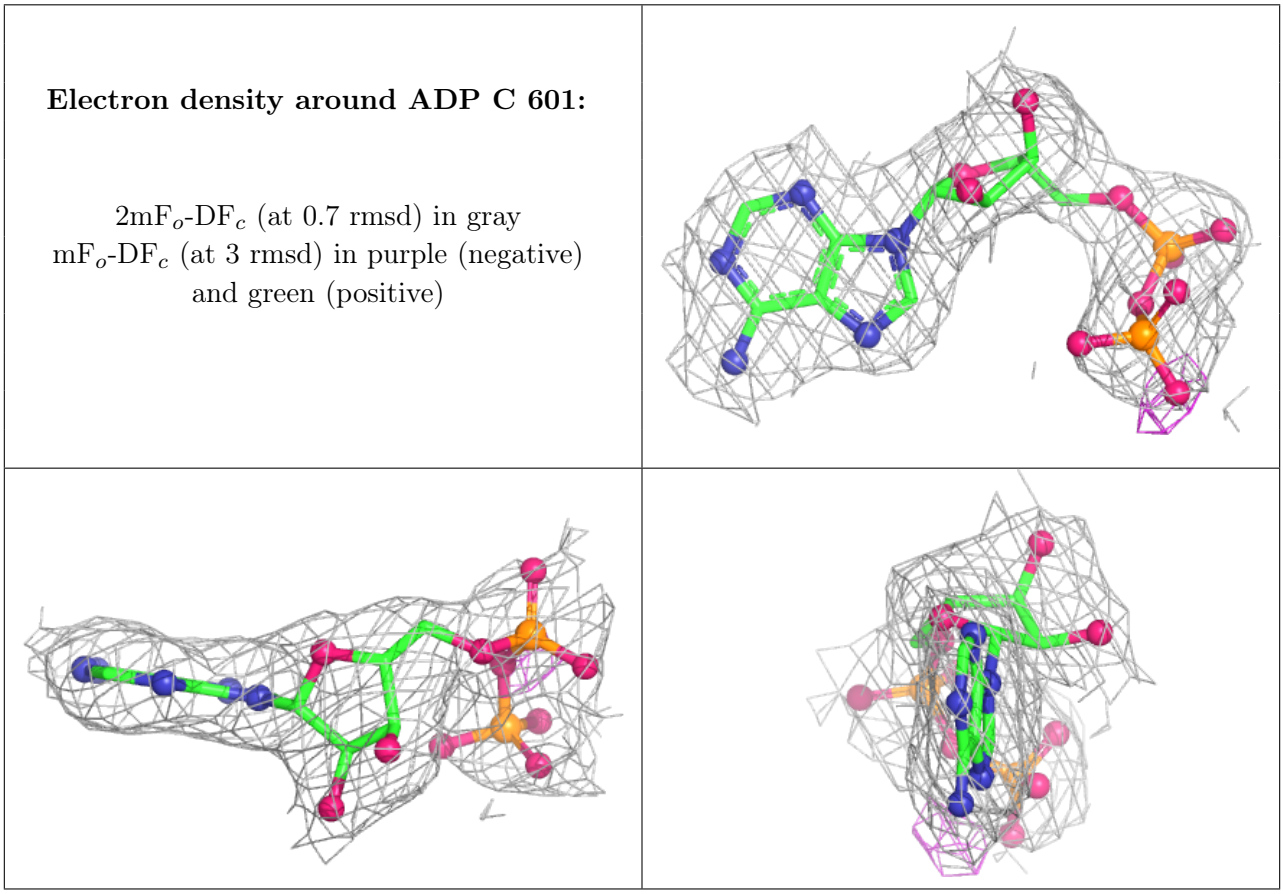
Electron density around ADP D 601:

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



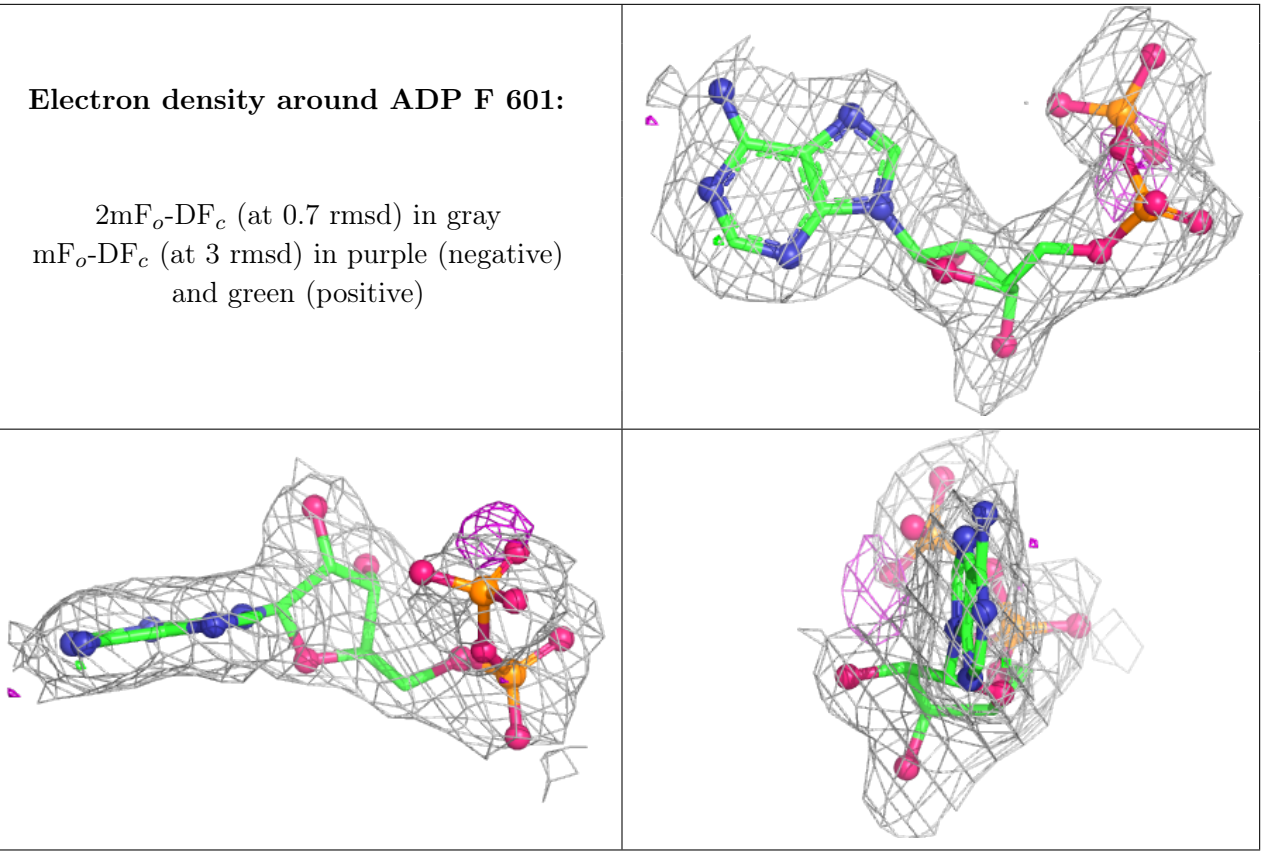
Electron density around ADP C 601:

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



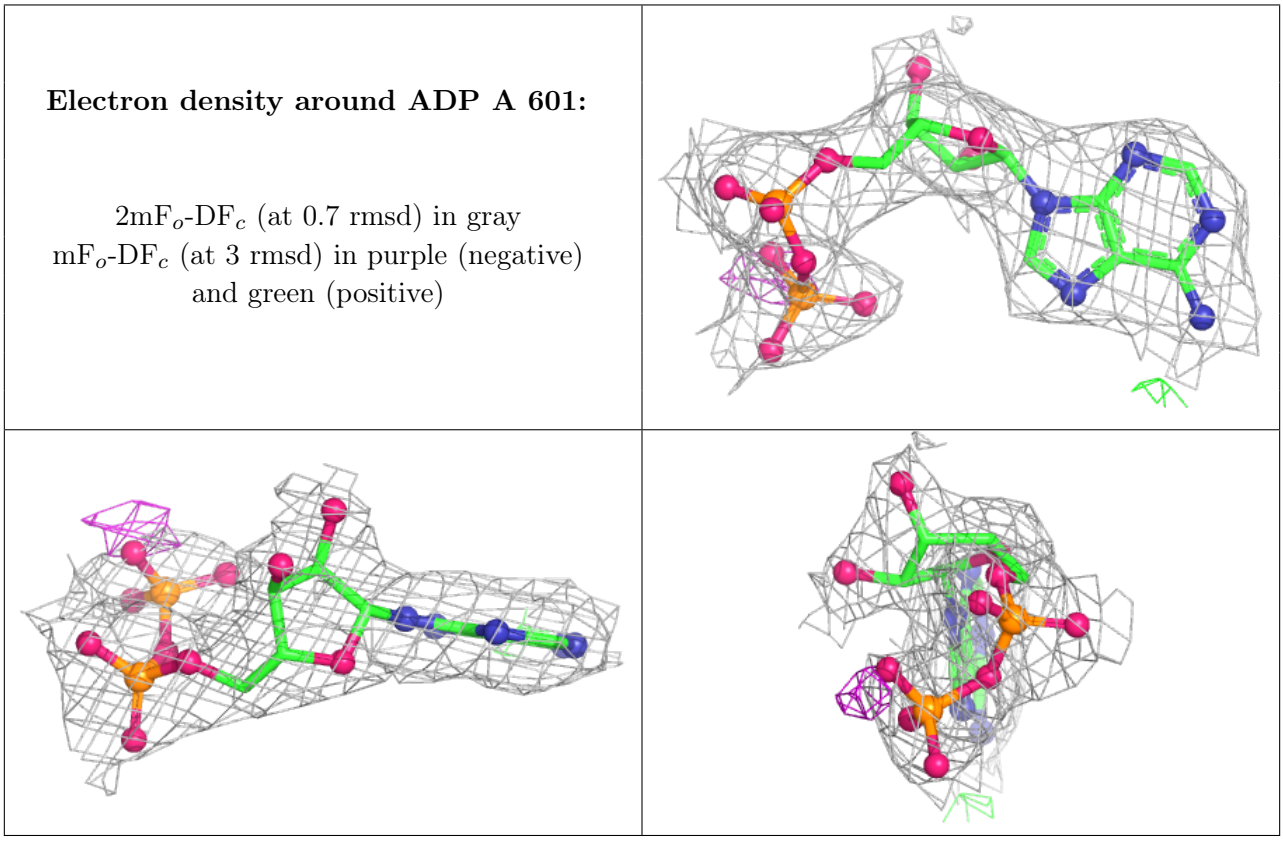
Electron density around ADP F 601:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.