



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:35 am BST

PDB ID : 4LRZ  
Title : Crystal Structure of the E.coli DhaR(N)-DhaL complex  
Authors : Shi, R.; McDonald, L.; Cygler, M.; Ekiel, I.  
Deposited on : 2013-07-21  
Resolution : 2.32 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

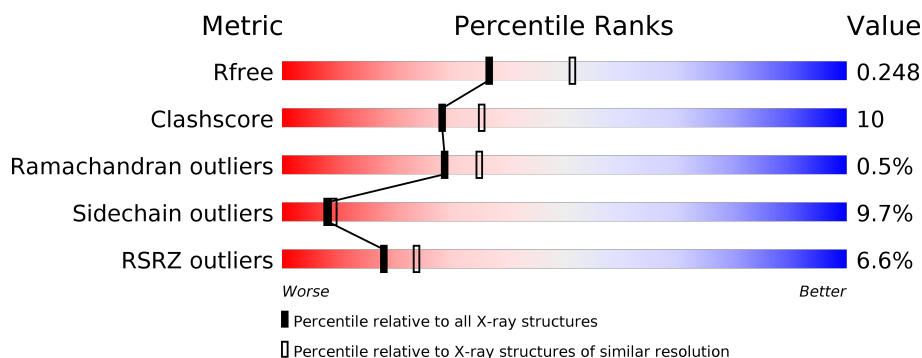
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	211	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
1	B	211	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>•</div> </div> </div>
1	C	211	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
1	D	211	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
2	E	318	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>5%</div> <div>8%</div> </div> </div>
2	F	318	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	318	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>8%</div> </div> </div>
2	H	318	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15955 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 PTS-dependent dihydroxyacetone kinase, ADP-binding subunit DhaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1584	982	277	314	11			
1	B	211	Total	C	N	O	S	0	0	0
			1584	982	277	314	11			
1	C	211	Total	C	N	O	S	0	0	0
			1584	982	277	314	11			
1	D	211	Total	C	N	O	S	0	0	0
			1584	982	277	314	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P76014
A	1	SER	-	EXPRESSION TAG	UNP P76014
B	0	GLY	-	EXPRESSION TAG	UNP P76014
B	1	SER	-	EXPRESSION TAG	UNP P76014
C	0	GLY	-	EXPRESSION TAG	UNP P76014
C	1	SER	-	EXPRESSION TAG	UNP P76014
D	0	GLY	-	EXPRESSION TAG	UNP P76014
D	1	SER	-	EXPRESSION TAG	UNP P76014

- Molecule 2 is a protein called PTS-dependent dihydroxyacetone kinase operon regulatory protein.

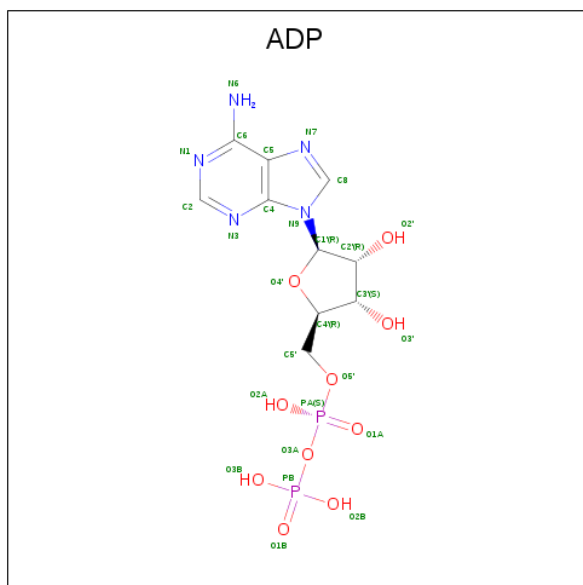
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	294	Total	C	N	O	S	0	2	0
			2275	1442	394	427	12			
2	F	294	Total	C	N	O	S	0	1	0
			2269	1438	393	426	12			
2	G	294	Total	C	N	O	S	0	2	0
			2275	1442	393	428	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	291	Total	C	N	O	S	0	0	0
			2239	1421	386	420	12			

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



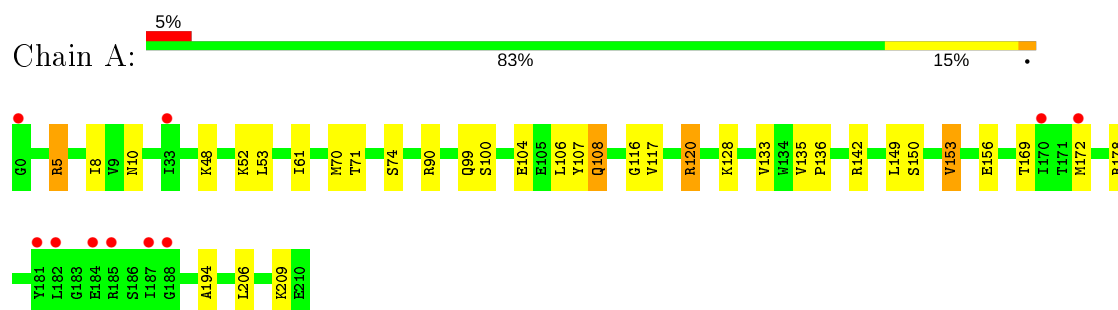
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	47	Total 47	O 47	0	0
5	C	59	Total 59	O 59	0	0
5	D	49	Total 49	O 49	0	0
5	E	59	Total 59	O 59	0	0
5	F	51	Total 51	O 51	0	0
5	G	60	Total 60	O 60	0	0
5	H	62	Total 62	O 62	0	0

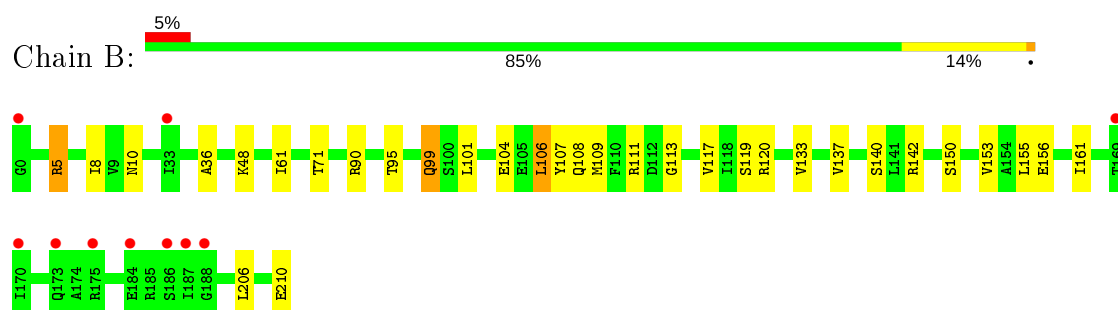
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

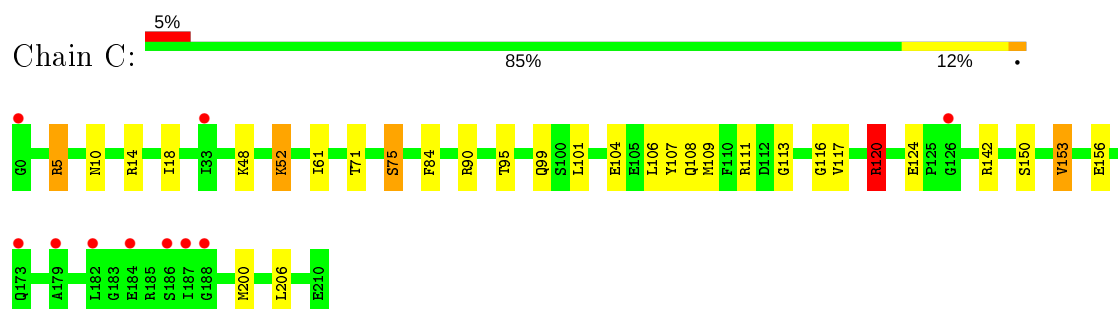
- Molecule 1: PTS-dependent dihydroxyacetone kinase, ADP-binding subunit DhaL



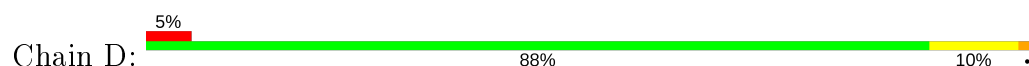
- Molecule 1: PTS-dependent dihydroxyacetone kinase, ADP-binding subunit DhaL

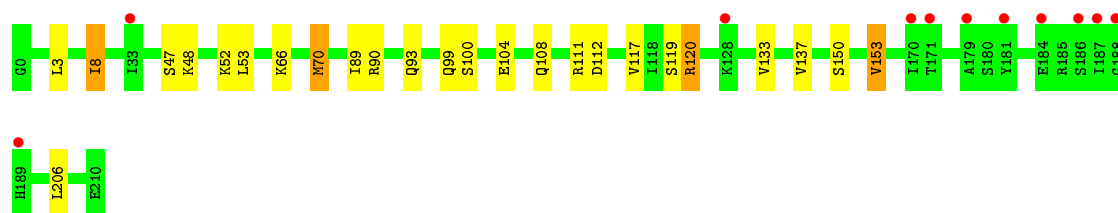


- Molecule 1: PTS-dependent dihydroxyacetone kinase, ADP-binding subunit DhaL

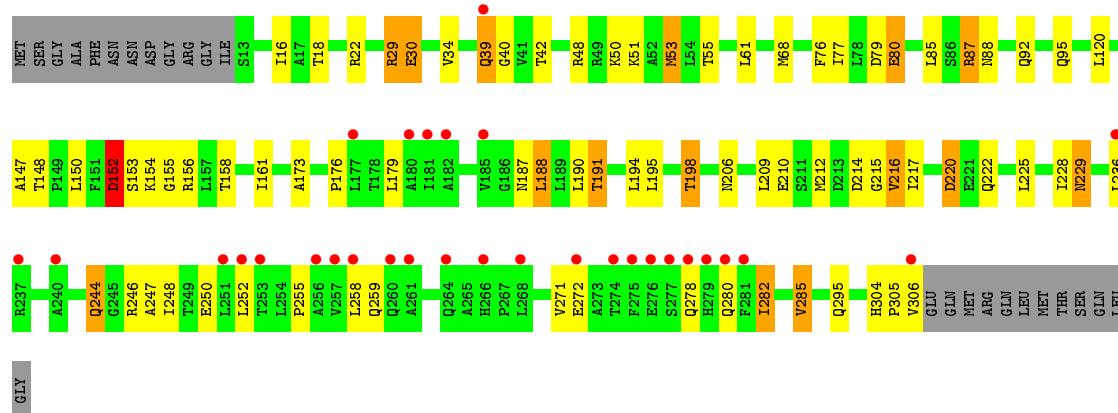


- Molecule 1: PTS-dependent dihydroxyacetone kinase, ADP-binding subunit DhaL

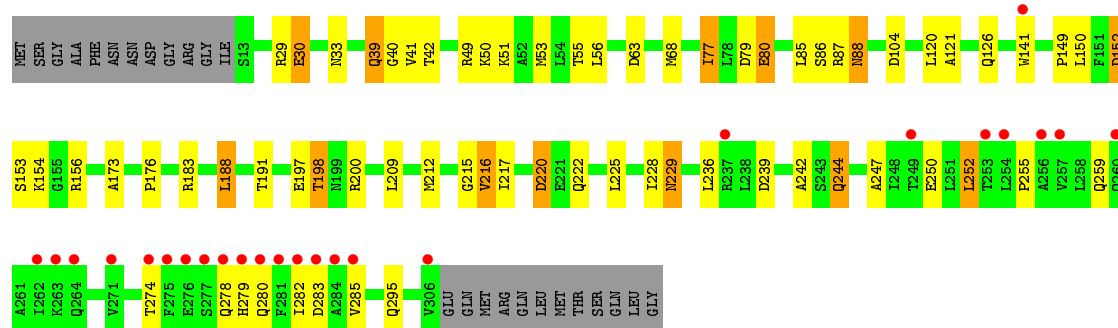




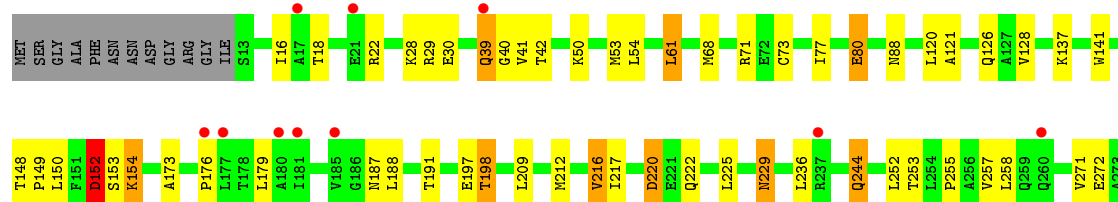
- Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein



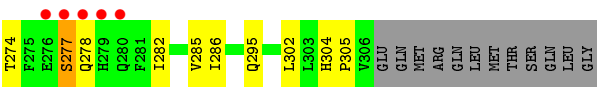
- Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein



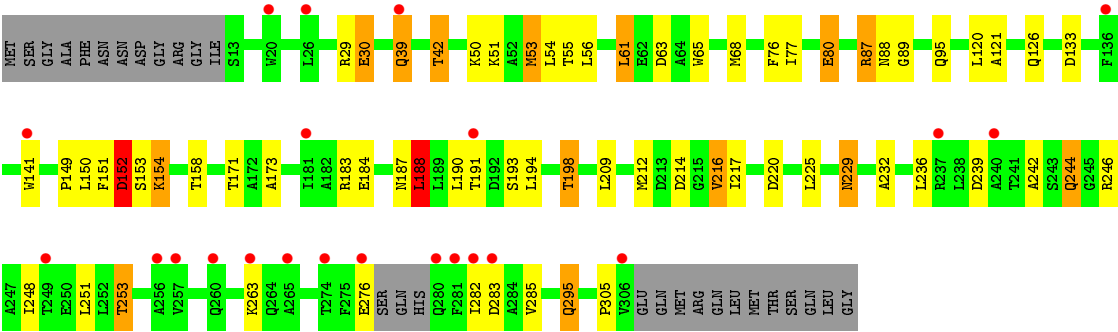
- Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein







● Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.77Å 91.50Å 93.81Å 84.15° 72.42° 90.01°	Depositor
Resolution (Å)	90.91 – 2.32 45.49 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.3 (90.91-2.32) 97.3 (45.49-2.32)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.200 , 0.247 0.200 , 0.248	Depositor DCC
$R_{free}$ test set	6008 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, 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	0.82	0/1606	0.83	1/2163 (0.0%)
1	B	0.85	1/1606 (0.1%)	0.83	0/2163
1	C	0.85	0/1606	0.86	2/2163 (0.1%)
1	D	0.81	0/1606	0.78	1/2163 (0.0%)
2	E	0.79	1/2323 (0.0%)	0.85	4/3163 (0.1%)
2	F	0.80	1/2314 (0.0%)	0.84	1/3151 (0.0%)
2	G	0.84	3/2323 (0.1%)	0.88	3/3163 (0.1%)
2	H	0.84	0/2279	0.87	4/3102 (0.1%)
All	All	0.82	6/15663 (0.0%)	0.85	16/21231 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	197	GLU	CG-CD	5.69	1.60	1.51
2	G	220	ASP	CB-CG	-5.68	1.39	1.51
2	E	153	SER	CB-OG	5.35	1.49	1.42
1	B	36	ALA	CA-CB	5.31	1.63	1.52
2	G	197	GLU	CB-CG	5.22	1.62	1.52
2	G	197	GLU	CG-CD	5.04	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	220	ASP	CB-CG-OD2	-11.56	107.90	118.30
2	G	152	ASP	CB-CG-OD1	-7.76	111.31	118.30
2	H	152	ASP	CB-CG-OD1	-7.38	111.66	118.30
2	E	87	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	120	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	G	220	ASP	CB-CG-OD1	6.41	124.07	118.30
2	E	79	ASP	CB-CG-OD1	6.16	123.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	80	GLU	CA-CB-CG	5.94	126.47	113.40
2	H	188	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	53	LEU	CA-CB-CG	5.39	127.71	115.30
2	H	220	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	14	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	E	188	LEU	CB-CG-CD1	5.08	119.64	111.00
2	H	87	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	E	152	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	D	53	LEU	CA-CB-CG	5.02	126.84	115.30

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	1584	0	1577	28	0
1	B	1584	0	1577	23	0
1	C	1584	0	1577	21	0
1	D	1584	0	1577	16	0
2	E	2275	0	2294	79	0
2	F	2269	0	2286	57	0
2	G	2275	0	2292	56	0
2	H	2239	0	2259	64	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	58	0	0	4	0
5	B	47	0	0	4	0
5	C	59	0	0	2	0
5	D	49	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	59	0	0	8	0
5	F	51	0	0	3	0
5	G	60	0	0	6	0
5	H	62	0	0	5	0
All	All	15955	0	15487	305	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 10.

All (305) 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)
2:E:209:LEU:HA	2:E:212:MET:HE1	1.18	1.12
2:E:209:LEU:HA	2:E:212:MET:CE	1.79	1.12
2:H:212:MET:HE3	2:H:216:VAL:CG1	1.83	1.08
2:G:209:LEU:HD23	2:G:212:MET:HE2	1.37	1.06
2:G:212:MET:HE1	2:G:216:VAL:CG1	1.86	1.04
2:G:212:MET:HE1	2:G:216:VAL:HG11	1.04	1.02
2:F:191:THR:HG22	2:H:191:THR:HG22	1.41	1.02
2:G:212:MET:CE	2:G:216:VAL:HG11	1.91	1.01
2:E:187[B]:ASN:HD22	2:G:187[B]:ASN:HD22	1.04	1.00
1:C:95:THR:HG21	1:C:109:MET:HE3	1.43	0.98
2:G:222:GLN:HG2	5:G:441:HOH:O	1.63	0.98
2:F:198:THR:HG21	5:H:411:HOH:O	1.65	0.97
2:E:191:THR:HG22	2:G:191:THR:HG22	1.47	0.96
2:H:244:GLN:HE21	2:H:244:GLN:H	1.09	0.96
1:B:95:THR:HG21	1:B:109:MET:CE	1.98	0.93
1:D:48:LYS:HE2	5:E:415:HOH:O	1.69	0.93
2:E:209:LEU:HD23	2:E:212:MET:HE3	1.51	0.92
1:B:10:ASN:HB3	5:B:403:HOH:O	1.69	0.92
1:C:120:ARG:HH11	1:C:120:ARG:HG3	1.31	0.91
2:E:187[B]:ASN:ND2	2:G:187[B]:ASN:HD22	1.67	0.90
1:C:95:THR:HG21	1:C:109:MET:CE	2.03	0.89
1:D:48:LYS:CE	5:E:415:HOH:O	2.22	0.86
2:F:209:LEU:HA	2:F:212:MET:HE2	1.57	0.86
2:G:152:ASP:HB3	2:G:154:LYS:H	1.39	0.86
2:H:212:MET:CE	2:H:216:VAL:HG11	2.05	0.86
1:B:48:LYS:HD3	1:B:71:THR:HG23	1.57	0.85
1:B:5:ARG:HG2	1:B:5:ARG:HH11	1.41	0.85
2:F:212:MET:HE3	2:F:216:VAL:CG1	2.07	0.85
2:H:217:ILE:HG23	2:H:225:LEU:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187[B]:ASN:ND2	2:G:187[B]:ASN:ND2	2.25	0.84
2:H:212:MET:CE	2:H:216:VAL:CG1	2.56	0.84
2:H:212:MET:HE3	2:H:216:VAL:HG11	1.58	0.83
1:B:95:THR:HG21	1:B:109:MET:HE3	1.59	0.82
2:E:187[B]:ASN:HD22	2:G:187[B]:ASN:ND2	1.78	0.81
2:E:209:LEU:CA	2:E:212:MET:HE1	2.09	0.80
2:G:244:GLN:HE21	2:G:244:GLN:H	1.28	0.80
2:G:255:PRO:HG3	2:G:274:THR:O	1.81	0.80
1:A:169:THR:HA	1:A:172:MET:CE	2.12	0.80
1:B:150:SER:OG	1:B:153:VAL:HG13	1.81	0.80
2:H:244:GLN:NE2	2:H:244:GLN:H	1.78	0.79
1:A:169:THR:HA	1:A:172:MET:HE2	1.64	0.79
2:H:152:ASP:HB3	2:H:154:LYS:H	1.46	0.79
2:F:212:MET:HE1	2:F:216:VAL:HG11	1.65	0.79
1:A:90:ARG:HD2	5:A:418:HOH:O	1.81	0.78
2:G:212:MET:CE	2:G:216:VAL:CG1	2.54	0.78
1:A:10:ASN:HB3	5:A:413:HOH:O	1.82	0.77
1:B:90:ARG:HD2	5:B:427:HOH:O	1.82	0.77
2:F:212:MET:CE	2:F:216:VAL:CG1	2.62	0.77
2:F:183:ARG:NH2	2:H:63:ASP:OD1	2.16	0.77
2:E:209:LEU:HD23	2:E:212:MET:CE	2.15	0.76
2:G:29:ARG:HH12	2:G:141:TRP:HZ2	1.33	0.76
2:F:225:LEU:HD23	2:F:244:GLN:HA	1.67	0.76
1:C:10:ASN:HB3	5:C:401:HOH:O	1.85	0.75
2:E:217:ILE:HD11	2:E:236:LEU:HD12	1.69	0.74
2:F:212:MET:CE	2:F:216:VAL:HG11	2.17	0.74
2:F:152:ASP:HB3	2:F:154:LYS:H	1.52	0.74
5:F:425:HOH:O	2:H:198:THR:HG21	1.86	0.74
2:E:198:THR:HG21	5:G:405:HOH:O	1.86	0.74
1:B:95:THR:HG21	1:B:109:MET:HE2	1.69	0.74
1:C:120:ARG:HH11	1:C:120:ARG:CG	2.00	0.73
2:G:217:ILE:HD11	2:G:236:LEU:HD12	1.69	0.73
2:H:212:MET:HE3	2:H:216:VAL:HG13	1.70	0.73
2:F:191:THR:CG2	2:H:191:THR:HG22	2.19	0.73
2:E:68:MET:HE3	2:G:173:ALA:HA	1.70	0.73
2:F:217:ILE:HD11	2:F:236:LEU:HD12	1.72	0.72
2:H:50:LYS:HE3	2:H:80:GLU:OE2	1.89	0.71
1:C:120:ARG:NH1	1:C:120:ARG:HG3	2.06	0.71
2:F:209:LEU:HD23	2:F:212:MET:HE1	1.72	0.70
1:B:99:GLN:HG2	5:B:423:HOH:O	1.90	0.70
2:G:209:LEU:HD23	2:G:212:MET:CE	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:ILE:HD11	2:H:236:LEU:HD12	1.72	0.69
2:E:152:ASP:HB3	2:E:154:LYS:H	1.55	0.69
1:C:108:GLN:OE1	1:C:111:ARG:NH1	2.24	0.69
1:A:128:LYS:HA	1:A:172:MET:HE1	1.75	0.69
2:F:191:THR:HG22	2:H:191:THR:CG2	2.20	0.69
2:E:214:ASP:OD2	5:E:447:HOH:O	2.11	0.68
2:E:217:ILE:CD1	2:E:236:LEU:HD12	2.24	0.68
5:B:432:HOH:O	2:G:41:VAL:HG12	1.94	0.67
2:H:209:LEU:HD23	2:H:212:MET:HE1	1.75	0.67
1:A:150:SER:OG	1:A:153:VAL:HG13	1.95	0.67
2:E:34:VAL:HG11	5:E:413:HOH:O	1.96	0.65
1:B:5:ARG:CG	1:B:5:ARG:HH11	2.08	0.65
1:A:169:THR:HG22	1:A:172:MET:HE2	1.79	0.65
2:E:173:ALA:HB3	2:G:173:ALA:HB3	1.79	0.65
2:E:187[A]:ASN:OD1	5:E:448:HOH:O	2.14	0.65
2:G:244:GLN:NE2	2:G:244:GLN:H	1.93	0.65
2:F:173:ALA:HA	2:H:68:MET:HE3	1.78	0.64
2:H:209:LEU:HD23	2:H:212:MET:CE	2.27	0.64
2:H:212:MET:HE1	2:H:216:VAL:HG11	1.80	0.64
2:H:209:LEU:HA	2:H:212:MET:HE2	1.79	0.64
2:E:244:GLN:H	2:E:244:GLN:HE21	1.45	0.64
2:H:30:GLU:CD	2:H:30:GLU:H	2.01	0.63
2:E:92:GLN:O	2:E:95:GLN:HG3	1.98	0.63
2:H:190:LEU:HD23	5:H:428:HOH:O	1.98	0.63
2:F:209:LEU:HD23	2:F:212:MET:CE	2.27	0.63
2:E:152:ASP:HB2	2:E:156:ARG:H	1.65	0.62
2:E:173:ALA:HA	2:G:68:MET:HE3	1.82	0.62
2:F:217:ILE:CD1	2:F:236:LEU:HD12	2.29	0.61
2:E:209:LEU:HA	2:E:212:MET:HE2	1.80	0.61
2:E:68:MET:CE	2:G:173:ALA:HA	2.29	0.61
1:A:104:GLU:O	1:A:108:GLN:HG2	2.01	0.60
5:E:418:HOH:O	2:G:198:THR:HG21	2.01	0.60
2:H:194:LEU:O	2:H:198:THR:HG22	2.02	0.60
1:C:104:GLU:O	1:C:108:GLN:HG2	2.02	0.60
2:G:29:ARG:NH1	2:G:141:TRP:HZ2	1.98	0.60
1:D:104:GLU:O	1:D:108:GLN:HG2	2.02	0.60
2:F:68:MET:HE3	2:H:173:ALA:HA	1.84	0.60
2:G:209:LEU:HA	2:G:212:MET:HE2	1.84	0.60
1:B:5:ARG:NH1	1:B:5:ARG:CG	2.65	0.59
2:E:18:THR:HG22	2:E:22:ARG:NH1	2.17	0.59
2:F:212:MET:HE3	2:F:216:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:216:VAL:H	2:H:229:ASN:ND2	2.00	0.59
2:F:216:VAL:H	2:F:229:ASN:ND2	1.98	0.59
1:D:120:ARG:HD2	5:G:439:HOH:O	2.03	0.59
2:F:173:ALA:HA	2:H:68:MET:CE	2.33	0.59
2:F:68:MET:CE	2:H:173:ALA:HB2	2.34	0.58
2:F:50:LYS:HD2	2:F:79:ASP:HB2	1.85	0.58
1:A:5:ARG:HB3	1:A:61:ILE:HG13	1.86	0.57
2:E:191:THR:HG22	2:G:191:THR:CG2	2.28	0.57
2:F:63:ASP:OD1	2:H:183:ARG:NH2	2.35	0.57
1:C:48:LYS:CE	5:G:436:HOH:O	2.51	0.57
1:A:74:SER:OG	5:A:444:HOH:O	2.18	0.57
1:C:48:LYS:HE3	5:G:436:HOH:O	2.04	0.57
2:E:173:ALA:HA	2:G:68:MET:CE	2.34	0.57
2:F:216:VAL:H	2:F:229:ASN:HD21	1.53	0.57
2:F:29:ARG:HH12	2:F:141:TRP:HZ2	1.52	0.57
2:H:225:LEU:HD23	2:H:244:GLN:HA	1.86	0.57
1:D:111:ARG:NH1	1:D:112:ASP:OD1	2.37	0.56
5:F:413:HOH:O	2:H:184:GLU:HG3	2.05	0.56
2:E:68:MET:HB2	2:G:176:PRO:HG3	1.87	0.56
2:E:206:ASN:O	2:E:210:GLU:HG3	2.05	0.56
2:F:29:ARG:NH1	2:F:141:TRP:HZ2	2.04	0.56
2:F:173:ALA:HB3	2:H:173:ALA:HB3	1.87	0.56
2:H:39:GLN:HG3	5:H:431:HOH:O	2.06	0.56
2:H:239:ASP:OD2	2:H:242:ALA:HB3	2.06	0.55
2:E:191:THR:CG2	2:G:187[B]:ASN:HD21	2.20	0.55
2:H:217:ILE:CD1	2:H:236:LEU:HD12	2.35	0.55
2:G:216:VAL:H	2:G:229:ASN:ND2	2.05	0.55
1:B:104:GLU:O	1:B:108:GLN:HG2	2.07	0.55
2:H:253:THR:HG23	2:H:276:GLU:HB3	1.88	0.54
1:A:128:LYS:HA	1:A:172:MET:CE	2.37	0.54
2:E:155:GLY:HA3	5:E:416:HOH:O	2.07	0.53
2:G:217:ILE:HG23	2:G:225:LEU:HD11	1.88	0.53
2:E:280:GLN:HE21	2:E:282:ILE:HD11	1.74	0.53
1:D:108:GLN:HG3	5:D:423:HOH:O	2.07	0.53
1:B:210:GLU:OE1	2:G:137:LYS:NZ	2.34	0.53
2:E:29:ARG:HB3	2:E:29:ARG:HH11	1.72	0.53
1:C:90:ARG:HB2	1:C:113:GLY:HA2	1.90	0.52
2:E:216:VAL:H	2:E:229:ASN:ND2	2.07	0.52
2:E:191:THR:CG2	2:G:191:THR:HG22	2.30	0.52
2:F:51:LYS:O	2:F:55:THR:HG23	2.09	0.52
2:H:30:GLU:HG3	5:H:444:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:244:GLN:NE2	2:E:244:GLN:H	2.07	0.52
2:E:217:ILE:HG23	2:E:225:LEU:HD11	1.92	0.52
2:G:61:LEU:HD22	2:G:77:ILE:HG12	1.91	0.52
2:G:217:ILE:CD1	2:G:236:LEU:HD12	2.36	0.52
1:B:101:LEU:HD11	1:B:109:MET:HE3	1.92	0.52
2:H:212:MET:CE	2:H:216:VAL:HG13	2.35	0.51
2:H:229:ASN:ND2	2:H:232:ALA:H	2.09	0.51
2:F:255:PRO:HG3	2:F:274:THR:O	2.10	0.51
2:F:30:GLU:H	2:F:30:GLU:CD	2.14	0.51
2:F:244:GLN:HE21	2:F:244:GLN:H	1.57	0.51
2:H:121:ALA:HB1	2:H:149:PRO:HD3	1.93	0.51
2:H:76:PHE:CE1	2:H:87:ARG:HG2	2.45	0.51
2:E:187[B]:ASN:OD1	2:E:190:LEU:HD23	2.11	0.51
1:A:169:THR:CA	1:A:172:MET:HE2	2.39	0.51
1:A:169:THR:HG22	1:A:172:MET:CE	2.41	0.51
2:F:220:ASP:HB3	2:F:222:GLN:H	1.75	0.50
2:F:200:ARG:NH1	2:H:295:GLN:HG3	2.25	0.50
2:H:216:VAL:H	2:H:229:ASN:HD21	1.57	0.50
2:E:50:LYS:NZ	2:E:158:THR:OG1	2.44	0.50
2:E:53:MET:HE1	2:E:85:LEU:CD1	2.41	0.50
1:C:107:TYR:CE1	1:C:142:ARG:HB2	2.46	0.50
2:F:215:GLY:HA2	2:F:229:ASN:HD21	1.77	0.50
2:E:39:GLN:HB2	5:E:420:HOH:O	2.12	0.49
2:G:216:VAL:H	2:G:229:ASN:HD21	1.57	0.49
2:H:214:ASP:OD1	2:H:305:PRO:HD3	2.13	0.49
2:H:61:LEU:HD22	2:H:77:ILE:HG12	1.93	0.49
1:D:90:ARG:HD2	1:D:93:GLN:HE21	1.77	0.49
2:E:220:ASP:HB3	2:E:222[A]:GLN:H	1.78	0.48
1:A:5:ARG:NH1	1:A:5:ARG:HG3	2.28	0.48
2:F:79:ASP:HB3	2:F:85:LEU:HD11	1.95	0.48
1:C:150:SER:OG	1:C:153:VAL:HG13	2.14	0.48
2:H:50:LYS:NZ	2:H:158:THR:OG1	2.46	0.48
2:E:212:MET:HE3	2:E:216:VAL:HG11	1.95	0.48
2:F:217:ILE:CD1	2:F:236:LEU:CD1	2.91	0.48
2:F:121:ALA:HB1	2:F:149:PRO:HD3	1.96	0.48
2:E:285:VAL:HG12	2:E:306:VAL:HG22	1.96	0.47
1:A:48:LYS:CD	1:A:71:THR:HG23	2.44	0.47
2:G:152:ASP:HB3	2:G:154:LYS:N	2.19	0.47
1:A:156:GLU:OE1	1:A:209:LYS:NZ	2.43	0.47
1:C:71:THR:O	1:C:75:SER:HB3	2.15	0.47
2:E:191:THR:HG21	2:G:187[B]:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:MET:HE3	2:G:216:VAL:CG1	2.44	0.47
2:G:50:LYS:HE3	2:G:80:GLU:OE2	2.15	0.47
2:H:187:ASN:O	2:H:191:THR:HG23	2.15	0.47
1:D:108:GLN:NE2	5:D:423:HOH:O	2.48	0.47
2:E:220:ASP:HB3	2:E:222[B]:GLN:H	1.79	0.47
2:E:53:MET:HE2	2:E:53:MET:HB3	1.66	0.47
2:H:30:GLU:CD	2:H:30:GLU:N	2.68	0.46
2:F:176:PRO:HG3	2:H:68:MET:HB2	1.97	0.46
2:E:176:PRO:HG3	2:G:68:MET:HB2	1.97	0.46
2:E:50:LYS:HE3	2:E:80:GLU:OE2	2.15	0.46
2:E:280:GLN:HE21	2:E:282:ILE:CD1	2.27	0.46
1:D:70:MET:HE3	1:D:89:ILE:HD11	1.98	0.46
1:B:106:LEU:HD11	1:B:155:LEU:HD21	1.98	0.46
1:A:133:VAL:CG2	1:A:194:ALA:HB1	2.46	0.46
2:E:76:PHE:CE1	2:E:87:ARG:HG2	2.52	0.45
1:A:149:LEU:HB3	1:A:153:VAL:HG22	1.99	0.45
2:E:194:LEU:O	2:E:198:THR:HG22	2.16	0.45
2:E:246:ARG:HG2	2:E:246:ARG:HH11	1.81	0.45
2:E:30:GLU:H	2:E:30:GLU:CD	2.19	0.45
2:E:68:MET:CE	2:G:173:ALA:CA	2.94	0.45
2:F:216:VAL:O	2:F:228:ILE:HA	2.16	0.45
2:F:68:MET:CE	2:H:173:ALA:CB	2.94	0.45
2:G:148:THR:HG21	2:G:179:LEU:HA	1.98	0.45
1:A:70:MET:SD	2:H:190:LEU:HD21	2.56	0.45
2:H:53:MET:HE2	2:H:53:MET:HB3	1.93	0.45
1:B:133:VAL:O	1:B:137:VAL:HG23	2.16	0.45
1:C:48:LYS:HE2	5:G:436:HOH:O	2.16	0.45
1:C:5:ARG:HB3	1:C:61:ILE:HG13	1.99	0.45
2:E:61:LEU:HD22	2:E:77:ILE:HG12	1.98	0.45
2:H:65:TRP:CD2	2:H:89:GLY:HA2	2.52	0.45
1:A:5:ARG:HG3	1:A:5:ARG:HH11	1.80	0.45
2:E:247:ALA:HB3	2:E:250:GLU:HG3	1.98	0.45
2:F:225:LEU:HD23	2:F:244:GLN:CA	2.43	0.45
2:F:244:GLN:NE2	2:F:244:GLN:H	2.15	0.45
1:A:135:VAL:HB	1:A:136:PRO:HD3	1.99	0.45
1:A:169:THR:HA	1:A:172:MET:HE3	1.94	0.44
1:B:90:ARG:HB2	1:B:113:GLY:HA2	1.99	0.44
2:F:56:LEU:HD13	2:F:188:LEU:HB3	1.98	0.44
2:F:87:ARG:HD3	2:F:104:ASP:OD2	2.17	0.44
2:E:217:ILE:CD1	2:E:236:LEU:CD1	2.95	0.44
2:E:198:THR:HB	2:G:198:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:217:ILE:CD1	2:G:236:LEU:CD1	2.95	0.44
1:A:90:ARG:HG3	1:A:116:GLY:HA3	2.00	0.44
1:D:70:MET:HG2	2:E:195:LEU:HD11	1.98	0.44
2:E:152:ASP:HB2	2:E:156:ARG:N	2.31	0.44
2:H:56:LEU:HD13	2:H:188:LEU:HB3	2.00	0.44
2:E:217:ILE:HG23	2:E:225:LEU:CD1	2.48	0.44
1:B:101:LEU:HD11	1:B:109:MET:CE	2.48	0.44
2:F:49:ARG:NE	5:F:414:HOH:O	2.51	0.44
2:E:216:VAL:H	2:E:229:ASN:HD21	1.66	0.43
2:F:239:ASP:OD2	2:F:242:ALA:HB3	2.18	0.43
2:F:77:ILE:HG13	2:F:86:SER:HB3	1.99	0.43
2:F:88:ASN:N	2:F:88:ASN:HD22	2.16	0.43
2:G:61:LEU:HD12	2:G:61:LEU:HA	1.83	0.43
1:D:90:ARG:HD2	1:D:93:GLN:NE2	2.33	0.43
1:B:140:SER:HB2	1:B:161:ILE:HG13	2.00	0.43
1:C:101:LEU:HD11	1:C:109:MET:HE3	2.00	0.43
1:C:52:LYS:HG2	5:C:427:HOH:O	2.17	0.43
2:E:285:VAL:HG13	2:E:304:HIS:HB2	2.00	0.43
2:G:18:THR:HG22	2:G:22:ARG:NH1	2.33	0.43
1:D:66:LYS:O	1:D:70:MET:HB2	2.19	0.43
2:G:277:SER:HB3	2:G:278:GLN:H	1.71	0.43
1:A:120:ARG:HG3	5:A:431:HOH:O	2.19	0.43
2:H:51:LYS:O	2:H:55:THR:HG23	2.18	0.43
1:B:107:TYR:CE1	1:B:142:ARG:HB2	2.54	0.42
1:B:5:ARG:HB3	1:B:61:ILE:HG13	2.01	0.42
2:E:148:THR:HG21	2:E:179:LEU:HA	2.02	0.42
2:F:39:GLN:HE21	2:F:39:GLN:HB3	1.61	0.42
2:H:39:GLN:O	2:H:42:THR:HG23	2.19	0.42
2:E:271:VAL:HG12	2:E:272:GLU:N	2.33	0.42
2:G:39:GLN:HE21	2:G:39:GLN:HB3	1.57	0.42
1:A:48:LYS:HD3	1:A:71:THR:HG23	2.02	0.42
2:E:152:ASP:OD2	2:E:156:ARG:HB2	2.20	0.42
2:E:215:GLY:HA2	2:E:229:ASN:HD21	1.84	0.42
2:G:304:HIS:HA	2:G:305:PRO:HD3	1.83	0.42
1:D:133:VAL:O	1:D:137:VAL:HG23	2.20	0.42
2:E:51:LYS:O	2:E:55:THR:HG23	2.20	0.42
1:B:101:LEU:CD1	1:B:109:MET:HE3	2.50	0.42
2:E:68:MET:HE1	2:G:173:ALA:HB2	2.02	0.42
1:A:107:TYR:CE1	1:A:142:ARG:HB2	2.55	0.42
2:G:126:GLN:O	2:G:128:VAL:HG23	2.20	0.42
2:E:304:HIS:HA	2:E:305:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:MET:CE	2:H:173:ALA:HA	2.49	0.41
1:C:95:THR:HG21	1:C:109:MET:HE2	1.98	0.41
2:F:212:MET:CE	2:F:216:VAL:HG13	2.44	0.41
2:G:286:ILE:HA	2:G:302:LEU:O	2.21	0.41
1:C:90:ARG:HG3	1:C:116:GLY:HA3	2.03	0.41
1:D:150:SER:OG	1:D:153:VAL:HG13	2.21	0.41
1:D:3:LEU:HD23	1:D:8:ILE:HD11	2.02	0.41
2:E:147:ALA:HA	2:E:161:ILE:O	2.21	0.41
2:H:217:ILE:HG23	2:H:225:LEU:CD1	2.40	0.41
2:F:173:ALA:CA	2:H:68:MET:CE	2.98	0.41
1:C:84:PHE:CE2	1:C:200:MET:CE	3.04	0.41
2:E:50:LYS:HD3	2:E:50:LYS:HA	1.80	0.41
2:F:30:GLU:N	2:F:30:GLU:CD	2.75	0.41
2:E:68:MET:CE	2:G:173:ALA:HB2	2.51	0.41
2:H:133:ASP:HA	2:H:141:TRP:CD1	2.56	0.41
2:E:216:VAL:O	2:E:228:ILE:HA	2.21	0.41
2:E:255:PRO:HG2	2:E:258:LEU:HD12	2.03	0.41
2:E:39:GLN:HE21	2:E:39:GLN:HB3	1.56	0.41
2:G:121:ALA:HB1	2:G:149:PRO:HD3	2.02	0.41
2:H:246:ARG:HE	2:H:251:LEU:HD21	1.86	0.41
1:D:108:GLN:CG	5:D:423:HOH:O	2.66	0.40
1:A:120:ARG:HD2	2:H:151:PHE:CZ	2.56	0.40
2:H:76:PHE:CD1	2:H:87:ARG:HG2	2.56	0.40
1:A:5:ARG:HB3	1:A:61:ILE:CG1	2.51	0.40
2:F:247:ALA:HB3	2:F:250:GLU:HG2	2.02	0.40
1:B:48:LYS:HE3	5:H:423:HOH:O	2.22	0.40
2:F:236:LEU:HD13	2:F:252:LEU:CD1	2.52	0.40
2:H:244:GLN:NE2	2:H:244:GLN:N	2.57	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	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
1	B	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
1	C	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
1	D	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
2	E	294/318 (92%)	284 (97%)	8 (3%)	2 (1%)	22	26
2	F	293/318 (92%)	284 (97%)	6 (2%)	3 (1%)	15	17
2	G	294/318 (92%)	285 (97%)	6 (2%)	3 (1%)	15	17
2	H	287/318 (90%)	280 (98%)	6 (2%)	1 (0%)	41	50
All	All	2004/2116 (95%)	1951 (97%)	44 (2%)	9 (0%)	29	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	152	ASP
2	F	152	ASP
2	G	152	ASP
2	H	152	ASP
2	E	40	GLY
2	F	40	GLY
2	F	278	GLN
2	G	40	GLY
2	G	71	ARG

### 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	169/169 (100%)	157 (93%)	12 (7%)	14	19
1	B	169/169 (100%)	159 (94%)	10 (6%)	19	26
1	C	169/169 (100%)	157 (93%)	12 (7%)	14	19
1	D	169/169 (100%)	158 (94%)	11 (6%)	17	22
2	E	243/260 (94%)	218 (90%)	25 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	242/260 (93%)	214 (88%)	28 (12%)	5	5
2	G	243/260 (94%)	212 (87%)	31 (13%)	4	4
2	H	238/260 (92%)	209 (88%)	29 (12%)	5	5
All	All	1642/1716 (96%)	1484 (90%)	158 (10%)	8	9

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	8	ILE
1	A	52	LYS
1	A	99	GLN
1	A	100	SER
1	A	106	LEU
1	A	108	GLN
1	A	117	VAL
1	A	120	ARG
1	A	153	VAL
1	A	178	ARG
1	A	206	LEU
1	B	5	ARG
1	B	8	ILE
1	B	99	GLN
1	B	106	LEU
1	B	111	ARG
1	B	117	VAL
1	B	119	SER
1	B	120	ARG
1	B	156	GLU
1	B	206	LEU
1	C	5	ARG
1	C	18	ILE
1	C	52	LYS
1	C	75	SER
1	C	99	GLN
1	C	106	LEU
1	C	117	VAL
1	C	120	ARG
1	C	124	GLU
1	C	153	VAL
1	C	156	GLU

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Mol	Chain	Res	Type
1	C	206	LEU
1	D	8	ILE
1	D	47	SER
1	D	52	LYS
1	D	70	MET
1	D	99	GLN
1	D	100	SER
1	D	117	VAL
1	D	119	SER
1	D	120	ARG
1	D	153	VAL
1	D	206	LEU
2	E	16	ILE
2	E	29	ARG
2	E	30	GLU
2	E	39	GLN
2	E	42	THR
2	E	48	ARG
2	E	53	MET
2	E	80	GLU
2	E	88	ASN
2	E	120	LEU
2	E	150	LEU
2	E	188	LEU
2	E	191	THR
2	E	198	THR
2	E	216	VAL
2	E	220	ASP
2	E	229	ASN
2	E	244	GLN
2	E	248	ILE
2	E	252	LEU
2	E	259	GLN
2	E	278	GLN
2	E	282	ILE
2	E	285	VAL
2	E	295	GLN
2	F	30	GLU
2	F	33	ASN
2	F	39	GLN
2	F	41	VAL
2	F	42	THR

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Mol	Chain	Res	Type
2	F	53	MET
2	F	77	ILE
2	F	80	GLU
2	F	88	ASN
2	F	120	LEU
2	F	126	GLN
2	F	150	LEU
2	F	153	SER
2	F	156	ARG
2	F	188	LEU
2	F	198	THR
2	F	216	VAL
2	F	220	ASP
2	F	229	ASN
2	F	244	GLN
2	F	252	LEU
2	F	259	GLN
2	F	279	HIS
2	F	280	GLN
2	F	282	ILE
2	F	283	ASP
2	F	285	VAL
2	F	295	GLN
2	G	16	ILE
2	G	28	LYS
2	G	30	GLU
2	G	39	GLN
2	G	42	THR
2	G	53	MET
2	G	54	LEU
2	G	61	LEU
2	G	73	CYS
2	G	80	GLU
2	G	88	ASN
2	G	120	LEU
2	G	150	LEU
2	G	153	SER
2	G	154	LYS
2	G	188	LEU
2	G	198	THR
2	G	216	VAL
2	G	220	ASP

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Mol	Chain	Res	Type
2	G	229	ASN
2	G	244	GLN
2	G	252	LEU
2	G	253	THR
2	G	257	VAL
2	G	258	LEU
2	G	271	VAL
2	G	272	GLU
2	G	277	SER
2	G	282	ILE
2	G	285	VAL
2	G	295	GLN
2	H	29	ARG
2	H	30	GLU
2	H	39	GLN
2	H	42	THR
2	H	53	MET
2	H	54	LEU
2	H	61	LEU
2	H	80	GLU
2	H	88	ASN
2	H	95	GLN
2	H	120	LEU
2	H	126	GLN
2	H	150	LEU
2	H	153	SER
2	H	154	LYS
2	H	171	THR
2	H	188	LEU
2	H	193	SER
2	H	198	THR
2	H	216	VAL
2	H	229	ASN
2	H	244	GLN
2	H	248	ILE
2	H	253	THR
2	H	263	LYS
2	H	282	ILE
2	H	283	ASP
2	H	285	VAL
2	H	295	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	67	ASN
1	A	96	GLN
1	A	108	GLN
1	A	143	GLN
1	A	189	HIS
1	B	41	ASN
1	B	67	ASN
1	B	96	GLN
1	B	143	GLN
1	B	173	GLN
1	C	41	ASN
1	C	67	ASN
1	C	96	GLN
1	C	143	GLN
1	C	189	HIS
1	D	41	ASN
1	D	96	GLN
1	D	143	GLN
1	D	173	GLN
1	D	189	HIS
2	E	39	GLN
2	E	88	ASN
2	E	226	GLN
2	E	229	ASN
2	E	244	GLN
2	E	280	GLN
2	E	295	GLN
2	F	39	GLN
2	F	88	ASN
2	F	226	GLN
2	F	229	ASN
2	F	244	GLN
2	G	39	GLN
2	G	88	ASN
2	G	126	GLN
2	G	226	GLN
2	G	229	ASN
2	G	244	GLN
2	H	88	ASN
2	H	226	GLN
2	H	229	ASN

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Mol	Chain	Res	Type
2	H	244	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
3	ADP	C	300	4	24,29,29	0.96	1 (4%)	29,45,45	1.42	7 (24%)
3	ADP	D	300	4	24,29,29	0.98	0	29,45,45	1.42	4 (13%)
3	ADP	A	300	4	24,29,29	1.00	1 (4%)	29,45,45	1.50	6 (20%)
3	ADP	B	300	4	24,29,29	0.95	1 (4%)	29,45,45	1.61	6 (20%)

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	C	300	4	-	0/12/32/32	0/3/3/3
3	ADP	D	300	4	-	0/12/32/32	0/3/3/3
3	ADP	A	300	4	-	0/12/32/32	0/3/3/3
3	ADP	B	300	4	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	300	ADP	O4'-C1'	2.41	1.44	1.41
3	B	300	ADP	C5-C4	2.12	1.46	1.40
3	A	300	ADP	C5-C4	2.01	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	300	ADP	N3-C2-N1	-3.79	122.75	128.68
3	B	300	ADP	N3-C2-N1	-3.77	122.79	128.68
3	A	300	ADP	N3-C2-N1	-3.64	122.98	128.68
3	C	300	ADP	N3-C2-N1	-3.33	123.47	128.68
3	A	300	ADP	C3'-C2'-C1'	3.20	105.80	100.98
3	B	300	ADP	PA-O3A-PB	-3.01	122.49	132.83
3	D	300	ADP	C3'-C2'-C1'	2.88	105.32	100.98
3	B	300	ADP	C2-N1-C6	2.79	123.53	118.75
3	C	300	ADP	C4-C5-N7	-2.73	106.55	109.40
3	D	300	ADP	C4-C5-N7	-2.70	106.59	109.40
3	B	300	ADP	C3'-C2'-C1'	2.61	104.91	100.98
3	C	300	ADP	C1'-N9-C4	-2.54	122.18	126.64
3	A	300	ADP	C4-C5-N7	-2.52	106.78	109.40
3	A	300	ADP	PA-O3A-PB	-2.51	124.21	132.83
3	B	300	ADP	C4-C5-N7	-2.49	106.80	109.40
3	C	300	ADP	PA-O3A-PB	-2.48	124.31	132.83
3	C	300	ADP	C3'-C2'-C1'	2.46	104.68	100.98
3	B	300	ADP	C1'-N9-C4	-2.34	122.54	126.64
3	A	300	ADP	C2-N1-C6	2.25	122.60	118.75
3	C	300	ADP	C2-N1-C6	2.22	122.56	118.75
3	D	300	ADP	C1'-N9-C4	-2.13	122.89	126.64
3	C	300	ADP	O2'-C2'-C1'	-2.07	103.20	110.85
3	A	300	ADP	O3B-PB-O2B	2.03	115.41	107.64

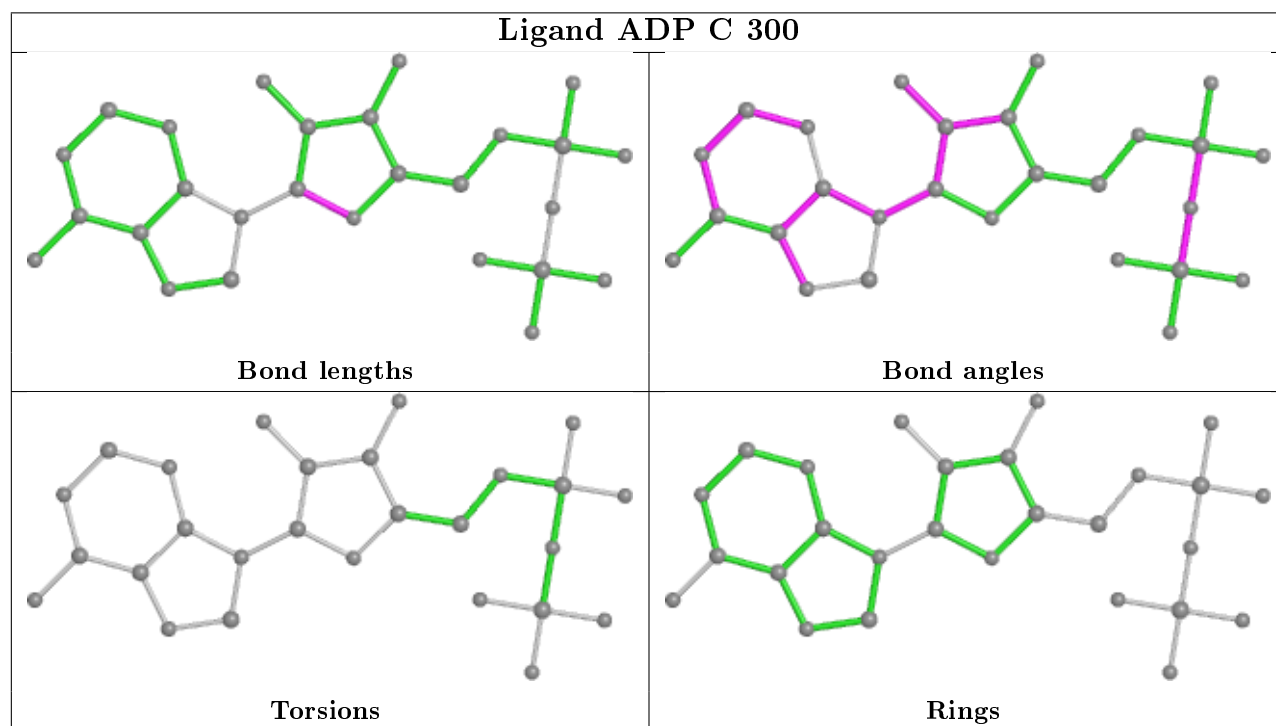
There are no chirality outliers.

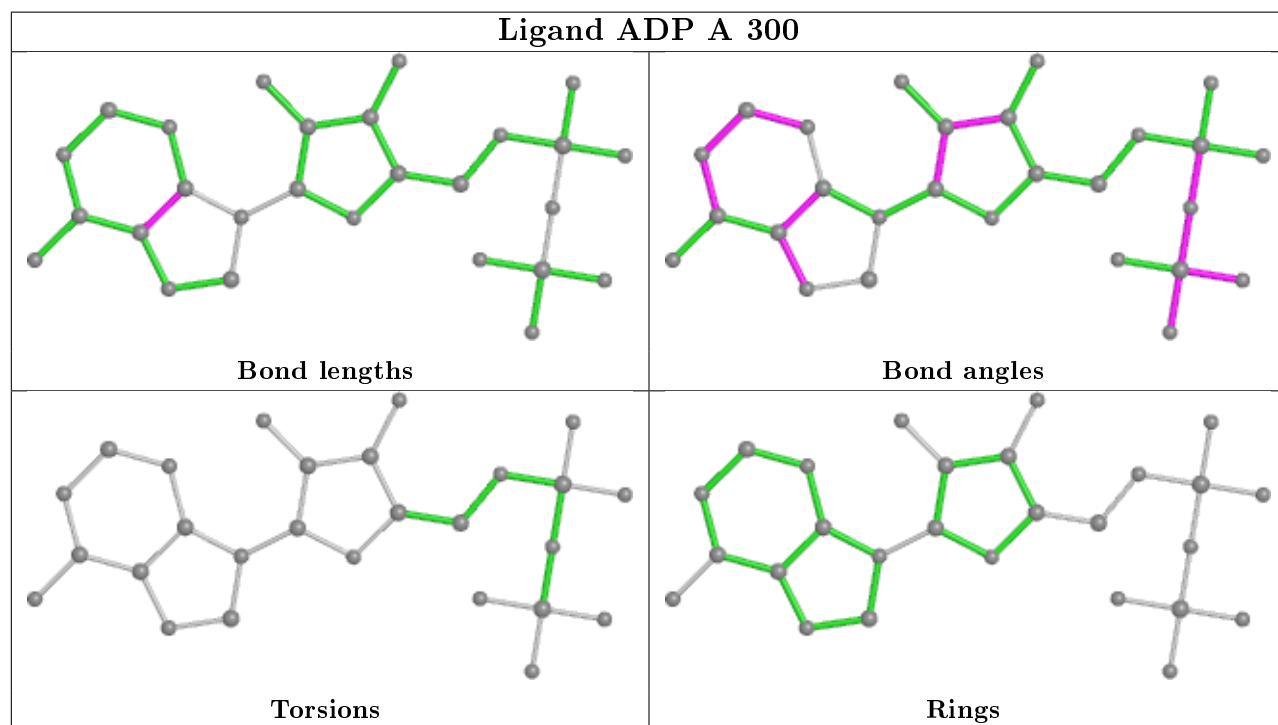
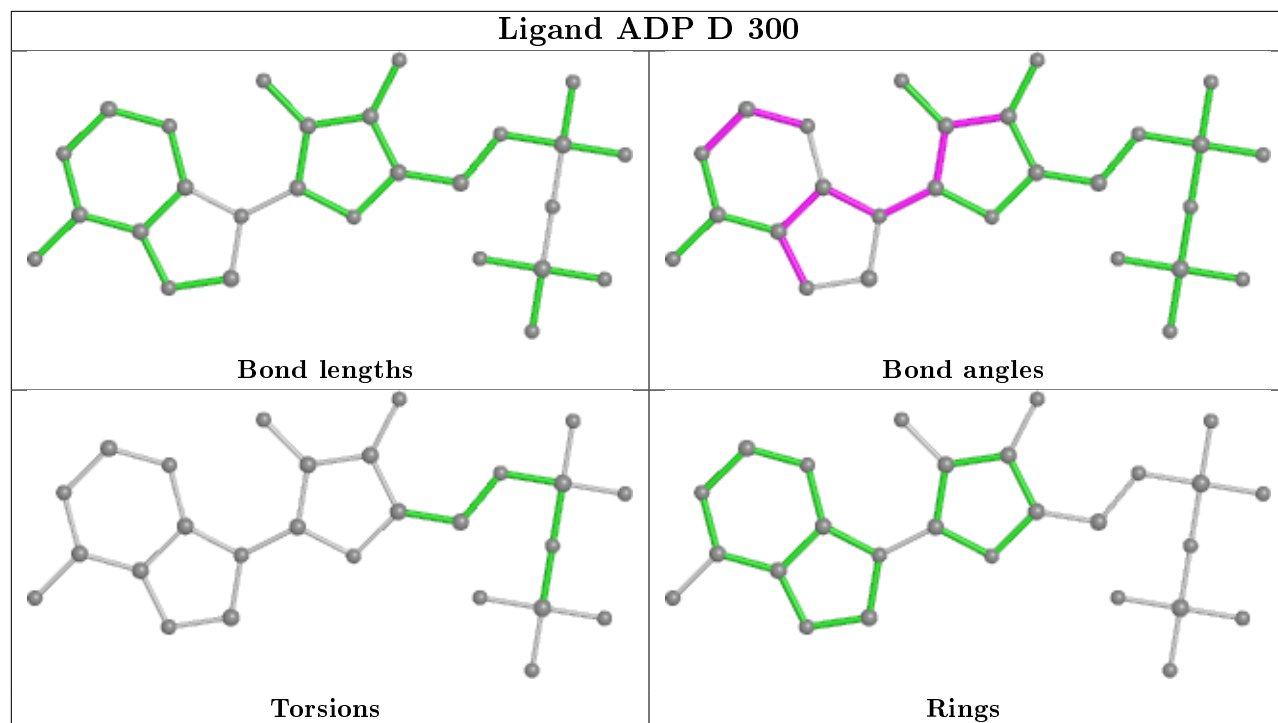
There are no torsion outliers.

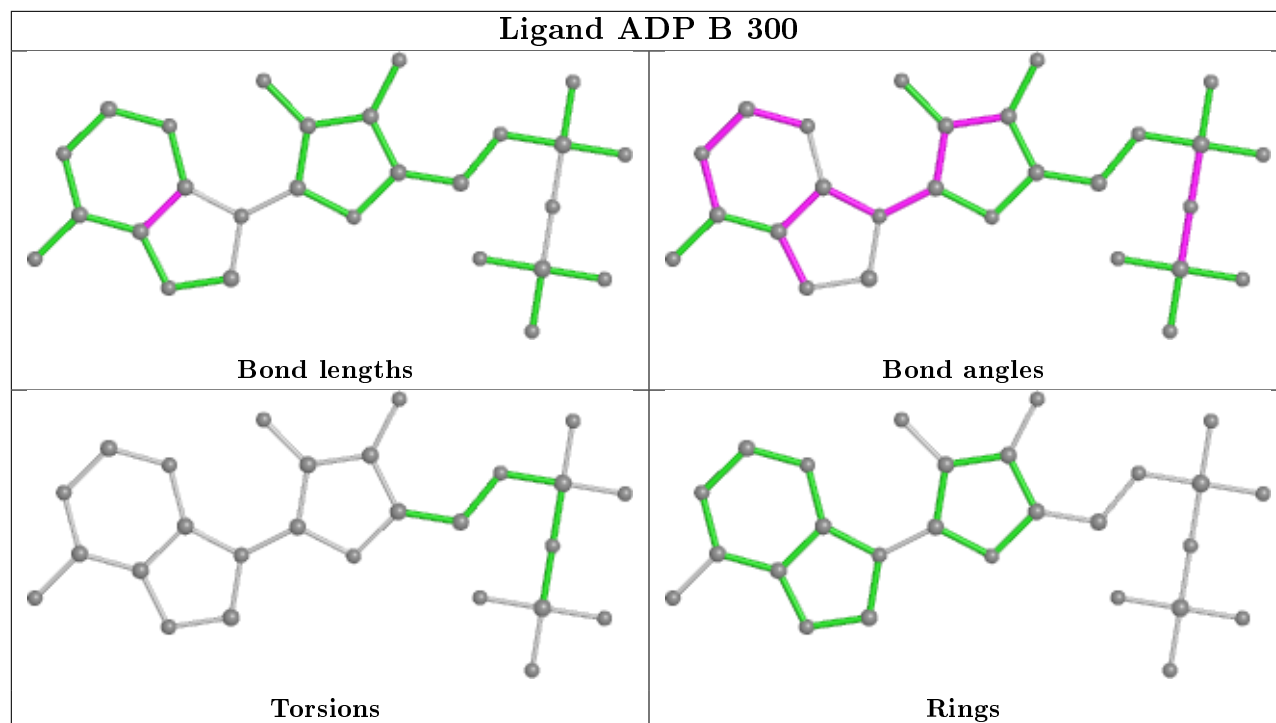
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/211 (100%)	0.29	10 (4%) 31 38	28, 39, 57, 69	0
1	B	211/211 (100%)	0.20	10 (4%) 31 38	28, 40, 56, 66	0
1	C	211/211 (100%)	0.25	10 (4%) 31 38	28, 39, 57, 68	0
1	D	211/211 (100%)	0.18	11 (5%) 27 34	28, 39, 56, 69	0
2	E	294/318 (92%)	0.59	30 (10%) 6 10	27, 45, 89, 116	0
2	F	294/318 (92%)	0.57	25 (8%) 10 15	29, 45, 89, 119	0
2	G	294/318 (92%)	0.34	15 (5%) 28 35	28, 44, 74, 97	0
2	H	291/318 (91%)	0.52	22 (7%) 13 18	29, 45, 79, 115	0
All	All	2017/2116 (95%)	0.39	133 (6%) 18 24	27, 42, 77, 119	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	281	PHE	7.2
2	E	277	SER	7.1
2	H	281	PHE	6.9
2	F	277	SER	6.5
2	F	279	HIS	6.2
2	E	279	HIS	5.7
2	F	306	VAL	5.4
2	H	276	GLU	5.3
2	F	278	GLN	5.0
2	H	282	ILE	4.9
1	D	187	ILE	4.5
2	G	279	HIS	4.4
2	E	278	GLN	4.3
2	F	276	GLU	4.2
2	E	306	VAL	4.2
2	H	306	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	33	ILE	4.1
2	G	277	SER	4.0
2	F	280	GLN	4.0
2	G	278	GLN	3.9
2	F	275	PHE	3.8
1	C	173	GLN	3.8
2	E	257	VAL	3.8
1	D	33	ILE	3.8
2	E	240	ALA	3.7
1	A	187	ILE	3.6
1	D	184	GLU	3.6
1	A	33	ILE	3.6
2	H	280	GLN	3.6
2	F	256	ALA	3.6
1	B	33	ILE	3.6
2	E	281	PHE	3.4
1	A	182	LEU	3.4
2	E	276	GLU	3.4
2	F	257	VAL	3.3
1	B	186	SER	3.3
2	E	180	ALA	3.1
1	C	187	ILE	3.1
2	F	282	ILE	3.1
2	E	280	GLN	3.0
2	F	274	THR	3.0
2	E	274	THR	3.0
2	H	136	PHE	3.0
1	A	185	ARG	2.9
1	C	179	ALA	2.9
2	H	265	ALA	2.9
2	H	260	GLN	2.8
2	G	280	GLN	2.7
2	F	262	ILE	2.7
2	E	236	LEU	2.7
2	F	253	THR	2.7
1	D	170	ILE	2.7
2	F	263	LYS	2.7
2	G	276	GLU	2.7
2	H	20	TRP	2.7
2	F	237	ARG	2.7
1	D	171	THR	2.7
2	H	249	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	187	ILE	2.6
1	C	184	GLU	2.6
2	E	181	ILE	2.6
2	E	177	LEU	2.6
2	H	39	GLN	2.6
2	F	284	ALA	2.6
2	G	260	GLN	2.6
1	C	188	GLY	2.6
2	E	39	GLN	2.6
1	B	0	GLY	2.5
2	E	258	LEU	2.5
1	A	181	TYR	2.5
1	B	173	GLN	2.5
2	H	237	ARG	2.5
2	G	180	ALA	2.5
1	A	188	GLY	2.5
2	H	141	TRP	2.5
2	E	256	ALA	2.5
1	A	170	ILE	2.5
1	B	184	GLU	2.4
2	F	283	ASP	2.4
1	C	186	SER	2.4
2	G	39	GLN	2.4
1	A	184	GLU	2.4
2	H	240	ALA	2.4
1	D	186	SER	2.4
1	D	181	TYR	2.4
2	H	283	ASP	2.4
1	D	188	GLY	2.3
2	E	251	LEU	2.3
2	G	21	GLU	2.3
2	E	260	GLN	2.3
2	E	264	GLN	2.3
1	B	170	ILE	2.3
2	F	254	LEU	2.3
2	F	264	GLN	2.3
2	E	266	HIS	2.3
2	G	185	VAL	2.3
2	H	257	VAL	2.3
2	H	256	ALA	2.3
2	E	185	VAL	2.2
2	F	141	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	189	HIS	2.2
2	G	176	PRO	2.2
1	A	0	GLY	2.2
1	B	169	THR	2.2
1	C	126	GLY	2.2
2	E	261	ALA	2.2
1	A	172	MET	2.2
1	C	0	GLY	2.2
1	B	175	ARG	2.2
2	F	271	VAL	2.2
2	E	253	THR	2.2
2	G	17	ALA	2.2
2	H	191	THR	2.2
2	H	274	THR	2.2
2	E	268	LEU	2.2
2	E	272	GLU	2.2
2	F	285	VAL	2.2
1	D	128	LYS	2.1
2	E	275	PHE	2.1
2	G	181	ILE	2.1
2	G	237	ARG	2.1
1	D	179	ALA	2.1
2	F	249	THR	2.1
2	E	237	ARG	2.1
1	C	182	LEU	2.1
1	B	188	GLY	2.1
2	H	263	LYS	2.1
2	E	182	ALA	2.1
2	F	260	GLN	2.0
2	E	252	LEU	2.0
2	H	26	LEU	2.0
2	H	181	ILE	2.0
2	G	177	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

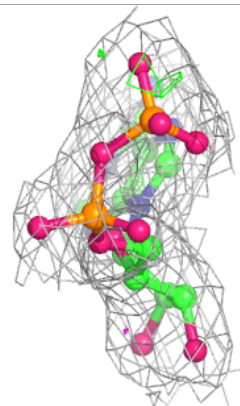
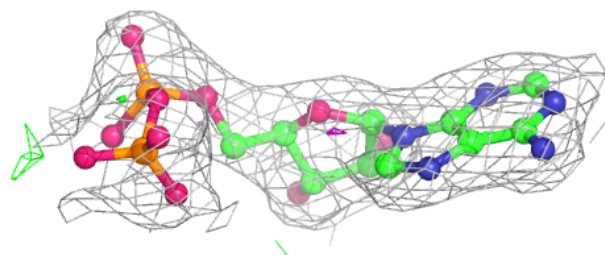
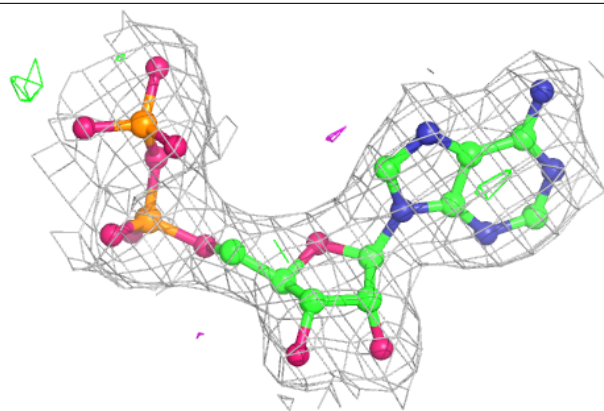
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	B	302	1/1	0.81	0.17	36,36,36,36	0
4	MG	D	301	1/1	0.91	0.06	35,35,35,35	0
4	MG	D	302	1/1	0.92	0.21	39,39,39,39	0
4	MG	A	302	1/1	0.93	0.13	36,36,36,36	0
4	MG	A	301	1/1	0.93	0.05	35,35,35,35	0
4	MG	C	302	1/1	0.94	0.15	40,40,40,40	0
4	MG	B	301	1/1	0.96	0.06	34,34,34,34	0
4	MG	C	301	1/1	0.96	0.07	34,34,34,34	0
3	ADP	D	300	27/27	0.98	0.14	31,36,39,41	0
3	ADP	A	300	27/27	0.98	0.14	29,36,39,40	0
3	ADP	B	300	27/27	0.98	0.15	32,34,38,40	0
3	ADP	C	300	27/27	0.98	0.13	32,35,38,38	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.

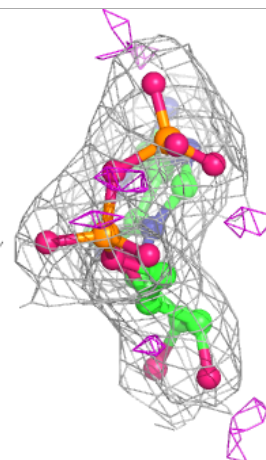
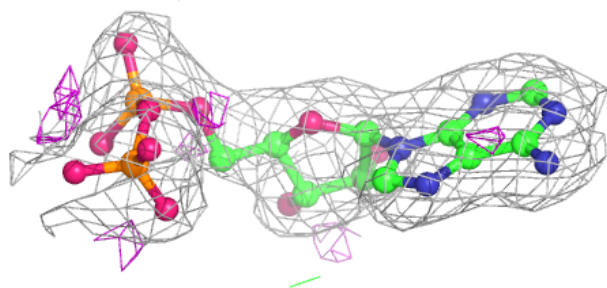
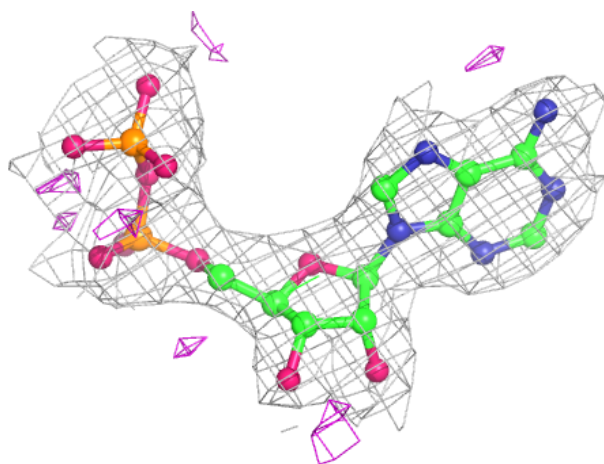
**Electron density around ADP D 300:**

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



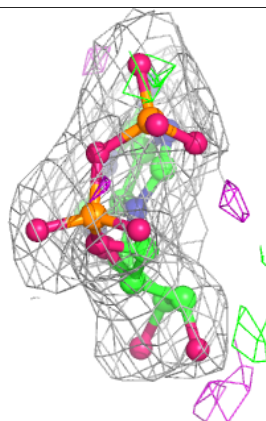
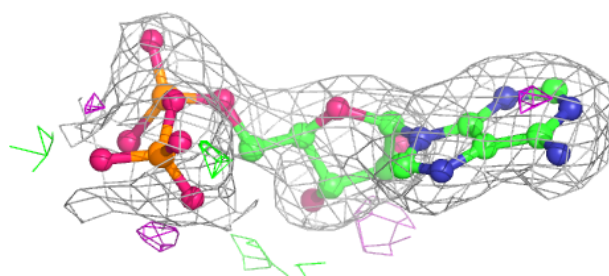
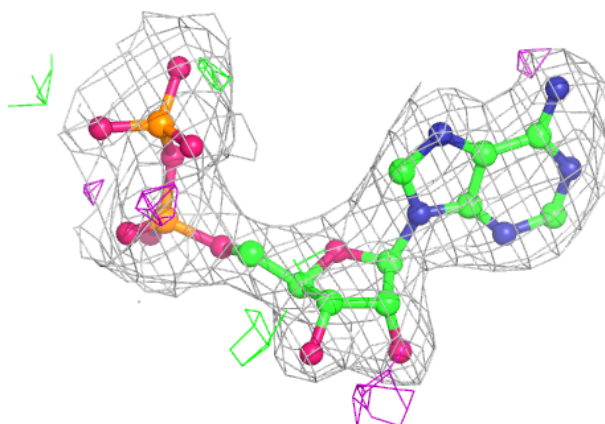
**Electron density around ADP A 300:**

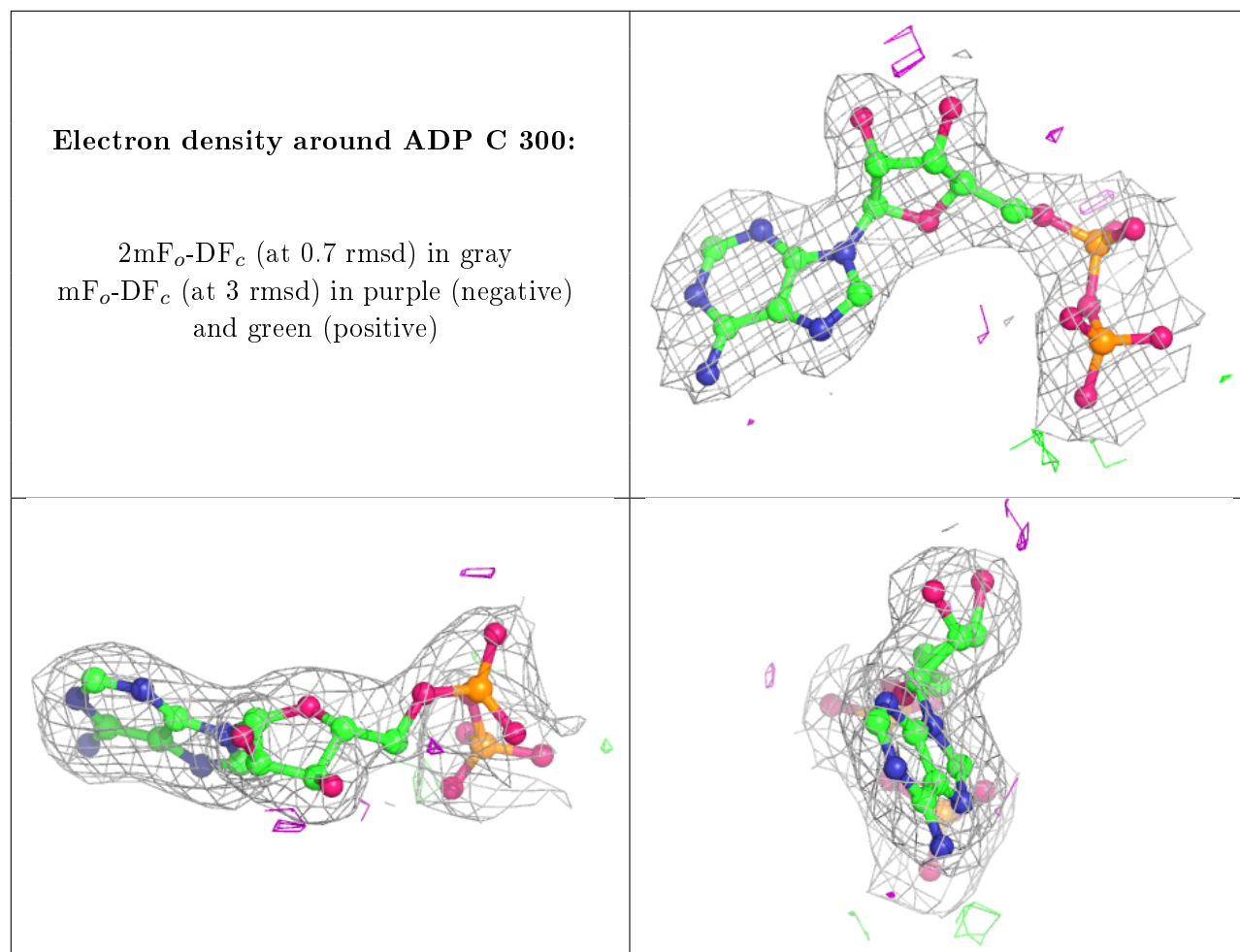
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADP B 300:**

$2mF_o - DF_c$  (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.