



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 10:49 AM EDT

PDB ID : 1Y8Q  
Title : SUMO E1 ACTIVATING ENZYME SAE1-SAE2-MG-ATP COMPLEX  
Authors : Lois, L.M.; Lima, C.D.  
Deposited on : 2004-12-13  
Resolution : 2.25 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 : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

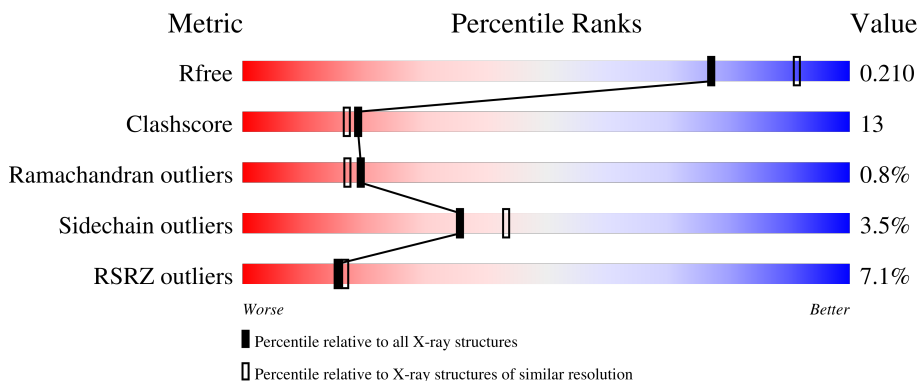
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	346	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">5%      67%      22%      • 10%</p>
1	C	346	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">4%      69%      19%      • 10%</p>
2	B	640	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">6%      59%      18%      • 20%</p>
2	D	640	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">7%      55%      23%      • 20%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13817 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 Ubiquitin-like 1 activating enzyme E1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2458	1557	417	471	13	0	0	0
1	C	311	2437	1544	414	466	13	0	0	0

- Molecule 2 is a protein called Ubiquitin-like 2 activating enzyme E1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	510	4005	2547	690	749	19	0	0	0
2	D	514	4031	2562	696	754	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ALA	CYS	engineered mutation	UNP Q9UBT2
D	173	ALA	CYS	engineered mutation	UNP Q9UBT2

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

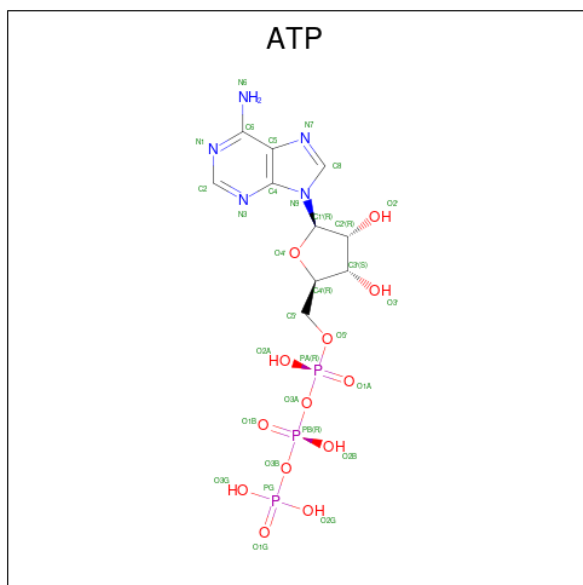
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Zn	0	0
			1	1		

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



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

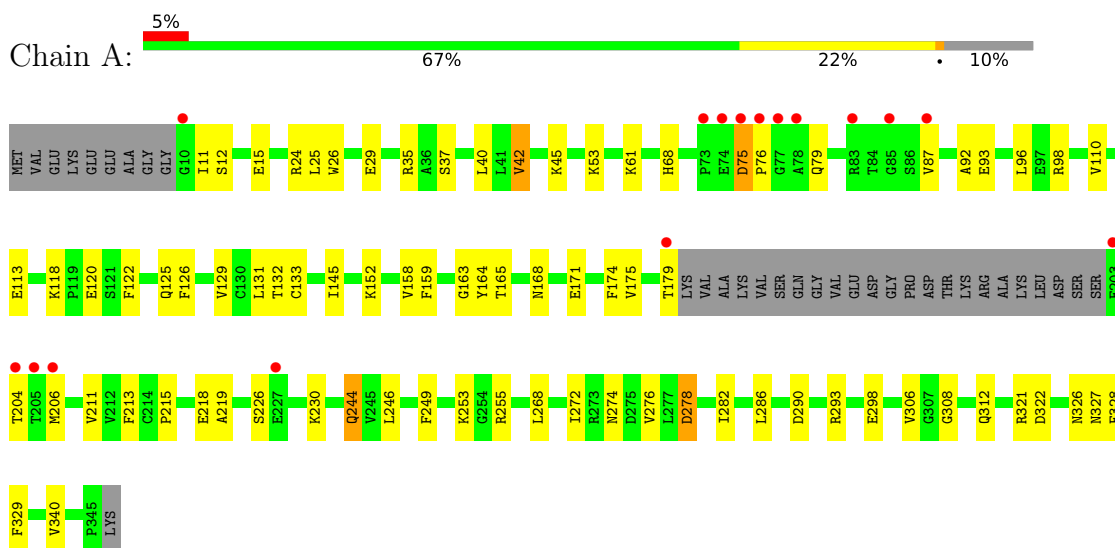
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	303	Total	O	0	0
			303	303		
6	C	158	Total	O	0	0
			158	158		
6	D	212	Total	O	0	0
			212	212		

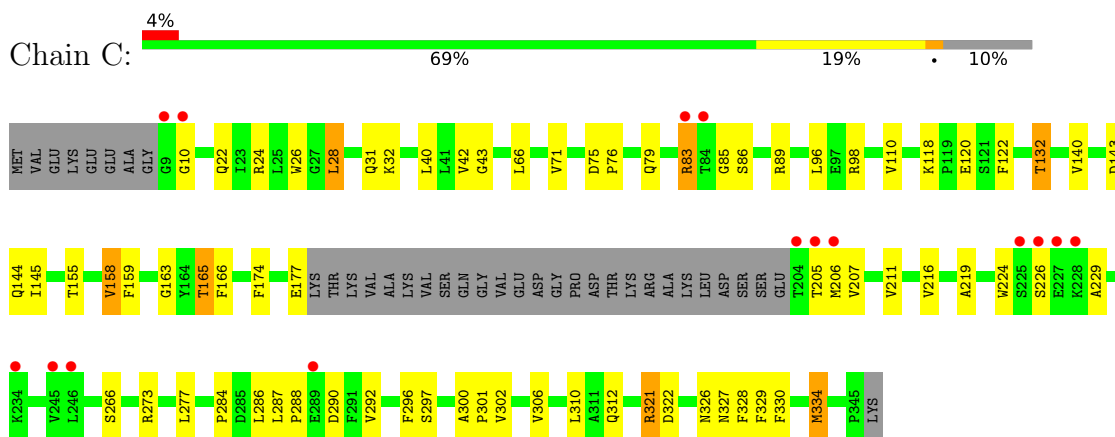
### 3 Residue-property plots i

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.

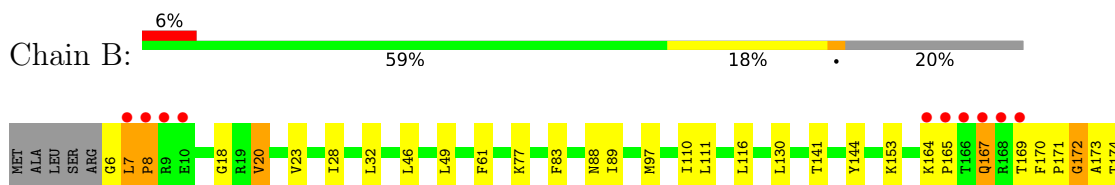
- Molecule 1: Ubiquitin-like 1 activating enzyme E1A

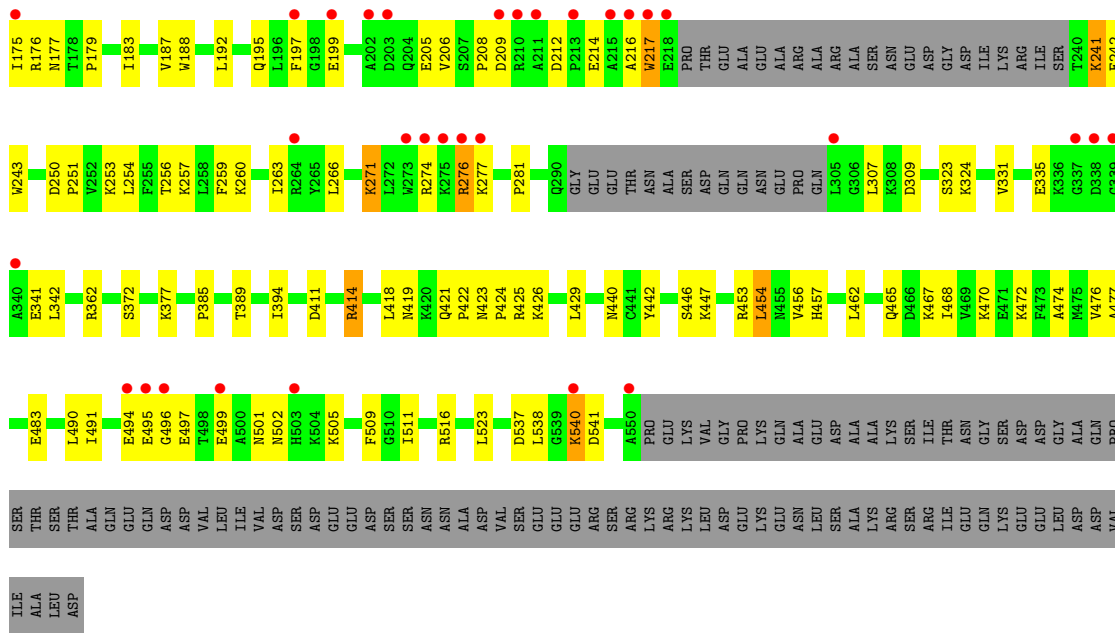


- Molecule 1: Ubiquitin-like 1 activating enzyme E1A

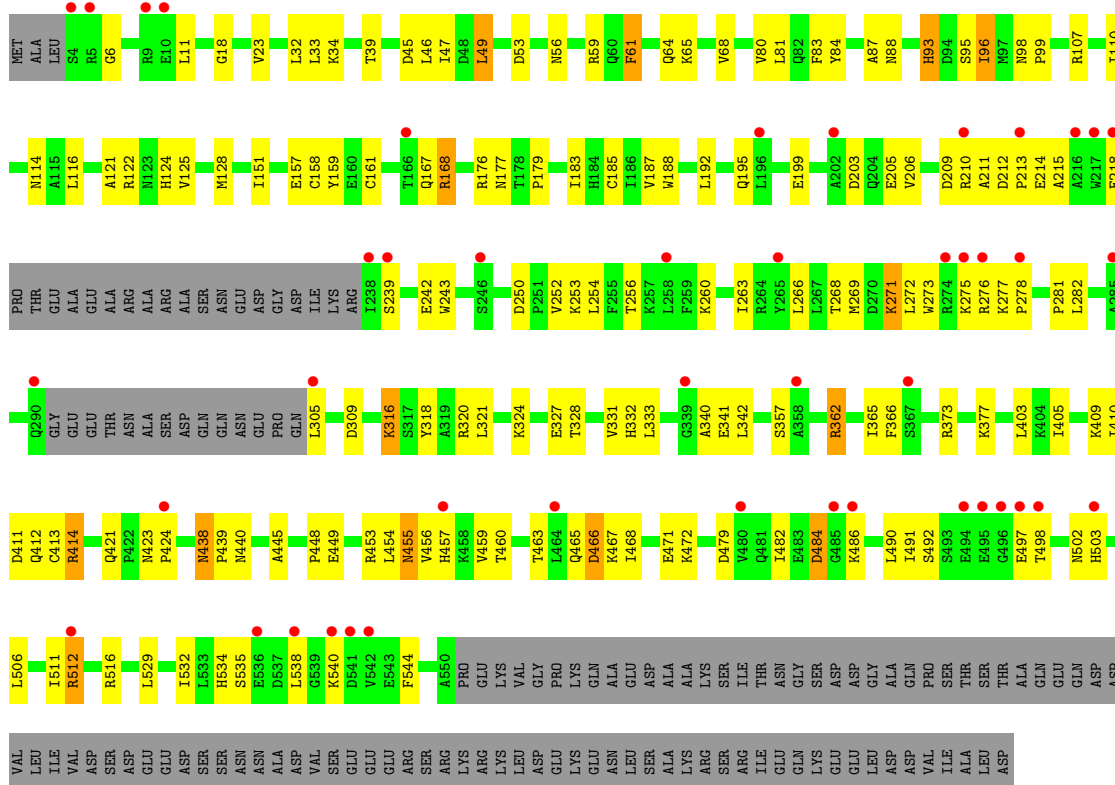


- Molecule 2: Ubiquitin-like 2 activating enzyme E1B





• Molecule 2: Ubiquitin-like 2 activating enzyme E1B



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.25Å 116.67Å 106.08Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	19.95 – 2.25 19.95 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.95-2.25) 95.8 (19.95-2.22)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.21Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.248 0.204 , 0.210	Depositor DCC
$R_{free}$ test set	5421 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0/2501	0.54	0/3374
1	C	0.37	0/2480	0.56	0/3346
2	B	0.34	0/4082	0.57	0/5526
2	D	0.33	0/4108	0.56	0/5560
All	All	0.35	0/13171	0.56	0/17806

There are no bond length outliers.

There are no bond angle outliers.

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	2458	0	2448	66	0
1	C	2437	0	2425	58	0
2	B	4005	0	4040	106	0
2	D	4031	0	4067	121	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	31	0	12	0	0
6	A	147	0	0	11	0
6	B	303	0	0	11	0
6	C	158	0	0	6	0
6	D	212	0	0	11	0
All	All	13817	0	13004	338	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 13.

All (338) 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:B:7:LEU:H	2:B:8:PRO:HA	1.22	1.03
1:C:165:THR:HG22	1:C:329:PHE:HB3	1.44	0.96
2:B:423:ASN:HB2	2:B:424:PRO:HD2	1.54	0.90
2:B:456:VAL:HG11	2:B:511:ILE:O	1.75	0.85
2:D:463:THR:HG23	2:D:467:LYS:HD3	1.60	0.83
1:A:312:GLN:HE21	2:B:389:THR:HG23	1.46	0.81
2:D:64:GLN:HG2	6:D:900:HOH:O	1.82	0.80
1:A:244:GLN:HE21	1:A:244:GLN:HA	1.47	0.79
2:B:170:PHE:HB2	2:B:175:ILE:HD11	1.63	0.79
2:D:456:VAL:HG21	2:D:511:ILE:O	1.84	0.76
1:A:274:ASN:O	1:A:278:ASP:HB2	1.85	0.76
2:B:276:ARG:HD3	2:B:277:LYS:H	1.49	0.76
2:B:167:GLN:H	2:B:167:GLN:NE2	1.84	0.76
2:D:506:LEU:HB3	2:D:511:ILE:HD12	1.68	0.76
2:D:53:ASP:H	2:D:56:ASN:ND2	1.84	0.75
1:C:143:ASP:CG	1:C:216:VAL:HG23	2.08	0.74
2:B:477:ALA:HB3	6:B:1021:HOH:O	1.85	0.74
2:D:273:TRP:HB3	2:D:278:PRO:HG3	1.67	0.74
1:C:22:GLN:HE21	1:C:31:GLN:HE22	1.34	0.73
2:D:465:GLN:HB2	2:D:491:ILE:HD13	1.71	0.72
1:A:45:LYS:HD3	1:A:133:CYS:SG	2.29	0.72
2:B:494:GLU:HB2	2:B:497:GLU:HG3	1.72	0.71
1:C:177:GLU:HG3	1:C:206:MET:H	1.55	0.71
2:B:7:LEU:H	2:B:8:PRO:CA	2.04	0.70
2:D:438:ASN:ND2	2:D:440:ASN:H	1.88	0.70
2:D:482:ILE:HD11	2:D:490:LEU:HD21	1.73	0.69
2:B:164:LYS:N	2:B:164:LYS:HD2	2.08	0.68
1:A:40:LEU:HD12	1:A:129:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:THR:HG22	1:C:207:VAL:HG23	1.75	0.68
1:C:334:MET:CE	1:C:334:MET:HA	2.23	0.67
1:A:25:LEU:HD11	2:B:144:TYR:CZ	2.29	0.67
1:C:83:ARG:HG3	1:C:86:SER:OG	1.95	0.67
2:D:23:VAL:HG12	2:D:116:LEU:HD21	1.75	0.67
2:B:141:THR:HG22	2:B:394:ILE:HG13	1.75	0.66
1:C:132:THR:HG21	6:C:348:HOH:O	1.94	0.66
1:A:215:PRO:HD2	1:A:218:GLU:OE2	1.96	0.65
2:B:490:LEU:HD11	2:B:511:ILE:HD11	1.77	0.65
1:C:28:LEU:HD22	1:C:32:LYS:HD2	1.76	0.65
1:C:79:GLN:HA	6:C:467:HOH:O	1.96	0.65
1:C:334:MET:HA	1:C:334:MET:HE3	1.76	0.65
2:B:496:GLY:HA2	2:B:499:GLU:CG	2.26	0.65
2:B:23:VAL:HG12	2:B:116:LEU:HD21	1.77	0.65
1:C:166:PHE:CE2	1:C:216:VAL:HG22	2.30	0.65
2:D:18:GLY:HA3	2:D:110:ILE:HD13	1.79	0.64
2:B:454:LEU:HA	2:B:538:LEU:HD11	1.80	0.64
2:B:462:LEU:HD12	2:B:502:ASN:HD22	1.62	0.63
1:C:286:LEU:O	1:C:286:LEU:HD23	1.97	0.63
1:A:226:SER:O	1:A:230:LYS:HG3	1.98	0.63
2:B:174:THR:HG21	6:B:912:HOH:O	1.97	0.63
1:A:165:THR:OG1	1:A:329:PHE:HB3	1.98	0.62
2:B:453:ARG:HG2	2:B:538:LEU:HD21	1.81	0.62
2:D:239:SER:HB3	2:D:242:GLU:HG3	1.82	0.62
1:A:312:GLN:HE21	2:B:389:THR:CG2	2.11	0.62
2:B:18:GLY:HA3	2:B:110:ILE:HD13	1.82	0.62
1:A:92:ALA:HB1	1:A:110:VAL:HG13	1.82	0.62
2:D:168:ARG:HB2	6:D:943:HOH:O	2.00	0.62
2:D:179:PRO:HG3	2:D:362:ARG:NH1	2.15	0.62
2:B:276:ARG:HD3	2:B:277:LYS:N	2.14	0.61
1:A:244:GLN:HA	1:A:244:GLN:NE2	2.14	0.61
2:D:275:LYS:HG3	2:D:276:ARG:HG3	1.83	0.61
1:A:174:PHE:HE2	1:A:211:VAL:HG23	1.66	0.60
2:B:197:PHE:HB3	2:B:342:LEU:HD12	1.82	0.60
2:D:492:SER:N	2:D:498:THR:HG21	2.16	0.60
1:C:42:VAL:O	1:C:132:THR:HB	2.01	0.60
1:A:75:ASP:H	1:A:76:PRO:CD	2.15	0.60
2:B:467:LYS:NZ	2:B:467:LYS:HB3	2.17	0.60
1:A:132:THR:HG21	6:A:351:HOH:O	2.02	0.59
2:D:188:TRP:CE3	2:D:362:ARG:HG3	2.37	0.59
1:A:25:LEU:HD11	2:B:144:TYR:CE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:535:SER:HA	6:D:947:HOH:O	2.00	0.59
1:C:277:LEU:HD12	1:C:284:PRO:HA	1.83	0.59
2:D:33:LEU:HG	2:D:80:VAL:HG21	1.86	0.58
1:A:158:VAL:HG12	6:A:383:HOH:O	2.03	0.58
2:B:167:GLN:H	2:B:167:GLN:HE21	1.50	0.58
2:D:484:ASP:OD1	2:D:486:LYS:HB3	2.04	0.58
1:C:120:GLU:HG3	1:C:145:ILE:HG23	1.84	0.58
2:D:177:ASN:HD21	2:D:209:ASP:HB3	1.69	0.58
1:C:177:GLU:HG3	1:C:206:MET:N	2.19	0.58
2:D:438:ASN:HD22	2:D:439:PRO:HD2	1.69	0.58
2:B:241:LYS:HB2	6:B:916:HOH:O	2.03	0.58
1:C:277:LEU:CD1	1:C:284:PRO:HA	2.34	0.57
1:C:26:TRP:HE1	1:C:31:GLN:NE2	2.02	0.57
2:D:252:VAL:HG23	6:D:877:HOH:O	2.05	0.57
1:A:312:GLN:HG3	2:B:389:THR:HG21	1.87	0.57
2:D:309:ASP:OD1	2:D:373:ARG:HD3	2.04	0.57
2:D:211:ALA:O	2:D:213:PRO:HD3	2.05	0.57
1:A:159:PHE:CG	1:A:246:LEU:HD13	2.40	0.57
2:B:216:ALA:HB3	2:B:271:LYS:NZ	2.19	0.56
2:B:253:LYS:HE3	6:B:1082:HOH:O	2.05	0.56
1:C:26:TRP:HE1	1:C:31:GLN:HE21	1.51	0.56
2:D:107:ARG:HD2	6:D:807:HOH:O	2.04	0.56
2:D:179:PRO:HG3	2:D:362:ARG:HH11	1.71	0.56
2:D:456:VAL:HG13	2:D:457:HIS:ND1	2.20	0.56
2:B:192:LEU:HD13	2:B:206:VAL:HG21	1.86	0.56
1:C:177:GLU:HA	1:C:205:THR:HB	1.88	0.56
1:A:11:ILE:HG22	1:A:35:ARG:HE	1.70	0.56
2:D:250:ASP:HB3	2:D:253:LYS:HB2	1.86	0.56
2:B:77:LYS:HE3	2:B:89:ILE:O	2.05	0.56
1:C:312:GLN:HB3	6:C:437:HOH:O	2.05	0.56
2:D:438:ASN:HD22	2:D:439:PRO:CD	2.19	0.56
1:C:155:THR:HG22	1:C:166:PHE:HB3	1.87	0.55
2:D:167:GLN:HB2	6:D:957:HOH:O	2.05	0.55
2:B:457:HIS:O	2:B:505:LYS:HG2	2.07	0.55
2:B:414:ARG:HD2	6:B:974:HOH:O	2.07	0.55
1:C:22:GLN:HE21	1:C:31:GLN:NE2	2.02	0.55
1:C:75:ASP:N	1:C:76:PRO:HD2	2.22	0.55
2:D:199:GLU:HA	2:D:341:GLU:OE2	2.06	0.55
1:A:79:GLN:HA	6:A:390:HOH:O	2.07	0.55
1:A:152:LYS:HE3	6:A:442:HOH:O	2.06	0.54
1:C:71:VAL:HG13	1:C:75:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:THR:CG2	1:C:329:PHE:HB3	2.28	0.54
2:D:466:ASP:O	2:D:471:GLU:HG3	2.08	0.54
1:A:308:GLY:O	2:B:389:THR:OG1	2.24	0.54
2:B:242:GLU:HG3	6:B:847:HOH:O	2.06	0.54
2:B:164:LYS:HD2	2:B:164:LYS:H	1.73	0.54
2:B:309:ASP:O	2:B:372:SER:HB2	2.07	0.54
2:B:18:GLY:HA3	2:B:110:ILE:CD1	2.38	0.53
1:A:11:ILE:HG22	1:A:35:ARG:NE	2.23	0.53
1:A:113:GLU:HG3	6:A:366:HOH:O	2.07	0.53
2:D:47:ILE:HD13	2:D:96:ILE:HG23	1.90	0.53
2:B:7:LEU:N	2:B:8:PRO:HA	2.06	0.53
2:B:177:ASN:HD21	2:B:209:ASP:HB3	1.74	0.53
2:B:20:VAL:CG2	2:B:111:LEU:HB3	2.38	0.53
2:B:423:ASN:CB	2:B:424:PRO:HD2	2.33	0.52
2:D:277:LYS:HB2	2:D:277:LYS:NZ	2.25	0.52
2:D:215:ALA:HB1	2:D:269:MET:HB3	1.92	0.52
2:D:449:GLU:HG3	2:D:529:LEU:HB2	1.90	0.52
1:C:118:LYS:HG2	1:C:122:PHE:CD2	2.45	0.52
2:B:183:ILE:O	2:B:187:VAL:HG23	2.10	0.52
2:D:188:TRP:NE1	2:D:206:VAL:HG13	2.25	0.51
2:B:540:LYS:HE3	2:B:540:LYS:HA	1.91	0.51
2:D:271:LYS:H	2:D:271:LYS:HD2	1.76	0.51
1:C:300:ALA:HB3	1:C:301:PRO:HD3	1.92	0.51
2:D:438:ASN:HD22	2:D:438:ASN:C	2.13	0.51
1:C:143:ASP:OD1	1:C:216:VAL:HG23	2.09	0.51
2:B:212:ASP:OD2	2:B:214:GLU:HB3	2.11	0.51
1:C:85:GLY:HA2	6:C:378:HOH:O	2.11	0.51
1:A:68:HIS:HB2	6:A:445:HOH:O	2.09	0.51
1:A:163:GLY:HA3	1:A:306:VAL:HG21	1.92	0.51
2:B:263:ILE:HG22	2:B:281:PRO:HG3	1.91	0.51
2:B:418:LEU:HD13	2:B:429:LEU:HD21	1.93	0.51
2:D:268:THR:HG22	2:D:268:THR:O	2.10	0.51
2:D:11:LEU:HD21	2:D:403:LEU:HD22	1.93	0.50
2:D:516:ARG:HH22	2:D:529:LEU:HD13	1.75	0.50
1:A:24:ARG:NH2	2:B:377:LYS:HD3	2.26	0.50
2:B:61:PHE:HD2	6:B:936:HOH:O	1.94	0.50
2:D:263:ILE:HD12	2:D:365:ILE:HG21	1.92	0.50
2:D:413:CYS:C	2:D:414:ARG:HG2	2.31	0.50
2:B:256:THR:O	2:B:260:LYS:HB3	2.11	0.50
2:D:454:LEU:HD21	2:D:532:ILE:HG23	1.94	0.50
2:B:476:VAL:HG21	2:B:523:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:HG22	1:C:302:VAL:HG12	1.92	0.50
2:D:445:ALA:O	2:D:448:PRO:HD3	2.11	0.50
2:B:171:PRO:C	2:B:173:ALA:H	2.15	0.50
2:D:177:ASN:ND2	2:D:209:ASP:HB3	2.25	0.50
1:C:163:GLY:HA3	1:C:306:VAL:HG21	1.94	0.50
2:D:423:ASN:HB2	2:D:424:PRO:HD2	1.94	0.50
2:D:468:ILE:O	2:D:472:LYS:HB3	2.12	0.50
2:B:446:SER:O	2:B:447:LYS:HD2	2.12	0.49
2:D:65:LYS:O	2:D:68:VAL:HG23	2.13	0.49
2:D:93:HIS:HD2	6:D:915:HOH:O	1.94	0.49
2:B:216:ALA:HB3	2:B:271:LYS:HZ3	1.76	0.49
2:D:318:TYR:O	2:D:357:SER:HB2	2.13	0.49
2:B:456:VAL:HG12	2:B:456:VAL:O	2.11	0.49
1:C:321:ARG:O	1:C:322:ASP:HB2	2.12	0.49
2:D:179:PRO:HD2	2:D:366:PHE:CE2	2.47	0.49
1:A:249:PHE:CE1	1:A:268:LEU:HD23	2.47	0.49
2:D:34:LYS:HB2	2:D:61:PHE:HZ	1.78	0.49
2:D:438:ASN:HD22	2:D:439:PRO:N	2.11	0.49
2:B:217:TRP:HE3	2:B:217:TRP:HA	1.78	0.49
2:B:495:GLU:CD	2:B:495:GLU:H	2.16	0.49
2:B:217:TRP:HA	2:B:217:TRP:CE3	2.48	0.49
2:D:405:ILE:HG12	2:D:410:ILE:CD1	2.43	0.49
1:A:96:LEU:HD13	1:A:110:VAL:HG23	1.95	0.48
1:A:244:GLN:HE21	1:A:244:GLN:CA	2.15	0.48
2:D:423:ASN:HB2	2:D:424:PRO:CD	2.43	0.48
2:D:195:GLN:HG3	2:D:206:VAL:HG23	1.96	0.48
2:D:266:LEU:HG	2:D:273:TRP:HZ2	1.78	0.48
2:B:179:PRO:HG3	2:B:362:ARG:HH11	1.79	0.48
2:D:33:LEU:CD2	2:D:80:VAL:HG21	2.43	0.48
2:D:263:ILE:HG22	2:D:281:PRO:HG3	1.95	0.48
2:B:171:PRO:O	2:B:173:ALA:N	2.47	0.48
2:B:465:GLN:HB2	2:B:491:ILE:HD13	1.95	0.48
2:D:88:ASN:HB3	6:D:973:HOH:O	2.13	0.48
2:B:6:GLY:O	2:B:7:LEU:HG	2.14	0.48
2:D:438:ASN:ND2	2:D:438:ASN:C	2.68	0.48
1:A:321:ARG:O	1:A:322:ASP:HB2	2.14	0.48
2:B:276:ARG:HA	2:B:276:ARG:HH11	1.79	0.48
1:C:96:LEU:HD13	1:C:110:VAL:HG13	1.96	0.47
1:A:158:VAL:CG1	6:A:383:HOH:O	2.59	0.47
2:D:263:ILE:HG13	2:D:365:ILE:HD13	1.96	0.47
2:D:333:LEU:HD11	2:D:340:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:OG1	1:A:204:THR:HA	2.15	0.47
2:B:195:GLN:O	2:B:241:LYS:HG2	2.14	0.47
2:D:405:ILE:HG12	2:D:410:ILE:HD13	1.97	0.47
2:D:512:ARG:H	2:D:512:ARG:HD2	1.79	0.47
1:A:253:LYS:C	1:A:255:ARG:H	2.18	0.47
1:C:165:THR:OG1	1:C:310:LEU:HD13	2.15	0.47
2:D:124:HIS:O	2:D:128:MET:HG2	2.15	0.47
1:A:213:PHE:HB3	6:A:364:HOH:O	2.15	0.47
2:B:324:LYS:HG2	6:B:1009:HOH:O	2.15	0.47
2:D:459:VAL:HA	6:D:917:HOH:O	2.14	0.47
2:D:185:CYS:O	2:D:188:TRP:HB3	2.15	0.47
2:D:192:LEU:HA	2:D:206:VAL:HG21	1.96	0.46
1:C:98:ARG:NH1	2:D:83:PHE:HB3	2.30	0.46
1:C:288:PRO:C	1:C:290:ASP:H	2.17	0.46
2:D:215:ALA:HB2	2:D:272:LEU:HG	1.95	0.46
2:B:251:PRO:HB3	2:B:323:SER:HA	1.98	0.46
2:B:425:ARG:O	2:B:426:LYS:HB2	2.15	0.46
2:D:305:LEU:C	2:D:305:LEU:HD13	2.36	0.46
2:D:409:LYS:HD3	2:D:412:GLN:OE1	2.15	0.46
2:D:263:ILE:CG2	2:D:281:PRO:HG3	2.44	0.46
1:C:224:TRP:HA	1:C:229:ALA:HB1	1.98	0.46
1:A:118:LYS:HD2	1:A:122:PHE:CG	2.50	0.46
2:B:259:PHE:HA	2:B:263:ILE:HD13	1.98	0.46
2:D:183:ILE:O	2:D:187:VAL:HG23	2.15	0.46
1:A:164:TYR:HA	1:A:329:PHE:O	2.16	0.46
2:D:151:ILE:HG23	2:D:158:CYS:HA	1.98	0.46
1:A:290:ASP:OD2	1:A:293:ARG:HD3	2.15	0.46
1:A:298:GLU:HA	6:A:383:HOH:O	2.16	0.46
1:A:53:LYS:HB3	1:A:53:LYS:HE2	1.76	0.45
2:B:28:ILE:HD11	2:B:141:THR:HG23	1.98	0.45
1:C:166:PHE:HE2	1:C:216:VAL:HG22	1.81	0.45
2:B:172:GLY:O	2:B:176:ARG:HD3	2.16	0.45
2:B:243:TRP:CH2	2:B:254:LEU:HA	2.51	0.45
1:C:28:LEU:O	1:C:32:LYS:HG3	2.16	0.45
2:D:96:ILE:HD11	2:D:121:ALA:HB1	1.98	0.45
1:A:75:ASP:N	1:A:76:PRO:CD	2.79	0.45
2:B:141:THR:CG2	2:B:394:ILE:HG13	2.46	0.45
2:D:49:LEU:HD23	2:D:95:SER:HB2	1.98	0.45
2:D:260:LYS:HB2	2:D:282:LEU:O	2.16	0.45
1:A:98:ARG:HD2	6:A:367:HOH:O	2.15	0.45
1:A:120:GLU:HG2	1:A:145:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:GLU:HB2	2:D:161:CYS:SG	2.56	0.45
2:D:122:ARG:HD3	2:D:159:TYR:OH	2.17	0.45
1:C:177:GLU:OE1	1:C:206:MET:SD	2.75	0.45
2:D:516:ARG:NH2	2:D:529:LEU:HD13	2.32	0.45
2:D:18:GLY:HA3	2:D:110:ILE:CD1	2.46	0.44
2:D:34:LYS:HD3	2:D:61:PHE:CZ	2.52	0.44
2:D:210:ARG:C	2:D:212:ASP:H	2.20	0.44
1:A:11:ILE:HD11	2:B:307:LEU:HD21	1.99	0.44
1:C:328:PHE:HB3	1:C:330:PHE:CE1	2.52	0.44
1:A:40:LEU:HB2	1:A:126:PHE:CG	2.52	0.44
1:A:122:PHE:O	1:A:125:GLN:HG2	2.17	0.44
2:B:496:GLY:HA2	2:B:499:GLU:CD	2.38	0.44
1:C:165:THR:HG23	6:C:353:HOH:O	2.18	0.44
2:D:176:ARG:HG3	2:D:176:ARG:HH11	1.83	0.44
2:D:114:ASN:OD1	2:D:125:VAL:HG11	2.18	0.44
2:D:538:LEU:N	2:D:538:LEU:HD22	2.33	0.44
1:A:75:ASP:H	1:A:76:PRO:HD2	1.81	0.44
2:B:440:ASN:HA	6:B:970:HOH:O	2.17	0.44
2:D:328:THR:HG22	2:D:332:HIS:CD2	2.52	0.44
1:A:175:VAL:CG2	1:A:206:MET:HB2	2.48	0.43
2:B:418:LEU:HD13	2:B:429:LEU:CD2	2.48	0.43
1:C:66:LEU:C	1:C:66:LEU:HD23	2.38	0.43
1:C:219:ALA:HB1	1:C:328:PHE:HE1	1.83	0.43
1:C:10:GLY:H	1:C:32:LYS:HE3	1.83	0.43
2:B:271:LYS:HD2	2:B:271:LYS:H	1.82	0.43
2:D:321:LEU:HD12	2:D:324:LYS:HE3	2.01	0.43
1:A:25:LEU:HB2	2:B:385:PRO:HB3	2.00	0.43
2:D:23:VAL:CG1	2:D:96:ILE:HG12	2.49	0.43
2:B:419:ASN:HB2	6:B:814:HOH:O	2.19	0.43
2:D:453:ARG:O	2:D:544:PHE:HA	2.18	0.43
2:D:460:THR:HG21	2:D:503:HIS:CD2	2.54	0.43
1:A:12:SER:OG	1:A:15:GLU:HG3	2.19	0.43
2:B:169:THR:HG22	2:B:170:PHE:N	2.34	0.43
2:D:479:ASP:OD1	2:D:492:SER:HA	2.18	0.43
1:A:29:GLU:HB3	6:A:402:HOH:O	2.19	0.43
2:B:176:ARG:NH1	2:B:205:GLU:HB2	2.33	0.43
2:B:483:GLU:OE1	2:B:516:ARG:HD3	2.18	0.43
2:D:455:ASN:ND2	2:D:534:HIS:HE1	2.17	0.43
2:B:20:VAL:HG23	2:B:111:LEU:HB3	2.01	0.43
2:D:39:THR:O	2:D:39:THR:HG22	2.19	0.43
2:D:250:ASP:OD2	2:D:253:LYS:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:456:VAL:HG12	2:D:534:HIS:ND1	2.33	0.42
1:A:37:SER:O	1:A:61:LYS:HB3	2.18	0.42
2:B:130:LEU:O	2:B:153:LYS:HD2	2.19	0.42
2:B:476:VAL:HG23	2:B:477:ALA:N	2.34	0.42
1:C:158:VAL:CG2	1:C:302:VAL:HG12	2.49	0.42
1:C:174:PHE:HE2	1:C:211:VAL:HG23	1.84	0.42
1:C:273:ARG:HG3	1:C:287:LEU:HD23	2.00	0.42
2:D:84:TYR:HD2	2:D:87:ALA:HB2	1.84	0.42
1:A:219:ALA:HB1	1:A:328:PHE:CE1	2.55	0.42
1:A:219:ALA:HB1	1:A:328:PHE:HE1	1.83	0.42
1:A:340:VAL:HG21	2:B:422:PRO:HG3	2.00	0.42
1:C:24:ARG:NH2	2:D:377:LYS:HD2	2.35	0.42
1:C:266:SER:HB3	1:C:292:VAL:HG11	2.01	0.42
1:A:98:ARG:HH12	2:B:83:PHE:HD2	1.67	0.42
1:A:272:ILE:O	1:A:276:VAL:HG23	2.20	0.42
1:A:206:MET:O	1:A:206:MET:HG3	2.20	0.42
1:A:282:ILE:HG21	1:A:286:LEU:HD22	2.01	0.42
1:C:89:ARG:HG3	1:C:89:ARG:HH11	1.84	0.42
2:D:316:LYS:HD3	2:D:320:ARG:HH11	1.85	0.42
1:A:93:GLU:HG3	1:A:110:VAL:HG11	2.01	0.41
2:B:208:PRO:HB3	2:B:266:LEU:HD13	2.01	0.41
2:B:331:VAL:O	2:B:335:GLU:HG3	2.19	0.41
2:D:243:TRP:CH2	2:D:254:LEU:HD23	2.55	0.41
2:D:405:ILE:HG23	2:D:410:ILE:HD11	2.02	0.41
1:C:43:GLY:HA3	1:C:132:THR:HG22	2.01	0.41
2:D:277:LYS:HB2	2:D:277:LYS:HZ2	1.84	0.41
2:B:414:ARG:HE	2:B:414:ARG:HB3	1.48	0.41
2:D:98:ASN:HA	2:D:99:PRO:HD3	1.94	0.41
2:D:454:LEU:N	2:D:454:LEU:HD23	2.35	0.41
2:B:167:GLN:HE21	2:B:167:GLN:N	2.16	0.41
2:B:199:GLU:HA	2:B:341:GLU:OE2	2.21	0.41
2:B:243:TRP:CH2	2:B:257:LYS:HB3	2.55	0.41
2:D:59:ARG:HH11	2:D:59:ARG:HG2	1.86	0.41
2:B:171:PRO:C	2:B:173:ALA:N	2.73	0.41
2:B:467:LYS:HB3	2:B:467:LYS:HZ3	1.84	0.41
2:D:316:LYS:HE3	2:D:316:LYS:HB3	1.92	0.41
2:D:203:ASP:OD2	2:D:203:ASP:N	2.54	0.41
2:B:188:TRP:NE1	2:B:206:VAL:HG23	2.35	0.41
2:D:96:ILE:H	2:D:96:ILE:HG13	1.68	0.41
1:A:326:ASN:HA	1:A:327:ASN:HA	1.75	0.41
2:B:250:ASP:HB3	2:B:253:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:540:LYS:HD3	6:D:839:HOH:O	2.20	0.41
1:A:25:LEU:HD12	1:A:26:TRP:CE3	2.56	0.41
1:A:42:VAL:HG22	1:A:131:LEU:HA	2.02	0.41
2:B:263:ILE:N	2:B:263:ILE:HD12	2.35	0.41
2:D:455:ASN:HD22	2:D:534:HIS:HE1	1.69	0.41
1:A:92:ALA:CB	1:A:110:VAL:HG13	2.50	0.41
1:C:140:VAL:O	1:C:144:GLN:HG3	2.21	0.41
1:C:158:VAL:HG13	6:C:356:HOH:O	2.20	0.41
2:D:256:THR:HG23	2:D:260:LYS:HE2	2.03	0.41
2:B:164:LYS:HB3	2:B:165:PRO:HD2	2.03	0.40
2:B:465:GLN:OE1	2:B:491:ILE:HG23	2.20	0.40
2:B:468:ILE:O	2:B:472:LYS:HB3	2.21	0.40
2:B:501:ASN:HB3	2:B:509:PHE:CZ	2.56	0.40
2:D:6:GLY:HA3	6:D:976:HOH:O	2.20	0.40
2:D:218:GLU:O	2:D:268:THR:HG22	2.21	0.40
2:D:333:LEU:HD13	2:D:342:LEU:HG	2.03	0.40
2:B:442:TYR:HD2	6:B:1060:HOH:O	2.04	0.40
2:D:33:LEU:CG	2:D:80:VAL:HG21	2.49	0.40
2:D:327:GLU:O	2:D:331:VAL:HG23	2.21	0.40
2:B:470:LYS:O	2:B:474:ALA:HA	2.21	0.40
1:C:296:PHE:O	1:C:297:SER:HB2	2.22	0.40
1:C:326:ASN:HA	1:C:327:ASN:HA	1.68	0.40
1:A:168:ASN:ND2	1:A:215:PRO:HA	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	309/346 (89%)	287 (93%)	20 (6%)	2 (1%)	25 25
1	C	307/346 (89%)	282 (92%)	23 (8%)	2 (1%)	22 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	504/640 (79%)	469 (93%)	31 (6%)	4 (1%)	19	17
2	D	508/640 (79%)	476 (94%)	27 (5%)	5 (1%)	15	13
All	All	1628/1972 (83%)	1514 (93%)	101 (6%)	13 (1%)	19	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
2	B	7	LEU
2	B	274	ARG
1	C	83	ARG
2	D	214	GLU
1	A	87	VAL
2	B	8	PRO
2	B	172	GLY
2	D	497	GLU
2	D	502	ASN
1	C	226	SER
2	D	61	PHE
2	D	484	ASP

### 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	270/296 (91%)	266 (98%)	4 (2%)	65	75
1	C	267/296 (90%)	259 (97%)	8 (3%)	41	50
2	B	440/551 (80%)	422 (96%)	18 (4%)	30	36
2	D	443/551 (80%)	424 (96%)	19 (4%)	29	33
All	All	1420/1694 (84%)	1371 (96%)	49 (4%)	36	43

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

Mol	Chain	Res	Type
1	A	42	VAL
1	A	171	GLU
1	A	244	GLN
1	A	278	ASP
2	B	20	VAL
2	B	32	LEU
2	B	46	LEU
2	B	49	LEU
2	B	88	ASN
2	B	97	MET
2	B	167	GLN
2	B	217	TRP
2	B	241	LYS
2	B	271	LYS
2	B	276	ARG
2	B	411	ASP
2	B	414	ARG
2	B	421	GLN
2	B	454	LEU
2	B	537	ASP
2	B	540	LYS
2	B	541	ASP
1	C	28	LEU
1	C	40	LEU
1	C	132	THR
1	C	158	VAL
1	C	159	PHE
1	C	165	THR
1	C	321	ARG
1	C	334	MET
2	D	32	LEU
2	D	45	ASP
2	D	46	LEU
2	D	49	LEU
2	D	81	LEU
2	D	93	HIS
2	D	96	ILE
2	D	168	ARG
2	D	205	GLU
2	D	271	LYS
2	D	316	LYS
2	D	362	ARG
2	D	411	ASP

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Mol	Chain	Res	Type
2	D	414	ARG
2	D	421	GLN
2	D	438	ASN
2	D	455	ASN
2	D	466	ASP
2	D	512	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	244	GLN
1	A	312	GLN
1	A	325	HIS
2	B	123	ASN
2	B	167	GLN
2	B	369	ASN
2	B	412	GLN
2	B	421	GLN
2	B	457	HIS
2	B	502	ASN
1	C	31	GLN
1	C	244	GLN
1	C	312	GLN
1	C	320	GLN
1	C	325	HIS
2	D	56	ASN
2	D	204	GLN
2	D	438	ASN
2	D	455	ASN
2	D	481	GLN
2	D	502	ASN
2	D	503	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
5	ATP	D	801	3	26,33,33	1.32	2 (7%)	31,52,52	1.70	6 (19%)
5	ATP	B	802	3	26,33,33	1.20	3 (11%)	31,52,52	1.72	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
5	ATP	D	801	3	-	6/18/38/38	0/3/3/3
5	ATP	B	802	3	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	801	ATP	C2-N3	4.66	1.39	1.32
5	B	802	ATP	C2-N3	3.67	1.38	1.32
5	B	802	ATP	C2'-C1'	-2.24	1.50	1.53
5	D	801	ATP	C2'-C1'	-2.16	1.50	1.53
5	B	802	ATP	C2-N1	2.13	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ATP	N3-C2-N1	-5.58	119.95	128.68
5	B	802	ATP	N3-C2-N1	-5.40	120.24	128.68
5	D	801	ATP	C4-C5-N7	-3.99	105.24	109.40
5	B	802	ATP	C4-C5-N7	-3.97	105.26	109.40
5	B	802	ATP	C5-C6-N6	3.91	126.30	120.35
5	D	801	ATP	C5-C6-N6	3.54	125.74	120.35
5	B	802	ATP	O2'-C2'-C3'	2.19	118.91	111.82
5	D	801	ATP	O2G-PG-O3B	2.18	111.95	104.64
5	D	801	ATP	PB-O3B-PG	-2.05	125.80	132.83
5	D	801	ATP	O2'-C2'-C3'	2.05	118.45	111.82
5	B	802	ATP	N6-C6-N1	-2.04	114.35	118.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

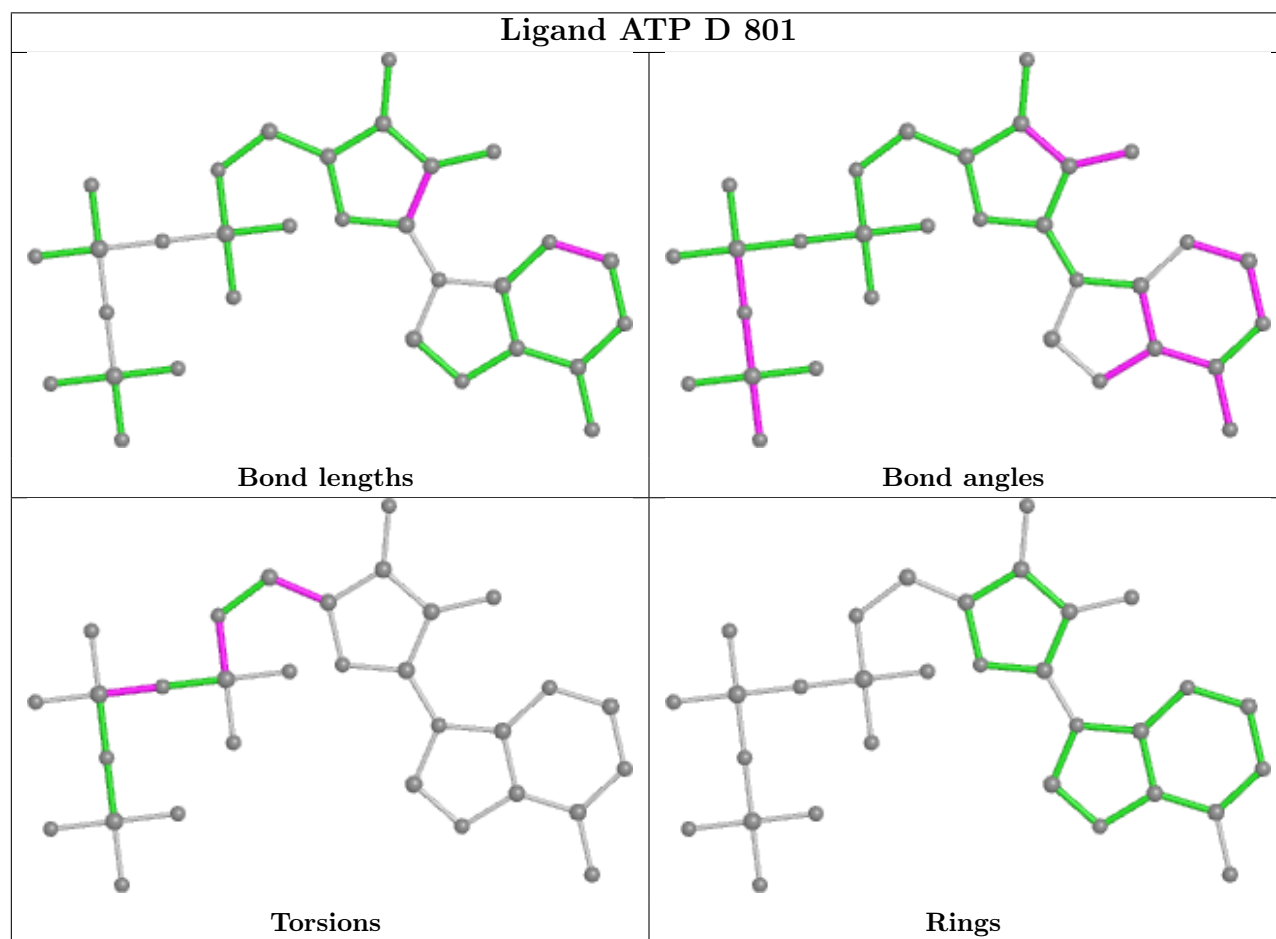
Mol	Chain	Res	Type	Atoms
5	B	802	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	C5'-O5'-PA-O2A
5	D	801	ATP	C5'-O5'-PA-O2A
5	D	801	ATP	PA-O3A-PB-O1B
5	B	802	ATP	C5'-O5'-PA-O3A
5	D	801	ATP	C5'-O5'-PA-O3A
5	D	801	ATP	C5'-O5'-PA-O1A
5	D	801	ATP	O4'-C4'-C5'-O5'
5	B	802	ATP	PA-O3A-PB-O1B
5	D	801	ATP	PA-O3A-PB-O2B
5	B	802	ATP	O4'-C4'-C5'-O5'

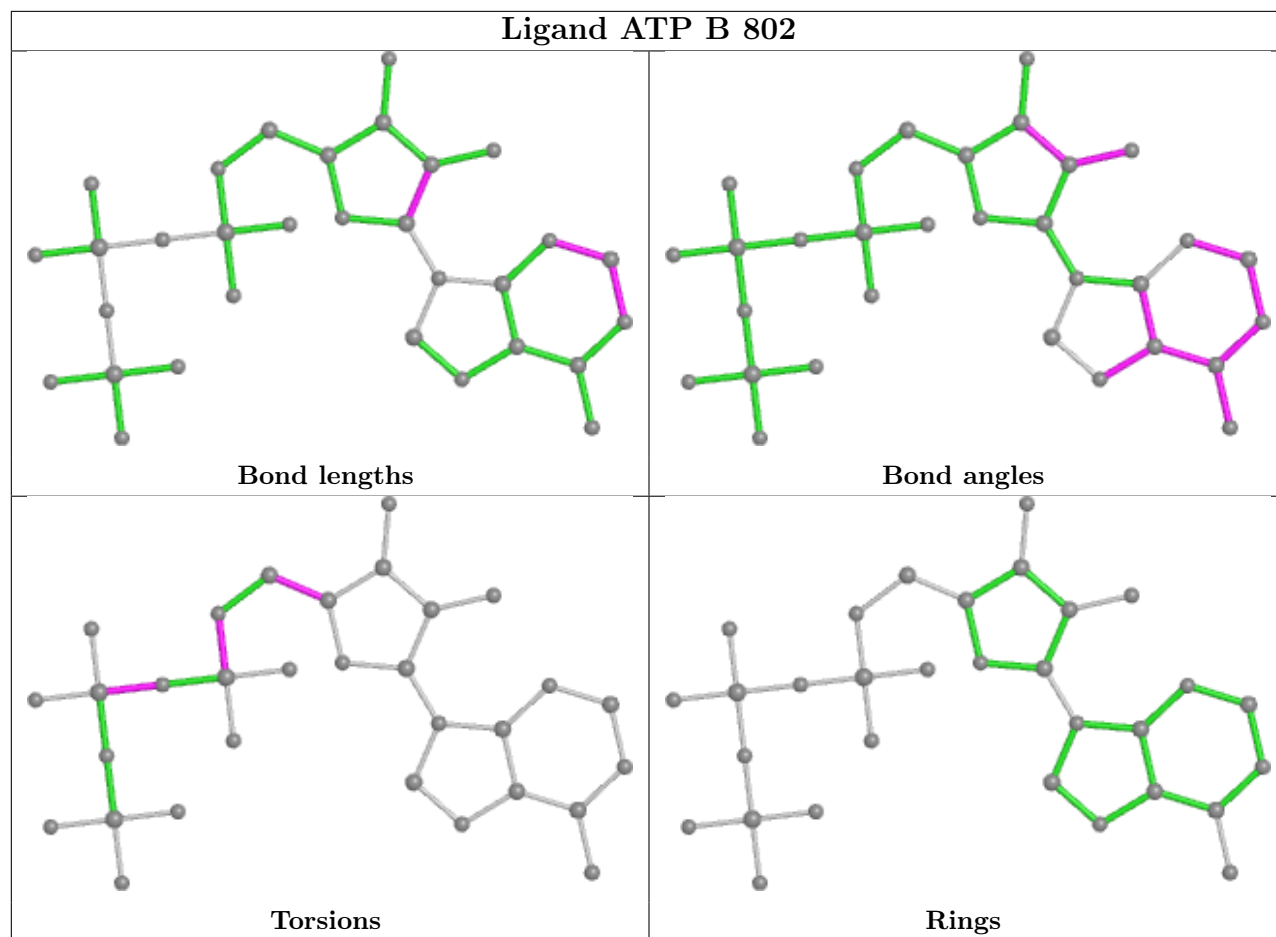
There are no ring outliers.

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	313/346 (90%)	0.04	16 (5%) 28 30	25, 42, 79, 109	0
1	C	311/346 (89%)	-0.00	15 (4%) 30 33	20, 40, 74, 104	0
2	B	510/640 (79%)	0.18	41 (8%) 12 13	20, 42, 94, 116	0
2	D	514/640 (80%)	0.31	45 (8%) 10 11	20, 51, 97, 120	0
All	All	1648/1972 (83%)	0.16	117 (7%) 16 17	20, 44, 92, 120	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	TRP	8.6
1	A	204	THR	6.2
2	D	238	ILE	6.1
2	B	165	PRO	6.1
2	B	217	TRP	6.1
1	A	203	GLU	6.0
2	D	216	ALA	5.8
1	A	205	THR	5.4
1	C	206	MET	5.4
1	C	204	THR	5.3
2	B	9	ARG	5.0
2	B	340	ALA	4.9
2	B	276	ARG	4.8
2	D	305	LEU	4.8
1	A	74	GLU	4.8
1	C	9	GLY	4.7
1	A	78	ALA	4.5
2	D	9	ARG	4.5
2	D	5	ARG	4.4
2	B	305	LEU	4.3
1	C	205	THR	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	485	GLY	4.2
2	D	275	LYS	4.0
1	A	73	PRO	4.0
2	B	275	LYS	3.9
2	B	218	GLU	3.9
2	B	210	ARG	3.9
2	D	274	ARG	3.9
1	A	75	ASP	3.8
1	C	10	GLY	3.8
2	B	338	ASP	3.7
2	D	541	ASP	3.7
1	A	179	THR	3.7
2	D	210	ARG	3.7
2	B	495	GLU	3.6
1	A	77	GLY	3.5
1	C	84	THR	3.5
2	B	540	LYS	3.5
2	B	7	LEU	3.4
1	C	227	GLU	3.4
2	B	339	GLY	3.3
2	D	540	LYS	3.3
2	D	542	VAL	3.3
2	D	486	LYS	3.3
1	A	76	PRO	3.2
2	D	367	SER	3.2
2	B	216	ALA	3.2
2	D	496	GLY	3.2
2	B	168	ARG	3.2
2	D	166	THR	3.2
2	D	536	GLU	3.2
2	B	213	PRO	3.1
2	B	496	GLY	3.1
2	B	203	ASP	3.0
1	A	206	MET	3.0
2	B	274	ARG	3.0
2	D	290	GLN	3.0
2	B	202	ALA	3.0
2	B	197	PHE	3.0
2	D	339	GLY	2.9
1	C	225	SER	2.9
2	D	218	GLU	2.9
2	B	8	PRO	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	166	THR	2.8
2	B	167	GLN	2.8
1	C	234	LYS	2.8
2	D	457	HIS	2.8
2	D	276	ARG	2.8
2	D	464	LEU	2.7
2	B	503	HIS	2.7
2	D	512	ARG	2.7
2	D	196	LEU	2.7
2	D	480	VAL	2.6
2	B	199	GLU	2.6
2	B	273	TRP	2.6
2	D	213	PRO	2.6
2	B	209	ASP	2.6
2	D	278	PRO	2.6
1	C	83	ARG	2.6
2	D	358	ALA	2.6
2	B	215	ALA	2.6
2	D	202	ALA	2.5
1	C	245	VAL	2.5
2	D	265	TYR	2.5
2	B	337	GLY	2.5
2	B	10	GLU	2.4
1	A	83	ARG	2.4
2	D	495	GLU	2.4
2	B	277	LYS	2.4
2	D	258	LEU	2.4
2	B	550	ALA	2.4
2	D	10	GLU	2.4
2	B	175	ILE	2.3
2	D	239	SER	2.3
1	A	227	GLU	2.3
1	C	289	GLU	2.3
2	B	211	ALA	2.3
2	B	169	THR	2.3
2	B	264	ARG	2.2
2	D	424	PRO	2.2
2	B	164	LYS	2.2
1	A	85	GLY	2.2
2	B	494	GLU	2.2
2	D	503	HIS	2.2
1	C	228	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	538	LEU	2.2
2	D	497	GLU	2.2
2	D	285	ALA	2.1
1	A	87	VAL	2.1
1	C	246	LEU	2.1
2	B	499	GLU	2.0
2	D	494	GLU	2.0
2	D	4	SER	2.0
2	D	246	SER	2.0
1	C	226	SER	2.0
1	A	10	GLY	2.0
2	D	498	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

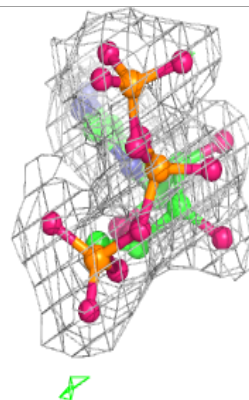
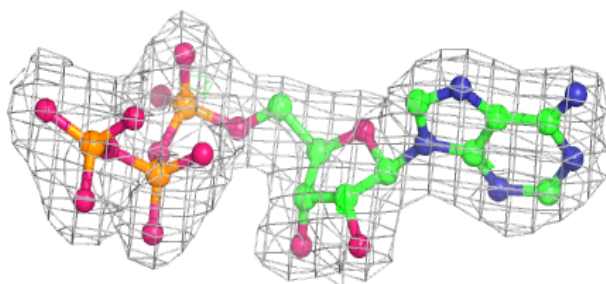
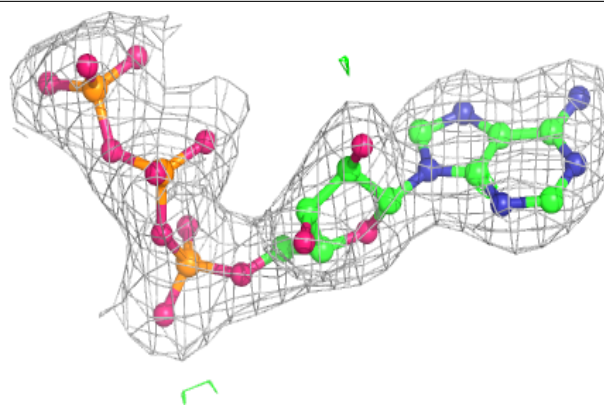
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	641	1/1	0.95	0.07	33,33,33,33	0
3	MG	B	641	1/1	0.98	0.03	35,35,35,35	0
5	ATP	B	802	31/31	0.99	0.09	25,29,31,31	0
5	ATP	D	801	31/31	0.99	0.07	18,23,29,30	0
4	ZN	B	642	1/1	1.00	0.07	26,26,26,26	0
4	ZN	D	642	1/1	1.00	0.07	31,31,31,31	0

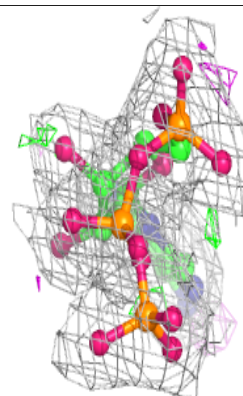
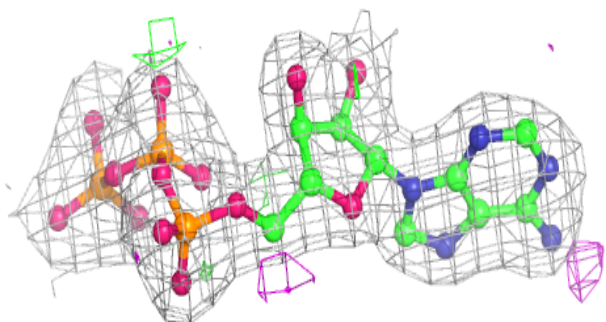
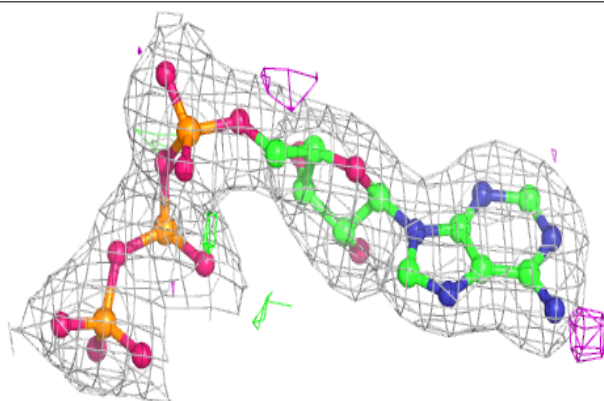
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 802:**

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

**Electron density around ATP D 801:**

$2mF_o-DF_c$  (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.