



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2024 – 11:48 am BST

PDB ID : 2CH6  
Title : Crystal structure of human N-acetylglucosamine kinase in complex with ADP and glucose  
Authors : Weihofen, W.A.; Berger, M.; Chen, H.; Saenger, W.; Hinderlich, S.  
Deposited on : 2006-03-13  
Resolution : 2.72 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

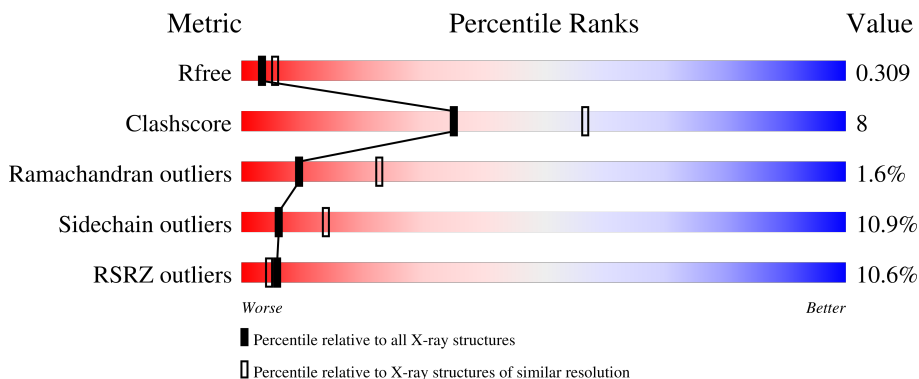
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	344	 4% 80% 15% .
1	B	344	 21% 66% 19% 5% 10%
1	C	344	 13% 73% 21% 5% .
1	D	344	 3% 81% 15% .

## 2 Entry composition [i](#)

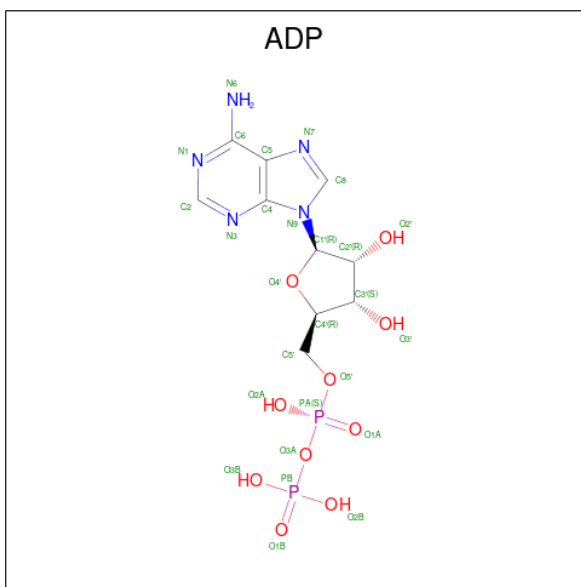
There are 3 unique types of molecules in this entry. The entry contains 10315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-ACETYL-D-GLUCOSAMINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	Total	C	N	O	S	0	0	0
			2623	1665	456	489	13			
1	B	310	Total	C	N	O	S	0	0	0
			2363	1497	409	444	13			
1	C	337	Total	C	N	O	S	0	0	0
			2559	1622	446	478	13			
1	D	343	Total	C	N	O	S	0	0	0
			2614	1660	455	486	13			

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



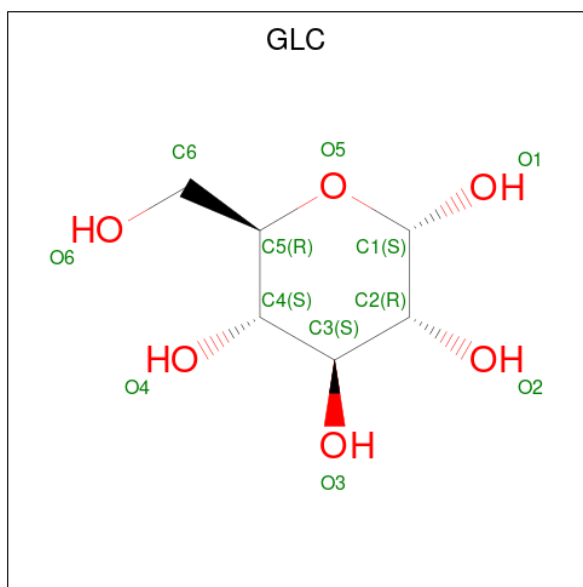
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
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		

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

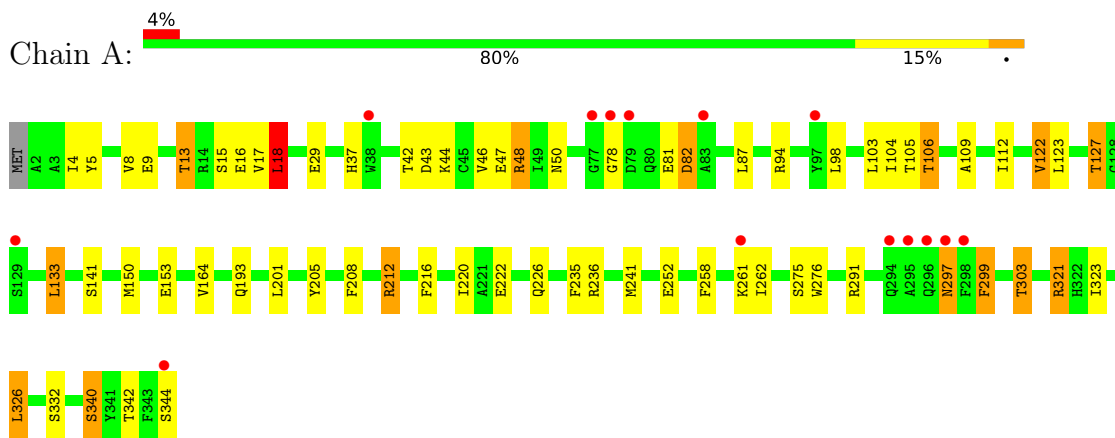


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

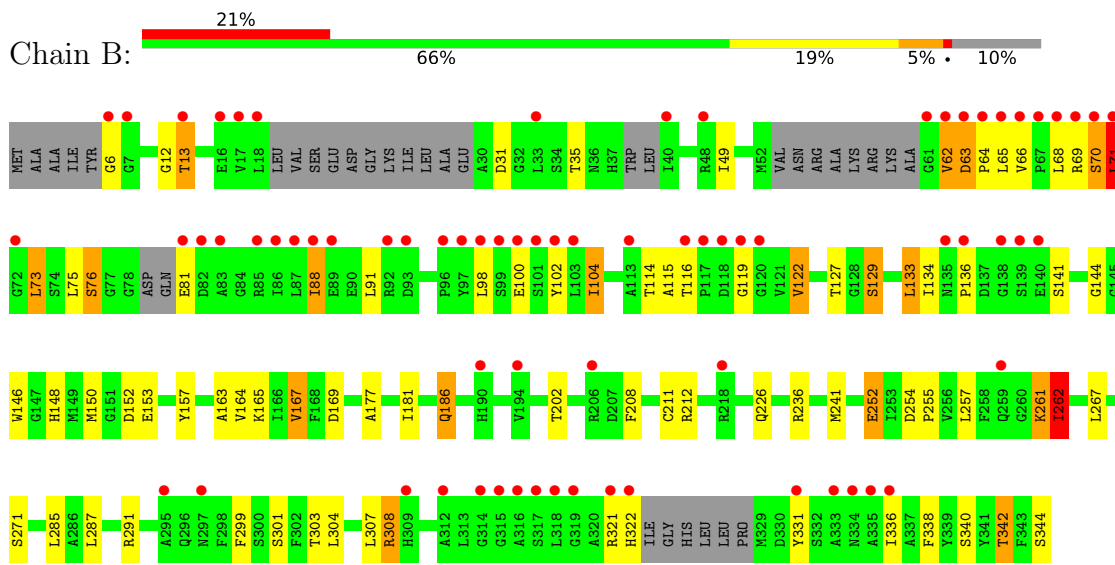
### 3 Residue-property plots [i](#)

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.

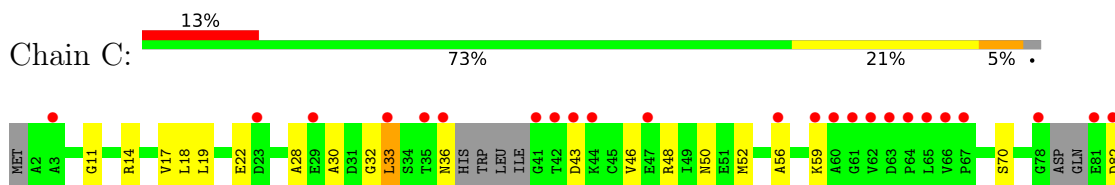
- Molecule 1: N-ACETYL-D-GLUCOSAMINE KINASE

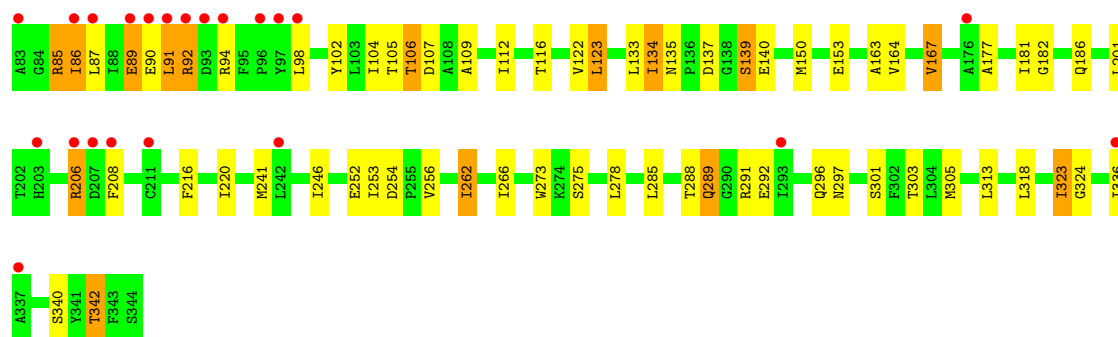


- Molecule 1: N-ACETYL-D-GLUCOSAMINE KINASE

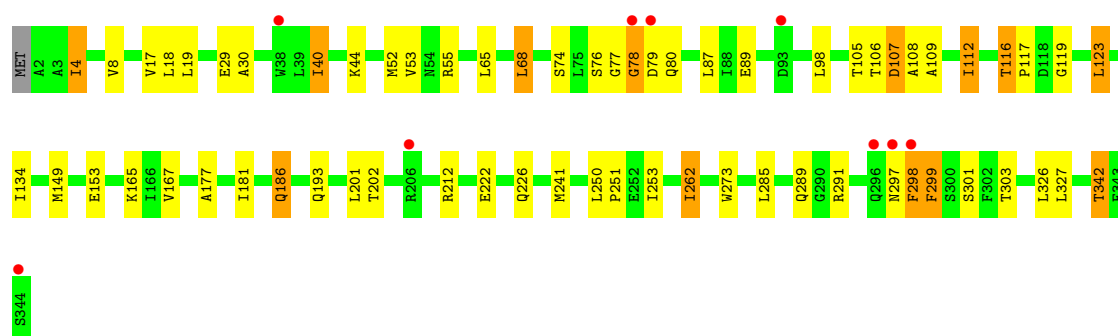
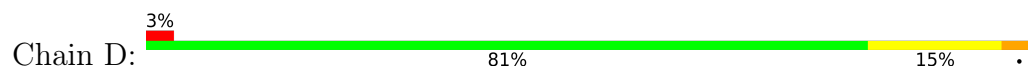


- Molecule 1: N-ACETYL-D-GLUCOSAMINE KINASE





● Molecule 1: N-ACETYL-D-GLUCOSAMINE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.71Å 101.99Å 110.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.72 29.80 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.80-2.72) 99.1 (29.80-2.72)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	49.60 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.227 , 0.289 0.260 , 0.309	Depositor DCC
$R_{free}$ test set	2093 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 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	0.53	0/2680	0.70	1/3621 (0.0%)
1	B	0.52	0/2410	0.65	0/3247
1	C	0.49	0/2611	0.64	0/3523
1	D	0.52	0/2671	0.69	0/3608
All	All	0.52	0/10372	0.67	1/13999 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	18	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ASN	Peptide
1	A	81	GLU	Peptide
1	A	82	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	297	ASN	Peptide

## 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	2623	0	2588	39	0
1	B	2363	0	2309	50	0
1	C	2559	0	2522	55	0
1	D	2614	0	2578	37	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
All	All	10315	0	10093	168	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 8.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:THR:HG22	2:B:470:ADP:O3B	1.69	0.92
1:C:135:ASN:HD22	1:C:139:SER:HB3	1.37	0.90
1:C:30:ALA:HB2	1:C:56:ALA:HB2	1.54	0.89
1:B:88:ILE:HG12	1:B:104:ILE:HD13	1.55	0.87
1:B:165:LYS:HA	1:C:150:MET:HE1	1.62	0.81
1:C:303:THR:HG22	1:C:340:SER:HB3	1.62	0.80
1:A:8:VAL:HG22	1:A:17:VAL:HG22	1.62	0.79
1:B:70:SER:O	1:B:71:LEU:HB2	1.81	0.79
1:D:105:THR:HG22	1:D:106:THR:O	1.82	0.78
1:C:46:VAL:HG21	1:C:91:LEU:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLY:HA2	1:B:134:ILE:HG23	1.66	0.78
1:D:262:ILE:O	1:D:303:THR:HG23	1.85	0.77
1:B:308:ARG:HE	1:B:336:ILE:HG23	1.49	0.77
1:C:262:ILE:O	1:C:303:THR:HG23	1.85	0.74
1:A:13:THR:HG23	2:A:470:ADP:O3B	1.90	0.72
1:B:165:LYS:HA	1:C:150:MET:CE	2.19	0.71
1:A:18:LEU:HD22	1:A:29:GLU:HG2	1.72	0.70
1:D:53:VAL:HG11	1:D:98:LEU:HD11	1.74	0.70
1:B:267:LEU:HD21	1:B:307:LEU:HD21	1.77	0.67
1:A:50:ASN:HD22	1:A:98:LEU:HD13	1.60	0.66
1:A:127:THR:HG22	2:A:470:ADP:H5'1	1.77	0.66
1:B:177:ALA:HB2	1:B:181:ILE:HD11	1.77	0.65
1:C:33:LEU:HB2	1:C:48:ARG:HD3	1.78	0.65
1:C:275:SER:HB3	1:C:278:LEU:HD12	1.79	0.64
1:C:106:THR:HG22	1:C:109:ALA:H	1.61	0.64
1:B:76:SER:HB2	3:B:1001:GLC:H4	1.80	0.64
1:C:32:GLY:HA3	1:C:52:MET:SD	2.37	0.64
1:A:205:TYR:CE1	1:D:149:MET:HG3	2.33	0.63
1:A:262:ILE:HG23	1:A:303:THR:HG23	1.80	0.62
1:B:261:LYS:HD3	1:B:262:ILE:H	1.65	0.62
1:C:70:SER:HB2	1:C:323:ILE:HD11	1.81	0.62
1:A:127:THR:HG23	2:A:470:ADP:O3B	2.00	0.61
1:A:193:GLN:HE21	1:A:212:ARG:HH12	1.48	0.61
1:A:44:LYS:O	1:A:48:ARG:HG2	2.00	0.61
1:C:163:ALA:O	1:C:167:VAL:HG12	2.01	0.61
1:A:303:THR:HG22	1:A:340:SER:OG	2.01	0.61
1:B:261:LYS:HD3	1:B:262:ILE:N	2.15	0.61
1:C:92:ARG:C	1:C:94:ARG:H	2.02	0.61
1:D:8:VAL:HG22	1:D:17:VAL:HG22	1.84	0.60
1:D:4:ILE:HD11	1:D:19:LEU:HD22	1.84	0.60
1:B:133:LEU:HD23	1:B:141:SER:HB2	1.84	0.60
1:B:291:ARG:NH1	1:B:299:PHE:O	2.35	0.59
1:C:177:ALA:HB2	1:C:181:ILE:HD11	1.84	0.59
1:C:82:ASP:HA	1:C:85:ARG:NH1	2.17	0.59
1:D:105:THR:HG23	1:D:109:ALA:HB3	1.86	0.58
1:A:9:GLU:O	1:A:15:SER:HA	2.04	0.58
1:C:137:ASP:OD2	1:C:139:SER:HB2	2.04	0.58
1:D:116:THR:HG22	1:D:117:PRO:HD2	1.85	0.57
1:C:206:ARG:N	1:C:206:ARG:HD3	2.18	0.57
1:A:201:LEU:HD22	1:A:205:TYR:HE2	1.69	0.57
1:D:40:ILE:HG23	1:D:44:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLU:O	1:D:226:GLN:HG2	2.05	0.56
1:C:48:ARG:O	1:C:52:MET:HB2	2.05	0.56
1:C:92:ARG:HD2	1:C:92:ARG:N	2.21	0.55
1:B:6:GLY:O	1:B:71:LEU:HA	2.06	0.55
1:A:258:PHE:CD2	1:A:299:PHE:HB3	2.40	0.55
1:D:17:VAL:HG23	1:D:52:MET:HE1	1.88	0.55
1:A:133:LEU:HD23	1:A:141:SER:HB3	1.89	0.55
1:C:246:ILE:HD12	1:C:266:ILE:HD13	1.89	0.54
1:C:301:SER:HB3	1:C:342:THR:HB	1.90	0.53
1:B:165:LYS:HD2	1:C:150:MET:HE3	1.91	0.53
1:D:250:LEU:HA	1:D:253:ILE:HD12	1.89	0.53
1:B:146:TRP:HE3	1:C:201:LEU:HD21	1.73	0.53
1:C:18:LEU:HD12	1:C:313:LEU:HB2	1.91	0.53
1:C:106:THR:CG2	1:C:109:ALA:H	2.21	0.53
1:A:106:THR:HG22	1:A:109:ALA:H	1.72	0.53
1:C:135:ASN:ND2	1:C:139:SER:HB3	2.17	0.52
1:B:6:GLY:N	1:B:70:SER:HG	2.06	0.52
1:C:134:ILE:HD13	1:C:140:GLU:HG3	1.92	0.52
1:A:220:ILE:HG22	1:A:235:PHE:HE1	1.74	0.51
1:C:56:ALA:HA	1:C:59:LYS:HB2	1.92	0.51
1:D:77:GLY:O	1:D:78:GLY:O	2.28	0.51
1:A:222:GLU:O	1:A:226:GLN:HG2	2.10	0.51
1:C:216:PHE:O	1:C:220:ILE:HD12	2.09	0.51
1:C:46:VAL:CG2	1:C:91:LEU:HD13	2.39	0.51
1:B:129:SER:HB2	1:B:152:ASP:HA	1.93	0.51
1:A:193:GLN:NE2	1:A:212:ARG:HH12	2.09	0.51
1:D:285:LEU:O	1:D:289:GLN:HG2	2.11	0.51
1:C:11:GLY:O	1:C:36:ASN:HA	2.12	0.50
1:A:78:GLY:HA2	3:A:1001:GLC:O2	2.11	0.50
1:A:205:TYR:HE1	1:D:149:MET:HG3	1.73	0.50
1:A:220:ILE:HG22	1:A:235:PHE:CE1	2.47	0.50
1:B:150:MET:SD	1:C:164:VAL:HG23	2.51	0.50
1:B:62:VAL:HG12	1:B:63:ASP:H	1.76	0.49
1:B:63:ASP:HB3	1:B:66:VAL:HB	1.94	0.49
1:D:177:ALA:HB2	1:D:181:ILE:HD11	1.92	0.49
1:B:153:GLU:HG2	1:B:241:MET:CE	2.42	0.49
1:C:92:ARG:HG2	1:C:102:TYR:CE2	2.48	0.49
1:A:262:ILE:HG23	1:A:303:THR:CG2	2.42	0.49
1:A:106:THR:CG2	1:A:109:ALA:H	2.24	0.49
1:D:53:VAL:HG11	1:D:98:LEU:CD1	2.42	0.49
1:D:301:SER:HB3	1:D:342:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:HIS:HB2	1:B:157:TYR:CE2	2.48	0.48
1:A:321:ARG:NH1	1:B:344:SER:O	2.46	0.48
1:D:18:LEU:HD23	1:D:29:GLU:HB3	1.94	0.48
1:D:74:SER:HA	1:D:105:THR:HB	1.94	0.48
1:C:14:ARG:HB3	1:C:14:ARG:CZ	2.43	0.48
1:A:16:GLU:OE1	1:A:18:LEU:HD21	2.14	0.48
1:C:323:ILE:HG22	1:C:324:GLY:H	1.79	0.47
1:B:13:THR:HB	1:B:211:CYS:SG	2.54	0.47
1:A:216:PHE:CE2	1:A:220:ILE:HD11	2.49	0.47
1:A:42:THR:O	1:A:46:VAL:HG23	2.15	0.47
1:A:321:ARG:HD2	1:B:344:SER:O	2.14	0.47
1:C:92:ARG:C	1:C:94:ARG:N	2.69	0.47
1:C:303:THR:HG22	1:C:340:SER:CB	2.40	0.47
1:B:13:THR:HG21	2:B:470:ADP:H5'1	1.96	0.47
1:B:153:GLU:HB3	1:B:241:MET:HB3	1.96	0.47
1:B:141:SER:OG	1:B:252:GLU:HG2	2.15	0.47
1:D:78:GLY:O	1:D:80:GLN:N	2.48	0.47
1:A:153:GLU:HB3	1:A:241:MET:HG3	1.97	0.46
1:D:53:VAL:CG1	1:D:98:LEU:HD11	2.43	0.46
1:A:326:LEU:HD21	1:B:285:LEU:HD12	1.97	0.46
1:D:123:LEU:HD13	1:D:273:TRP:HZ2	1.81	0.46
1:B:146:TRP:CE3	1:C:201:LEU:HD21	2.51	0.46
1:A:205:TYR:HE1	1:D:149:MET:CG	2.29	0.45
1:B:115:ALA:HB2	1:B:267:LEU:HD22	1.99	0.45
1:B:163:ALA:O	1:B:167:VAL:HG13	2.15	0.45
1:D:119:GLY:HA3	1:D:134:ILE:O	2.16	0.45
1:A:258:PHE:CD2	1:A:299:PHE:CB	3.00	0.45
1:D:108:ALA:O	1:D:112:ILE:HG13	2.17	0.45
1:D:76:SER:HA	1:D:107:ASP:HB3	1.97	0.45
1:B:62:VAL:HG12	1:B:63:ASP:N	2.32	0.45
1:D:4:ILE:HD12	1:D:68:LEU:HD12	1.98	0.45
1:B:68:LEU:O	1:B:69:ARG:HG2	2.16	0.44
1:B:116:THR:HG22	1:B:331:TYR:HB2	1.99	0.44
1:B:165:LYS:HE3	1:B:169:ASP:OD2	2.17	0.44
1:B:262:ILE:O	1:B:303:THR:OG1	2.24	0.44
1:C:105:THR:HG21	1:C:318:LEU:HD13	2.00	0.44
1:C:133:LEU:O	1:C:140:GLU:HA	2.17	0.44
1:B:153:GLU:HG2	1:B:241:MET:HE1	2.00	0.43
1:A:5:TYR:N	1:A:5:TYR:CD2	2.86	0.43
1:B:122:VAL:HG12	1:B:267:LEU:HB3	2.01	0.43
1:B:304:LEU:HB3	1:B:338:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:HE1	1:D:165:LYS:HA	2.01	0.42
1:D:250:LEU:N	1:D:251:PRO:CD	2.81	0.42
1:D:298:PHE:O	1:D:299:PHE:CB	2.66	0.42
1:C:17:VAL:HG23	1:C:52:MET:CE	2.49	0.42
1:C:112:ILE:H	1:C:112:ILE:HG13	1.74	0.42
1:C:112:ILE:HG23	1:C:122:VAL:HG22	2.01	0.42
1:C:107:ASP:OD1	1:C:107:ASP:N	2.52	0.42
1:D:186:GLN:HE21	1:D:186:GLN:HA	1.84	0.42
1:B:13:THR:CG2	1:B:127:THR:HB	2.50	0.42
1:C:153:GLU:HB3	1:C:241:MET:HG3	2.02	0.41
1:C:19:LEU:HD23	1:C:28:ALA:HB3	2.01	0.41
1:C:291:ARG:HH12	1:C:297:ASN:HA	1.85	0.41
1:A:275:SER:O	1:A:276:TRP:C	2.58	0.41
1:B:254:ASP:HA	1:B:255:PRO:HD3	1.80	0.41
1:C:133:LEU:HD13	1:C:253:ILE:HG12	2.02	0.41
1:C:254:ASP:OD1	1:C:256:VAL:HG22	2.21	0.41
1:D:134:ILE:N	1:D:134:ILE:HD12	2.36	0.41
1:D:109:ALA:HA	1:D:112:ILE:HD11	2.02	0.41
1:A:18:LEU:HD22	1:A:29:GLU:CG	2.48	0.41
1:C:85:ARG:C	1:C:87:LEU:H	2.24	0.41
1:A:112:ILE:HD11	1:A:122:VAL:HG22	2.03	0.41
1:C:296:GLN:O	1:C:297:ASN:HB2	2.21	0.41
1:B:49:ILE:HD13	1:B:73:LEU:HD13	2.03	0.41
1:D:153:GLU:HB3	1:D:241:MET:HB3	2.02	0.41
1:B:186:GLN:HE21	1:B:186:GLN:HA	1.85	0.40
1:B:321:ARG:HD3	1:B:321:ARG:HA	1.95	0.40
1:A:16:GLU:OE1	1:A:18:LEU:CD2	2.69	0.40
1:B:12:GLY:HA3	1:B:127:THR:HG21	2.03	0.40
1:B:271:SER:OG	2:B:470:ADP:O2A	2.36	0.40
1:B:301:SER:HB3	1:B:342:THR:HB	2.04	0.40
1:C:177:ALA:CB	1:C:181:ILE:HD11	2.50	0.40
1:D:167:VAL:HB	1:D:181:ILE:HG23	2.04	0.40
1:C:285:LEU:O	1:C:289:GLN:HG2	2.21	0.40
1:C:123:LEU:HD13	1:C:273:TRP:CZ2	2.56	0.40
1:D:30:ALA:HB1	1:D:55:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

## 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	341/344 (99%)	322 (94%)	16 (5%)	3 (1%)	17	38
1	B	298/344 (87%)	262 (88%)	27 (9%)	9 (3%)	4	9
1	C	331/344 (96%)	301 (91%)	24 (7%)	6 (2%)	8	20
1	D	341/344 (99%)	318 (93%)	20 (6%)	3 (1%)	17	38
All	All	1311/1376 (95%)	1203 (92%)	87 (7%)	21 (2%)	9	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	208	PHE
1	B	71	LEU
1	B	100	GLU
1	B	208	PHE
1	B	262	ILE
1	C	208	PHE
1	D	78	GLY
1	B	144	GLY
1	D	79	ASP
1	A	323	ILE
1	B	98	LEU
1	D	299	PHE
1	C	22	GLU
1	B	62	VAL
1	C	33	LEU
1	C	89	GLU
1	B	64	PRO
1	B	136	PRO
1	C	86	ILE
1	C	182	GLY

### 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	272/273 (100%)	240 (88%)	32 (12%)	5 11
1	B	246/273 (90%)	211 (86%)	35 (14%)	3 7
1	C	264/273 (97%)	237 (90%)	27 (10%)	7 16
1	D	270/273 (99%)	249 (92%)	21 (8%)	12 28
All	All	1052/1092 (96%)	937 (89%)	115 (11%)	6 14

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	13	THR
1	A	18	LEU
1	A	37	HIS
1	A	43	ASP
1	A	47	GLU
1	A	48	ARG
1	A	87	LEU
1	A	94	ARG
1	A	103	LEU
1	A	104	ILE
1	A	105	THR
1	A	106	THR
1	A	122	VAL
1	A	123	LEU
1	A	127	THR
1	A	133	LEU
1	A	164	VAL
1	A	212	ARG
1	A	236	ARG
1	A	252	GLU
1	A	261	LYS
1	A	291	ARG
1	A	297	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	299	PHE
1	A	303	THR
1	A	321	ARG
1	A	326	LEU
1	A	332	SER
1	A	340	SER
1	A	342	THR
1	A	344	SER
1	B	13	THR
1	B	31	ASP
1	B	35	THR
1	B	63	ASP
1	B	65	LEU
1	B	70	SER
1	B	71	LEU
1	B	73	LEU
1	B	75	LEU
1	B	76	SER
1	B	81	GLU
1	B	88	ILE
1	B	91	LEU
1	B	102	TYR
1	B	104	ILE
1	B	114	THR
1	B	122	VAL
1	B	129	SER
1	B	133	LEU
1	B	164	VAL
1	B	167	VAL
1	B	186	GLN
1	B	202	THR
1	B	212	ARG
1	B	226	GLN
1	B	236	ARG
1	B	252	GLU
1	B	257	LEU
1	B	261	LYS
1	B	262	ILE
1	B	287	LEU
1	B	308	ARG
1	B	322	HIS
1	B	340	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	342	THR
1	C	43	ASP
1	C	50	ASN
1	C	85	ARG
1	C	86	ILE
1	C	89	GLU
1	C	90	GLU
1	C	91	LEU
1	C	92	ARG
1	C	98	LEU
1	C	104	ILE
1	C	106	THR
1	C	116	THR
1	C	123	LEU
1	C	134	ILE
1	C	139	SER
1	C	167	VAL
1	C	186	GLN
1	C	206	ARG
1	C	252	GLU
1	C	262	ILE
1	C	288	THR
1	C	289	GLN
1	C	292	GLU
1	C	305	MET
1	C	323	ILE
1	C	336	ILE
1	C	342	THR
1	D	4	ILE
1	D	40	ILE
1	D	65	LEU
1	D	68	LEU
1	D	87	LEU
1	D	89	GLU
1	D	107	ASP
1	D	112	ILE
1	D	116	THR
1	D	123	LEU
1	D	186	GLN
1	D	193	GLN
1	D	201	LEU
1	D	202	THR

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Mol	Chain	Res	Type
1	D	212	ARG
1	D	262	ILE
1	D	291	ARG
1	D	298	PHE
1	D	326	LEU
1	D	327	LEU
1	D	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	173	ASN
1	A	179	HIS
1	A	186	GLN
1	A	193	GLN
1	A	226	GLN
1	A	259	GLN
1	A	294	GLN
1	A	309	HIS
1	B	37	HIS
1	B	186	GLN
1	B	226	GLN
1	B	334	ASN
1	C	135	ASN
1	C	173	ASN
1	C	186	GLN
1	C	289	GLN
1	C	325	HIS
1	D	173	ASN
1	D	186	GLN
1	D	193	GLN
1	D	289	GLN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	B	470	-	24,29,29	1.03	2 (8%)	29,45,45	1.36	5 (17%)
3	GLC	D	1001	-	12,12,12	0.75	0	17,17,17	1.02	0
3	GLC	B	1001	-	12,12,12	0.71	0	17,17,17	0.95	0
2	ADP	C	470	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	6 (20%)
2	ADP	A	470	-	24,29,29	0.98	1 (4%)	29,45,45	1.30	2 (6%)
2	ADP	D	470	-	24,29,29	1.04	2 (8%)	29,45,45	1.32	3 (10%)
3	GLC	C	1001	-	12,12,12	0.69	0	17,17,17	0.79	0
3	GLC	A	1001	-	12,12,12	0.76	0	17,17,17	0.99	1 (5%)

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	B	470	-	-	0/12/32/32	0/3/3/3
3	GLC	D	1001	-	-	0/2/22/22	0/1/1/1
3	GLC	B	1001	-	-	1/2/22/22	0/1/1/1
2	ADP	C	470	-	-	1/12/32/32	0/3/3/3
2	ADP	A	470	-	-	1/12/32/32	0/3/3/3
2	ADP	D	470	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	C	1001	-	-	0/2/22/22	0/1/1/1
3	GLC	A	1001	-	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	470	ADP	C5-C4	2.78	1.48	1.40
2	B	470	ADP	C5-C4	2.62	1.47	1.40
2	C	470	ADP	C5-C4	2.47	1.47	1.40
2	D	470	ADP	C2-N3	2.38	1.35	1.32
2	A	470	ADP	C5-C4	2.28	1.47	1.40
2	B	470	ADP	C2-N3	2.19	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	470	ADP	N3-C2-N1	-4.06	122.33	128.68
2	B	470	ADP	N3-C2-N1	-3.41	123.34	128.68
2	D	470	ADP	N3-C2-N1	-3.38	123.40	128.68
2	A	470	ADP	N3-C2-N1	-3.33	123.48	128.68
2	C	470	ADP	C3'-C2'-C1'	3.28	105.92	100.98
2	A	470	ADP	C4-C5-N7	-3.20	106.07	109.40
2	C	470	ADP	C4-C5-N7	-3.17	106.09	109.40
2	D	470	ADP	C3'-C2'-C1'	2.98	105.47	100.98
2	B	470	ADP	C3'-C2'-C1'	2.48	104.71	100.98
2	C	470	ADP	C2-N1-C6	2.38	122.82	118.75
2	C	470	ADP	PA-O3A-PB	-2.36	124.73	132.83
2	B	470	ADP	C4-C5-N7	-2.25	107.06	109.40
2	D	470	ADP	C4-C5-N7	-2.13	107.17	109.40
2	C	470	ADP	C1'-N9-C4	-2.12	122.92	126.64
2	B	470	ADP	O2A-PA-O1A	2.09	122.59	112.24
3	A	1001	GLC	O5-C5-C4	-2.05	105.97	109.69
2	B	470	ADP	PA-O3A-PB	-2.02	125.90	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	470	ADP	PB-O3A-PA-O5'
2	A	470	ADP	PA-O3A-PB-O3B
2	D	470	ADP	PA-O3A-PB-O3B

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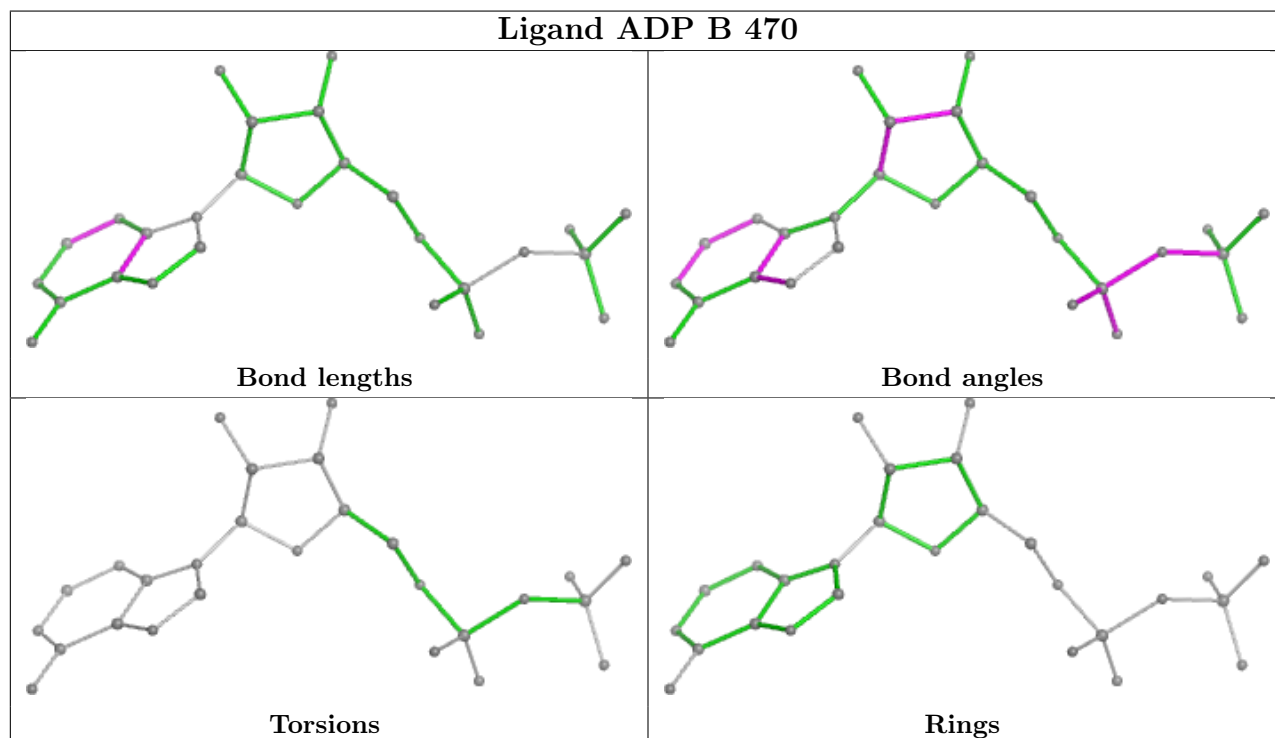
Mol	Chain	Res	Type	Atoms
3	B	1001	GLC	O5-C5-C6-O6

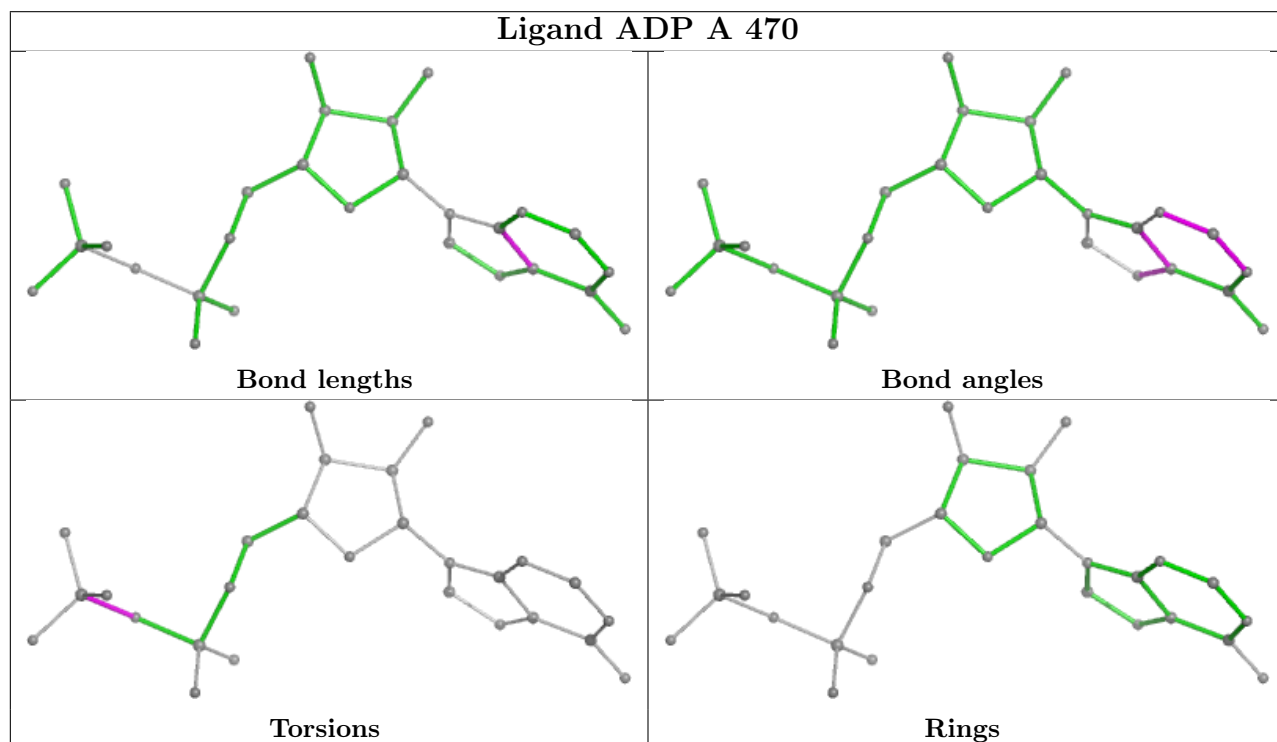
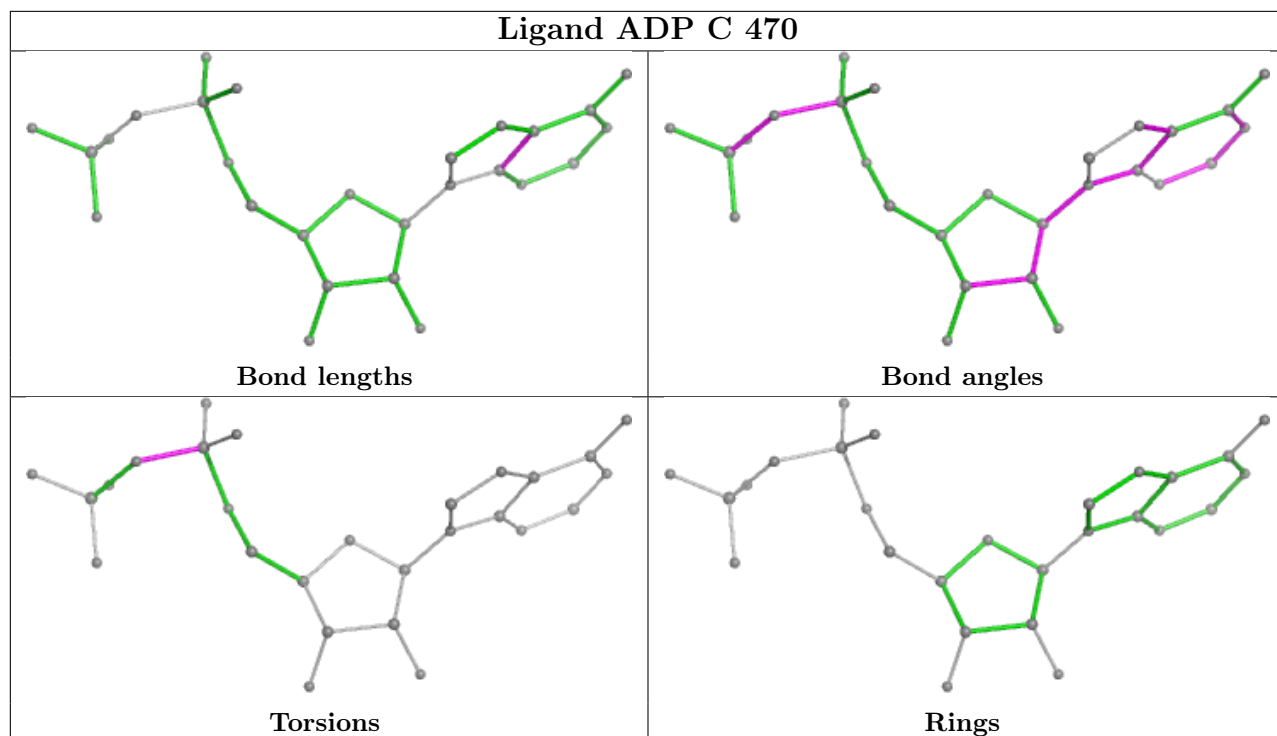
There are no ring outliers.

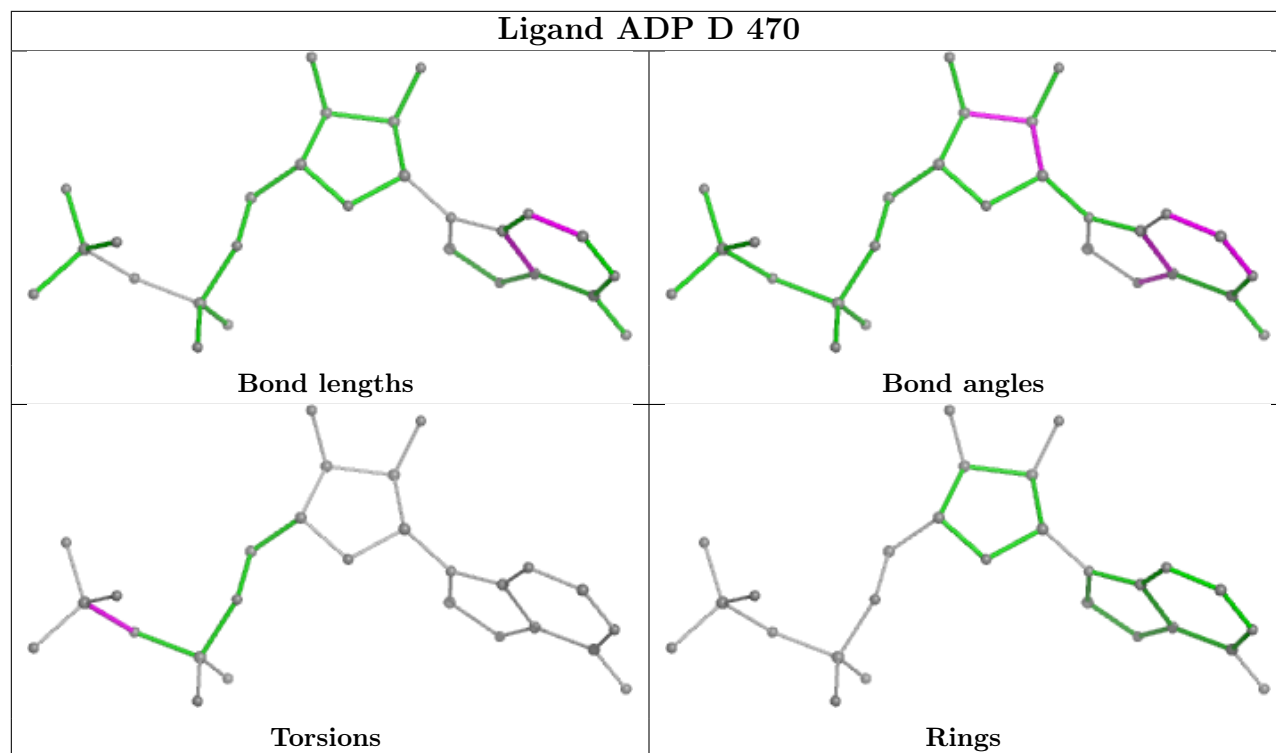
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	470	ADP	3	0
3	B	1001	GLC	1	0
2	A	470	ADP	3	0
3	A	1001	GLC	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	343/344 (99%)	0.45	14 (4%) 37 36	36, 52, 73, 88	0
1	B	310/344 (90%)	1.20	72 (23%) 0 0	41, 56, 85, 96	0
1	C	337/344 (97%)	0.65	46 (13%) 3 2	40, 51, 73, 90	0
1	D	343/344 (99%)	0.25	9 (2%) 56 57	30, 46, 62, 79	0
All	All	1333/1376 (96%)	0.62	141 (10%) 6 4	30, 51, 75, 96	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	SER	10.8
1	B	71	LEU	9.3
1	B	62	VAL	8.2
1	B	64	PRO	7.8
1	B	83	ALA	7.4
1	A	298	PHE	6.9
1	B	65	LEU	6.7
1	B	6	GLY	6.4
1	B	81	GLU	6.2
1	C	66	VAL	6.0
1	B	101	SER	5.8
1	D	79	ASP	5.5
1	C	65	LEU	5.3
1	C	94	ARG	5.3
1	B	88	ILE	5.3
1	B	66	VAL	5.2
1	B	335	ALA	5.0
1	C	92	ARG	4.8
1	B	69	ARG	4.7
1	B	116	THR	4.6
1	B	98	LEU	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	100	GLU	4.5
1	C	23	ASP	4.5
1	B	314	GLY	4.4
1	C	89	GLU	4.3
1	B	67	PRO	4.3
1	C	203	HIS	4.3
1	B	117	PRO	4.3
1	B	103	LEU	4.2
1	C	33	LEU	4.2
1	C	43	ASP	4.2
1	B	63	ASP	4.1
1	A	83	ALA	4.0
1	B	97	TYR	3.9
1	B	113	ALA	3.8
1	A	344	SER	3.8
1	B	297	ASN	3.8
1	A	79	ASP	3.7
1	B	40	ILE	3.7
1	C	206	ARG	3.7
1	D	78	GLY	3.7
1	C	83	ALA	3.7
1	B	17	VAL	3.7
1	C	97	TYR	3.7
1	B	136	PRO	3.7
1	B	68	LEU	3.6
1	B	119	GLY	3.6
1	C	63	ASP	3.6
1	B	331	TYR	3.6
1	C	78	GLY	3.6
1	D	38	TRP	3.6
1	B	334	ASN	3.6
1	D	297	ASN	3.6
1	A	296	GLN	3.5
1	C	56	ALA	3.4
1	B	93	ASP	3.4
1	B	317	SER	3.4
1	B	33	LEU	3.4
1	C	86	ILE	3.4
1	B	61	GLY	3.4
1	B	140	GLU	3.3
1	C	91	LEU	3.3
1	B	206	ARG	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	47	GLU	3.2
1	B	139	SER	3.2
1	B	102	TYR	3.2
1	B	322	HIS	3.1
1	B	321	ARG	3.1
1	D	298	PHE	3.1
1	C	41	GLY	3.0
1	D	206	ARG	3.0
1	C	64	PRO	3.0
1	B	336	ILE	3.0
1	C	90	GLU	3.0
1	B	92	ARG	3.0
1	B	89	GLU	2.9
1	B	85	ARG	2.9
1	B	118	ASP	2.8
1	C	207	ASP	2.8
1	B	318	LEU	2.8
1	C	29	GLU	2.8
1	C	93	ASP	2.8
1	C	87	LEU	2.7
1	C	176	ALA	2.7
1	C	82	ASP	2.7
1	B	295	ALA	2.7
1	B	16	GLU	2.7
1	C	293	ILE	2.7
1	D	93	ASP	2.7
1	B	120	GLY	2.7
1	B	86	ILE	2.6
1	A	295	ALA	2.6
1	D	344	SER	2.6
1	C	96	PRO	2.5
1	A	297	ASN	2.5
1	C	59	LYS	2.5
1	C	44	LYS	2.5
1	B	82	ASP	2.5
1	B	87	LEU	2.5
1	B	333	ALA	2.4
1	C	36	ASN	2.4
1	A	261	LYS	2.4
1	B	48	ARG	2.4
1	C	208	PHE	2.4
1	A	294	GLN	2.4

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	218	ARG	2.4
1	B	190	HIS	2.3
1	B	316	ALA	2.3
1	C	242	LEU	2.3
1	C	337	ALA	2.3
1	B	319	GLY	2.3
1	C	67	PRO	2.3
1	B	312	ALA	2.3
1	C	42	THR	2.3
1	A	77	GLY	2.2
1	C	61	GLY	2.2
1	B	315	GLY	2.2
1	C	35	THR	2.2
1	C	60	ALA	2.2
1	B	309	HIS	2.2
1	B	194	VAL	2.2
1	C	62	VAL	2.2
1	B	99	SER	2.1
1	B	96	PRO	2.1
1	A	97	TYR	2.1
1	B	72	GLY	2.1
1	B	18	LEU	2.1
1	B	13	THR	2.1
1	B	138	GLY	2.1
1	C	81	GLU	2.1
1	B	135	ASN	2.1
1	B	7	GLY	2.1
1	C	98	LEU	2.1
1	D	296	GLN	2.0
1	C	336	ILE	2.0
1	C	3	ALA	2.0
1	A	78	GLY	2.0
1	C	211	CYS	2.0
1	A	129	SER	2.0
1	B	259	GLN	2.0
1	A	38	TRP	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](#)

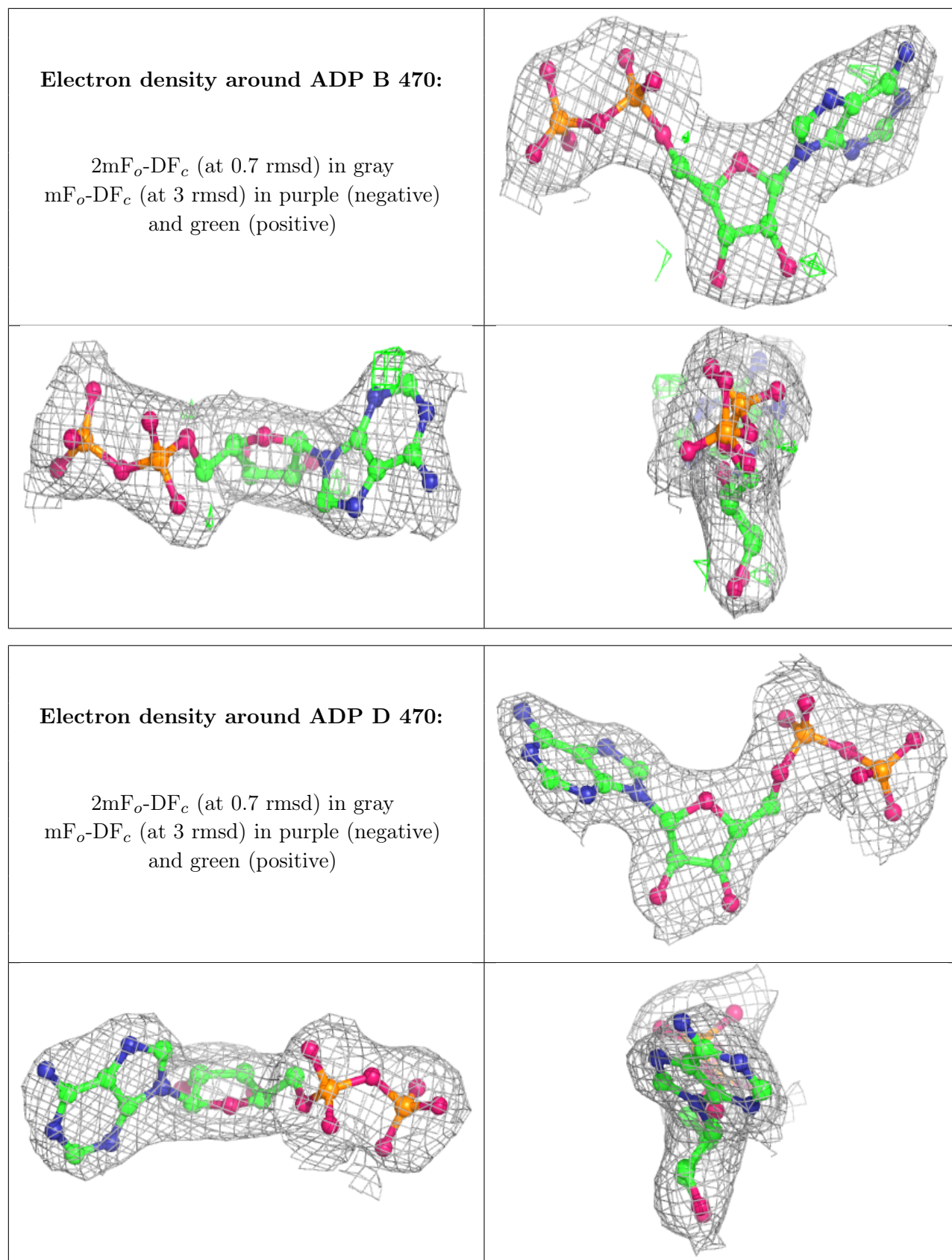
There are no monosaccharides in this entry.

### 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<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.

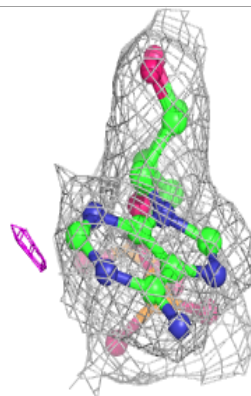
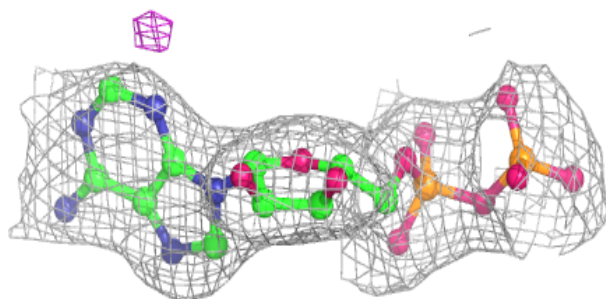
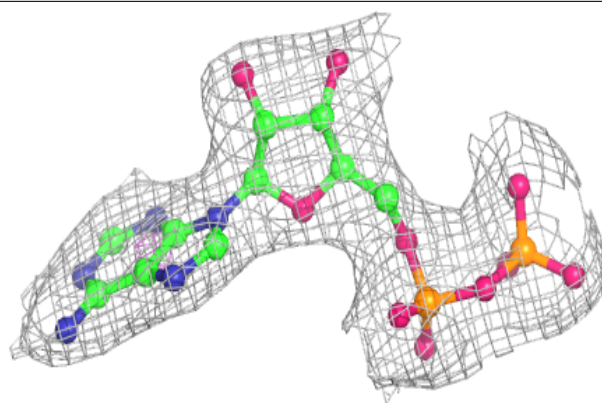
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	B	1001	12/12	0.90	0.25	59,60,62,62	0
3	GLC	C	1001	12/12	0.93	0.17	57,58,60,61	0
2	ADP	B	470	27/27	0.94	0.17	49,54,58,58	0
3	GLC	D	1001	12/12	0.95	0.14	43,45,46,48	0
3	GLC	A	1001	12/12	0.96	0.17	38,41,44,44	0
2	ADP	D	470	27/27	0.96	0.13	47,49,52,53	0
2	ADP	C	470	27/27	0.97	0.12	39,42,46,47	0
2	ADP	A	470	27/27	0.97	0.14	24,27,32,34	0

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

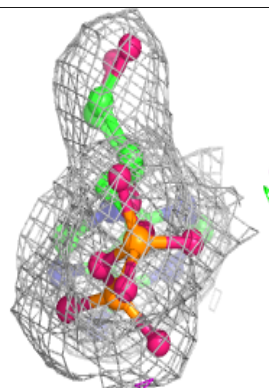
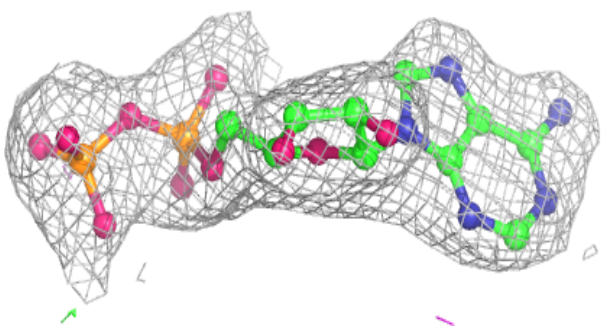
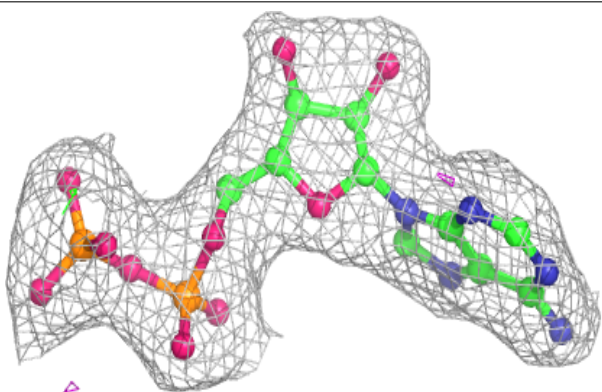


**Electron density around ADP C 470:**

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

**Electron density around ADP A 470:**

$2mF_o-DF_c$  (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.