



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:21 pm BST

PDB ID : 1Y4S  
Title : Conformation rearrangement of heat shock protein 90 upon ADP binding  
Authors : Huai, Q.; Wang, H.; Liu, Y.; Kim, H.; Toft, D.; Ke, H.  
Deposited on : 2004-12-01  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

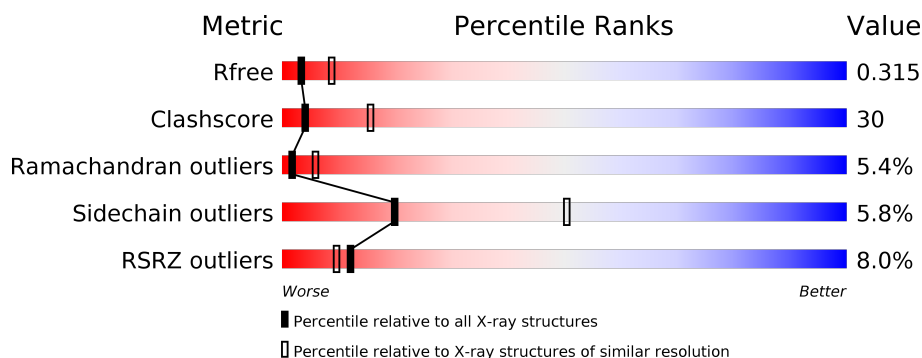
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	<div> <div>8%</div> <div> <div></div> <div>43%</div> <div>36%</div> <div>6%</div> <div>15%</div> </div> </div>
1	B	559	<div> <div>6%</div> <div> <div></div> <div>37%</div> <div>43%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7784 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.

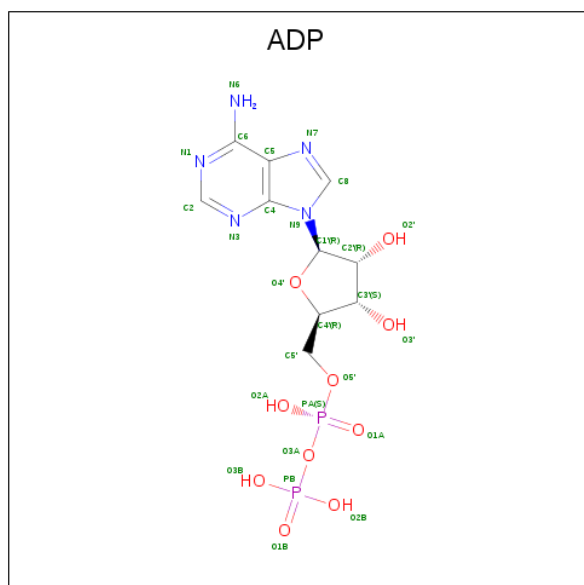
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			
1	B	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			

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

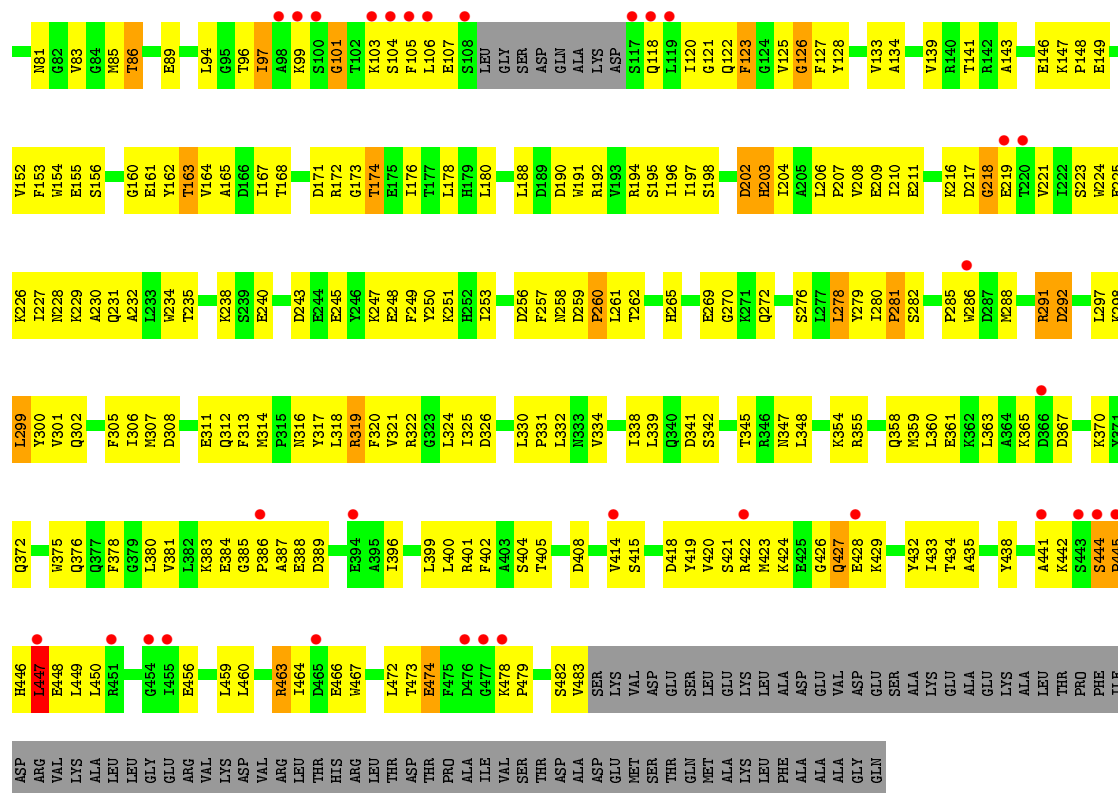
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.50 Å 84.18 Å 212.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 78.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 88.4 (78.28-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.82 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.269 , 0.314 0.267 , 0.315	Depositor DCC
$R_{free}$ test set	5232 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5801e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.52	0/3941	0.78	3/5314 (0.1%)
1	B	0.48	0/3941	0.71	2/5314 (0.0%)
All	All	0.50	0/7882	0.75	5/10628 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	N-CA-C	-8.81	91.07	113.10
1	B	426	GLY	N-CA-C	-6.12	97.81	113.10
1	A	123	PHE	N-CA-C	5.89	126.89	111.00
1	B	447	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	400	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3864	0	3786	215	0
1	B	3864	0	3786	245	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	0	0
3	B	27	0	12	0	0
All	All	7784	0	7596	460	1

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 30.

All (460) 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:402:PHE:HD1	1:B:460:LEU:HD21	1.11	1.14
1:A:463:ARG:H	1:A:463:ARG:HD2	1.17	1.06
1:B:402:PHE:CD1	1:B:460:LEU:HD21	1.92	1.02
1:B:2:LYS:H	1:B:2:LYS:HD3	1.25	0.98
1:A:242:THR:HG22	1:A:244:GLU:H	1.27	0.96
1:A:407:THR:HG22	1:A:409:SER:H	1.36	0.89
1:A:29:GLU:HG3	1:A:192:ARG:HH22	1.38	0.88
1:A:97:ILE:HG22	1:A:98:ALA:H	1.37	0.88
1:A:107:GLU:HG2	1:A:108:SER:H	1.39	0.86
1:A:314:MET:HE1	1:A:356:VAL:HG21	1.56	0.86
1:A:96:THR:HG22	1:A:97:ILE:H	1.40	0.86
1:A:460:LEU:HD13	1:A:465:ASP:HB3	1.59	0.85
1:A:419:TYR:HE2	1:A:430:ILE:HA	1.41	0.85
1:A:62:GLU:HA	1:A:62:GLU:OE1	1.74	0.85
1:B:203:HIS:H	1:B:203:HIS:CD2	1.93	0.84
1:B:331:PRO:O	1:B:334:VAL:HG23	1.76	0.84
1:A:346:ARG:HG3	1:A:349:ARG:HH21	1.42	0.83
1:A:386:PRO:HD3	1:A:396:ILE:HG21	1.61	0.81
1:A:444:SER:HB3	1:A:445:PRO:HD2	1.61	0.81
1:A:419:TYR:CE2	1:A:430:ILE:HA	2.15	0.81
1:B:152:VAL:HG12	1:B:153:PHE:H	1.47	0.80
1:A:99:LYS:NZ	1:A:123:PHE:HB2	1.97	0.79
1:B:97:ILE:HD11	1:B:125:VAL:HG21	1.62	0.79
1:B:420:VAL:HG22	1:B:423:MET:HE2	1.66	0.77
1:B:285:PRO:HG2	1:B:288:MET:HB2	1.66	0.76
1:A:266:ASN:ND2	1:A:355:ARG:HD3	2.01	0.76
1:A:397:ALA:HA	1:A:400:LEU:HD11	1.67	0.76
1:A:401:ARG:HG2	1:A:415:SER:HA	1.65	0.76
1:B:190:ASP:O	1:B:194:ARG:HB2	1.86	0.75
1:B:372:GLN:O	1:B:376:GLN:HG3	1.86	0.75
1:B:30:ILE:HD11	1:B:257:PHE:CE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLN:O	1:B:428:GLU:HB2	1.89	0.72
1:B:332:LEU:HD23	1:B:332:LEU:O	1.88	0.72
1:A:463:ARG:H	1:A:463:ARG:CD	1.99	0.71
1:B:238:LYS:HE2	1:B:265:HIS:O	1.89	0.71
1:B:96:THR:HG22	1:B:97:ILE:H	1.54	0.71
1:B:203:HIS:H	1:B:203:HIS:HD2	1.39	0.71
1:B:334:VAL:CG1	1:B:339:LEU:HG	2.22	0.70
1:B:297:LEU:N	1:B:297:LEU:HD12	2.07	0.70
1:A:463:ARG:HD2	1:A:463:ARG:N	2.00	0.69
1:A:99:LYS:HZ1	1:A:123:PHE:HB2	1.55	0.69
1:A:431:TYR:HE2	1:A:481:GLN:HE21	1.38	0.69
1:B:36:ILE:HG22	1:B:204:ILE:CD1	2.22	0.69
1:A:397:ALA:HA	1:A:400:LEU:CD1	2.23	0.69
1:A:247:LYS:HG2	1:A:260:PRO:HD2	1.73	0.68
1:A:301:VAL:HB	1:A:306:ILE:CD1	2.23	0.68
1:A:419:TYR:HE1	1:A:456:GLU:HB2	1.58	0.68
1:A:97:ILE:HG22	1:A:98:ALA:N	2.08	0.68
1:B:2:LYS:N	1:B:2:LYS:HD3	2.02	0.68
1:B:152:VAL:HG12	1:B:153:PHE:N	2.08	0.68
1:A:106:LEU:HD13	1:A:106:LEU:O	1.94	0.67
1:B:396:ILE:O	1:B:400:LEU:HG	1.93	0.67
1:B:423:MET:HE1	1:B:478:LYS:HG3	1.76	0.67
1:A:50:ALA:HB1	1:A:57:TYR:CE1	2.30	0.67
1:B:104:SER:HB2	1:B:286:TRP:NE1	2.09	0.67
1:B:262:THR:CG2	1:B:363:LEU:HD13	2.25	0.67
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.59	0.67
1:A:192:ARG:NH1	1:A:196:ILE:HD11	2.09	0.67
1:A:426:GLY:O	1:A:427:GLN:HB3	1.96	0.66
1:A:324:LEU:C	1:A:324:LEU:HD12	2.16	0.66
1:B:74:ARG:HA	1:B:188:LEU:HD11	1.77	0.66
1:B:375:TRP:HZ2	1:B:383:LYS:HE3	1.58	0.66
1:A:318:LEU:HD13	1:A:356:VAL:HG11	1.77	0.65
1:B:35:LEU:CD1	1:B:78:ILE:HD12	2.25	0.65
1:A:242:THR:HB	1:A:245:GLU:HG3	1.79	0.65
1:A:428:GLU:HG3	1:A:428:GLU:O	1.96	0.65
1:B:104:SER:HA	1:B:107:GLU:OE1	1.96	0.65
1:A:242:THR:HG22	1:A:244:GLU:N	2.06	0.64
1:B:297:LEU:HD11	1:B:314:MET:HG2	1.77	0.64
1:B:121:GLY:O	1:B:122:GLN:HG3	1.96	0.64
1:B:97:ILE:CD1	1:B:125:VAL:HG21	2.28	0.64
1:B:278:LEU:HD12	1:B:278:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HB	1:B:89:GLU:HG3	1.81	0.63
1:B:297:LEU:HD11	1:B:314:MET:CG	2.28	0.63
1:A:344:VAL:O	1:A:348:LEU:HG	1.98	0.63
1:B:1:MET:HG3	1:B:167:ILE:CG2	2.29	0.63
1:A:407:THR:CG2	1:A:409:SER:H	2.09	0.63
1:A:331:PRO:C	1:A:333:ASN:H	2.02	0.63
1:B:375:TRP:CZ2	1:B:383:LYS:HE3	2.33	0.62
1:B:276:SER:HB2	1:B:278:LEU:CD1	2.29	0.62
1:B:388:GLU:O	1:B:388:GLU:HG2	1.98	0.62
1:A:261:LEU:HD12	1:A:280:ILE:HG22	1.82	0.62
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.63	0.62
1:A:192:ARG:O	1:A:196:ILE:HG13	2.00	0.62
1:A:434:THR:HG22	1:A:435:ALA:N	2.14	0.62
1:B:318:LEU:O	1:B:321:VAL:HG23	1.99	0.62
1:B:106:LEU:O	1:B:107:GLU:HG3	2.00	0.62
1:B:234:TRP:CE3	1:B:324:LEU:HD21	2.35	0.62
1:B:194:ARG:HG3	1:B:227:ILE:HD11	1.81	0.62
1:A:210:ILE:CG2	1:A:227:ILE:HD11	2.30	0.61
1:B:262:THR:HG21	1:B:363:LEU:HD13	1.82	0.61
1:A:210:ILE:HG21	1:A:227:ILE:HD11	1.83	0.61
1:A:190:ASP:O	1:A:194:ARG:HB2	2.01	0.61
1:A:29:GLU:H	1:A:29:GLU:CD	2.04	0.61
1:A:261:LEU:HD21	1:A:282:SER:HA	1.82	0.61
1:B:319:ARG:NH1	1:B:381:VAL:HG22	2.15	0.60
1:B:30:ILE:HD11	1:B:257:PHE:HE1	1.65	0.60
1:B:441:ALA:O	1:B:459:LEU:HD22	2.01	0.60
1:A:23:SER:HB3	1:A:119:LEU:O	2.02	0.60
1:A:145:GLY:O	1:A:146:GLU:HG2	2.02	0.60
1:B:191:TRP:O	1:B:195:SER:HB2	2.02	0.60
1:B:104:SER:HB2	1:B:286:TRP:CE2	2.37	0.60
1:B:297:LEU:HD22	1:B:325:ILE:HD11	1.82	0.60
1:B:70:ASP:OD1	1:B:73:LYS:N	2.32	0.60
1:A:234:TRP:NE1	1:A:326:ASP:HB2	2.17	0.59
1:A:435:ALA:HB3	1:A:441:ALA:HB2	1.84	0.59
1:B:192:ARG:O	1:B:196:ILE:HG13	2.02	0.59
1:B:272:GLN:NE2	1:B:347:ASN:HB3	2.17	0.59
1:B:473:THR:O	1:B:474:GLU:CB	2.51	0.59
1:A:325:ILE:HD12	1:A:352:LEU:HD11	1.83	0.59
1:A:346:ARG:HG3	1:A:349:ARG:NH2	2.16	0.59
1:B:281:PRO:HG2	1:B:378:PHE:CE1	2.38	0.59
1:A:272:GLN:NE2	1:A:347:ASN:HB3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD12	1:A:313:PHE:HB2	1.85	0.59
1:A:372:GLN:O	1:A:376:GLN:HG3	2.03	0.59
1:A:35:LEU:CD1	1:A:78:ILE:HD12	2.32	0.59
1:B:280:ILE:HG13	1:B:359:MET:HE3	1.84	0.59
1:A:211:GLU:HG2	1:A:212:LYS:N	2.18	0.58
1:A:57:TYR:O	1:A:58:GLU:C	2.40	0.58
1:B:96:THR:HG22	1:B:97:ILE:N	2.18	0.58
1:A:219:GLU:HG2	1:A:220:THR:N	2.19	0.58
1:A:232:ALA:O	1:A:235:THR:HB	2.04	0.58
1:A:346:ARG:CG	1:A:349:ARG:HH21	2.14	0.58
1:B:51:LEU:HD13	1:B:332:LEU:HD21	1.84	0.58
1:A:64:ARG:HD3	1:A:81:ASN:OD1	2.02	0.58
1:B:36:ILE:HG22	1:B:204:ILE:HD13	1.85	0.58
1:A:234:TRP:HE1	1:A:326:ASP:HB2	1.68	0.58
1:A:211:GLU:HB2	1:A:224:TRP:CZ3	2.39	0.58
1:B:380:LEU:HD12	1:B:380:LEU:H	1.69	0.58
1:A:27:ASN:O	1:A:30:ILE:HB	2.03	0.57
1:B:35:LEU:HD13	1:B:78:ILE:HD12	1.86	0.57
1:B:387:ALA:HB1	1:B:467:TRP:CH2	2.39	0.57
1:A:263:TRP:HB3	1:A:279:TYR:CD2	2.39	0.57
1:A:301:VAL:HB	1:A:306:ILE:HD11	1.86	0.57
1:A:107:GLU:CG	1:A:108:SER:H	2.13	0.57
1:B:194:ARG:HG3	1:B:227:ILE:CD1	2.34	0.57
1:B:334:VAL:HG13	1:B:339:LEU:HG	1.87	0.57
1:B:64:ARG:HG3	1:B:64:ARG:HH11	1.70	0.57
1:A:449:LEU:O	1:A:449:LEU:HD23	2.05	0.57
1:A:29:GLU:CG	1:A:192:ARG:HH22	2.13	0.56
1:B:250:TYR:HB2	1:B:279:TYR:CE2	2.40	0.56
1:B:446:HIS:O	1:B:449:LEU:HG	2.05	0.56
1:B:203:HIS:HB2	1:B:249:PHE:HD1	1.71	0.56
1:B:216:LYS:HB2	1:B:221:VAL:HG21	1.88	0.56
1:B:299:LEU:HD23	1:B:300:TYR:N	2.21	0.56
1:B:312:GLN:HA	1:B:312:GLN:OE1	2.05	0.56
1:A:290:ASN:O	1:A:292:ASP:N	2.39	0.56
1:A:125:VAL:CG1	1:A:129:SER:HB3	2.36	0.56
1:A:70:ASP:OD2	1:A:73:LYS:HB2	2.06	0.56
1:A:103:LYS:HB3	1:A:105:PHE:CD2	2.40	0.56
1:A:281:PRO:HG2	1:A:378:PHE:CZ	2.41	0.55
1:A:142:ARG:HB2	1:A:169:LYS:HB3	1.88	0.55
1:A:178:LEU:N	1:A:178:LEU:HD12	2.21	0.55
1:A:317:TYR:OH	1:A:357:LEU:HD21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:SER:HB2	1:B:278:LEU:HD11	1.87	0.55
1:A:73:LYS:O	1:A:74:ARG:HB2	2.06	0.55
1:A:107:GLU:HG2	1:A:108:SER:N	2.17	0.55
1:B:32:LEU:CD1	1:B:78:ILE:HD11	2.36	0.55
1:A:389:ASP:CG	1:A:392:ASN:HD22	2.10	0.55
1:B:34:GLU:HG3	1:B:126:GLY:HA2	1.87	0.55
1:B:306:ILE:HG22	1:B:307:MET:N	2.22	0.55
1:B:122:GLN:O	1:B:123:PHE:O	2.25	0.55
1:B:64:ARG:NH1	1:B:64:ARG:HG3	2.22	0.55
1:B:12:GLU:HA	1:B:15:GLN:HE21	1.70	0.55
1:A:5:GLU:OE2	1:A:87:ARG:NH2	2.40	0.55
1:A:212:LYS:HB2	1:A:223:SER:HB2	1.89	0.54
1:A:96:THR:HG22	1:A:97:ILE:N	2.18	0.54
1:B:297:LEU:CD1	1:B:297:LEU:N	2.70	0.54
1:A:103:LYS:HD3	1:A:105:PHE:HE2	1.71	0.54
1:B:435:ALA:HB3	1:B:441:ALA:HB2	1.89	0.54
1:B:7:ARG:HD3	1:B:162:TYR:OH	2.07	0.54
1:A:431:TYR:HE2	1:A:481:GLN:NE2	2.05	0.54
1:A:211:GLU:HG2	1:A:212:LYS:H	1.72	0.54
1:A:261:LEU:O	1:A:262:THR:HG23	2.08	0.54
1:A:29:GLU:HG3	1:A:192:ARG:NH2	2.16	0.54
1:A:460:LEU:HD22	1:A:465:ASP:OD1	2.08	0.54
1:B:261:LEU:HG	1:B:281:PRO:O	2.08	0.54
1:B:301:VAL:HG12	1:B:302:GLN:HG3	1.89	0.54
1:A:383:LYS:C	1:A:385:GLY:H	2.11	0.53
1:B:419:TYR:CE1	1:B:456:GLU:HB3	2.43	0.53
1:A:420:VAL:HA	1:A:423:MET:HE3	1.89	0.53
1:A:280:ILE:HD13	1:A:360:LEU:HD21	1.89	0.53
1:A:103:LYS:CD	1:A:105:PHE:HE2	2.21	0.53
1:A:433:ILE:HD11	1:A:457:VAL:HG11	1.90	0.53
1:B:330:LEU:HB3	1:B:334:VAL:HG21	1.91	0.53
1:B:316:ASN:O	1:B:319:ARG:HG3	2.09	0.53
1:B:380:LEU:HD12	1:B:380:LEU:N	2.23	0.53
1:A:317:TYR:CE1	1:A:318:LEU:HG	2.43	0.53
1:A:99:LYS:O	1:A:99:LYS:HD3	2.08	0.53
1:B:211:GLU:HB2	1:B:224:TRP:CZ3	2.44	0.53
1:B:433:ILE:HD11	1:B:447:LEU:HB3	1.89	0.53
1:A:406:HIS:CE1	1:A:422:ARG:HH11	2.26	0.52
1:B:104:SER:HB2	1:B:286:TRP:HE1	1.74	0.52
1:B:176:ILE:HG22	1:B:178:LEU:CD1	2.40	0.52
1:B:209:GLU:HA	1:B:226:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:H	1:B:203:HIS:HD2	1.57	0.52
1:B:2:LYS:CD	1:B:2:LYS:H	2.11	0.52
1:B:272:GLN:HE21	1:B:347:ASN:HB3	1.72	0.52
1:B:423:MET:HE1	1:B:478:LYS:NZ	2.24	0.52
1:B:94:LEU:HD22	1:B:127:PHE:CE2	2.45	0.52
1:B:133:VAL:HG12	1:B:180:LEU:CD2	2.40	0.52
1:B:330:LEU:CD1	1:B:339:LEU:HD21	2.39	0.52
1:B:311:GLU:CD	1:B:311:GLU:H	2.13	0.52
1:B:420:VAL:HA	1:B:423:MET:HE2	1.91	0.52
1:A:135:ASP:HB3	1:A:181:ARG:HG2	1.91	0.52
1:A:261:LEU:CD2	1:A:282:SER:HA	2.40	0.52
1:B:361:GLU:HG3	1:B:365:LYS:HE3	1.91	0.52
1:B:97:ILE:O	1:B:97:ILE:HG23	2.09	0.52
1:B:30:ILE:O	1:B:33:ARG:N	2.42	0.52
1:A:99:LYS:HZ1	1:A:123:PHE:CB	2.22	0.51
1:A:238:LYS:HE2	1:A:265:HIS:O	2.09	0.51
1:A:97:ILE:CG2	1:A:98:ALA:H	2.17	0.51
1:B:2:LYS:CD	1:B:2:LYS:N	2.73	0.51
1:A:434:THR:O	1:A:435:ALA:HB2	2.11	0.51
1:B:172:ARG:HG2	1:B:173:GLY:N	2.26	0.51
1:B:420:VAL:HG13	1:B:423:MET:CE	2.41	0.51
1:A:331:PRO:O	1:A:333:ASN:N	2.44	0.51
1:B:428:GLU:C	1:B:429:LYS:HG3	2.29	0.51
1:A:235:THR:HG21	1:A:303:ARG:NH2	2.26	0.51
1:A:31:PHE:CG	1:A:32:LEU:N	2.79	0.51
1:B:432:TYR:O	1:B:483:VAL:HG23	2.10	0.51
1:B:7:ARG:HG2	1:B:7:ARG:HH11	1.75	0.51
1:A:169:LYS:NZ	1:A:171:ASP:HB2	2.25	0.50
1:A:434:THR:CG2	1:A:435:ALA:N	2.73	0.50
1:B:248:GLU:OE1	1:B:251:LYS:HE3	2.11	0.50
1:A:106:LEU:O	1:A:106:LEU:HD22	2.11	0.50
1:A:62:GLU:OE1	1:A:62:GLU:CA	2.53	0.50
1:A:404:SER:HB2	1:A:414:VAL:HG21	1.92	0.50
1:A:86:THR:H	1:A:89:GLU:HB2	1.76	0.50
1:B:321:VAL:HG12	1:B:322:ARG:N	2.27	0.50
1:A:135:ASP:OD1	1:A:179:HIS:ND1	2.32	0.50
1:B:342:SER:HB3	1:B:345:THR:OG1	2.12	0.50
1:B:35:LEU:HD12	1:B:78:ILE:HD12	1.92	0.50
1:B:428:GLU:O	1:B:479:PRO:HD2	2.11	0.50
1:A:118:GLN:HG3	1:A:120:ILE:HG13	1.94	0.50
1:A:154:TRP:CH2	1:A:156:SER:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:THR:CG2	1:A:363:LEU:HD13	2.42	0.50
1:A:35:LEU:HD13	1:A:78:ILE:HD12	1.94	0.50
1:B:9:PHE:HB3	1:B:13:VAL:HB	1.93	0.50
1:A:324:LEU:HD12	1:A:325:ILE:N	2.26	0.50
1:B:383:LYS:C	1:B:385:GLY:H	2.14	0.50
1:A:28:LYS:C	1:A:30:ILE:H	2.15	0.49
1:B:298:LYS:O	1:B:324:LEU:HA	2.12	0.49
1:B:464:ILE:O	1:B:464:ILE:HG12	2.10	0.49
1:B:278:LEU:H	1:B:278:LEU:HD12	1.76	0.49
1:B:74:ARG:NH1	1:B:74:ARG:HG2	2.25	0.49
1:B:234:TRP:NE1	1:B:326:ASP:HB2	2.27	0.49
1:A:427:GLN:NE2	1:A:431:TYR:OH	2.45	0.49
1:B:41:ASP:O	1:B:45:LYS:HG2	2.13	0.49
1:A:177:THR:C	1:A:178:LEU:HD12	2.33	0.49
1:A:148:PRO:HB3	1:A:170:GLU:HA	1.95	0.49
1:B:96:THR:CG2	1:B:97:ILE:H	2.17	0.49
1:A:312:GLN:NE2	1:A:340:GLN:OE1	2.46	0.49
1:B:234:TRP:HE1	1:B:326:ASP:HB2	1.78	0.49
1:B:249:PHE:CE2	1:B:253:ILE:HD13	2.48	0.48
1:B:44:ASP:HB3	1:B:305:PHE:CB	2.43	0.48
1:B:152:VAL:CG1	1:B:153:PHE:H	2.23	0.48
1:B:104:SER:HB2	1:B:286:TRP:CZ2	2.47	0.48
1:B:253:ILE:HG22	1:B:298:LYS:HD2	1.95	0.48
1:A:125:VAL:HG12	1:A:129:SER:HB3	1.94	0.48
1:A:393:GLN:HE21	1:A:472:LEU:HA	1.79	0.48
1:A:301:VAL:HG12	1:A:332:LEU:HD23	1.95	0.48
1:B:26:SER:HB2	1:B:118:GLN:HG2	1.94	0.48
1:A:406:HIS:ND1	1:A:422:ARG:NH1	2.62	0.48
1:A:397:ALA:HB2	1:A:472:LEU:HD21	1.94	0.48
1:B:281:PRO:HG2	1:B:378:PHE:CZ	2.48	0.48
1:A:272:GLN:HE21	1:A:347:ASN:HB3	1.77	0.48
1:B:288:MET:O	1:B:288:MET:HG2	2.13	0.48
1:B:44:ASP:HB3	1:B:305:PHE:HB3	1.95	0.48
1:A:226:LYS:HG3	1:A:228:ASN:H	1.78	0.48
1:A:449:LEU:C	1:A:449:LEU:HD23	2.34	0.48
1:B:15:GLN:HB3	1:B:105:PHE:CZ	2.49	0.48
1:B:299:LEU:HD23	1:B:300:TYR:O	2.13	0.48
1:B:203:HIS:N	1:B:203:HIS:CD2	2.71	0.48
1:B:361:GLU:OE1	1:B:361:GLU:HA	2.13	0.47
1:A:251:LYS:HE2	1:A:257:PHE:O	2.14	0.47
1:A:342:SER:HB3	1:A:345:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HA	1:B:188:LEU:HD13	1.96	0.47
1:B:278:LEU:N	1:B:278:LEU:CD1	2.78	0.47
1:A:6:THR:HG22	1:A:7:ARG:N	2.29	0.47
1:B:319:ARG:HH11	1:B:381:VAL:HG22	1.78	0.47
1:B:206:LEU:O	1:B:228:ASN:ND2	2.48	0.47
1:A:360:LEU:O	1:A:363:LEU:HB3	2.15	0.47
1:B:217:ASP:O	1:B:218:GLY:C	2.53	0.47
1:B:280:ILE:HG13	1:B:359:MET:CE	2.45	0.47
1:A:444:SER:CB	1:A:445:PRO:HD2	2.32	0.47
1:B:367:ASP:OD2	1:B:370:LYS:HG3	2.15	0.47
1:A:317:TYR:CD1	1:A:318:LEU:HG	2.50	0.47
1:A:56:LEU:C	1:A:58:GLU:H	2.18	0.47
1:A:219:GLU:HG2	1:A:220:THR:H	1.79	0.47
1:B:11:SER:O	1:B:15:GLN:HG3	2.15	0.47
1:A:103:LYS:HB3	1:A:105:PHE:CE2	2.50	0.46
1:A:148:PRO:O	1:A:168:THR:HA	2.14	0.46
1:B:232:ALA:O	1:B:235:THR:HB	2.14	0.46
1:B:120:ILE:HD13	1:B:257:PHE:HE2	1.80	0.46
1:B:259:ASP:HB3	1:B:260:PRO:HD2	1.97	0.46
1:A:363:LEU:C	1:A:365:LYS:H	2.17	0.46
1:A:462:ASP:HB2	1:A:465:ASP:OD2	2.15	0.46
1:B:423:MET:CE	1:B:478:LYS:HG3	2.42	0.46
1:A:99:LYS:HZ2	1:A:123:PHE:HB2	1.78	0.46
1:A:439:ALA:O	1:A:441:ALA:N	2.49	0.46
1:B:280:ILE:HA	1:B:281:PRO:HD2	1.81	0.46
1:B:28:LYS:C	1:B:30:ILE:H	2.19	0.46
1:A:65:VAL:CG1	1:A:208:VAL:HG22	2.46	0.46
1:B:280:ILE:O	1:B:281:PRO:O	2.34	0.46
1:A:268:VAL:HG21	1:A:274:TYR:CZ	2.50	0.46
1:A:280:ILE:HD13	1:A:360:LEU:CD2	2.45	0.46
1:A:315:PRO:HD3	1:A:353:THR:OG1	2.15	0.46
1:B:250:TYR:HB2	1:B:279:TYR:CD2	2.51	0.46
1:B:297:LEU:HD11	1:B:314:MET:HG3	1.98	0.46
1:B:46:LEU:N	1:B:83:VAL:HG13	2.31	0.46
1:B:141:THR:HB	1:B:174:THR:HG23	1.97	0.46
1:B:386:PRO:HD3	1:B:396:ILE:HG21	1.97	0.46
1:A:289:TRP:O	1:A:290:ASN:HB2	2.15	0.46
1:A:481:GLN:HG2	1:A:482:SER:N	2.30	0.46
1:B:229:LYS:O	1:B:230:ALA:HB3	2.15	0.46
1:B:29:GLU:CG	1:B:192:ARG:HH22	2.28	0.46
1:A:103:LYS:HD3	1:A:105:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:C	1:B:30:ILE:N	2.70	0.45
1:B:262:THR:HG23	1:B:363:LEU:HD13	1.97	0.45
1:A:427:GLN:HG3	1:A:429:LYS:CG	2.46	0.45
1:B:155:GLU:HG3	1:B:156:SER:N	2.31	0.45
1:B:7:ARG:NH1	1:B:7:ARG:HG2	2.30	0.45
1:A:291:ARG:O	1:A:292:ASP:HB2	2.16	0.45
1:A:389:ASP:OD1	1:A:392:ASN:HB2	2.17	0.45
1:B:133:VAL:HG12	1:B:180:LEU:HD22	1.99	0.45
1:B:133:VAL:CG1	1:B:180:LEU:HD22	2.46	0.45
1:A:229:LYS:HE2	1:A:231:GLN:OE1	2.17	0.45
1:A:329:ASP:HB2	1:A:344:VAL:HG11	1.98	0.45
1:A:402:PHE:CD2	1:A:402:PHE:N	2.84	0.45
1:B:103:LYS:HG2	1:B:103:LYS:O	2.17	0.45
1:B:15:GLN:OE1	1:B:105:PHE:CE2	2.69	0.45
1:A:268:VAL:HG12	1:A:272:GLN:O	2.16	0.45
1:B:278:LEU:H	1:B:278:LEU:CD1	2.30	0.45
1:B:434:THR:HG21	1:B:466:GLU:HB2	1.99	0.45
1:A:331:PRO:C	1:A:333:ASN:N	2.69	0.45
1:A:448:GLU:O	1:A:451:ARG:HB3	2.17	0.45
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.32	0.45
1:A:28:LYS:C	1:A:30:ILE:N	2.70	0.45
1:A:283:GLN:HA	1:A:377:GLN:HG3	1.98	0.45
1:A:435:ALA:CB	1:A:441:ALA:HB2	2.47	0.45
1:B:256:ASP:OD1	1:B:258:ASN:ND2	2.50	0.45
1:B:321:VAL:O	1:B:322:ARG:HG2	2.17	0.45
1:A:289:TRP:CZ2	1:A:380:LEU:HD23	2.51	0.44
1:A:318:LEU:HD13	1:A:356:VAL:CG1	2.46	0.44
1:A:480:PHE:O	1:A:481:GLN:HB2	2.16	0.44
1:A:424:LYS:C	1:A:426:GLY:H	2.20	0.44
1:A:434:THR:CG2	1:A:435:ALA:H	2.30	0.44
1:B:147:LYS:C	1:B:149:GLU:H	2.21	0.44
1:B:300:TYR:O	1:B:301:VAL:HG23	2.17	0.44
1:A:178:LEU:N	1:A:178:LEU:CD1	2.80	0.44
1:A:237:ASN:ND2	1:A:240:GLU:OE1	2.47	0.44
1:B:194:ARG:NH2	1:B:225:GLU:OE2	2.46	0.44
1:B:279:TYR:N	1:B:322:ARG:O	2.47	0.44
1:B:354:LYS:O	1:B:358:GLN:HG3	2.18	0.44
1:B:85:MET:O	1:B:143:ALA:HB2	2.17	0.44
1:B:447:LEU:HD12	1:B:448:GLU:N	2.32	0.44
1:B:154:TRP:HA	1:B:163:THR:O	2.17	0.44
1:B:312:GLN:OE1	1:B:312:GLN:CA	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:TYR:OH	1:B:442:LYS:HD2	2.18	0.44
1:A:378:PHE:O	1:A:379:GLY:C	2.54	0.44
1:A:427:GLN:HG3	1:A:429:LYS:HG3	1.98	0.44
1:B:194:ARG:NH2	1:B:225:GLU:CD	2.71	0.44
1:A:406:HIS:CE1	1:A:422:ARG:NH1	2.86	0.43
1:B:414:VAL:HG13	1:B:418:ASP:HB2	2.00	0.43
1:A:262:THR:HG21	1:A:363:LEU:HD13	2.01	0.43
1:A:345:THR:O	1:A:348:LEU:N	2.47	0.43
1:A:261:LEU:HD13	1:A:374:PHE:HB2	1.99	0.43
1:B:1:MET:HG2	1:B:1:MET:O	2.17	0.43
1:B:207:PRO:HA	1:B:228:ASN:HD22	1.84	0.43
1:B:330:LEU:HD13	1:B:339:LEU:HD21	2.00	0.43
1:B:389:ASP:O	1:B:389:ASP:OD1	2.35	0.43
1:A:278:LEU:N	1:A:278:LEU:HD12	2.34	0.43
1:A:414:VAL:HG13	1:A:422:ARG:NH2	2.33	0.43
1:B:231:GLN:O	1:B:232:ALA:C	2.56	0.43
1:B:243:ASP:O	1:B:247:LYS:HG3	2.18	0.43
1:B:404:SER:OG	1:B:405:THR:N	2.52	0.43
1:A:7:ARG:HD3	1:A:162:TYR:OH	2.18	0.43
1:A:35:LEU:HD12	1:A:78:ILE:HD12	1.99	0.43
1:B:197:ILE:HD12	1:B:210:ILE:HD12	2.00	0.43
1:B:360:LEU:HB3	1:B:399:LEU:HD22	2.00	0.43
1:B:202:ASP:H	1:B:203:HIS:CD2	2.37	0.43
1:B:473:THR:O	1:B:474:GLU:HB2	2.18	0.43
1:B:5:GLU:CD	1:B:7:ARG:HE	2.22	0.43
1:A:68:SER:HB3	1:A:211:GLU:HB2	2.01	0.43
1:B:463:ARG:O	1:B:463:ARG:NE	2.43	0.43
1:A:6:THR:CG2	1:A:7:ARG:N	2.82	0.43
1:B:57:TYR:HA	1:B:172:ARG:HH12	1.84	0.43
1:B:396:ILE:O	1:B:396:ILE:HG22	2.19	0.43
1:B:65:VAL:CG1	1:B:208:VAL:HG22	2.49	0.43
1:B:203:HIS:HB3	1:B:249:PHE:HB2	2.00	0.42
1:A:164:VAL:CG1	1:A:165:ALA:N	2.82	0.42
1:A:232:ALA:HB1	1:A:234:TRP:CZ3	2.54	0.42
1:B:139:VAL:HG22	1:B:176:ILE:HG12	1.99	0.42
1:B:31:PHE:CG	1:B:32:LEU:N	2.87	0.42
1:A:217:ASP:C	1:A:219:GLU:H	2.23	0.42
1:A:422:ARG:HG2	1:A:456:GLU:OE2	2.19	0.42
1:A:143:ALA:O	1:A:146:GLU:HB2	2.19	0.42
1:A:423:MET:SD	1:A:478:LYS:HG3	2.60	0.42
1:B:316:ASN:C	1:B:318:LEU:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:O	1:B:450:LEU:HB2	2.20	0.42
1:A:371:TYR:OH	1:A:399:LEU:HB3	2.20	0.42
1:A:419:TYR:O	1:A:423:MET:HB2	2.19	0.42
1:A:397:ALA:CB	1:A:472:LEU:HD21	2.49	0.42
1:B:400:LEU:O	1:B:401:ARG:HD3	2.20	0.42
1:A:74:ARG:HH12	1:A:185:ASP:CG	2.22	0.41
1:A:28:LYS:O	1:A:30:ILE:N	2.53	0.41
1:B:1:MET:HG3	1:B:167:ILE:HG22	2.01	0.41
1:A:51:LEU:O	1:A:54:PRO:HD3	2.20	0.41
1:B:195:SER:O	1:B:198:SER:HB3	2.19	0.41
1:A:383:LYS:C	1:A:385:GLY:N	2.73	0.41
1:A:81:ASN:HA	1:A:172:ARG:O	2.20	0.41
1:B:66:ARG:NE	1:B:209:GLU:OE1	2.50	0.41
1:B:57:TYR:O	1:B:59:GLY:N	2.54	0.41
1:A:393:GLN:NE2	1:A:472:LEU:HA	2.35	0.41
1:B:94:LEU:HD22	1:B:127:PHE:CZ	2.55	0.41
1:B:153:PHE:O	1:B:164:VAL:HA	2.20	0.41
1:B:423:MET:O	1:B:424:LYS:HG2	2.20	0.41
1:B:401:ARG:HA	1:B:401:ARG:HD3	1.88	0.41
1:B:63:LEU:HD22	1:B:81:ASN:O	2.20	0.41
1:A:337:GLU:O	1:A:338:ILE:C	2.58	0.41
1:B:94:LEU:O	1:B:128:TYR:OH	2.37	0.41
1:A:447:LEU:HD23	1:A:447:LEU:O	2.21	0.41
1:B:19:LEU:HD22	1:B:105:PHE:CE1	2.55	0.41
1:B:164:VAL:HG12	1:B:165:ALA:N	2.35	0.41
1:B:415:SER:O	1:B:418:ASP:HB2	2.21	0.41
1:B:444:SER:N	1:B:445:PRO:HD3	2.36	0.41
1:A:131:PHE:CE2	1:A:137:VAL:HG23	2.56	0.41
1:A:197:ILE:O	1:A:200:TYR:N	2.54	0.41
1:A:317:TYR:O	1:A:318:LEU:HD23	2.21	0.41
1:A:333:ASN:O	1:A:334:VAL:C	2.59	0.41
1:B:134:ALA:HB2	1:B:178:LEU:HB3	2.03	0.41
1:B:230:ALA:O	1:B:231:GLN:HG3	2.21	0.41
1:B:288:MET:CG	1:B:288:MET:O	2.69	0.41
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.86	0.41
1:B:423:MET:HE1	1:B:478:LYS:HZ2	1.86	0.41
1:A:169:LYS:HZ3	1:A:171:ASP:HB2	1.86	0.41
1:B:101:GLY:HA2	1:B:286:TRP:CZ3	2.55	0.41
1:A:1:MET:HE2	1:A:4:GLN:HE22	1.84	0.40
1:B:208:VAL:HB	1:B:228:ASN:HB2	2.02	0.40
1:B:313:PHE:CE2	1:B:348:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:NH2	1:B:456:GLU:OE1	2.55	0.40
1:B:60:ASP:O	1:B:60:ASP:OD2	2.39	0.40
1:A:285:PRO:HG2	1:A:288:MET:HB2	2.03	0.40
1:A:409:SER:HB3	1:A:411:ALA:H	1.85	0.40
1:A:74:ARG:NH1	1:A:185:ASP:OD1	2.54	0.40
1:B:202:ASP:HB2	1:B:245:GLU:OE1	2.21	0.40
1:B:321:VAL:HG12	1:B:322:ARG:H	1.85	0.40
1:A:428:GLU:H	1:A:428:GLU:HG2	1.60	0.40
1:B:197:ILE:CD1	1:B:210:ILE:HD12	2.51	0.40
1:B:208:VAL:H	1:B:228:ASN:CB	2.35	0.40
1:B:29:GLU:H	1:B:29:GLU:CD	2.23	0.40
1:B:299:LEU:HD13	1:B:307:MET:HG2	2.03	0.40
1:B:354:LYS:HB3	1:B:354:LYS:HE2	1.92	0.40
1:B:383:LYS:C	1:B:385:GLY:N	2.75	0.40
1:B:420:VAL:CG2	1:B:423:MET:HE2	2.44	0.40
1:A:428:GLU:CG	1:A:428:GLU:O	2.67	0.40
1:B:190:ASP:O	1:B:194:ARG:CB	2.65	0.40
1:A:334:VAL:HA	1:A:338:ILE:HD12	2.04	0.40
1:B:384:GLU:HA	1:B:464:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:CD1	1:B:338:ILE:CD1[2_655]	2.15	0.05

## 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	471/559 (84%)	368 (78%)	78 (17%)	25 (5%)	<b>2</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	471/559 (84%)	366 (78%)	79 (17%)	26 (6%)	2	5
All	All	942/1118 (84%)	734 (78%)	157 (17%)	51 (5%)	2	6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	125	VAL
1	A	288	MET
1	A	290	ASN
1	A	292	ASP
1	A	435	ALA
1	A	439	ALA
1	A	445	PRO
1	A	475	PHE
1	A	476	ASP
1	B	58	GLU
1	B	97	ILE
1	B	123	PHE
1	B	281	PRO
1	B	291	ARG
1	B	445	PRO
1	B	463	ARG
1	B	474	GLU
1	A	332	LEU
1	A	425	GLU
1	A	430	ILE
1	A	446	HIS
1	A	463	ARG
1	B	17	LEU
1	B	126	GLY
1	B	218	GLY
1	B	282	SER
1	B	292	ASP
1	B	317	TYR
1	B	320	PHE
1	A	51	LEU
1	A	291	ARG
1	A	441	ALA
1	B	101	GLY
1	B	160	GLY
1	B	427	GLN

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Mol	Chain	Res	Type
1	B	444	SER
1	A	217	ASP
1	A	252	HIS
1	A	364	ALA
1	A	440	ALA
1	B	99	LYS
1	B	146	GLU
1	B	219	GLU
1	B	421	SER
1	A	289	TRP
1	A	380	LEU
1	B	54	PRO
1	A	338	ILE
1	B	148	PRO
1	B	270	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/488 (86%)	395 (94%)	24 (6%)	20	51
1	B	419/488 (86%)	394 (94%)	25 (6%)	19	49
All	All	838/976 (86%)	789 (94%)	49 (6%)	20	50

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	30	ILE
1	A	32	LEU
1	A	52	SER
1	A	55	ASP
1	A	62	GLU
1	A	64	ARG
1	A	141	THR

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Mol	Chain	Res	Type
1	A	168	THR
1	A	171	ASP
1	A	215	GLU
1	A	228	ASN
1	A	256	ASP
1	A	282	SER
1	A	291	ARG
1	A	317	TYR
1	A	325	ILE
1	A	353	THR
1	A	394	GLU
1	A	400	LEU
1	A	402	PHE
1	A	429	LYS
1	A	445	PRO
1	A	468	MET
1	B	2	LYS
1	B	7	ARG
1	B	86	THR
1	B	161	GLU
1	B	163	THR
1	B	168	THR
1	B	171	ASP
1	B	174	THR
1	B	202	ASP
1	B	203	HIS
1	B	223	SER
1	B	240	GLU
1	B	260	PRO
1	B	269	GLU
1	B	278	LEU
1	B	291	ARG
1	B	292	ASP
1	B	299	LEU
1	B	308	ASP
1	B	319	ARG
1	B	341	ASP
1	B	408	ASP
1	B	447	LEU
1	B	472	LEU
1	B	482	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	228	ASN
1	A	266	ASN
1	A	272	GLN
1	A	290	ASN
1	A	393	GLN
1	A	427	GLN
1	A	481	GLN
1	B	4	GLN
1	B	15	GLN
1	B	203	HIS
1	B	228	ASN
1	B	266	ASN
1	B	272	GLN
1	B	350	ASN
1	B	358	GLN
1	B	427	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	A	701	2	24,29,29	0.72	0	29,45,45	1.48	2 (6%)
3	ADP	B	702	2	24,29,29	0.76	0	29,45,45	1.38	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	701	2	-	2/12/32/32	0/3/3/3
3	ADP	B	702	2	-	6/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	701	ADP	PA-O3A-PB	-6.81	109.44	132.83
3	B	702	ADP	PA-O3A-PB	-6.43	110.75	132.83
3	A	701	ADP	C5'-C6-N6	2.44	124.06	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

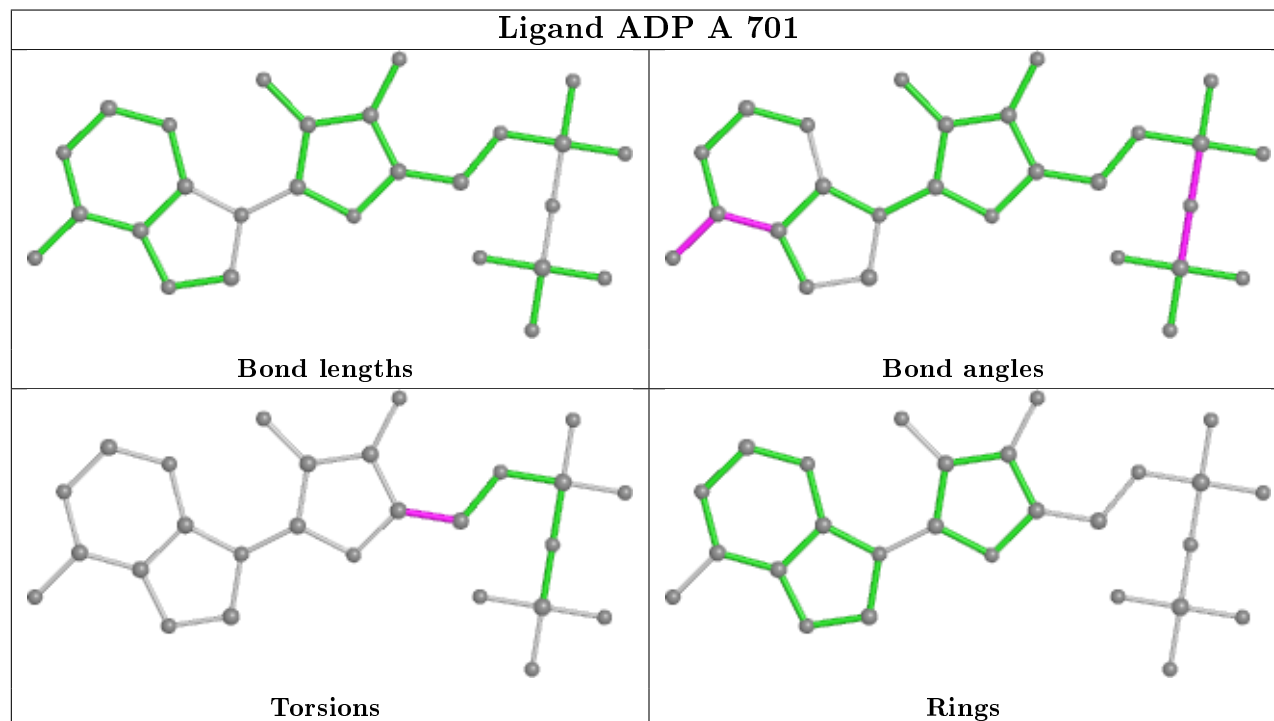
Mol	Chain	Res	Type	Atoms
3	B	702	ADP	C5'-O5'-PA-O3A
3	A	701	ADP	O4'-C4'-C5'-O5'
3	A	701	ADP	C3'-C4'-C5'-O5'
3	B	702	ADP	C5'-O5'-PA-O2A
3	B	702	ADP	PA-O3A-PB-O1B
3	B	702	ADP	PA-O3A-PB-O2B
3	B	702	ADP	PA-O3A-PB-O3B
3	B	702	ADP	C5'-O5'-PA-O1A

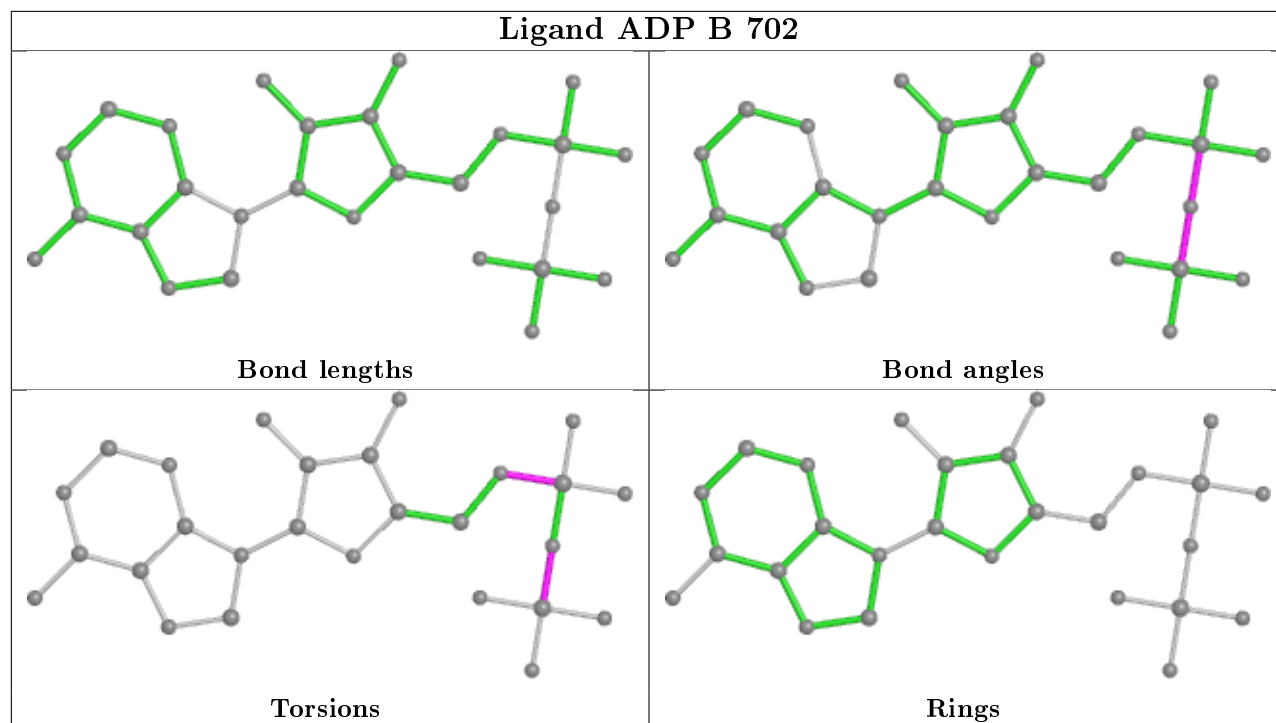
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	475/559 (84%)	0.58	42 (8%) 10 7	9, 58, 100, 100	0
1	B	475/559 (84%)	0.53	34 (7%) 15 11	33, 70, 98, 100	0
All	All	950/1118 (84%)	0.55	76 (8%) 12 9	9, 65, 100, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	SER	13.2
1	A	108	SER	8.1
1	A	107	GLU	7.6
1	B	105	PHE	7.3
1	A	118	GLN	6.6
1	B	100	SER	6.6
1	B	99	LYS	6.1
1	A	117	SER	5.7
1	A	99	LYS	5.5
1	A	119	LEU	5.3
1	A	475	PHE	5.1
1	A	106	LEU	5.1
1	A	480	PHE	4.9
1	B	108	SER	4.8
1	B	118	GLN	4.8
1	A	98	ALA	4.7
1	A	440	ALA	4.7
1	B	119	LEU	4.7
1	B	98	ALA	4.7
1	A	104	SER	4.6
1	B	220	THR	4.0
1	B	219	GLU	4.0
1	B	454	GLY	3.9
1	A	105	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	424	LYS	3.9
1	A	459	LEU	3.9
1	B	476	ASP	3.7
1	A	432	TYR	3.7
1	A	472	LEU	3.6
1	B	104	SER	3.5
1	A	447	LEU	3.5
1	B	455	ILE	3.4
1	A	428	GLU	3.4
1	A	441	ALA	3.3
1	A	455	ILE	3.3
1	A	444	SER	3.2
1	A	481	GLN	3.2
1	A	400	LEU	3.2
1	A	433	ILE	3.2
1	A	476	ASP	3.2
1	A	100	SER	3.2
1	A	473	THR	3.0
1	A	286	TRP	3.0
1	B	478	LYS	2.9
1	B	106	LEU	2.8
1	B	441	ALA	2.8
1	A	465	ASP	2.8
1	A	466	GLU	2.7
1	B	428	GLU	2.6
1	B	386	PRO	2.6
1	B	465	ASP	2.5
1	B	414	VAL	2.5
1	A	436	ASP	2.5
1	A	123	PHE	2.4
1	B	477	GLY	2.4
1	B	1	MET	2.4
1	B	445	PRO	2.3
1	A	446	HIS	2.3
1	A	120	ILE	2.3
1	A	460	LEU	2.3
1	B	394	GLU	2.3
1	A	60	ASP	2.3
1	A	443	SER	2.3
1	B	103	LYS	2.2
1	B	366	ASP	2.2
1	A	386	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	2.2
1	B	58	GLU	2.2
1	A	435	ALA	2.2
1	B	451	ARG	2.2
1	B	443	SER	2.1
1	B	422	ARG	2.1
1	B	444	SER	2.1
1	A	431	TYR	2.0
1	B	286	TRP	2.0
1	A	474	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

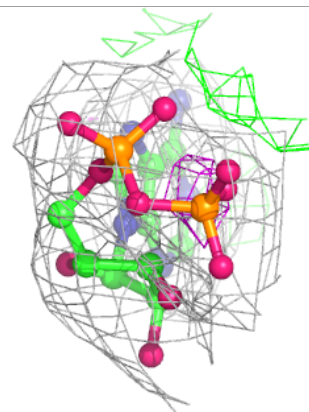
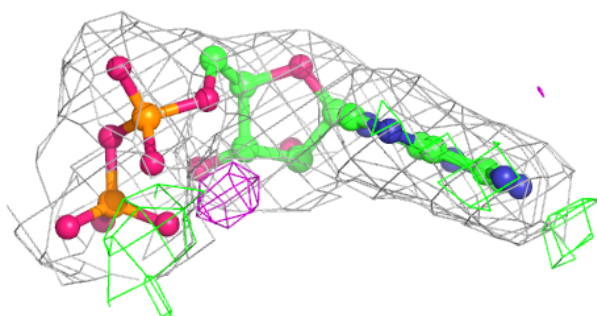
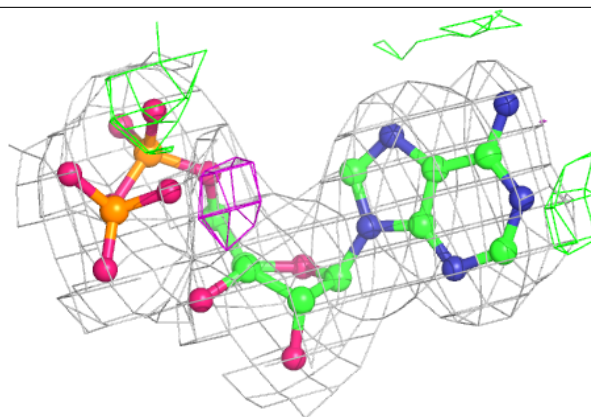
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MG	B	704	1/1	0.94	0.31	28,28,28,28	0
3	ADP	A	701	27/27	0.96	0.19	22,26,28,29	0
3	ADP	B	702	27/27	0.96	0.16	27,35,38,39	0
2	MG	A	703	1/1	0.99	0.32	26,26,26,26	0

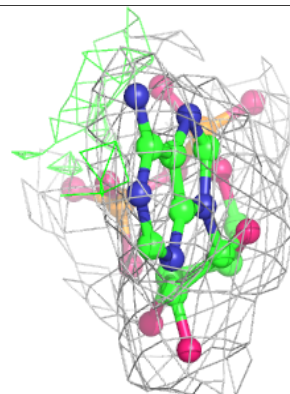
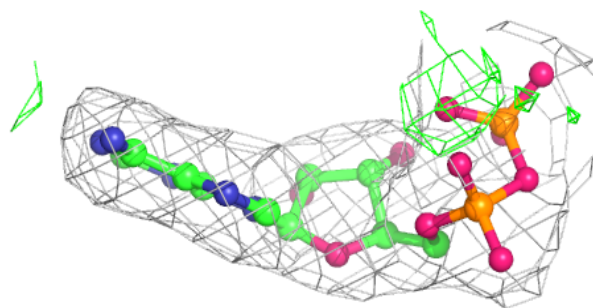
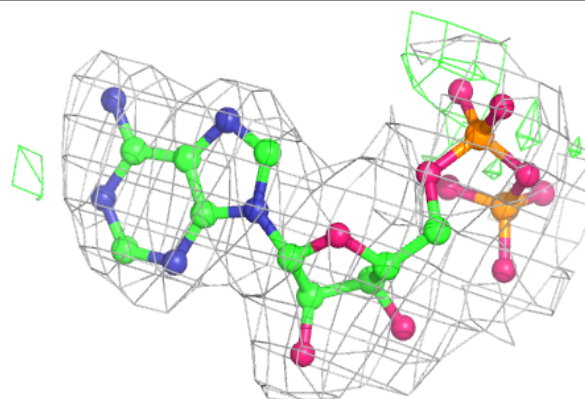
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP 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)

**Electron density around ADP 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)



## 6.5 Other polymers

There are no such residues in this entry.