Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:39 PM BST

PDB ID	:	5YH3
Title	:	The structure of hFam20C and hFam20A complex
Authors	:	Zhu, Q.; Xiao, J.
Deposited on	:	2017-09-27
Resolution	:	3.30 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:

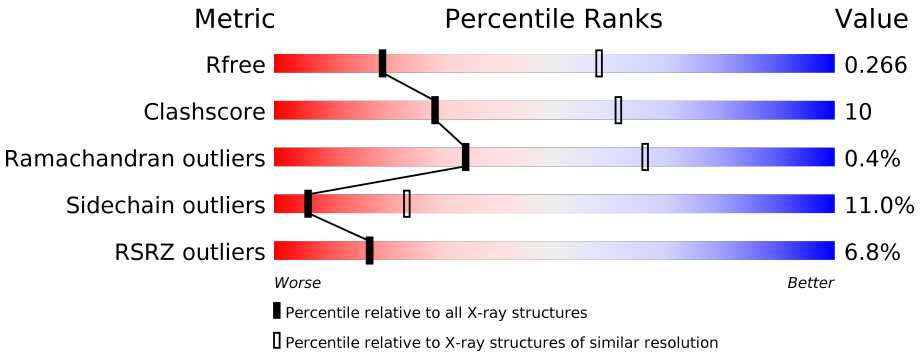
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

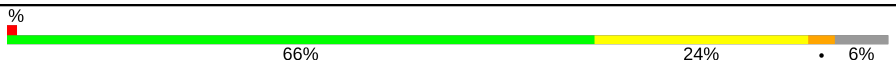
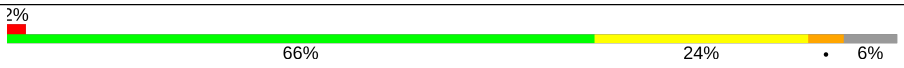
The reported resolution of this entry is 3.30 Å.

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	467	
1	B	467	
2	C	438	
2	D	438	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13012 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 Pseudokinase FAM20A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3545	2267	623	634	21			
1	B	438	Total	C	N	O	S	0	0	0
			3545	2267	623	634	21			

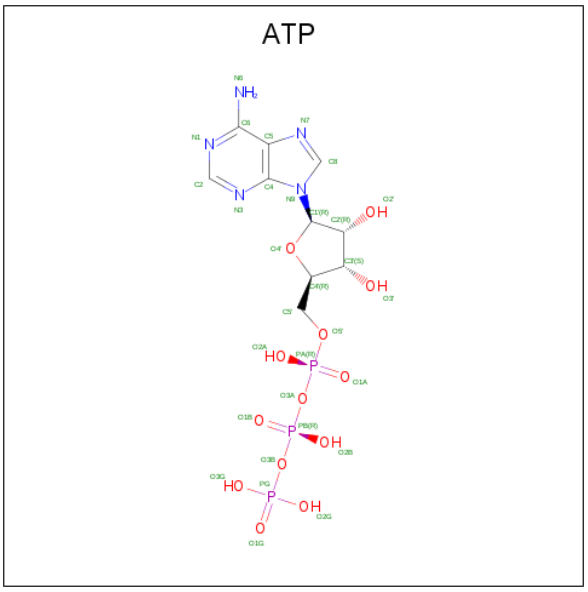
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	LYS	ASN	engineered mutation	UNP Q96MK3
B	332	LYS	ASN	engineered mutation	UNP Q96MK3

- Molecule 2 is a protein called Extracellular serine/threonine protein kinase FAM20C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	385	Total	C	N	O	S	0	0	0
			3184	2029	562	575	18			
2	D	314	Total	C	N	O	S	0	0	0
			2614	1660	468	468	18			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



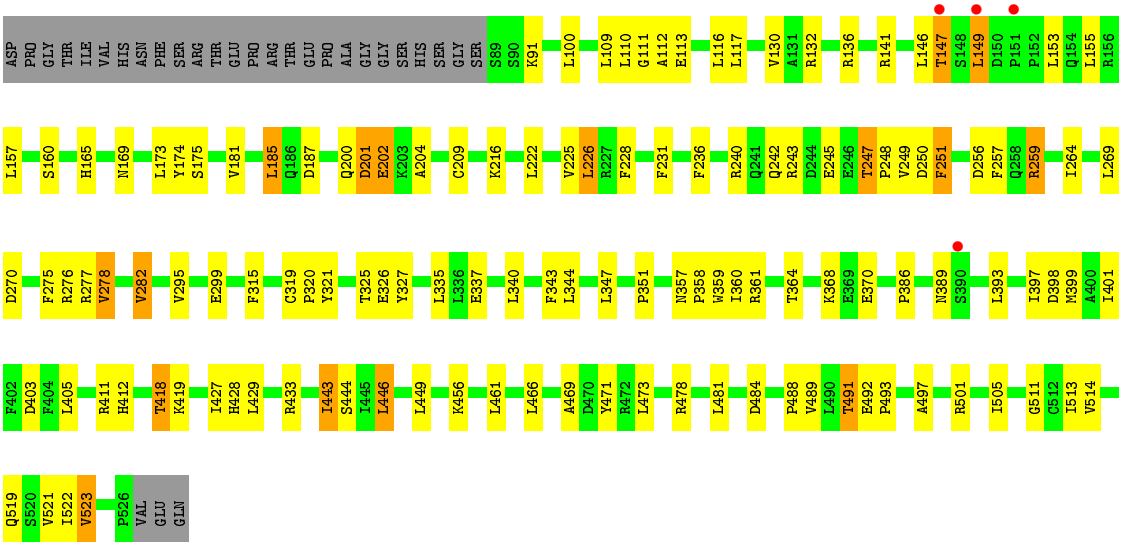
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

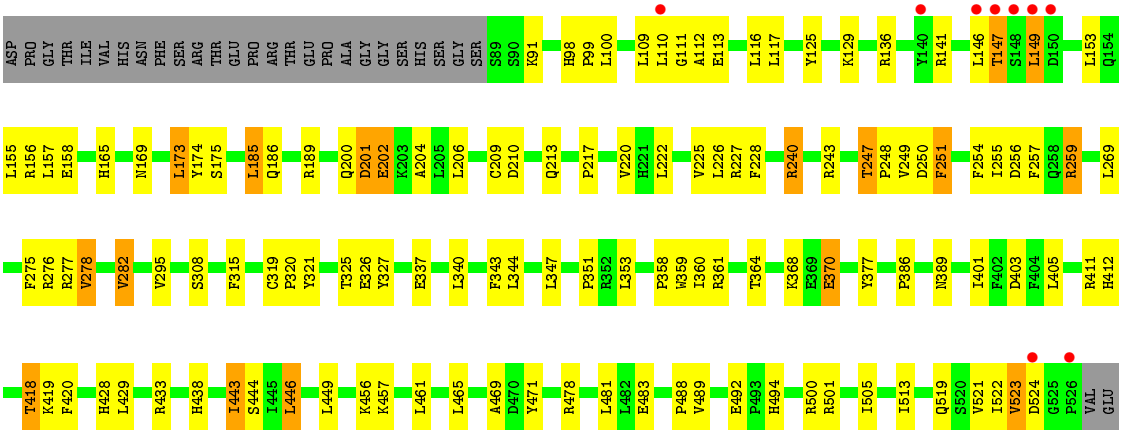
- Molecule 1: Pseudokinase FAM20A

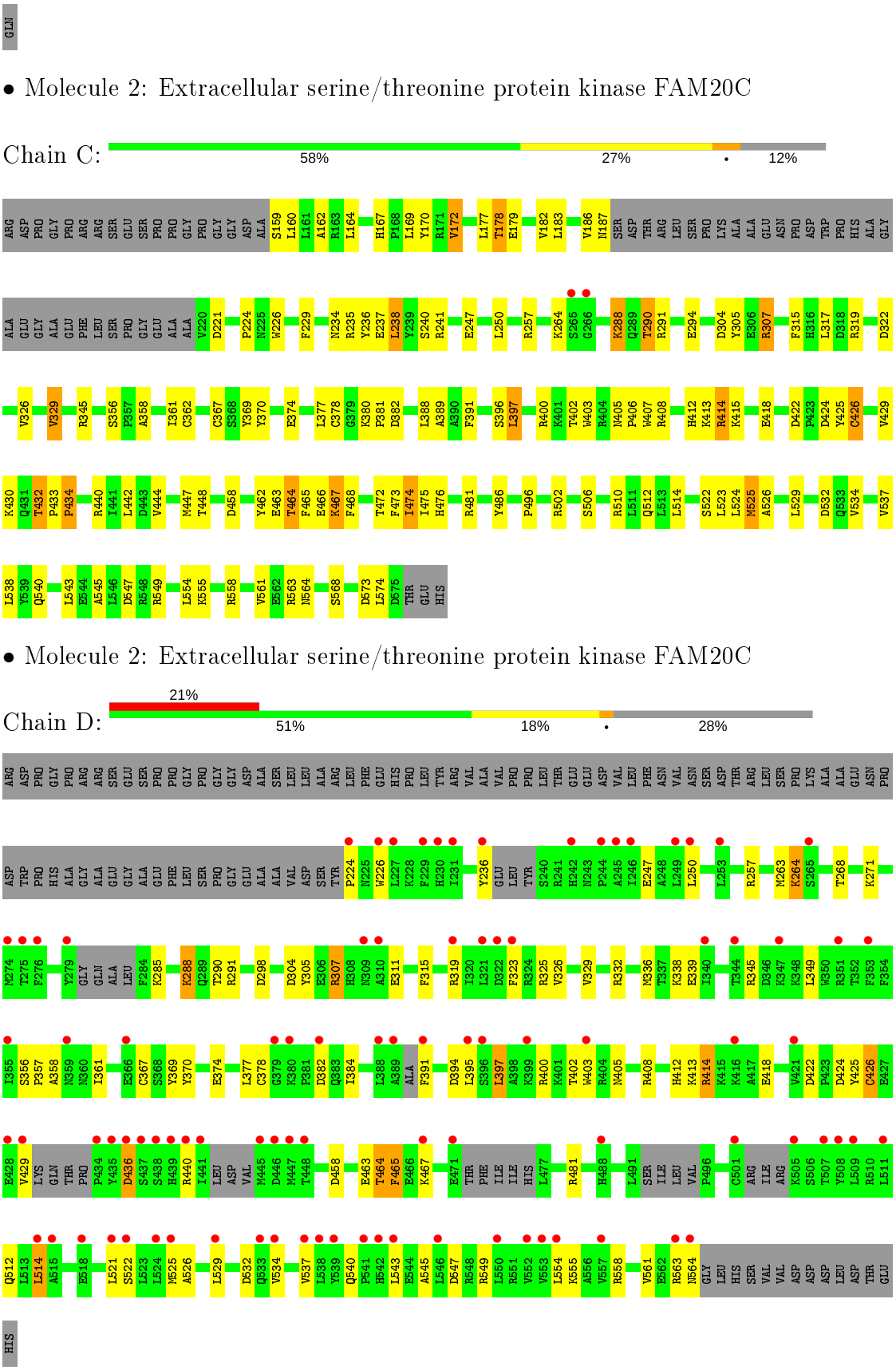
Chain A:



- Molecule 1: Pseudokinase FAM20A

Chain B:




GLN
• Molecule 2: Extracellular serine/threonine protein kinase FAM20C
Chain C:
58%
27%
12%
• Molecule 2: Extracellular serine/threonine protein kinase FAM20C
Chain D:
21%
51%
18%
28%
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.47Å 192.75Å 226.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.30 48.56 – 3.30	Depositor EDS
% Data completeness (in resolution range)	75.9 (48.56-3.30) 83.5 (48.56-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.233 , 0.266 0.233 , 0.266	Depositor DCC
R_{free} test set	2160 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	13012	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.28	0/3633	0.47	0/4923
1	B	0.27	0/3633	0.45	0/4923
2	C	0.28	0/3265	0.47	0/4415
2	D	0.26	0/2675	0.42	0/3592
All	All	0.27	0/13206	0.45	0/17853

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ASP	Peptide
1	B	201	ASP	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	3545	0	3533	66	0
1	B	3545	0	3533	67	0
2	C	3184	0	3121	78	0
2	D	2614	0	2545	48	0
3	A	62	0	24	4	0
3	B	62	0	24	5	0
All	All	13012	0	12780	251	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 (251) 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:C:235:ARG:HG3	2:C:472:THR:HG22	1.42	1.02
2:C:167:HIS:HD2	2:C:169:LEU:H	1.21	0.88
2:C:468:PHE:HB3	2:C:472:THR:HG21	1.59	0.84
1:B:136:ARG:NH2	3:B:702:ATP:O2B	2.11	0.84
1:A:327:TYR:HH	2:C:305:TYR:HH	1.16	0.83
1:B:327:TYR:HH	2:D:305:TYR:HH	1.07	0.82
2:C:315:PHE:HA	2:C:326:VAL:HG21	1.64	0.78
2:C:288:LYS:HE2	2:C:377:LEU:HD21	1.66	0.77
1:A:256:ASP:OD1	1:A:259:ARG:NH2	2.21	0.74
1:B:227:ARG:NH1	3:B:702:ATP:O3G	2.20	0.74
1:A:401:ILE:HG23	1:A:505:ILE:HD13	1.69	0.74
1:A:116:LEU:HA	1:A:419:LYS:HD3	1.71	0.73
2:C:400:ARG:NH1	2:C:463:GLU:OE1	2.22	0.73
1:A:136:ARG:NH1	3:A:702:ATP:O2A	2.16	0.73
1:B:401:ILE:HG23	1:B:505:ILE:HD13	1.71	0.72
1:B:202:GLU:O	1:B:204:ALA:N	2.22	0.72
2:C:403:TRP:NE1	2:C:464:THR:OG1	2.19	0.72
1:B:116:LEU:HA	1:B:419:LYS:HD3	1.71	0.71
2:C:522:SER:OG	2:C:547:ASP:OD2	2.06	0.71
1:A:202:GLU:O	1:A:204:ALA:N	2.21	0.70
2:C:468:PHE:HB3	2:C:472:THR:CG2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:555:LYS:HD2	2:D:558:ARG:HE	1.56	0.69
2:D:315:PHE:HA	2:D:326:VAL:HG21	1.73	0.69
1:A:243:ARG:NH1	1:A:488:PRO:O	2.26	0.68
1:A:278:VAL:HG12	1:A:428:HIS:HB2	1.74	0.68
2:C:304:ASP:O	2:C:481:ARG:NH1	2.28	0.67
2:C:167:HIS:CD2	2:C:169:LEU:H	2.10	0.67
2:C:433:PRO:HB2	2:C:434:PRO:HD3	1.76	0.67
2:C:555:LYS:HD2	2:C:558:ARG:HE	1.59	0.67
1:B:256:ASP:OD1	1:B:259:ARG:NH2	2.27	0.66
1:B:243:ARG:NH1	1:B:488:PRO:O	2.27	0.66
1:B:386:PRO:O	1:B:389:ASN:ND2	2.28	0.66
2:D:288:LYS:HE2	2:D:377:LEU:HD21	1.77	0.66
1:A:481:LEU:HD22	1:A:489:VAL:HG21	1.78	0.66
1:A:446:LEU:HD13	1:A:449:LEU:HB3	1.78	0.65
2:D:400:ARG:NH1	2:D:463:GLU:OE1	2.28	0.65
1:A:250:ASP:HA	2:C:356:SER:HB2	1.78	0.64
2:C:182:VAL:O	2:C:467:LYS:NZ	2.28	0.64
2:D:403:TRP:NE1	2:D:464:THR:OG1	2.28	0.64
1:B:446:LEU:HD13	1:B:449:LEU:HB3	1.78	0.64
1:A:361:ARG:NH2	1:A:444:SER:OG	2.30	0.64
1:A:111:GLY:O	1:A:113:GLU:N	2.32	0.62
2:D:436:ASP:N	2:D:436:ASP:OD1	2.33	0.62
1:B:481:LEU:HD22	1:B:489:VAL:HG21	1.81	0.62
1:A:136:ARG:NH2	3:A:702:ATP:O1B	2.34	0.61
1:B:250:ASP:HA	2:D:356:SER:HB2	1.83	0.61
2:C:512:GLN:HA	2:C:554:LEU:HD21	1.82	0.60
2:D:263:MET:HB2	2:D:349:LEU:HD12	1.82	0.60
1:A:344:LEU:HD11	1:A:429:LEU:HD21	1.83	0.60
1:B:111:GLY:O	1:B:113:GLU:N	2.32	0.60
1:B:125:TYR:OH	3:B:701:ATP:O2G	2.11	0.60
2:C:468:PHE:CB	2:C:472:THR:HG21	2.31	0.60
1:B:109:LEU:HD11	1:B:169:ASN:HD22	1.67	0.60
1:A:109:LEU:HD11	1:A:169:ASN:HD22	1.66	0.59
2:D:304:ASP:O	2:D:481:ARG:NH1	2.35	0.59
1:B:278:VAL:HG12	1:B:428:HIS:HB2	1.85	0.59
2:C:164:LEU:HD22	2:C:524:LEU:HD13	1.83	0.59
1:A:256:ASP:O	1:A:433:ARG:NH1	2.36	0.58
1:A:478:ARG:NH1	1:A:492:GLU:OE2	2.35	0.58
1:B:478:ARG:NH1	1:B:492:GLU:OE2	2.36	0.58
1:B:129:LYS:NZ	3:B:702:ATP:O1G	2.37	0.57
1:B:249:VAL:HB	2:D:358:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PRO:O	1:A:389:ASN:ND2	2.38	0.56
2:C:564:ASN:O	2:C:568:SER:OG	2.24	0.56
1:B:243:ARG:NH2	1:B:337:GLU:OE2	2.37	0.56
1:A:327:TYR:OH	2:C:305:TYR:OH	2.00	0.56
1:A:357:ASN:OD1	1:A:359:TRP:N	2.26	0.55
1:B:344:LEU:HD11	1:B:429:LEU:HD21	1.87	0.55
2:D:522:SER:OG	2:D:547:ASP:OD2	2.20	0.55
1:A:91:LYS:NZ	1:A:469:ALA:O	2.35	0.55
2:C:563:ARG:HG3	2:C:564:ASN:OD1	2.07	0.55
2:C:224:PRO:HB2	2:C:226:TRP:CD1	2.42	0.55
2:C:172:VAL:HG13	2:C:241:ARG:HH22	1.71	0.55
1:B:186:GLN:OE1	1:B:189:ARG:NH2	2.25	0.54
2:D:264:LYS:HD2	2:D:271:LYS:HE3	1.90	0.54
2:C:361:ILE:HD12	2:C:382:ASP:HB3	1.90	0.54
1:A:185:LEU:HD23	1:A:282:VAL:HG12	1.90	0.54
2:C:170:TYR:HE1	2:C:510:ARG:HD3	1.73	0.54
2:D:512:GLN:HA	2:D:554:LEU:HD21	1.90	0.54
1:B:136:ARG:NH1	3:B:702:ATP:O1A	2.38	0.53
2:C:426:CYS:HA	2:C:429:VAL:HG12	1.90	0.53
1:B:256:ASP:O	1:B:433:ARG:NH1	2.42	0.53
2:D:422:ASP:HB3	2:D:425:TYR:HB2	1.89	0.53
1:A:248:PRO:HG2	1:A:251:PHE:CD1	2.44	0.52
1:B:308:SER:HB3	2:D:298:ASP:HA	1.91	0.52
2:C:447:MET:HG3	2:C:476:HIS:CD2	2.43	0.52
1:A:117:LEU:HD22	1:A:165:HIS:HB3	1.90	0.52
1:B:250:ASP:HA	2:D:357:PRO:HD2	1.91	0.52
2:D:563:ARG:NE	2:D:563:ARG:O	2.42	0.52
1:A:243:ARG:NH2	1:A:337:GLU:OE2	2.41	0.52
1:B:91:LYS:NZ	1:B:469:ALA:O	2.40	0.52
1:A:403:ASP:OD2	1:A:411:ARG:HD2	2.10	0.51
2:C:466:GLU:C	2:C:468:PHE:H	2.13	0.51
2:C:429:VAL:O	2:C:432:THR:OG1	2.28	0.51
2:D:412:HIS:ND1	2:D:413:LYS:O	2.43	0.51
1:A:456:LYS:HA	1:A:523:VAL:HG23	1.92	0.51
1:B:456:LYS:HA	1:B:523:VAL:HG23	1.93	0.51
2:C:369:TYR:HB3	2:C:370:TYR:HD1	1.76	0.51
2:C:170:TYR:CE1	2:C:510:ARG:HD3	2.45	0.50
2:C:407:TRP:CZ3	2:C:444:VAL:HG11	2.46	0.50
1:A:228:PHE:HZ	1:A:340:LEU:HD22	1.76	0.50
1:A:405:LEU:O	1:A:501:ARG:NH1	2.44	0.50
1:A:247:THR:HG22	1:A:259:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:CYS:HB3	1:B:320:PRO:HD3	1.94	0.50
2:C:529:LEU:HD13	2:C:537:VAL:HG22	1.94	0.49
1:B:117:LEU:HD22	1:B:165:HIS:HB3	1.93	0.49
2:C:545:ALA:O	2:C:549:ARG:HD2	2.12	0.49
1:B:513:ILE:HA	1:B:521:VAL:HG21	1.94	0.49
2:D:369:TYR:HB3	2:D:370:TYR:HD1	1.77	0.49
2:C:164:LEU:O	2:C:170:TYR:HD2	1.96	0.49
2:C:422:ASP:HB3	2:C:425:TYR:HB2	1.94	0.49
1:A:242:GLN:HB2	1:A:245:GLU:HG3	1.94	0.49
1:B:405:LEU:O	1:B:501:ARG:NH1	2.46	0.49
1:A:466:LEU:HD13	1:A:473:LEU:HD13	1.94	0.49
1:B:247:THR:HG22	1:B:259:ARG:NH2	2.26	0.49
2:C:177:LEU:HD12	2:C:177:LEU:H	1.77	0.49
2:C:315:PHE:HD1	2:C:326:VAL:HG23	1.78	0.49
2:C:234:ASN:OD1	2:C:237:GLU:HG2	2.13	0.49
1:A:174:TYR:CE2	1:A:276:ARG:HG3	2.49	0.48
2:C:406:PRO:HG2	2:C:407:TRP:CZ3	2.47	0.48
2:C:407:TRP:HZ2	2:C:426:CYS:SG	2.35	0.48
1:A:248:PRO:O	1:A:251:PHE:HB2	2.14	0.48
1:B:228:PHE:HZ	1:B:340:LEU:HD22	1.77	0.48
2:C:396:SER:HB2	2:C:397:LEU:HD13	1.95	0.48
2:D:250:LEU:HD11	2:D:315:PHE:CE2	2.49	0.48
1:B:248:PRO:O	1:B:251:PHE:HB2	2.13	0.48
1:B:403:ASP:OD2	1:B:411:ARG:HD2	2.14	0.48
1:A:399:MET:SD	1:A:411:ARG:HD3	2.54	0.47
1:B:100:LEU:HD12	1:B:465:LEU:HD12	1.97	0.47
1:B:174:TYR:CE2	1:B:276:ARG:HG3	2.49	0.47
1:B:361:ARG:NH2	1:B:444:SER:OG	2.47	0.47
2:D:465:PHE:O	2:D:467:LYS:N	2.46	0.47
1:A:320:PRO:HB2	1:A:326:GLU:HG2	1.94	0.47
1:A:200:GLN:O	1:A:202:GLU:N	2.47	0.47
2:C:412:HIS:HD1	2:C:415:LYS:HB2	1.80	0.47
1:B:185:LEU:HD23	1:B:282:VAL:HG12	1.96	0.47
1:B:248:PRO:HG2	1:B:251:PHE:CD1	2.49	0.47
2:D:361:ILE:HD12	2:D:382:ASP:HB3	1.96	0.47
1:A:256:ASP:HB3	1:A:433:ARG:HD3	1.96	0.46
2:C:247:GLU:HG2	2:C:319:ARG:HH22	1.80	0.46
2:C:444:VAL:O	2:C:448:THR:HG23	2.15	0.46
2:D:545:ALA:O	2:D:549:ARG:HD2	2.15	0.46
2:C:241:ARG:NH2	2:C:322:ASP:OD2	2.49	0.46
1:A:160:SER:OG	1:A:187:ASP:OD2	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PRO:HB2	1:A:359:TRP:CE3	2.50	0.46
2:C:169:LEU:O	2:C:510:ARG:NH1	2.47	0.46
2:D:558:ARG:HA	2:D:561:VAL:HG12	1.97	0.46
2:C:532:ASP:C	2:C:534:VAL:H	2.18	0.46
1:B:275:PHE:O	1:B:277:ARG:HG3	2.16	0.45
2:C:412:HIS:ND1	2:C:413:LYS:O	2.49	0.45
2:D:304:ASP:OD1	2:D:307:ARG:NH2	2.49	0.45
2:D:250:LEU:HD11	2:D:315:PHE:HE2	1.80	0.45
2:D:413:LYS:O	2:D:414:ARG:HG2	2.16	0.45
1:A:443:ILE:H	1:A:443:ILE:HD12	1.81	0.45
1:B:320:PRO:HB2	1:B:326:GLU:HG2	1.98	0.45
2:C:526:ALA:HB2	2:C:543:LEU:HD13	1.98	0.45
1:A:429:LEU:HA	1:A:429:LEU:HD23	1.75	0.45
1:A:319:CYS:HB3	1:A:320:PRO:HD3	1.98	0.45
2:D:338:LYS:HG3	2:D:339:GLU:HG3	1.98	0.45
1:B:200:GLN:O	1:B:202:GLU:N	2.48	0.45
2:D:394:ASP:HB3	2:D:397:LEU:HD21	1.99	0.45
2:C:304:ASP:OD1	2:C:307:ARG:NH2	2.50	0.45
2:C:563:ARG:NE	2:C:563:ARG:O	2.50	0.45
2:D:332:ARG:NH2	2:D:339:GLU:OE1	2.50	0.45
1:A:275:PHE:O	1:A:277:ARG:HG3	2.16	0.45
2:C:426:CYS:O	2:C:430:LYS:HG3	2.16	0.45
1:A:270:ASP:OD2	1:A:278:VAL:N	2.38	0.44
1:B:141:ARG:HG3	1:B:146:LEU:HD23	1.99	0.44
1:B:429:LEU:HA	1:B:429:LEU:HD23	1.73	0.44
2:C:317:LEU:HA	2:C:525:MET:HE1	1.98	0.44
2:C:463:GLU:O	2:C:475:ILE:HG13	2.17	0.44
2:C:506:SER:O	2:C:510:ARG:HG3	2.17	0.44
2:C:380:LYS:HA	2:C:381:PRO:HA	1.69	0.44
2:C:462:TYR:CD1	2:C:474:ILE:HG13	2.52	0.44
2:D:563:ARG:HG3	2:D:564:ASN:OD1	2.18	0.44
2:C:182:VAL:HG22	2:C:183:LEU:H	1.82	0.44
1:B:256:ASP:OD1	1:B:257:PHE:N	2.47	0.43
1:A:109:LEU:CD1	1:A:169:ASN:HD22	2.31	0.43
2:C:448:THR:HG21	2:C:496:PRO:HB2	1.99	0.43
1:A:398:ASP:OD2	1:A:456:LYS:HE2	2.18	0.43
2:C:523:LEU:HD12	2:C:523:LEU:H	1.84	0.43
1:A:132:ARG:NH2	3:A:702:ATP:O1B	2.51	0.43
2:C:304:ASP:OD1	2:C:305:TYR:N	2.51	0.43
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.84	0.43
2:C:178:THR:OG1	2:C:179:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:329:VAL:HB	2:C:389:ALA:HA	1.99	0.43
2:C:442:LEU:HD21	2:C:502:ARG:HG2	2.00	0.43
2:C:159:SER:HA	2:C:162:ALA:HB3	2.00	0.43
2:D:532:ASP:C	2:D:534:VAL:H	2.21	0.43
1:A:513:ILE:HA	1:A:521:VAL:HG21	2.00	0.43
1:B:173:LEU:HD22	1:B:277:ARG:O	2.18	0.42
1:B:351:PRO:O	1:B:418:THR:HG22	2.19	0.42
1:B:147:THR:O	1:B:149:LEU:HD22	2.19	0.42
2:C:466:GLU:C	2:C:468:PHE:N	2.71	0.42
2:C:538:LEU:HA	2:C:538:LEU:HD23	1.93	0.42
2:D:268:THR:O	2:D:271:LYS:HE2	2.19	0.42
2:D:247:GLU:HG2	2:D:319:ARG:HH22	1.83	0.42
2:D:323:PHE:HB3	2:D:325:ARG:HG2	2.02	0.42
1:A:226:LEU:HD22	1:A:236:PHE:HB2	2.02	0.42
1:A:446:LEU:HD22	1:A:446:LEU:HA	1.88	0.42
1:B:100:LEU:HD11	1:B:461:LEU:HB3	2.02	0.42
1:B:217:PRO:O	1:B:220:VAL:HG22	2.19	0.42
2:C:458:ASP:CB	2:C:481:ARG:HD2	2.49	0.42
2:D:224:PRO:HB2	2:D:226:TRP:CD1	2.54	0.42
1:B:438:HIS:HB3	1:B:494:HIS:ND1	2.35	0.42
2:D:426:CYS:HA	2:D:429:VAL:HG12	2.01	0.42
2:D:529:LEU:HD13	2:D:537:VAL:HG22	2.00	0.42
1:A:351:PRO:O	1:A:418:THR:HG22	2.20	0.42
1:B:370:GLU:HB3	1:B:377:TYR:CE1	2.54	0.42
1:A:181:VAL:O	1:A:185:LEU:HD12	2.20	0.41
1:A:264:ILE:HG21	1:A:484:ASP:OD2	2.19	0.41
1:B:457:LYS:HB2	1:B:524:ASP:HA	2.02	0.41
2:C:229:PHE:CE1	2:C:238:LEU:HD12	2.55	0.41
2:C:468:PHE:CG	2:C:472:THR:HG21	2.54	0.41
2:D:526:ALA:HB2	2:D:543:LEU:HD13	2.02	0.41
2:D:336:MET:HE3	2:D:384:ILE:HG12	2.01	0.41
1:A:130:VAL:HG22	1:A:231:PHE:CD1	2.55	0.41
1:B:116:LEU:HB3	1:B:420:PHE:CZ	2.55	0.41
1:B:478:ARG:HH12	1:B:492:GLU:CD	2.24	0.41
1:B:156:ARG:HD2	1:B:158:GLU:OE2	2.21	0.41
1:B:98:HIS:CG	1:B:99:PRO:HD2	2.56	0.41
2:D:304:ASP:OD1	2:D:305:TYR:N	2.54	0.41
1:A:491:THR:OG1	1:A:493:PRO:HD2	2.21	0.41
2:C:250:LEU:HD11	2:C:315:PHE:CE2	2.55	0.41
1:A:141:ARG:HG3	1:A:146:LEU:HD23	2.02	0.41
1:B:210:ASP:HB3	1:B:213:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:554:LEU:HD12	2:C:554:LEU:HA	1.85	0.41
1:A:249:VAL:HB	2:C:358:ALA:HB2	2.03	0.41
1:A:393:LEU:O	1:A:397:ILE:HG12	2.21	0.41
1:B:500:ARG:HE	1:B:500:ARG:HB3	1.63	0.41
2:C:413:LYS:O	2:C:414:ARG:HG2	2.19	0.41
1:B:173:LEU:HD21	1:B:344:LEU:HD21	2.03	0.41
2:C:172:VAL:N	2:C:241:ARG:HH12	2.18	0.41
2:D:458:ASP:CB	2:D:481:ARG:HD2	2.51	0.41
2:D:554:LEU:HA	2:D:554:LEU:HD12	1.89	0.41
1:A:147:THR:O	1:A:149:LEU:HD22	2.20	0.40
1:A:256:ASP:OD1	1:A:257:PHE:N	2.53	0.40
1:B:240:ARG:HB3	1:B:240:ARG:HE	1.61	0.40
1:B:254:PHE:CD1	1:B:255:ILE:HG23	2.57	0.40
1:B:443:ILE:H	1:B:443:ILE:HD12	1.85	0.40
2:C:294:GLU:HG3	2:C:486:TYR:CE1	2.56	0.40
1:A:511:GLY:O	1:A:514:VAL:HG22	2.21	0.40
3:A:702:ATP:H8	3:A:702:ATP:C5'	2.34	0.40
1:A:100:LEU:HD11	1:A:461:LEU:HB3	2.04	0.40
1:A:497:ALA:O	1:A:501:ARG:HG3	2.21	0.40
1:B:358:PRO:HB2	1:B:359:TRP:CE3	2.57	0.40
2:D:315:PHE:HD1	2:D:326:VAL:HG23	1.87	0.40
2:D:514:LEU:HB3	2:D:521:LEU:HG	2.03	0.40
1:A:335:LEU:HA	1:A:335:LEU:HD13	1.88	0.40
2:D:285:LYS:HD2	2:D:311:GLU:HG3	2.02	0.40
2:D:394:ASP:OD1	2:D:395:LEU:N	2.55	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	436/467 (93%)	397 (91%)	38 (9%)	1 (0%)	47 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	436/467 (93%)	397 (91%)	38 (9%)	1 (0%)	47 77
2	C	381/438 (87%)	337 (88%)	41 (11%)	3 (1%)	19 51
2	D	296/438 (68%)	263 (89%)	32 (11%)	1 (0%)	41 71
All	All	1549/1810 (86%)	1394 (90%)	149 (10%)	6 (0%)	34 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	397	LEU
2	C	467	LYS
1	A	112	ALA
2	C	290	THR
1	B	112	ALA
2	C	434	PRO

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	394/418 (94%)	350 (89%)	44 (11%)	6 23
1	B	394/418 (94%)	352 (89%)	42 (11%)	6 25
2	C	349/387 (90%)	306 (88%)	43 (12%)	4 20
2	D	284/387 (73%)	257 (90%)	27 (10%)	8 29
All	All	1421/1610 (88%)	1265 (89%)	156 (11%)	6 24

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	147	THR
1	A	149	LEU
1	A	153	LEU
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	173	LEU
1	A	175	SER
1	A	185	LEU
1	A	201	ASP
1	A	202	GLU
1	A	209	CYS
1	A	216	LYS
1	A	222	LEU
1	A	225	VAL
1	A	226	LEU
1	A	240	ARG
1	A	247	THR
1	A	251	PHE
1	A	259	ARG
1	A	269	LEU
1	A	278	VAL
1	A	282	VAL
1	A	295	VAL
1	A	299	GLU
1	A	315	PHE
1	A	321	TYR
1	A	325	THR
1	A	343	PHE
1	A	347	LEU
1	A	360	ILE
1	A	364	THR
1	A	368	LYS
1	A	370	GLU
1	A	412	HIS
1	A	418	THR
1	A	427	ILE
1	A	443	ILE
1	A	446	LEU
1	A	471	TYR
1	A	491	THR
1	A	519	GLN
1	A	522	ILE
1	A	523	VAL
2	C	160	LEU
2	C	172	VAL
2	C	178	THR

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Mol	Chain	Res	Type
2	C	186	VAL
2	C	187	ASN
2	C	221	ASP
2	C	236	TYR
2	C	238	LEU
2	C	240	SER
2	C	257	ARG
2	C	264	LYS
2	C	288	LYS
2	C	290	THR
2	C	291	ARG
2	C	307	ARG
2	C	329	VAL
2	C	345	ARG
2	C	362	CYS
2	C	367	CYS
2	C	374	GLU
2	C	378	CYS
2	C	388	LEU
2	C	391	PHE
2	C	397	LEU
2	C	402	THR
2	C	405	ASN
2	C	408	ARG
2	C	414	ARG
2	C	418	GLU
2	C	424	ASP
2	C	426	CYS
2	C	432	THR
2	C	440	ARG
2	C	464	THR
2	C	465	PHE
2	C	473	PHE
2	C	474	ILE
2	C	514	LEU
2	C	525	MET
2	C	540	GLN
2	C	561	VAL
2	C	573	ASP
2	C	574	LEU
1	B	110	LEU
1	B	147	THR

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Mol	Chain	Res	Type
1	B	149	LEU
1	B	153	LEU
1	B	155	LEU
1	B	157	LEU
1	B	173	LEU
1	B	175	SER
1	B	185	LEU
1	B	201	ASP
1	B	202	GLU
1	B	209	CYS
1	B	222	LEU
1	B	225	VAL
1	B	226	LEU
1	B	240	ARG
1	B	247	THR
1	B	251	PHE
1	B	259	ARG
1	B	269	LEU
1	B	278	VAL
1	B	282	VAL
1	B	295	VAL
1	B	315	PHE
1	B	321	TYR
1	B	325	THR
1	B	343	PHE
1	B	347	LEU
1	B	353	LEU
1	B	360	ILE
1	B	364	THR
1	B	368	LYS
1	B	370	GLU
1	B	412	HIS
1	B	418	THR
1	B	443	ILE
1	B	446	LEU
1	B	471	TYR
1	B	483	GLU
1	B	519	GLN
1	B	522	ILE
1	B	523	VAL
2	D	236	TYR
2	D	257	ARG

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Mol	Chain	Res	Type
2	D	264	LYS
2	D	288	LYS
2	D	290	THR
2	D	291	ARG
2	D	307	ARG
2	D	329	VAL
2	D	345	ARG
2	D	367	CYS
2	D	374	GLU
2	D	378	CYS
2	D	391	PHE
2	D	402	THR
2	D	405	ASN
2	D	408	ARG
2	D	414	ARG
2	D	418	GLU
2	D	424	ASP
2	D	426	CYS
2	D	436	ASP
2	D	440	ARG
2	D	464	THR
2	D	465	PHE
2	D	514	LEU
2	D	525	MET
2	D	540	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	167	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	ATP	A	701	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	5 (16%)
3	ATP	A	702	-	26,33,33	0.98	1 (3%)	31,52,52	1.41	4 (12%)
3	ATP	B	702	-	26,33,33	0.95	1 (3%)	31,52,52	1.27	3 (9%)
3	ATP	B	701	-	26,33,33	0.97	1 (3%)	31,52,52	1.58	5 (16%)

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	ATP	A	701	-	-	7/18/38/38	0/3/3/3
3	ATP	A	702	-	-	6/18/38/38	0/3/3/3
3	ATP	B	702	-	-	8/18/38/38	0/3/3/3
3	ATP	B	701	-	-	9/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ATP	C5-C4	2.67	1.48	1.40
3	B	702	ATP	C5-C4	2.65	1.47	1.40
3	B	701	ATP	C5-C4	2.62	1.47	1.40
3	A	701	ATP	C5-C4	2.33	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	ATP	PA-O3A-PB	-3.98	119.17	132.83
3	B	701	ATP	PB-O3B-PG	-3.71	120.10	132.83
3	B	701	ATP	PA-O3A-PB	-3.67	120.24	132.83
3	A	702	ATP	C3'-C2'-C1'	3.41	106.12	100.98
3	B	701	ATP	N3-C2-N1	-3.16	123.74	128.68
3	A	701	ATP	C3'-C2'-C1'	3.15	105.72	100.98
3	B	702	ATP	N3-C2-N1	-3.08	123.87	128.68
3	A	701	ATP	N3-C2-N1	-3.06	123.89	128.68
3	B	702	ATP	C3'-C2'-C1'	3.01	105.50	100.98
3	A	702	ATP	N3-C2-N1	-2.99	124.01	128.68
3	A	701	ATP	C4-C5-N7	-2.80	106.48	109.40
3	B	701	ATP	C3'-C2'-C1'	2.78	105.16	100.98
3	B	701	ATP	C4-C5-N7	-2.61	106.68	109.40
3	B	702	ATP	C4-C5-N7	-2.57	106.72	109.40
3	A	702	ATP	PB-O3B-PG	-2.53	124.15	132.83
3	A	702	ATP	C4-C5-N7	-2.38	106.92	109.40
3	A	701	ATP	PB-O3B-PG	-2.29	124.95	132.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PB-O3B-PG-O3G
3	A	701	ATP	C5'-O5'-PA-O1A
3	A	701	ATP	C5'-O5'-PA-O2A
3	A	701	ATP	C3'-C4'-C5'-O5'
3	A	702	ATP	PB-O3A-PA-O5'
3	A	702	ATP	C5'-O5'-PA-O1A
3	A	702	ATP	C5'-O5'-PA-O2A
3	A	702	ATP	O4'-C4'-C5'-O5'
3	A	702	ATP	C3'-C4'-C5'-O5'
3	B	702	ATP	PB-O3B-PG-O2G
3	B	702	ATP	C5'-O5'-PA-O1A
3	B	701	ATP	PB-O3B-PG-O3G
3	B	701	ATP	C5'-O5'-PA-O1A
3	B	701	ATP	O4'-C4'-C5'-O5'
3	B	701	ATP	C3'-C4'-C5'-O5'
3	A	701	ATP	O4'-C4'-C5'-O5'
3	B	702	ATP	C3'-C4'-C5'-O5'
3	B	701	ATP	C4'-C5'-O5'-PA
3	A	701	ATP	C5'-O5'-PA-O3A
3	A	702	ATP	C5'-O5'-PA-O3A
3	B	702	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	B	701	ATP	C5'-O5'-PA-O3A
3	B	701	ATP	C5'-O5'-PA-O2A
3	B	702	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	C4'-C5'-O5'-PA
3	B	702	ATP	PG-O3B-PB-O1B
3	B	701	ATP	PB-O3B-PG-O1G
3	B	701	ATP	PB-O3B-PG-O2G
3	B	702	ATP	PG-O3B-PB-O2B
3	B	702	ATP	C5'-O5'-PA-O2A

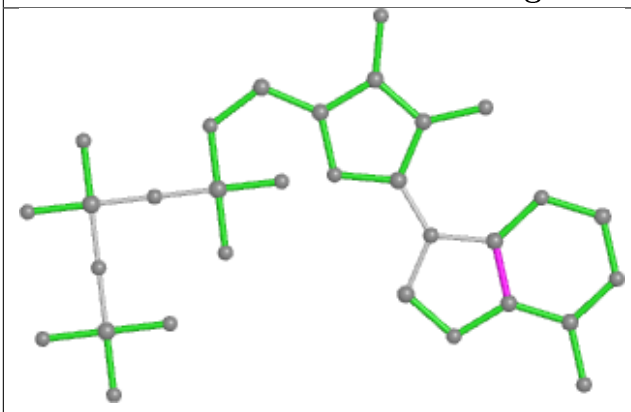
There are no ring outliers.

3 monomers are involved in 9 short contacts:

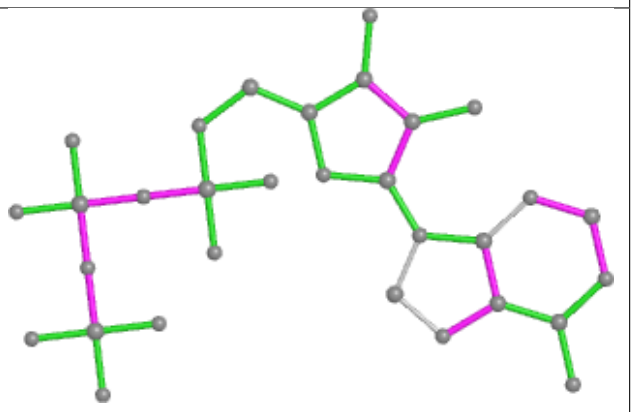
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ATP	4	0
3	B	702	ATP	4	0
3	B	701	ATP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

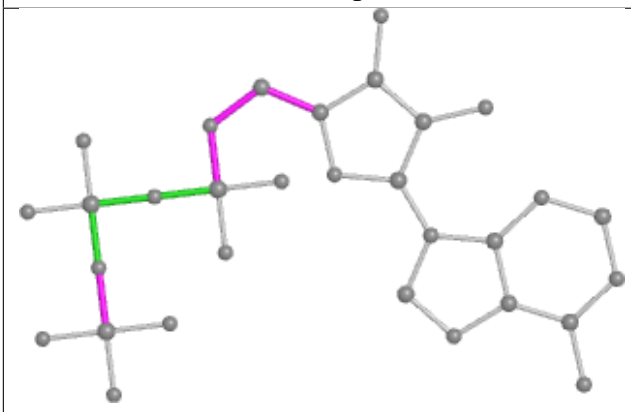
Ligand ATP A 701



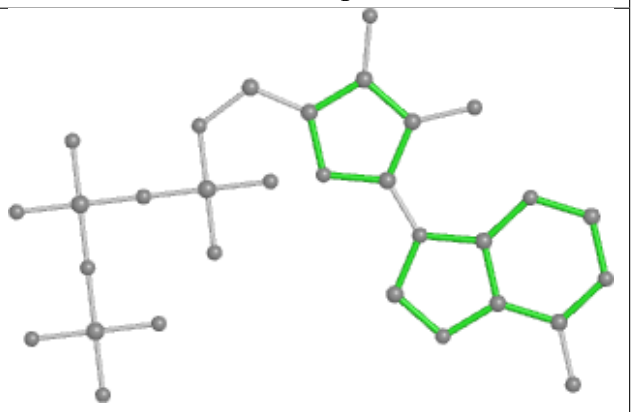
Bond lengths



Bond angles

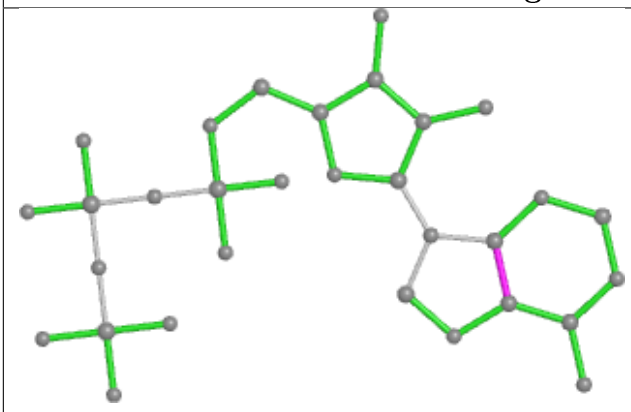


Torsions

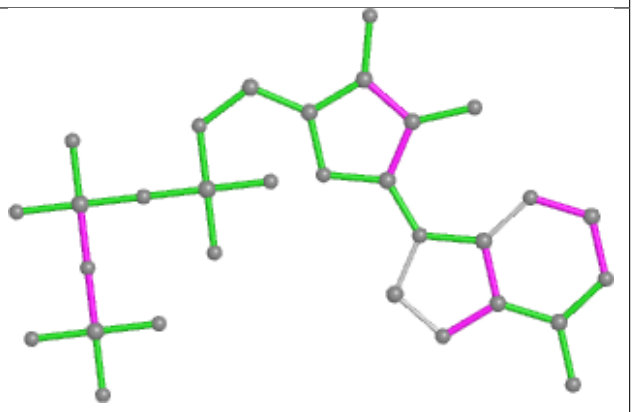


Rings

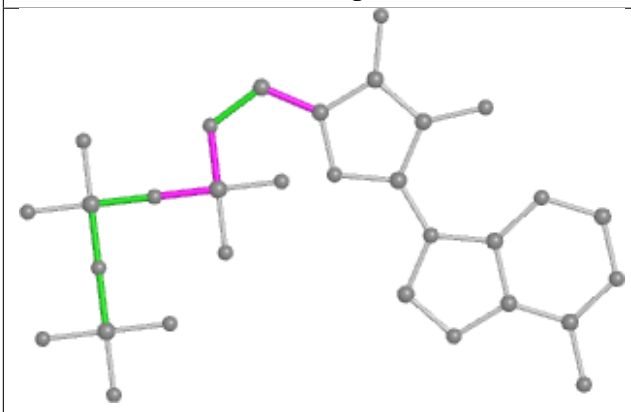
Ligand ATP A 702



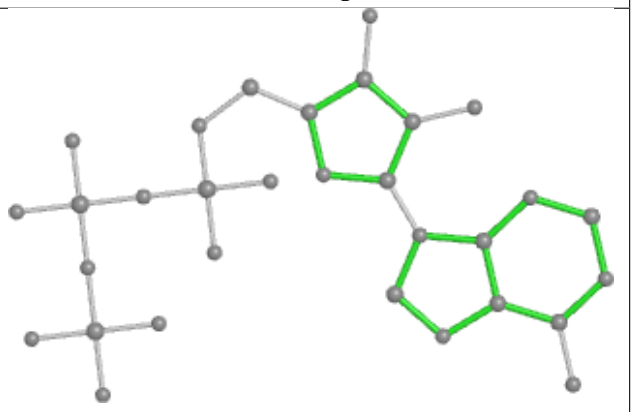
Bond lengths



Bond angles

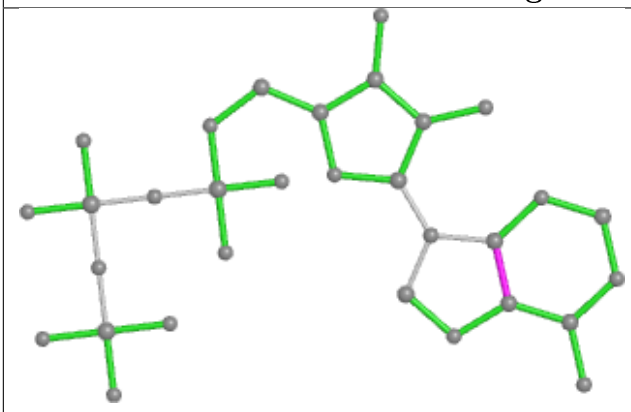


Torsions

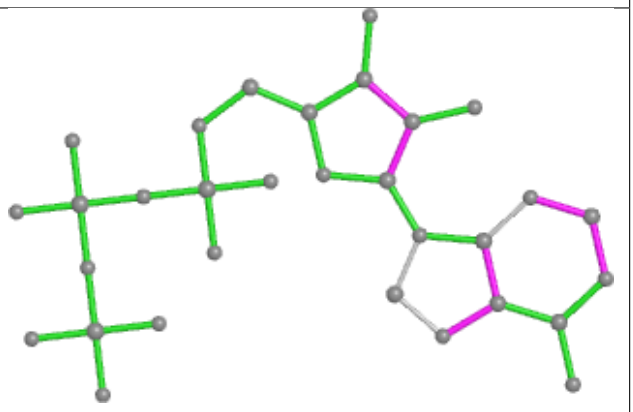


Rings

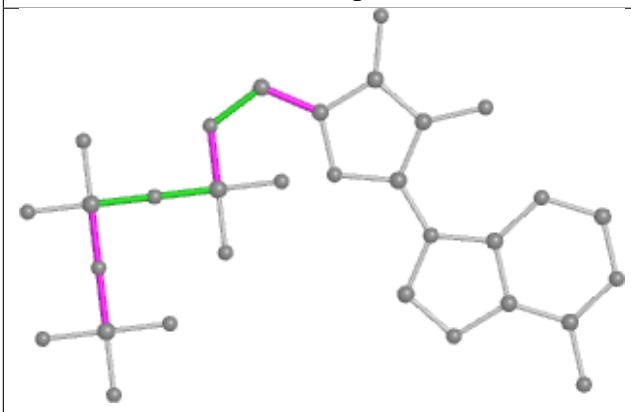
Ligand ATP B 702



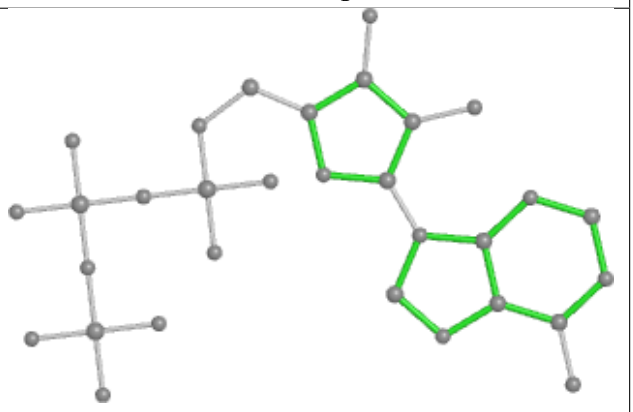
Bond lengths



Bond angles

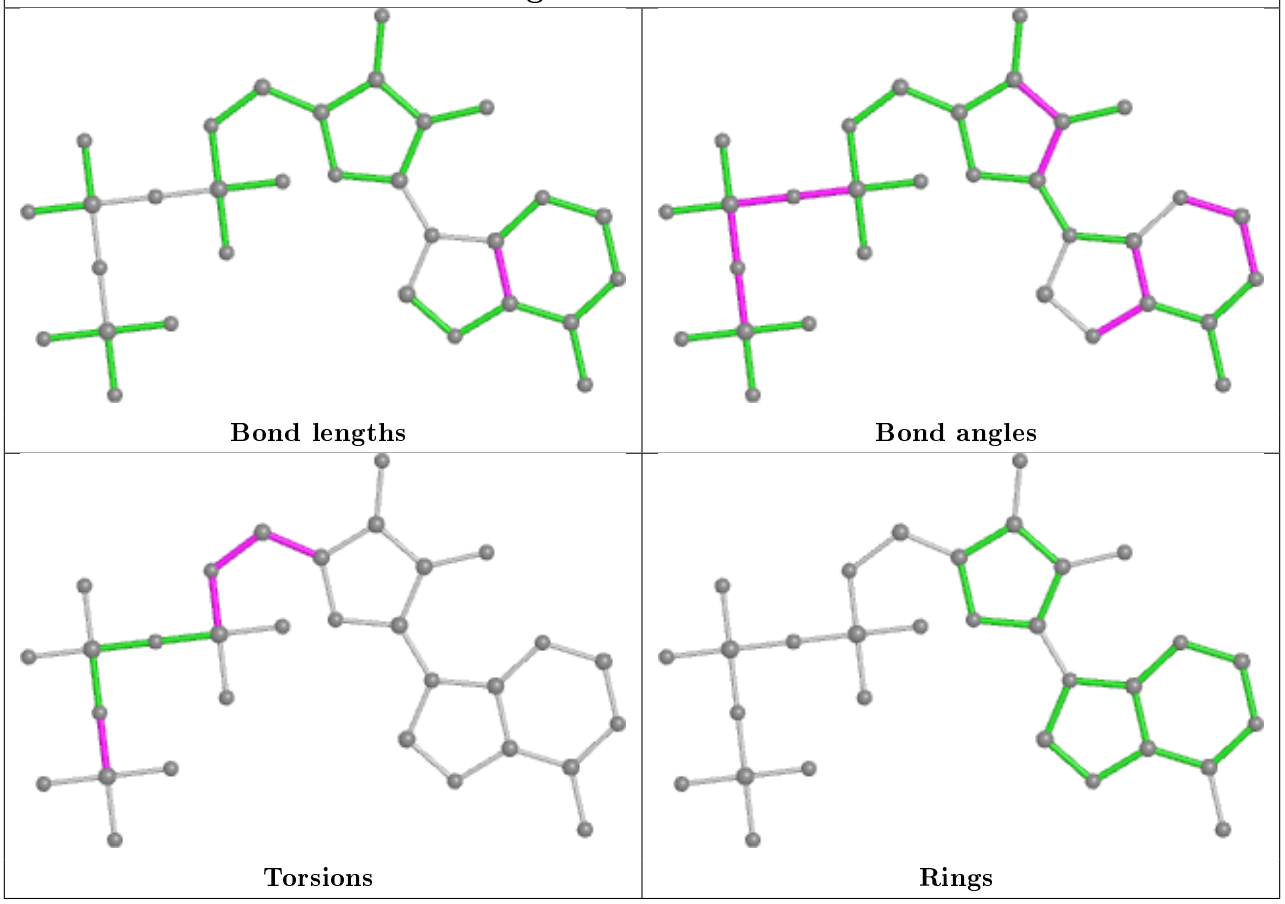


Torsions



Rings

Ligand ATP B 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	438/467 (93%)	-0.28	4 (0%) 84 84	28, 39, 76, 131	0
1	B	438/467 (93%)	-0.03	9 (2%) 63 62	34, 63, 107, 146	0
2	C	385/438 (87%)	-0.26	2 (0%) 91 91	29, 45, 80, 143	0
2	D	314/438 (71%)	1.47	92 (29%) 0 0	77, 131, 151, 172	0
All	All	1575/1810 (87%)	0.15	107 (6%) 17 17	28, 54, 140, 172	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	511	LEU	5.6
2	D	236	TYR	5.5
2	D	244	PRO	5.4
2	D	507	THR	5.1
2	D	429	VAL	4.9
2	D	438	SER	4.9
2	D	246	ILE	4.8
2	D	521	LEU	4.5
1	A	390	SER	4.5
2	D	554	LEU	4.4
2	D	439	HIS	4.4
2	D	322	ASP	4.3
2	D	279	TYR	4.3
2	D	553	VAL	4.2
2	D	505	LYS	4.1
2	D	525	MET	4.0
2	D	245	ALA	4.0
2	D	509	LEU	4.0
2	D	253	LEU	3.9
2	D	539	TYR	3.8
2	D	274	MET	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	435	TYR	3.8
1	A	147	THR	3.6
2	D	550	LEU	3.6
2	D	276	PHE	3.6
2	D	379	GLY	3.6
2	D	448	THR	3.5
2	D	543	LEU	3.5
2	D	515	ALA	3.4
2	D	396	SER	3.3
2	D	529	LEU	3.3
2	D	323	PHE	3.3
2	D	447	MET	3.3
2	D	552	VAL	3.3
2	D	534	VAL	3.3
2	D	351	ARG	3.2
2	D	542	HIS	3.1
2	D	441	ILE	3.1
1	B	140	TYR	3.1
2	D	230	HIS	3.1
2	D	488	HIS	3.1
2	D	563	ARG	3.1
2	D	231	ILE	3.1
2	D	436	ASP	3.0
1	B	149	LEU	2.9
1	B	526	PRO	2.9
2	D	445	MET	2.9
2	D	437	SER	2.9
2	D	501	CYS	2.9
2	D	564	ASN	2.8
2	D	319	ARG	2.8
2	D	471	GLU	2.8
2	D	389	ALA	2.8
1	B	148	SER	2.8
2	D	514	LEU	2.8
2	D	310	ALA	2.8
2	D	395	LEU	2.7
2	D	353	PHE	2.7
2	D	391	PHE	2.6
2	D	309	ASN	2.6
2	D	446	ASP	2.6
1	B	146	LEU	2.6
2	D	538	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	147	THR	2.6
2	D	321	LEU	2.5
2	D	533	GLN	2.5
2	D	541	PRO	2.5
2	D	508	TYR	2.5
2	D	382	ASP	2.5
2	D	227	LEU	2.5
2	D	388	LEU	2.5
2	D	347	LYS	2.5
2	D	224	PRO	2.5
1	B	110	LEU	2.5
2	D	226	TRP	2.4
1	A	149	LEU	2.4
1	A	151	PRO	2.4
2	D	421	VAL	2.4
2	D	546	LEU	2.4
2	D	434	PRO	2.4
2	D	537	VAL	2.3
2	D	355	ILE	2.3
2	D	524	LEU	2.3
2	D	242	HIS	2.3
2	D	359	ASN	2.3
2	D	344	THR	2.3
2	D	275	THR	2.3
2	D	380	LYS	2.3
2	C	265	SER	2.2
2	C	266	GLY	2.2
2	D	366	GLU	2.2
1	B	150	ASP	2.2
2	D	416	LYS	2.2
2	D	250	LEU	2.2
2	D	399	LYS	2.2
2	D	522	SER	2.2
1	B	524	ASP	2.2
2	D	557	VAL	2.2
2	D	440	ARG	2.2
2	D	229	PHE	2.1
2	D	518	GLU	2.1
2	D	265	SER	2.1
2	D	403	TRP	2.1
2	D	340	ILE	2.1
2	D	467	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	249	LEU	2.0
2	D	428	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

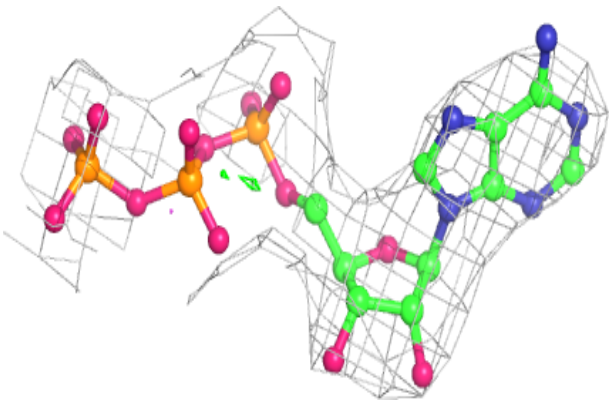
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

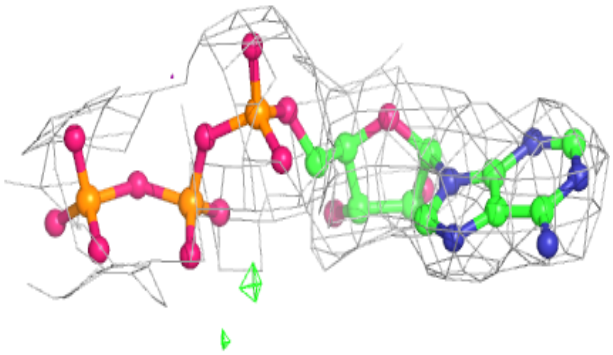
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ATP	B	702	31/31	0.87	0.22	84,113,170,205	0
3	ATP	B	701	31/31	0.90	0.20	57,88,147,174	0
3	ATP	A	702	31/31	0.94	0.17	43,54,77,105	0
3	ATP	A	701	31/31	0.96	0.20	28,39,60,63	0

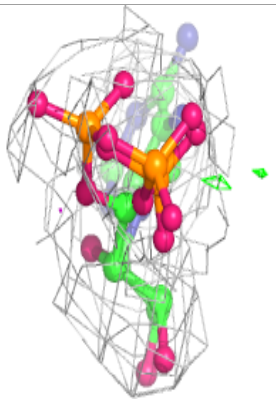
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 702:

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

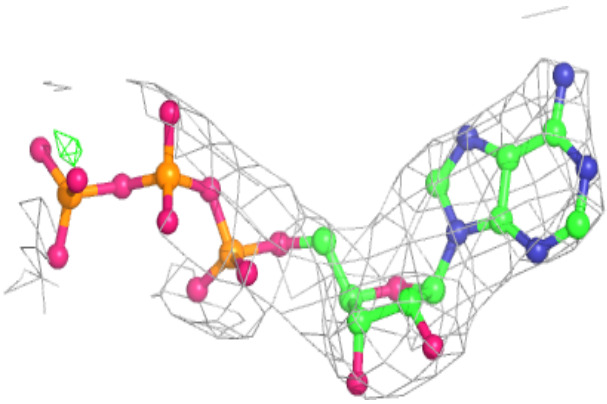


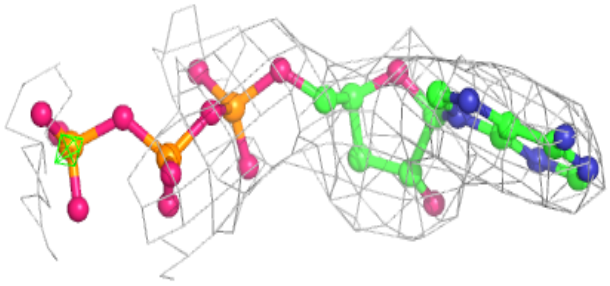


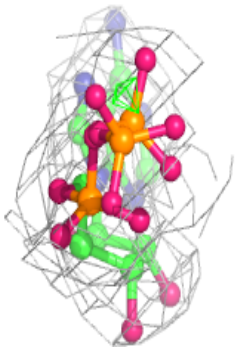


Electron density around ATP B 701:

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

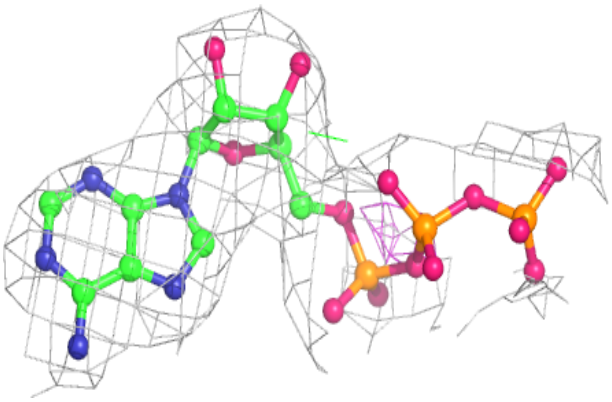


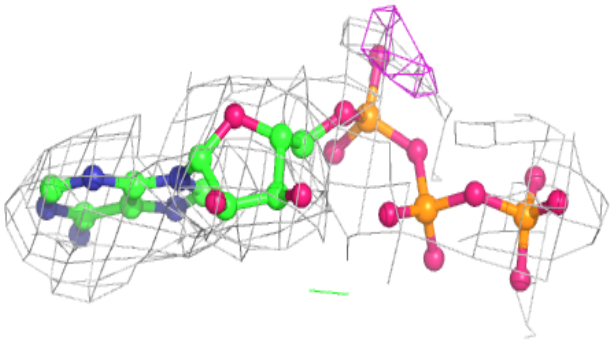


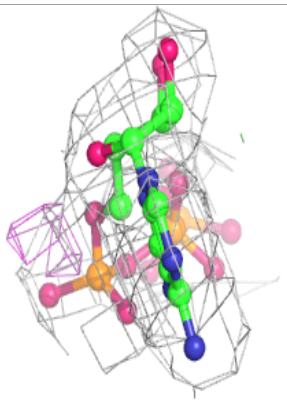


Electron density around ATP A 702:

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

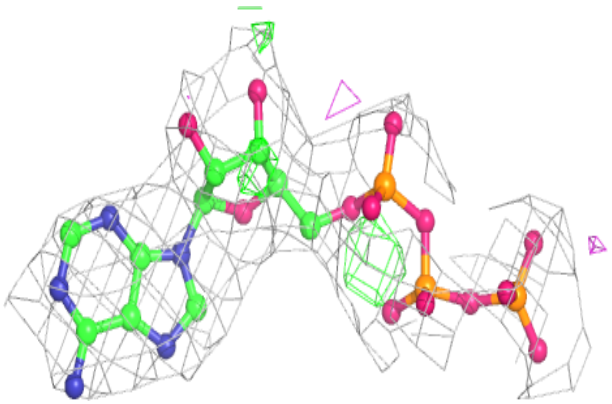


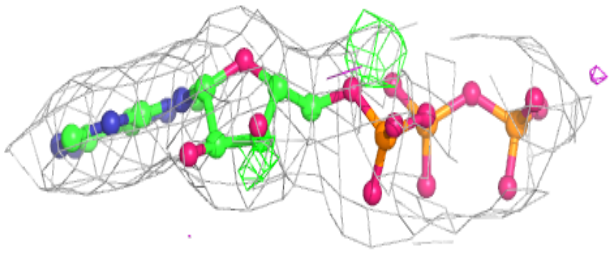


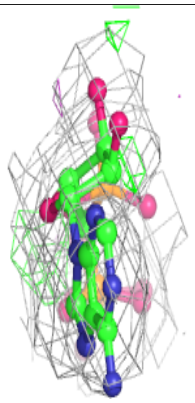


Electron density around ATP A 701:

$2mF_o$-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.