



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:54 am BST

PDB ID : 2FME
Title : Crystal structure of the mitotic kinesin eg5 (ksp) in complex with mg-adp and (r)-4-(3-hydroxyphenyl)-n,n,7,8-tetramethyl-3,4-dihydroisoquinoline-2(1h)-carboxamide
Authors : Sheriff, S.
Deposited on : 2006-01-09
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

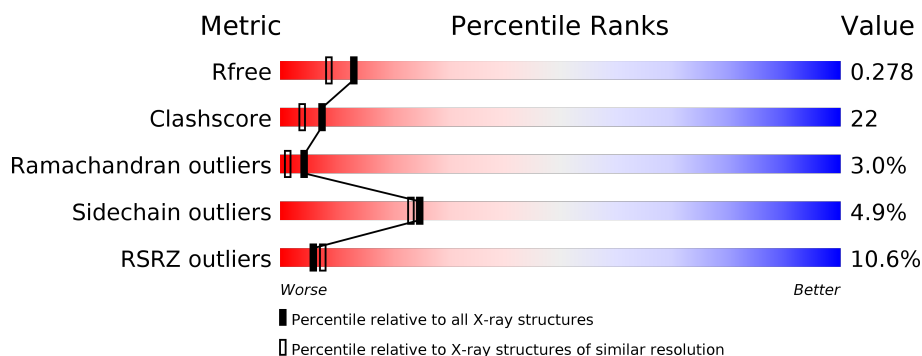
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	368	<div> <div>10%</div> <div>58%</div> <div>26%</div> <div>•</div> <div>13%</div> </div>
1	B	368	<div> <div>9%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5282 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.

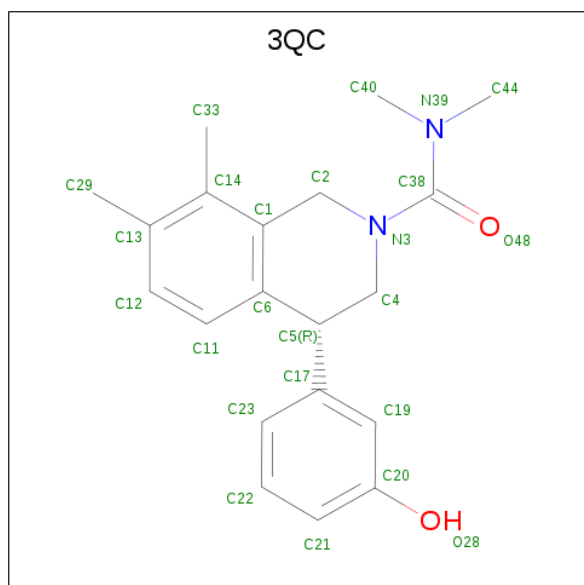
- Molecule 1 is a protein called Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	1
			2473	1549	430	484	10			
1	B	329	Total	C	N	O	S	0	0	1
			2527	1582	435	500	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

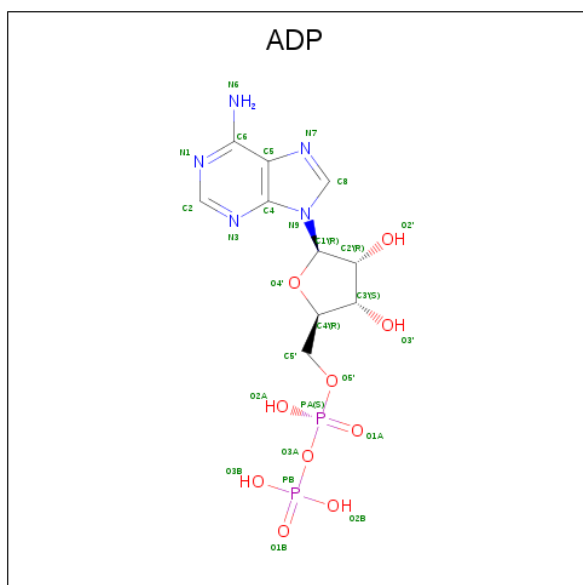
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (4R)-4-(3-HYDROXYPHENYL)-N,N,7,8-TETRAMETHYL-3,4-DIHYDROIS OQUINOLINE-2(1H)-CARBOXAMIDE (three-letter code: 3QC) (formula: C₂₀H₂₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

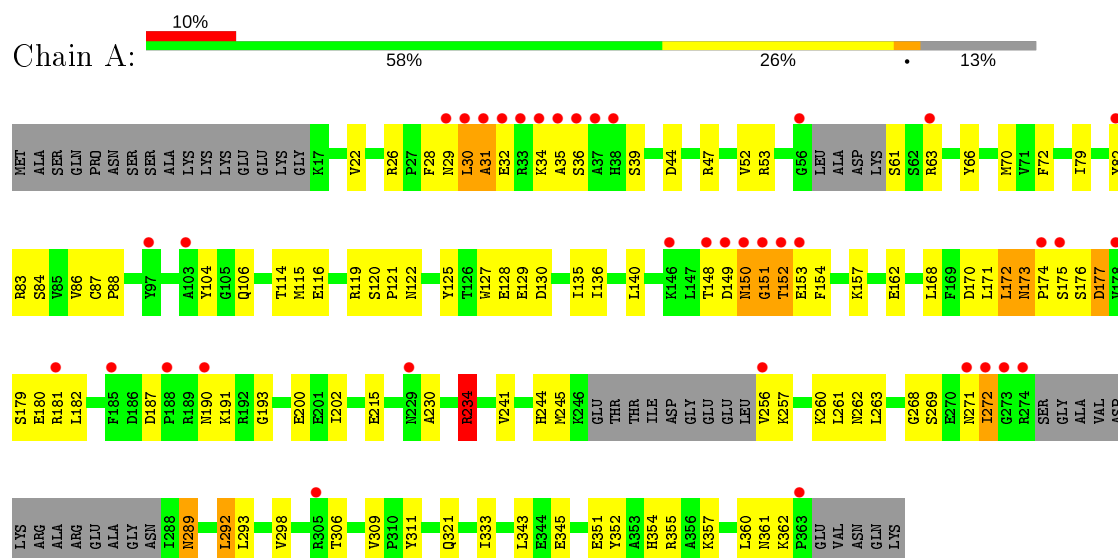
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	B	81	Total	O	0	0
			81	81		

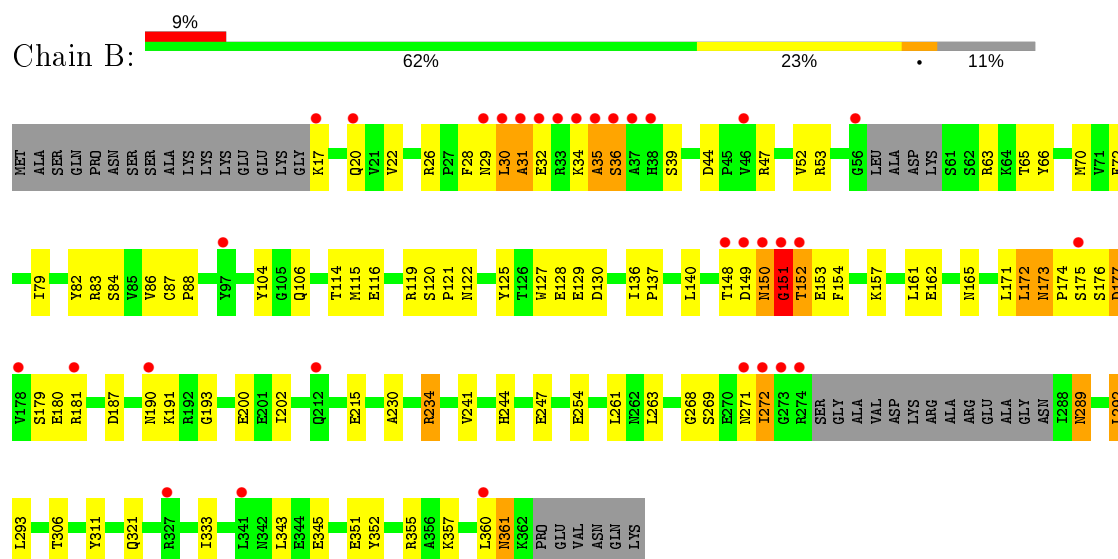
3 Residue-property plots [i](#)

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: Kinesin-like protein KIF11



• Molecule 1: Kinesin-like protein KIF11



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.80 Å 80.00 Å 69.20 Å 90.00° 96.50° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.00-2.10) 93.4 (40.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 2.10 Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, R_{free}	0.280 , 0.305 0.251 , 0.278	Depositor DCC
R_{free} test set	944 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5282	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3QC, 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	0.37	0/2509	0.73	3/3398 (0.1%)
1	B	0.35	0/2564	0.72	4/3476 (0.1%)
All	All	0.36	0/5073	0.72	7/6874 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	234	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	B	234	ARG	NE-CZ-NH1	-12.73	113.93	120.30
1	B	234	ARG	NE-CZ-NH2	11.42	126.01	120.30
1	A	234	ARG	CD-NE-CZ	6.23	132.33	123.60
1	B	234	ARG	CD-NE-CZ	5.77	131.68	123.60
1	B	151	GLY	N-CA-C	-5.27	99.92	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2473	0	2445	112	0
1	B	2527	0	2490	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	23	4	0
3	B	24	0	23	4	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	97	0	0	2	0
5	B	81	0	0	7	0
All	All	5282	0	5005	224	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 22.

All (224) 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:A:31:ALA:HA	1:A:34:LYS:HD3	1.30	1.13
1:B:31:ALA:HA	1:B:34:LYS:HD3	1.34	1.08
1:B:119:ARG:HH12	1:B:130:ASP:HB2	1.36	0.90
1:A:119:ARG:HH12	1:A:130:ASP:HB2	1.35	0.90
1:B:20:GLN:HG2	5:B:443:HOH:O	1.75	0.87
1:A:115:MET:HE1	1:A:333:ILE:HD12	1.68	0.76
1:A:173:ASN:HD22	1:A:174:PRO:N	1.84	0.75
3:B:370:3QC:H402	3:B:370:3QC:H22A	1.68	0.75
1:A:187:ASP:HB3	1:A:190:ASN:HB2	1.69	0.75
1:A:28:PHE:HA	1:A:32:GLU:OE1	1.87	0.75
3:A:370:3QC:H402	3:A:370:3QC:H22A	1.69	0.74
1:B:272:ILE:HG23	1:B:292:LEU:HD13	1.70	0.73
1:B:187:ASP:HB3	1:B:190:ASN:HB2	1.69	0.73
1:B:28:PHE:HA	1:B:32:GLU:OE1	1.89	0.72
1:A:272:ILE:HG23	1:A:292:LEU:HD13	1.70	0.72
1:B:173:ASN:HD22	1:B:174:PRO:CD	2.03	0.71
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.04	0.70
1:B:173:ASN:HD22	1:B:174:PRO:HD2	1.57	0.69
1:B:115:MET:HE1	1:B:333:ILE:HD12	1.73	0.69
1:B:152:THR:HG22	1:B:153:GLU:N	2.07	0.69
1:B:173:ASN:HD22	1:B:174:PRO:N	1.90	0.69
1:A:152:THR:HG22	1:A:153:GLU:N	2.06	0.69
1:A:53:ARG:NH1	1:A:63:ARG:HH22	1.90	0.69
1:B:152:THR:CG2	1:B:153:GLU:N	2.56	0.68
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:CG2	1:A:153:GLU:N	2.55	0.68
1:A:87:CYS:HB3	1:A:88:PRO:HD3	1.76	0.68
1:B:173:ASN:HA	1:B:200:GLU:HG3	1.74	0.68
1:B:53:ARG:NH1	1:B:63:ARG:HH22	1.91	0.67
1:A:31:ALA:CA	1:A:34:LYS:HD3	2.19	0.67
1:A:173:ASN:HA	1:A:200:GLU:HG3	1.76	0.67
1:B:119:ARG:HH12	1:B:130:ASP:CB	2.08	0.66
1:A:150:ASN:CG	1:A:151:GLY:N	2.48	0.66
1:B:29:ASN:OD1	1:B:29:ASN:O	2.14	0.65
1:A:150:ASN:CG	1:A:151:GLY:H	2.00	0.65
1:A:268:GLY:O	1:A:271:ASN:HB2	1.96	0.65
1:A:119:ARG:HH12	1:A:130:ASP:CB	2.10	0.65
1:B:152:THR:CG2	1:B:153:GLU:H	2.10	0.64
1:A:245:MET:O	1:A:256:VAL:O	2.16	0.64
1:B:150:ASN:CG	1:B:151:GLY:N	2.51	0.64
1:A:151:GLY:O	1:A:152:THR:CB	2.46	0.64
1:A:30:LEU:C	1:A:32:GLU:H	2.01	0.64
1:A:29:ASN:OD1	1:A:29:ASN:O	2.16	0.63
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.62	0.63
1:B:30:LEU:C	1:B:32:GLU:H	2.02	0.63
1:A:104:TYR:OH	1:A:272:ILE:HD11	1.98	0.62
1:B:268:GLY:O	1:B:271:ASN:HB2	1.99	0.62
1:B:104:TYR:OH	1:B:272:ILE:HD11	1.99	0.62
1:A:152:THR:CG2	1:A:153:GLU:H	2.13	0.62
1:B:176:SER:OG	1:B:180:GLU:HG3	2.00	0.61
1:A:176:SER:OG	1:A:180:GLU:HG3	2.00	0.61
1:A:173:ASN:ND2	1:A:175:SER:H	1.98	0.61
1:B:151:GLY:O	1:B:152:THR:CB	2.49	0.61
1:B:360:LEU:C	1:B:360:LEU:HD23	2.22	0.60
1:A:125:TYR:HB3	1:A:129:GLU:HG3	1.83	0.60
1:B:125:TYR:HB3	1:B:129:GLU:HG3	1.82	0.60
1:B:114:THR:HG22	1:B:115:MET:HE2	1.84	0.60
1:A:256:VAL:O	1:A:257:LYS:HB2	2.02	0.60
1:B:161:LEU:CD2	5:B:451:HOH:O	2.49	0.59
1:B:150:ASN:CG	1:B:151:GLY:H	2.04	0.59
1:B:173:ASN:ND2	1:B:175:SER:H	2.00	0.59
1:B:272:ILE:HG22	1:B:293:LEU:HD23	1.84	0.59
1:A:177:ASP:OD2	1:A:179:SER:HB3	2.03	0.58
1:B:151:GLY:O	1:B:152:THR:OG1	2.20	0.58
1:A:272:ILE:HG22	1:A:293:LEU:HD23	1.84	0.58
1:B:190:ASN:ND2	1:B:193:GLY:HA3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:ND2	1:B:174:PRO:HD2	2.18	0.57
1:B:360:LEU:C	1:B:361:ASN:HD22	2.08	0.57
1:A:360:LEU:HD23	1:A:360:LEU:C	2.25	0.57
1:A:119:ARG:NH1	1:A:130:ASP:HB2	2.14	0.56
1:A:151:GLY:O	1:A:152:THR:OG1	2.19	0.56
1:B:150:ASN:O	1:B:151:GLY:O	2.23	0.56
1:B:361:ASN:N	1:B:361:ASN:HD22	2.03	0.56
1:B:79:ILE:O	1:B:83:ARG:HG3	2.05	0.56
1:A:173:ASN:ND2	1:A:174:PRO:HD2	2.20	0.56
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.88	0.55
1:A:61:SER:HB3	1:B:65:THR:O	2.06	0.55
1:B:114:THR:HG22	1:B:115:MET:CE	2.37	0.55
1:B:272:ILE:CG2	1:B:292:LEU:HD13	2.36	0.55
1:A:79:ILE:O	1:A:83:ARG:HG3	2.06	0.55
1:A:190:ASN:ND2	1:A:193:GLY:HA3	2.21	0.55
1:A:311:TYR:CG	1:A:321:GLN:HG3	2.42	0.55
1:A:29:ASN:O	1:A:32:GLU:N	2.40	0.55
1:A:114:THR:HG22	1:A:115:MET:CE	2.37	0.54
1:A:272:ILE:CG2	1:A:292:LEU:HD13	2.38	0.54
1:B:29:ASN:O	1:B:32:GLU:N	2.41	0.54
1:B:177:ASP:OD2	1:B:179:SER:HB3	2.08	0.54
1:B:157:LYS:HA	1:B:202:ILE:O	2.08	0.54
1:A:187:ASP:OD1	1:A:190:ASN:ND2	2.41	0.54
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.42	0.54
1:A:173:ASN:C	1:A:173:ASN:HD22	2.11	0.53
1:A:154:PHE:HA	1:A:244:HIS:O	2.07	0.53
1:B:172:LEU:HB2	5:B:385:HOH:O	2.09	0.53
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.91	0.53
1:A:114:THR:HG22	1:A:115:MET:HE2	1.91	0.53
1:A:269:SER:C	1:A:271:ASN:H	2.11	0.53
1:A:152:THR:O	1:A:153:GLU:HB2	2.09	0.53
1:B:119:ARG:NH1	1:B:130:ASP:CB	2.72	0.52
1:B:154:PHE:HA	1:B:244:HIS:O	2.09	0.52
1:A:157:LYS:HA	1:A:202:ILE:O	2.09	0.52
1:A:61:SER:CB	1:B:65:THR:O	2.57	0.52
1:A:82:TYR:CE1	1:A:86:VAL:HG11	2.45	0.52
1:B:31:ALA:CA	1:B:34:LYS:HD3	2.24	0.52
1:B:357:LYS:HB3	1:B:357:LYS:NZ	2.24	0.52
1:A:357:LYS:HB3	1:A:357:LYS:NZ	2.25	0.52
1:B:269:SER:C	1:B:271:ASN:H	2.14	0.52
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HG3	1:A:171:LEU:HD13	1.92	0.51
1:A:150:ASN:ND2	1:A:151:GLY:H	2.07	0.51
1:A:119:ARG:NH1	1:A:130:ASP:CB	2.73	0.51
1:A:245:MET:O	1:A:256:VAL:C	2.49	0.51
1:A:52:VAL:O	1:A:63:ARG:HB2	2.11	0.51
1:A:150:ASN:O	1:A:151:GLY:O	2.29	0.51
1:B:63:ARG:NH1	1:B:63:ARG:HB3	2.26	0.50
1:B:152:THR:HG23	1:B:153:GLU:H	1.76	0.50
1:B:82:TYR:CE1	1:B:86:VAL:HG11	2.46	0.50
1:A:30:LEU:C	1:A:32:GLU:N	2.65	0.50
1:B:52:VAL:O	1:B:63:ARG:HB2	2.12	0.50
1:A:136:ILE:HG12	1:A:263:LEU:HD13	1.94	0.50
1:B:187:ASP:OD1	1:B:190:ASN:ND2	2.45	0.49
1:A:152:THR:HG23	1:A:153:GLU:H	1.77	0.49
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.42	0.49
3:A:370:3QC:C40	3:A:370:3QC:H22A	2.41	0.49
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.94	0.49
1:A:30:LEU:O	1:A:32:GLU:N	2.46	0.49
3:B:370:3QC:C40	3:B:370:3QC:H22A	2.40	0.49
1:B:149:ASP:O	1:B:150:ASN:O	2.31	0.48
1:B:150:ASN:ND2	1:B:151:GLY:H	2.11	0.48
1:A:149:ASP:O	1:A:150:ASN:O	2.31	0.48
1:A:119:ARG:NH1	1:A:130:ASP:OD1	2.46	0.48
1:B:17:LYS:HA	1:B:361:ASN:O	2.13	0.48
1:B:162:GLU:HG3	1:B:171:LEU:HD13	1.96	0.48
1:A:29:ASN:O	1:A:31:ALA:N	2.46	0.48
1:B:30:LEU:C	1:B:32:GLU:N	2.66	0.48
1:B:165:ASN:HB3	5:B:407:HOH:O	2.14	0.48
1:B:289:ASN:ND2	1:B:292:LEU:H	2.12	0.48
1:A:360:LEU:HD23	1:A:361:ASN:O	2.14	0.47
1:B:119:ARG:NH1	1:B:130:ASP:HB2	2.15	0.47
1:B:152:THR:O	1:B:153:GLU:HB2	2.13	0.47
1:B:241:VAL:CG1	1:B:261:LEU:HB3	2.44	0.47
1:A:63:ARG:NH1	1:A:63:ARG:HB3	2.28	0.47
1:B:360:LEU:HD23	1:B:361:ASN:N	2.29	0.47
1:B:30:LEU:O	1:B:32:GLU:N	2.48	0.47
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.76	0.47
1:B:44:ASP:OD2	1:B:47:ARG:HD2	2.14	0.47
1:B:119:ARG:NH1	1:B:130:ASP:OD1	2.47	0.47
1:A:152:THR:HG22	1:A:153:GLU:HG2	1.97	0.47
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD3	5:A:423:HOH:O	2.13	0.47
3:A:370:3QC:H331	3:A:370:3QC:H291	1.62	0.47
1:A:289:ASN:ND2	1:A:292:LEU:H	2.12	0.47
1:B:230:ALA:O	1:B:234:ARG:HG3	2.14	0.47
1:B:292:LEU:HA	1:B:292:LEU:HD23	1.74	0.47
1:B:116:GLU:HG2	1:B:136:ILE:HD12	1.97	0.46
1:B:173:ASN:HD22	1:B:173:ASN:C	2.18	0.46
1:A:241:VAL:CG1	1:A:261:LEU:HB3	2.46	0.46
1:A:269:SER:C	1:A:271:ASN:N	2.68	0.46
1:A:116:GLU:HG2	1:A:136:ILE:HD12	1.98	0.46
1:B:106:GLN:NE2	1:B:345:GLU:HG3	2.31	0.46
1:B:35:ALA:O	1:B:36:SER:O	2.34	0.46
1:B:173:ASN:CA	1:B:200:GLU:HG3	2.45	0.46
1:B:70:MET:HE1	1:B:84:SER:HB3	1.97	0.46
1:B:269:SER:C	1:B:271:ASN:N	2.70	0.45
1:A:119:ARG:NH1	1:A:127:TRP:HA	2.31	0.45
1:A:106:GLN:NE2	1:A:345:GLU:HG3	2.32	0.45
1:A:66:TYR:CE2	1:A:351:GLU:OE2	2.70	0.45
1:B:29:ASN:O	1:B:31:ALA:N	2.49	0.45
1:B:119:ARG:NH1	1:B:127:TRP:HA	2.32	0.45
1:A:28:PHE:CE1	1:A:39:SER:HB2	2.52	0.44
1:A:79:ILE:HG13	1:A:83:ARG:HD2	2.00	0.44
1:B:66:TYR:CE2	1:B:351:GLU:OE2	2.70	0.44
1:B:152:THR:HG22	1:B:153:GLU:HG2	2.00	0.44
1:B:28:PHE:CE1	1:B:39:SER:HB2	2.52	0.44
1:A:215:GLU:HA	3:A:370:3QC:H401	2.00	0.44
1:A:352:TYR:O	1:A:355:ARG:HG2	2.17	0.44
1:A:173:ASN:CA	1:A:200:GLU:HG3	2.46	0.43
1:A:29:ASN:O	1:A:30:LEU:C	2.56	0.43
1:B:357:LYS:HB3	5:B:419:HOH:O	2.18	0.43
1:B:79:ILE:HG13	1:B:83:ARG:HD2	1.99	0.43
1:A:70:MET:HE1	1:A:84:SER:HB3	2.01	0.43
1:B:352:TYR:O	1:B:355:ARG:HG2	2.18	0.43
1:A:172:LEU:HB2	5:A:382:HOH:O	2.19	0.43
1:B:120:SER:HA	1:B:121:PRO:HD3	1.86	0.43
1:A:187:ASP:HB3	1:A:190:ASN:HD22	1.84	0.43
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.48	0.43
1:B:190:ASN:HD22	1:B:193:GLY:HA3	1.83	0.43
1:B:28:PHE:HE1	1:B:39:SER:HB2	1.84	0.43
1:A:241:VAL:HG13	1:A:261:LEU:HB3	2.01	0.42
1:A:309:VAL:CG1	1:A:311:TYR:CE2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:O	1:A:357:LYS:HG3	2.18	0.42
1:A:115:MET:HE2	1:A:135:ILE:HD12	2.01	0.42
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.49	0.42
1:A:170:ASP:HB2	1:A:182:LEU:HD11	2.01	0.42
1:B:247:GLU:O	1:B:254:GLU:HA	2.19	0.42
1:A:187:ASP:HB3	1:A:190:ASN:ND2	2.34	0.42
1:B:215:GLU:HA	3:B:370:3QC:H401	2.02	0.42
1:B:66:TYR:HE2	1:B:351:GLU:OE2	2.03	0.42
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.85	0.42
1:B:187:ASP:HB3	1:B:190:ASN:ND2	2.34	0.42
1:B:26:ARG:HH22	1:B:32:GLU:CD	2.23	0.42
1:A:190:ASN:HD22	1:A:193:GLY:HA3	1.85	0.42
1:A:26:ARG:HH22	1:A:32:GLU:CD	2.23	0.42
1:A:70:MET:HE1	1:A:72:PHE:CZ	2.55	0.41
1:B:29:ASN:O	1:B:30:LEU:C	2.58	0.41
1:A:230:ALA:O	1:A:234:ARG:HG3	2.20	0.41
1:A:28:PHE:HE1	1:A:39:SER:HB2	1.84	0.41
1:A:298:VAL:HG13	1:A:309:VAL:CG2	2.49	0.41
1:A:66:TYR:HE2	1:A:351:GLU:OE2	2.03	0.41
1:A:357:LYS:CB	1:A:357:LYS:NZ	2.84	0.41
1:B:161:LEU:HD23	5:B:451:HOH:O	2.14	0.41
1:B:187:ASP:HB3	1:B:190:ASN:HD22	1.84	0.41
1:A:120:SER:HA	1:A:121:PRO:HD3	1.86	0.41
1:A:29:ASN:O	1:A:32:GLU:HB2	2.21	0.41
1:A:63:ARG:HG3	1:B:63:ARG:HG2	2.01	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.86	0.41
3:B:370:3QC:H291	3:B:370:3QC:H331	1.63	0.41
1:B:177:ASP:O	1:B:180:GLU:HG2	2.20	0.41
1:B:357:LYS:CB	1:B:357:LYS:NZ	2.84	0.41
1:A:245:MET:O	1:A:256:VAL:HA	2.21	0.40
1:A:309:VAL:HG13	1:A:311:TYR:CE2	2.57	0.40
1:B:161:LEU:HD22	5:B:451:HOH:O	2.20	0.40
1:A:257:LYS:HB2	1:A:257:LYS:HE3	1.86	0.40
1:B:70:MET:HE1	1:B:72:PHE:HZ	1.86	0.40
1:B:136:ILE:N	1:B:137:PRO:HD2	2.37	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	313/368 (85%)	291 (93%)	12 (4%)	10 (3%)	4	1
1	B	323/368 (88%)	304 (94%)	10 (3%)	9 (3%)	5	1
All	All	636/736 (86%)	595 (94%)	22 (4%)	19 (3%)	4	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	150	ASN
1	A	152	THR
1	A	191	LYS
1	A	362	LYS
1	B	30	LEU
1	B	150	ASN
1	B	152	THR
1	B	191	LYS
1	A	31	ALA
1	A	36	SER
1	A	151	GLY
1	B	31	ALA
1	B	35	ALA
1	B	36	SER
1	B	151	GLY
1	A	35	ALA
1	A	272	ILE
1	B	272	ILE

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	273/322 (85%)	259 (95%)	14 (5%)	24	22
1	B	279/322 (87%)	266 (95%)	13 (5%)	26	25
All	All	552/644 (86%)	525 (95%)	27 (5%)	25	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	128	GLU
1	A	140	LEU
1	A	148	THR
1	A	168	LEU
1	A	172	LEU
1	A	173	ASN
1	A	177	ASP
1	A	181	ARG
1	A	234	ARG
1	A	289	ASN
1	A	292	LEU
1	A	306	THR
1	A	343	LEU
1	B	122	ASN
1	B	128	GLU
1	B	140	LEU
1	B	148	THR
1	B	172	LEU
1	B	173	ASN
1	B	177	ASP
1	B	181	ARG
1	B	289	ASN
1	B	292	LEU
1	B	306	THR
1	B	343	LEU
1	B	361	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	122	ASN
1	A	141	HIS
1	A	142	GLN
1	A	173	ASN
1	A	190	ASN
1	A	205	HIS
1	A	262	ASN
1	A	289	ASN
1	B	18	ASN
1	B	98	ASN
1	B	122	ASN
1	B	141	HIS
1	B	142	GLN
1	B	173	ASN
1	B	190	ASN
1	B	205	HIS
1	B	262	ASN
1	B	289	ASN
1	B	361	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ADP	B	371	2	24,29,29	1.47	4 (16%)	29,45,45	1.82	4 (13%)
4	ADP	A	371	2	24,29,29	1.40	5 (20%)	29,45,45	1.92	4 (13%)
3	3QC	B	370	-	26,26,26	2.14	8 (30%)	35,38,38	2.19	9 (25%)
3	3QC	A	370	-	26,26,26	2.20	10 (38%)	35,38,38	2.20	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	371	2	-	0/12/32/32	0/3/3/3
4	ADP	A	371	2	-	0/12/32/32	0/3/3/3
3	3QC	B	370	-	-	0/12/24/24	0/3/3/3
3	3QC	A	370	-	-	0/12/24/24	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	370	3QC	C19-C20	5.02	1.46	1.39
3	A	370	3QC	C19-C20	4.64	1.46	1.39
3	A	370	3QC	C23-C17	4.54	1.46	1.39
3	B	370	3QC	C23-C17	4.20	1.45	1.39
4	B	371	ADP	C2-N3	4.13	1.38	1.32
3	A	370	3QC	C19-C17	3.76	1.45	1.39
3	A	370	3QC	C11-C6	3.73	1.44	1.39
3	A	370	3QC	C21-C20	3.70	1.46	1.38
3	B	370	3QC	C11-C6	3.59	1.44	1.39
3	B	370	3QC	C19-C17	3.54	1.44	1.39
4	A	371	ADP	C2-N3	3.40	1.37	1.32
3	B	370	3QC	C22-C21	3.12	1.45	1.38
3	B	370	3QC	C22-C23	3.03	1.45	1.38
3	B	370	3QC	C21-C20	2.71	1.44	1.38
3	A	370	3QC	C22-C23	2.70	1.44	1.38
4	B	371	ADP	C2-N1	2.61	1.38	1.33
4	B	371	ADP	C4-N3	2.58	1.39	1.35
4	A	371	ADP	C4-N3	2.57	1.39	1.35
3	A	370	3QC	C12-C11	2.54	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	371	ADP	PA-O2A	-2.51	1.43	1.55
3	B	370	3QC	C12-C11	2.49	1.43	1.38
3	A	370	3QC	C33-C14	-2.46	1.46	1.51
4	A	371	ADP	PB-O3B	-2.26	1.46	1.54
4	A	371	ADP	C2-N1	2.25	1.38	1.33
4	B	371	ADP	PB-O3B	-2.16	1.46	1.54
3	A	370	3QC	C22-C21	2.13	1.43	1.38
3	A	370	3QC	C12-C13	2.06	1.44	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	370	3QC	C17-C5-C6	7.97	123.67	113.32
4	A	371	ADP	N3-C2-N1	-7.57	116.84	128.68
3	B	370	3QC	C17-C5-C6	7.55	123.14	113.32
4	B	371	ADP	N3-C2-N1	-7.27	117.31	128.68
3	A	370	3QC	C4-C5-C17	4.70	119.06	110.63
3	B	370	3QC	C4-C5-C17	4.30	118.35	110.63
4	A	371	ADP	C2'-C3'-C4'	-3.83	95.21	102.64
3	A	370	3QC	C20-C19-C17	-3.80	116.85	120.11
4	B	371	ADP	C2'-C3'-C4'	-3.54	95.77	102.64
3	B	370	3QC	C20-C19-C17	-3.47	117.14	120.11
3	B	370	3QC	C23-C22-C21	-3.18	115.74	120.25
3	B	370	3QC	C4-C5-C6	3.10	115.27	110.60
4	A	371	ADP	C2-N1-C6	2.95	123.80	118.75
3	A	370	3QC	C23-C22-C21	-2.75	116.35	120.25
4	B	371	ADP	C2-N1-C6	2.50	123.02	118.75
4	B	371	ADP	O5'-C5'-C4'	2.48	117.54	108.99
4	A	371	ADP	O5'-C5'-C4'	2.47	117.50	108.99
3	A	370	3QC	C4-C5-C6	2.46	114.29	110.60
3	B	370	3QC	O48-C38-N3	-2.43	118.45	123.80
3	B	370	3QC	C22-C21-C20	2.40	122.70	119.31
3	B	370	3QC	C29-C13-C14	-2.37	117.49	121.17
3	B	370	3QC	C5-C4-N3	-2.29	101.57	111.28
3	A	370	3QC	C29-C13-C14	-2.18	117.78	121.17
3	A	370	3QC	C5-C4-N3	-2.14	102.21	111.28
3	A	370	3QC	C1-C2-N3	2.12	115.51	111.75
3	A	370	3QC	C22-C21-C20	2.06	122.22	119.31

There are no chirality outliers.

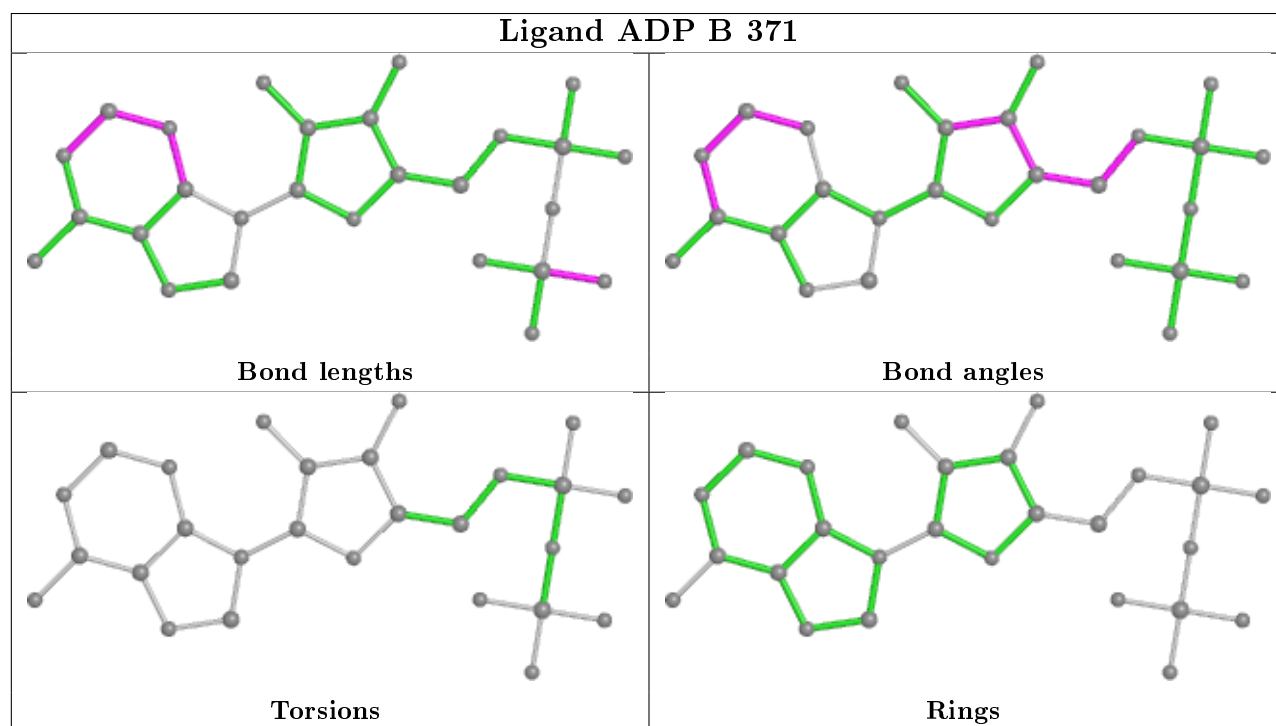
There are no torsion outliers.

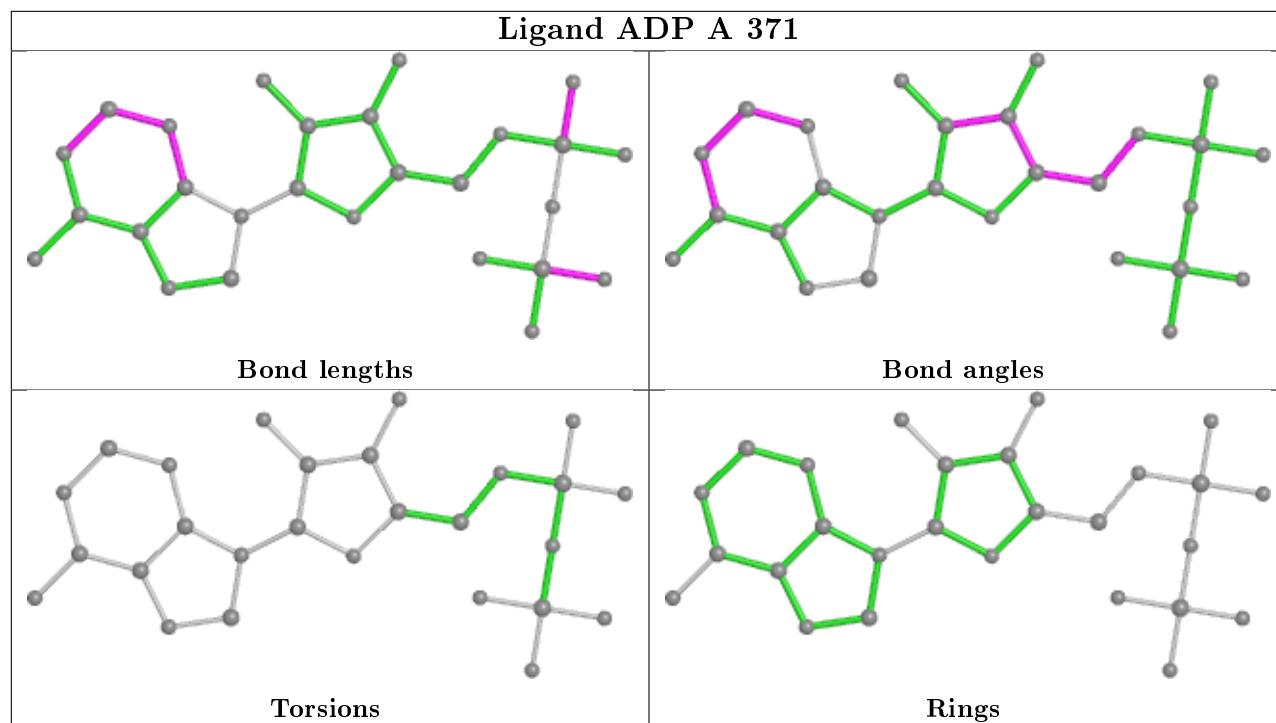
There are no ring outliers.

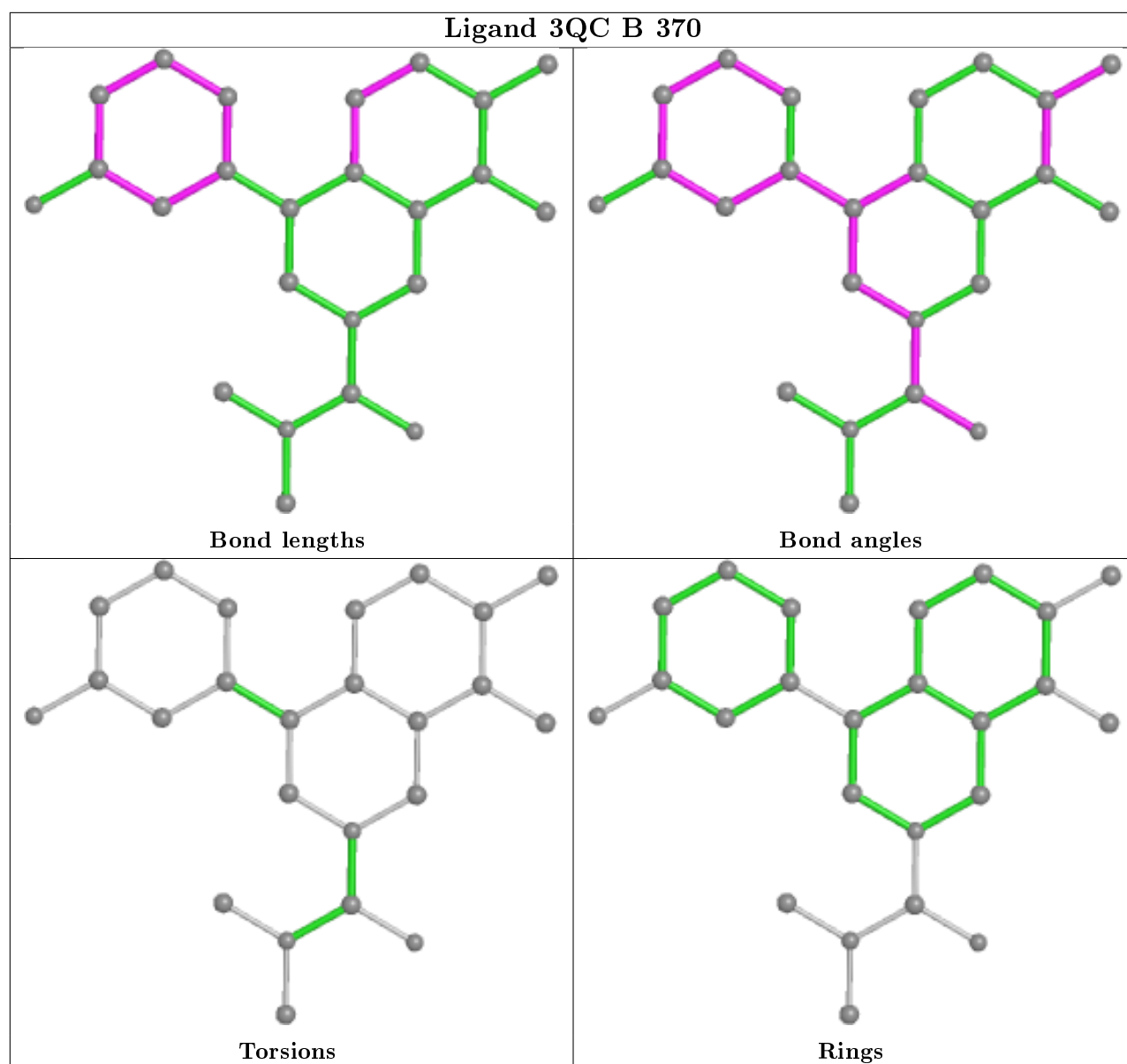
2 monomers are involved in 8 short contacts:

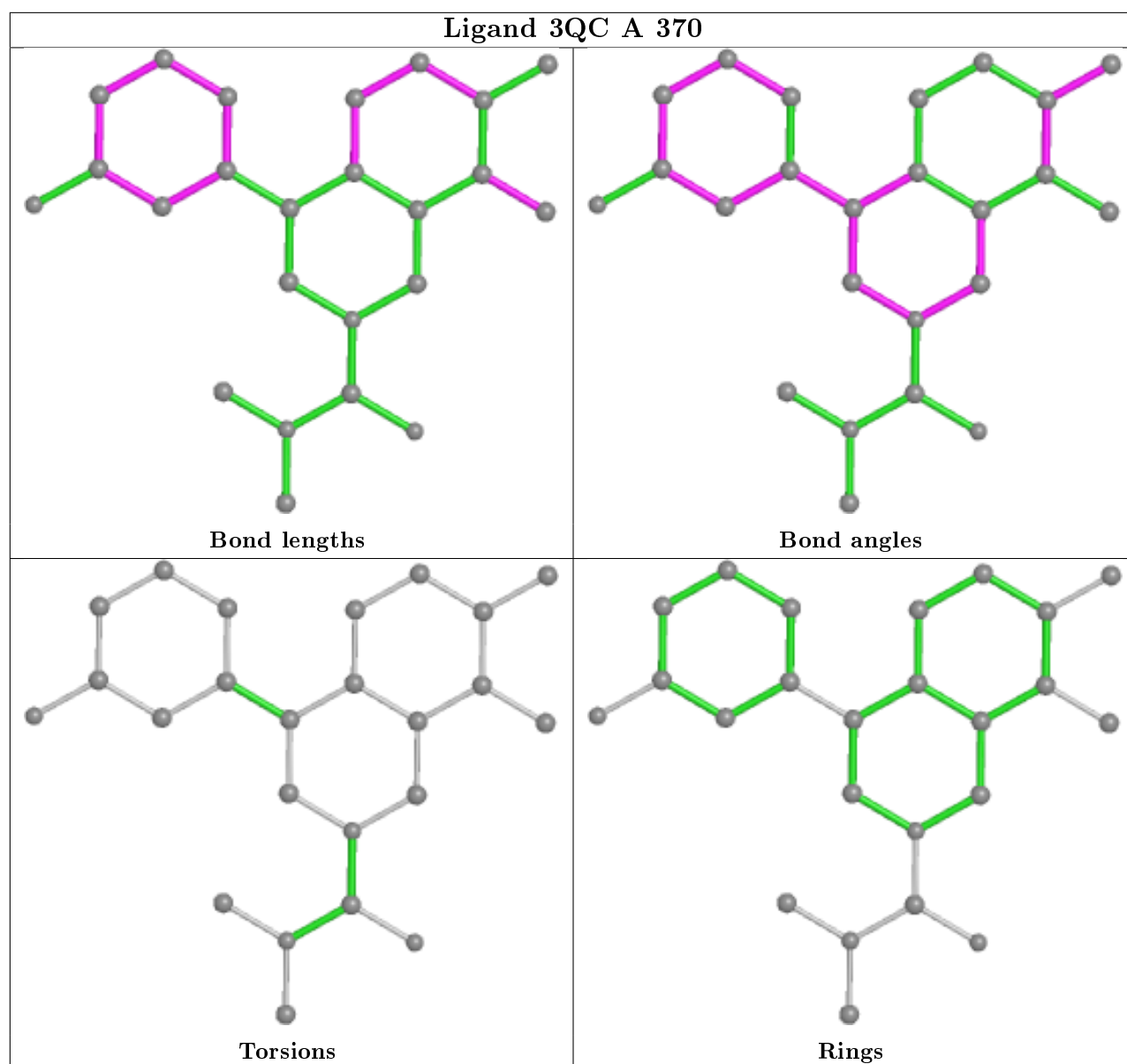
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	370	3QC	4	0
3	A	370	3QC	4	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/368 (87%)	1.07	37 (11%) 4 6	11, 25, 44, 53	0
1	B	329/368 (89%)	0.88	32 (9%) 7 10	13, 26, 46, 53	0
All	All	650/736 (88%)	0.97	69 (10%) 6 7	11, 26, 46, 53	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	19.3
1	B	36	SER	13.5
1	B	35	ALA	12.7
1	A	273	GLY	10.8
1	B	272	ILE	10.2
1	A	274	ARG	9.4
1	B	37	ALA	9.4
1	A	272	ILE	9.3
1	A	150	ASN	8.7
1	B	34	LYS	8.1
1	A	149	ASP	8.0
1	A	36	SER	7.7
1	A	31	ALA	7.7
1	A	151	GLY	7.5
1	B	273	GLY	7.4
1	B	31	ALA	7.0
1	A	34	LYS	6.9
1	B	274	ARG	6.8
1	A	30	LEU	6.0
1	A	38	HIS	5.9
1	B	38	HIS	5.8
1	A	56	GLY	5.7
1	A	148	THR	5.3
1	B	360	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	THR	5.1
1	A	190	ASN	4.9
1	B	33	ARG	4.9
1	A	97	TYR	4.9
1	A	33	ARG	4.8
1	A	32	GLU	4.8
1	B	152	THR	4.4
1	A	256	VAL	4.3
1	A	271	ASN	4.3
1	B	56	GLY	4.2
1	B	149	ASP	4.2
1	A	37	ALA	4.1
1	A	153	GLU	4.1
1	A	305	ARG	4.1
1	B	30	LEU	3.9
1	B	190	ASN	3.9
1	A	175	SER	3.7
1	B	151	GLY	3.3
1	A	174	PRO	3.3
1	B	271	ASN	3.3
1	B	32	GLU	3.2
1	B	97	TYR	3.2
1	A	188	PRO	3.1
1	A	82	TYR	3.1
1	A	29	ASN	3.1
1	B	178	VAL	2.9
1	B	20	GLN	2.9
1	B	17	LYS	2.9
1	B	150	ASN	2.8
1	B	29	ASN	2.8
1	A	178	VAL	2.7
1	B	46	VAL	2.6
1	B	341	LEU	2.6
1	B	148	THR	2.6
1	A	181	ARG	2.5
1	B	181	ARG	2.4
1	A	185	PHE	2.4
1	B	175	SER	2.3
1	A	363	PRO	2.2
1	B	212	GLN	2.1
1	A	229	ASN	2.1
1	A	63	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	146	LYS	2.0
1	A	103	ALA	2.0
1	B	327	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

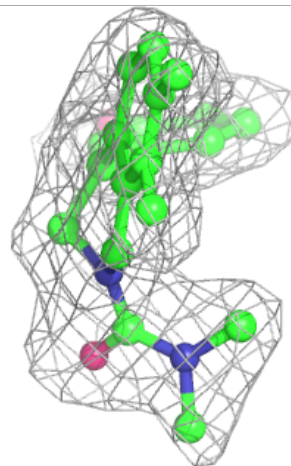
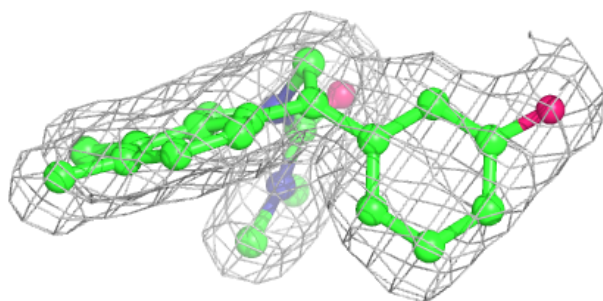
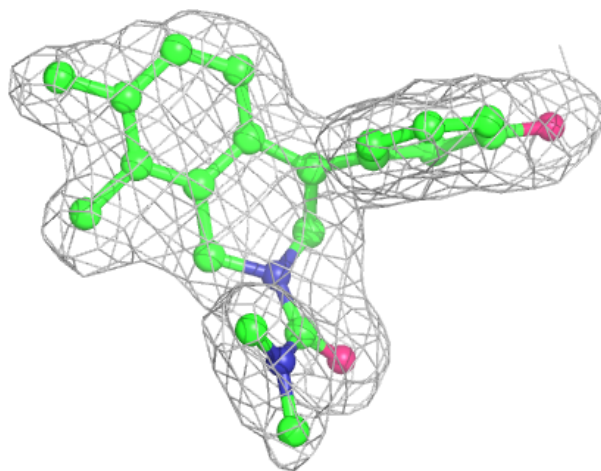
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3QC	B	370	24/24	0.93	0.16	14,19,20,21	0
3	3QC	A	370	24/24	0.93	0.19	14,20,21,22	0
4	ADP	B	371	27/27	0.96	0.14	13,23,25,29	0
4	ADP	A	371	27/27	0.97	0.14	14,19,21,23	0
2	MG	A	369	1/1	0.97	0.29	21,21,21,21	0
2	MG	B	369	1/1	0.97	0.23	21,21,21,21	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.

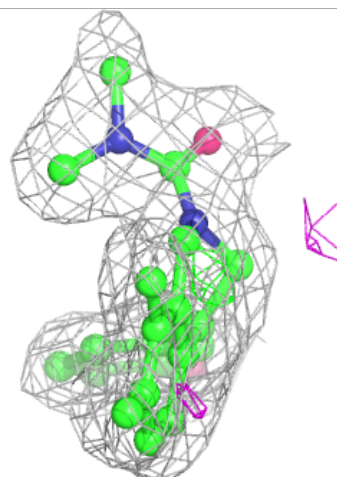
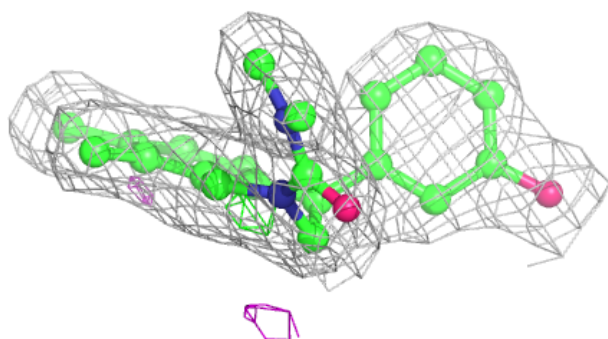
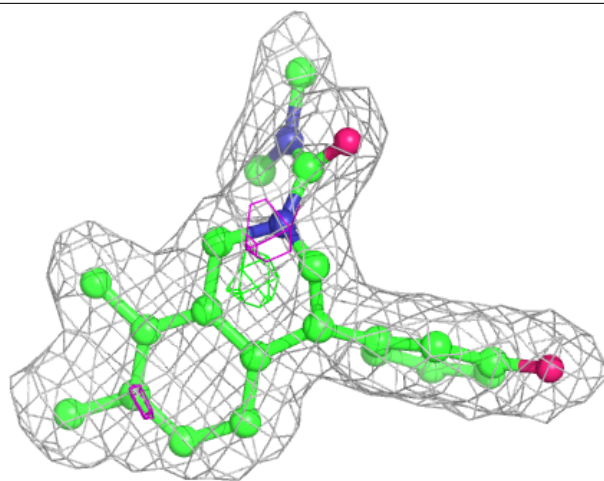
Electron density around 3QC B 370:

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



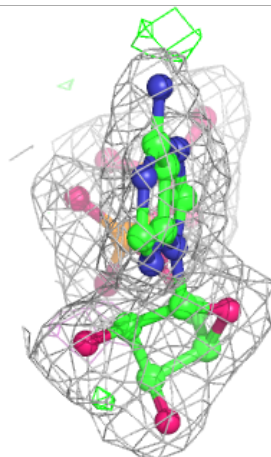
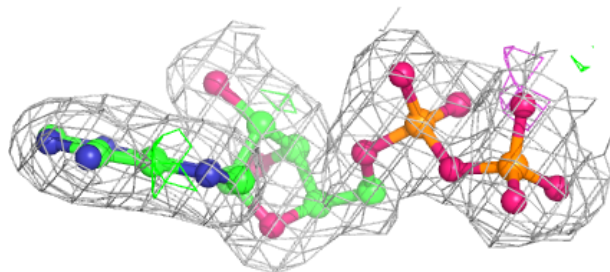
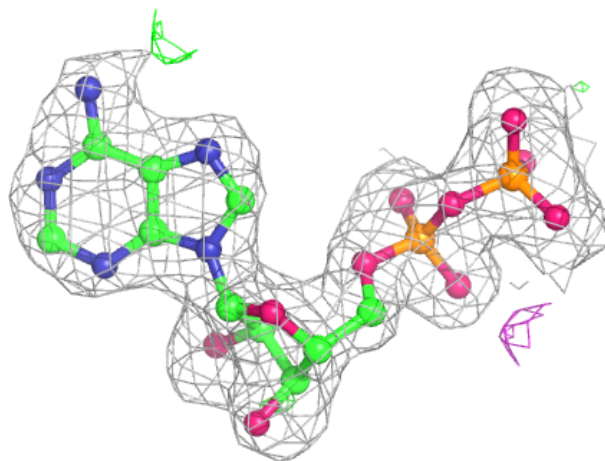
Electron density around 3QC A 370:

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



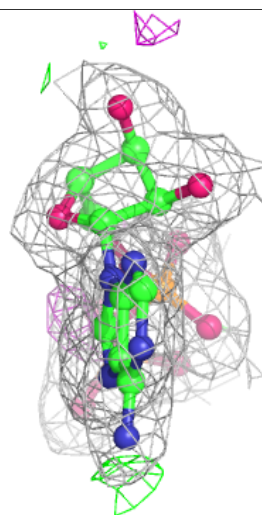
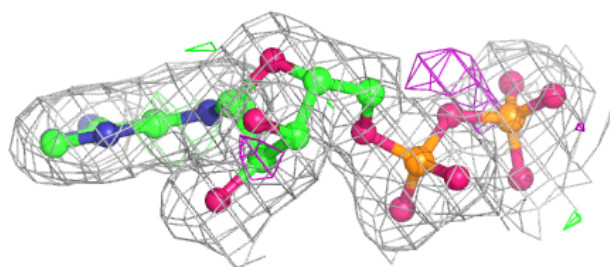
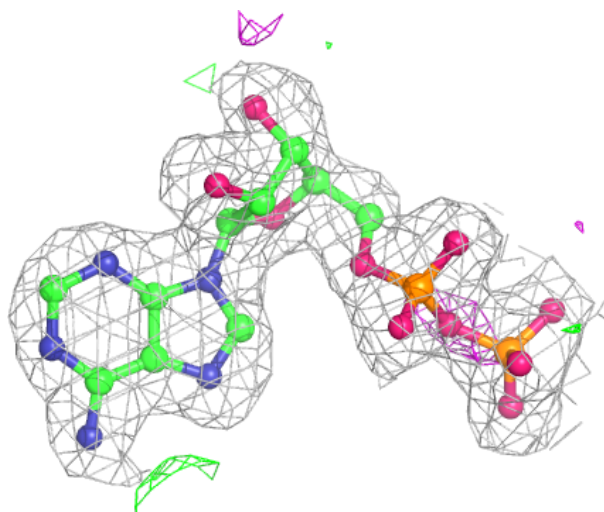
Electron density around ADP B 371:

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



Electron density around ADP A 371:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.