



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:35 pm BST

PDB ID : 6P8V  
Title : Structure of E. coli MS115-1 HORMA:CdnC:Trip13 complex  
Authors : Ye, Q.; Corbett, K.D.  
Deposited on : 2019-06-08  
Resolution : 2.64 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

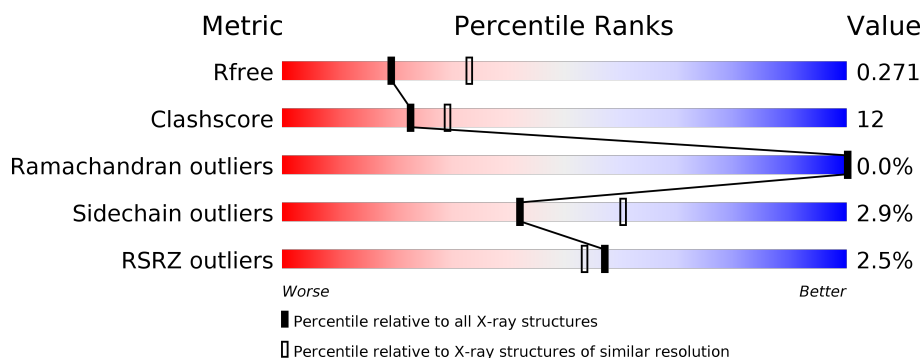
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	311	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	B	311	<div> <div>68%</div> <div>28%</div> <div>• •</div> </div>
1	C	311	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>•</div> </div>
1	D	311	<div> <div>3%</div> <div>66%</div> <div>31%</div> <div>•</div> </div>
1	E	311	<div> <div>4%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>
1	F	311	<div> <div>7%</div> <div>56%</div> <div>28%</div> <div>• 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	321	<div><div></div><div>84%</div><div>15%</div></div>
3	H	174	<div><div>2%</div><div></div><div>76%</div><div>20%</div><div>••</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 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 ATPase, AAA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2325	1465	421	434	1	4			
1	B	302	Total	C	N	O	S	Se	0	0	0
			2344	1477	425	437	1	4			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2352	1481	426	440	1	4			
1	D	303	Total	C	N	O	S	Se	0	0	0
			2352	1481	426	440	1	4			
1	E	298	Total	C	N	O	S	Se	0	0	0
			2308	1452	419	432	1	4			
1	F	270	Total	C	N	O	S	Se	0	0	0
			2092	1325	372	391	1	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP D7Y2H4
A	159	GLN	GLU	engineered mutation	UNP D7Y2H4
B	1	MSE	-	expression tag	UNP D7Y2H4
B	159	GLN	GLU	engineered mutation	UNP D7Y2H4
C	1	MSE	-	expression tag	UNP D7Y2H4
C	159	GLN	GLU	engineered mutation	UNP D7Y2H4
D	1	MSE	-	expression tag	UNP D7Y2H4
D	159	GLN	GLU	engineered mutation	UNP D7Y2H4
E	1	MSE	-	expression tag	UNP D7Y2H4
E	159	GLN	GLU	engineered mutation	UNP D7Y2H4
F	1	MSE	-	expression tag	UNP D7Y2H4
F	159	GLN	GLU	engineered mutation	UNP D7Y2H4

- Molecule 2 is a protein called E. coli MS115-1 CdnC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	320	Total	C	N	O	Se	0	0	0
			2550	1632	438	476	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MSE	-	expression tag	UNP D7Y2H2

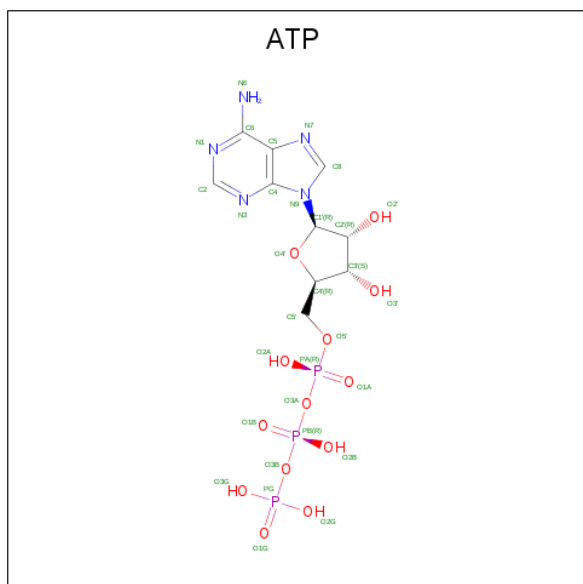
- Molecule 3 is a protein called E. coli MS115-1 HORMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	170	Total	C	N	O	Se	0	0	0
			1337	840	228	266	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	expression tag	UNP A0A1X1LKT4
H	0	ASN	-	expression tag	UNP A0A1X1LKT4
H	1	ALA	-	expression tag	UNP A0A1X1LKT4

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

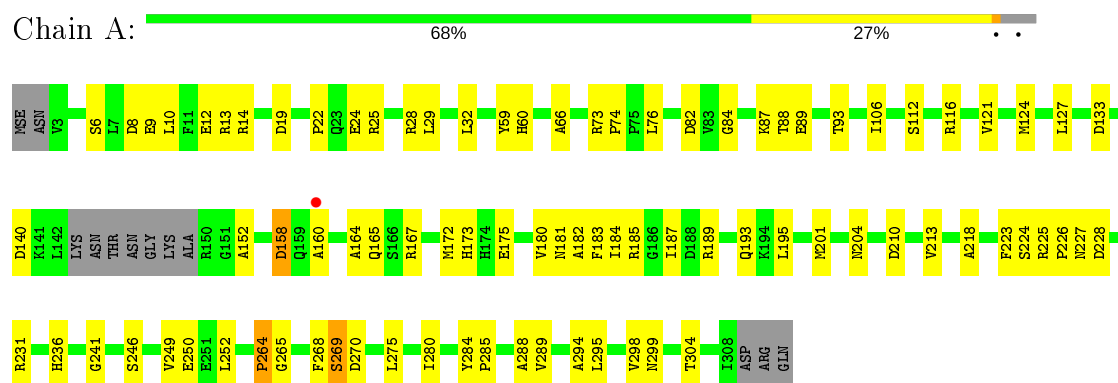
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		

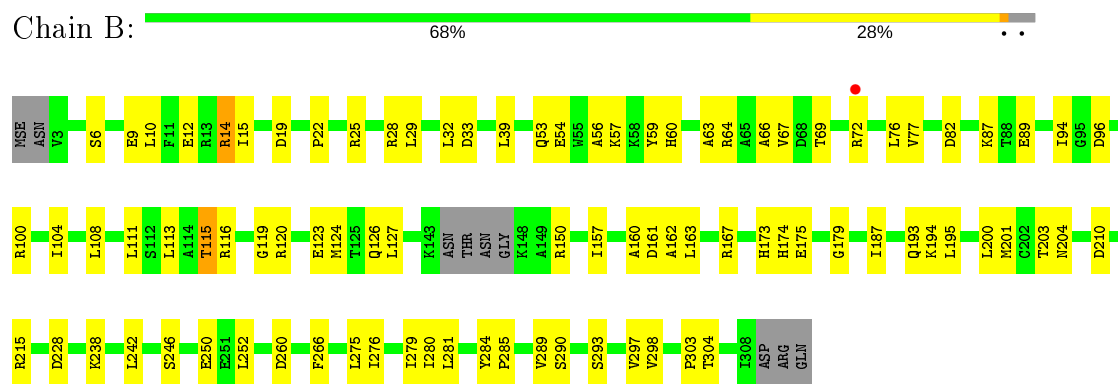
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

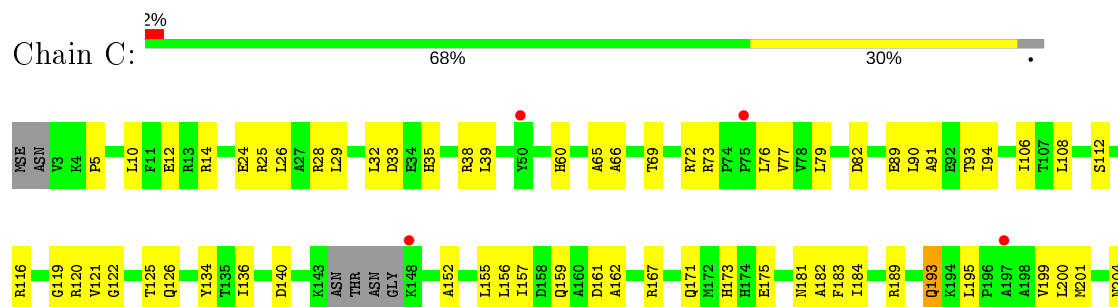
- Molecule 1: ATPase, AAA family



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- Molecule 1: ATPase, AAA family

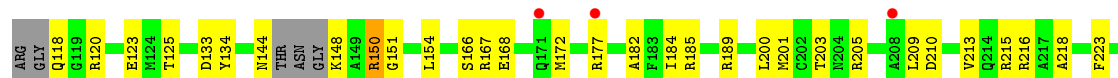
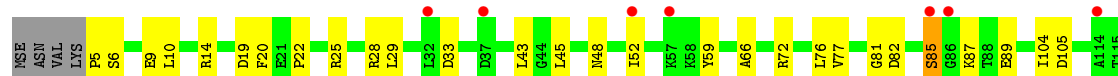




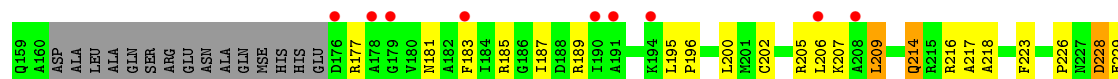
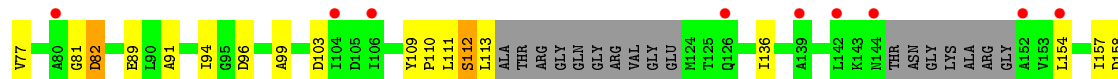
- Molecule 1: ATPase, AAA family



- Molecule 1: ATPase, AAA family




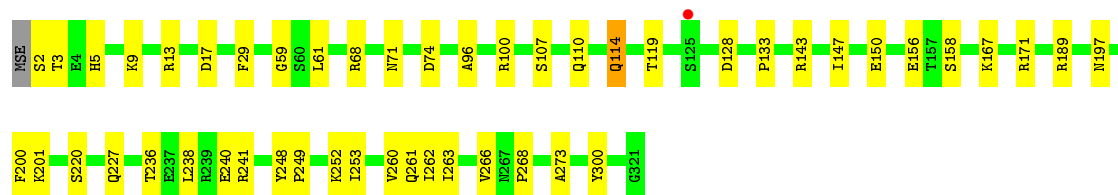
- Molecule 1: ATPase, AAA family






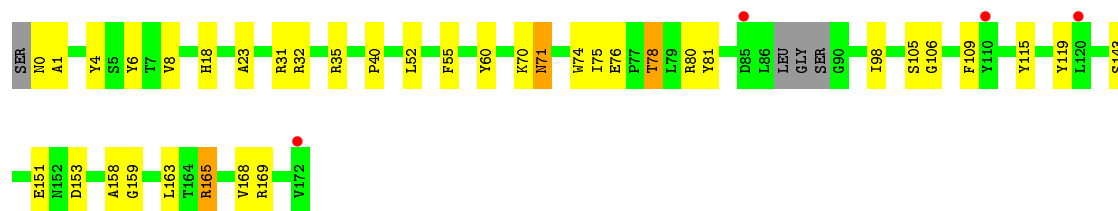
- Molecule 2: E. coli MS115-1 CdnC

Chain G:  84% 15%



- Molecule 3: E. coli MS115-1 HORMA

Chain H:  2% 76% 20% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.79Å 138.52Å 100.21Å 90.00° 98.18° 90.00°	Depositor
Resolution (Å)	88.88 – 2.64 99.19 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.1 (88.88-2.64) 99.1 (99.19-2.64)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.233 , 0.271 0.233 , 0.271	Depositor DCC
$R_{free}$ test set	3478 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

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	0.26	0/2362	0.43	0/3201
1	B	0.26	0/2381	0.44	0/3226
1	C	0.26	0/2389	0.43	0/3237
1	D	0.27	0/2389	0.43	0/3237
1	E	0.26	0/2343	0.44	0/3173
1	F	0.27	0/2125	0.43	0/2884
2	G	0.26	0/2605	0.43	0/3524
3	H	0.28	0/1363	0.47	0/1837
All	All	0.26	0/17957	0.44	0/24319

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	2325	0	2361	59	0
1	B	2344	0	2380	68	1
1	C	2352	0	2385	81	0
1	D	2352	0	2385	78	0
1	E	2308	0	2340	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2092	0	2125	74	0
2	G	2550	0	2536	36	1
3	H	1337	0	1279	23	0
4	B	62	0	24	5	0
4	C	31	0	12	0	0
4	D	31	0	12	4	0
4	G	31	0	12	2	0
5	G	1	0	0	0	0
All	All	17816	0	17851	410	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 12.

All (410) 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:C:277:PRO:HG2	1:D:73:ARG:HD3	1.46	0.94
1:A:289:VAL:H	1:B:60:HIS:HE1	1.24	0.85
1:B:275:LEU:HD11	1:B:298:VAL:HG22	1.61	0.81
1:D:280:ILE:HD11	1:E:66:ALA:HB1	1.62	0.80
1:A:275:LEU:HD11	1:A:298:VAL:HG22	1.62	0.80
1:A:133:ASP:OD1	1:A:189:ARG:NH1	2.16	0.77
1:A:280:ILE:HD11	1:B:66:ALA:HB1	1.67	0.77
1:F:275:LEU:HD11	1:F:298:VAL:HG22	1.66	0.77
1:C:25:ARG:NH1	1:C:89:GLU:OE2	2.18	0.76
2:G:114:GLN:NE2	2:G:119:THR:OG1	2.19	0.76
1:C:108:LEU:HD11	1:C:156:LEU:HB2	1.68	0.74
1:B:25:ARG:NH1	1:B:89:GLU:OE2	2.21	0.73
1:D:158:ASP:OD2	1:E:185:ARG:NH1	2.22	0.72
1:E:290:SER:HB3	1:E:293:SER:HB3	1.71	0.72
1:E:150:ARG:HH12	2:G:197:ASN:H	1.35	0.72
1:B:252:LEU:HD22	1:B:298:VAL:HG21	1.69	0.72
1:A:167:ARG:NH1	1:A:181:ASN:OD1	2.22	0.71
1:A:66:ALA:HB1	1:F:280:ILE:HD11	1.71	0.71
1:E:150:ARG:NH1	2:G:197:ASN:H	1.87	0.71
1:A:204:ASN:HD22	1:B:167:ARG:HH22	1.39	0.71
1:C:225:ARG:NH1	1:C:265:GLY:O	2.24	0.70
1:C:5:PRO:O	1:C:134:TYR:OH	2.09	0.70
1:C:252:LEU:HD22	1:C:298:VAL:HG21	1.74	0.70
1:D:122:GLY:N	1:D:175:GLU:OE2	2.19	0.69
1:C:106:ILE:HG12	1:C:152:ALA:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:HH12	1:C:122:GLY:HA2	1.59	0.68
1:B:289:VAL:H	1:C:60:HIS:CE1	2.12	0.68
1:A:289:VAL:H	1:B:60:HIS:CE1	2.11	0.68
1:D:96:ASP:OD1	1:D:100:ARG:NH1	2.26	0.68
1:B:162:ALA:HB2	1:C:181:ASN:HD22	1.59	0.68
1:A:76:LEU:HD11	1:A:201:MSE:HE3	1.76	0.67
1:D:133:ASP:OD1	1:D:189:ARG:NH2	2.26	0.67
1:F:260:ASP:N	1:F:260:ASP:OD1	2.26	0.67
4:B:402:ATP:O1G	1:C:216:ARG:NH2	2.27	0.67
1:F:205:ARG:HE	1:F:207:LYS:HE3	1.58	0.67
1:A:165:GLN:OE1	1:B:174:HIS:ND1	2.26	0.67
1:A:241:GLY:HA3	1:B:63:ALA:HB2	1.78	0.66
1:E:167:ARG:HG3	1:E:210:ASP:OD2	1.95	0.66
1:C:204:ASN:HD22	1:D:167:ARG:HH22	1.44	0.65
1:A:8:ASP:OD1	1:A:14:ARG:NH2	2.27	0.65
1:B:289:VAL:H	1:C:60:HIS:HE1	1.43	0.65
1:B:56:ALA:HB2	1:B:67:VAL:HG11	1.79	0.64
1:B:173:HIS:CD2	1:B:175:GLU:H	2.15	0.64
1:E:82:ASP:O	1:E:85:SER:OG	2.14	0.64
1:E:172:MSE:HE3	1:E:177:ARG:HG2	1.78	0.64
1:E:81:GLY:HA3	1:E:223:PHE:HB2	1.80	0.64
1:B:167:ARG:NH1	1:B:210:ASP:OD2	2.31	0.63
1:E:295:LEU:O	1:E:299:ASN:ND2	2.32	0.63
1:F:25:ARG:HD2	1:F:89:GLU:OE2	1.97	0.63
1:F:181:ASN:HB3	1:F:185:ARG:HE	1.62	0.63
1:E:105:ASP:OD2	2:G:189:ARG:NH1	2.31	0.63
1:A:210:ASP:HB3	1:A:213:VAL:HG23	1.80	0.63
1:E:167:ARG:HG2	1:E:172:MSE:HE2	1.81	0.63
1:F:39:LEU:HG	1:F:94:ILE:HG12	1.81	0.63
1:B:173:HIS:HD2	1:B:175:GLU:H	1.46	0.62
1:F:111:LEU:HD23	1:F:157:ILE:HG23	1.80	0.62
1:F:54:GLU:HG2	1:F:58:LYS:HE3	1.81	0.62
1:A:76:LEU:HD22	1:A:187:ILE:HD13	1.82	0.62
1:D:251:GLU:OE2	1:D:254:ARG:HD3	1.99	0.62
1:D:116:ARG:HA	1:D:124:MSE:HG3	1.82	0.62
1:A:295:LEU:O	1:A:299:ASN:ND2	2.33	0.62
1:A:173:HIS:HD2	1:A:175:GLU:H	1.47	0.61
1:B:120:ARG:NH2	1:B:126:GLN:OE1	2.33	0.61
1:D:161:ASP:OD1	1:D:203:THR:OG1	2.17	0.60
1:D:269:SER:OG	1:E:215:ARG:NH1	2.34	0.60
1:A:160:ALA:HB2	1:A:201:MSE:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASP:HB3	1:C:213:VAL:HG23	1.83	0.60
1:C:73:ARG:NH2	1:C:218:ALA:O	2.35	0.60
3:H:18:HIS:HB3	3:H:158:ALA:HB1	1.83	0.60
1:C:76:LEU:HD13	1:C:201:MSE:HE3	1.84	0.60
1:B:57:LYS:HG2	1:B:64:ARG:HH22	1.67	0.59
1:B:160:ALA:HB3	1:B:203:THR:HB	1.84	0.59
1:C:193:GLN:HB2	1:C:195:LEU:HG	1.84	0.59
1:F:181:ASN:HD22	1:F:185:ARG:HH21	1.50	0.59
1:A:164:ALA:HA	1:A:180:VAL:HG22	1.85	0.59
1:B:15:ILE:HD12	1:B:108:LEU:HD23	1.84	0.59
1:F:246:SER:O	1:F:250:GLU:HG2	2.02	0.59
1:D:173:HIS:HD2	1:D:175:GLU:H	1.50	0.59
1:C:12:GLU:HG3	1:C:112:SER:HB2	1.85	0.59
1:F:45:LEU:HD22	1:F:52:ILE:HB	1.84	0.58
1:D:25:ARG:NH1	1:D:89:GLU:OE1	2.37	0.58
1:D:76:LEU:HD11	1:D:201:MSE:HE3	1.84	0.58
1:F:295:LEU:O	1:F:299:ASN:ND2	2.37	0.58
1:C:125:THR:HG23	1:C:182:ALA:HB2	1.84	0.58
1:A:183:PHE:HE2	1:A:201:MSE:HE1	1.69	0.57
1:C:167:ARG:HD3	1:C:210:ASP:OD2	2.03	0.57
1:F:30:VAL:HG12	1:F:229:GLU:HB3	1.86	0.57
1:F:183:PHE:CZ	1:F:187:ILE:HD11	2.39	0.57
2:G:107:SER:HB2	2:G:110:GLN:HG3	1.86	0.57
1:C:28:ARG:NH1	1:D:72:ARG:HH12	2.02	0.57
1:B:281:LEU:CB	1:C:38:ARG:HH12	2.18	0.57
1:E:252:LEU:HD22	1:E:298:VAL:HG21	1.86	0.57
1:A:270:ASP:OD1	1:A:304:THR:OG1	2.23	0.56
1:B:116:ARG:NH1	1:C:122:GLY:HA2	2.19	0.56
2:G:9:LYS:O	2:G:13:ARG:HG3	2.05	0.56
1:D:281:LEU:HD22	1:E:45:LEU:HD13	1.87	0.56
1:F:111:LEU:HB3	1:F:157:ILE:HA	1.87	0.56
1:E:120:ARG:HB2	1:E:123:GLU:HG3	1.87	0.56
1:B:281:LEU:HB3	1:C:38:ARG:HH12	1.71	0.56
1:B:279:ILE:HG12	1:B:297:VAL:HG11	1.86	0.56
1:E:246:SER:O	1:E:250:GLU:HG2	2.06	0.56
1:D:275:LEU:HD11	1:D:298:VAL:HG22	1.88	0.56
1:F:292:HIS:NE2	1:F:296:GLN:OE1	2.39	0.55
1:B:124:MSE:HE2	1:B:179:GLY:HA3	1.88	0.55
1:E:48:ASN:HD21	1:E:148:LYS:HE2	1.70	0.55
1:C:24:GLU:O	1:C:28:ARG:HG3	2.07	0.55
1:C:295:LEU:O	1:C:299:ASN:ND2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:O	1:D:218:ALA:N	2.37	0.54
1:B:157:ILE:HD12	1:B:201:MSE:HE2	1.89	0.54
1:D:125:THR:HG23	1:D:182:ALA:HB2	1.90	0.54
1:B:304:THR:HG21	1:C:215:ARG:HA	1.88	0.54
1:A:6:SER:HB2	1:A:9:GLU:HG3	1.88	0.54
1:F:20:PHE:O	1:F:24:GLU:HG2	2.08	0.54
1:F:228:ASP:N	1:F:228:ASP:OD1	2.41	0.54
1:A:25:ARG:HB2	1:A:93:THR:HG21	1.90	0.53
1:D:252:LEU:CD2	1:D:298:VAL:HG21	2.37	0.53
1:E:104:ILE:HG13	1:E:151:GLY:HA2	1.90	0.53
1:D:296:GLN:HG3	1:D:300:LYS:HE3	1.90	0.53
1:F:74:PRO:O	1:F:218:ALA:HB2	2.08	0.53
1:B:157:ILE:HG23	1:B:163:LEU:HD12	1.90	0.53
1:F:77:VAL:HB	1:F:200:LEU:HD23	1.89	0.53
3:H:81:TYR:HB3	3:H:163:LEU:HD22	1.91	0.53
1:E:201:MSE:HE1	1:E:213:VAL:HG11	1.91	0.52
1:C:161:ASP:OD1	1:D:181:ASN:ND2	2.40	0.52
2:G:201:LYS:NZ	4:G:401:ATP:HN61	2.07	0.52
1:B:10:LEU:HD21	1:B:127:LEU:HD22	1.92	0.52
1:D:183:PHE:CZ	1:D:201:MSE:HE1	2.45	0.52
1:F:136:ILE:HG23	1:F:195:LEU:HD11	1.90	0.52
3:H:71:ASN:N	3:H:71:ASN:OD1	2.42	0.52
1:A:228:ASP:OD1	1:A:231:ARG:NH2	2.43	0.52
1:A:225:ARG:NH1	1:A:265:GLY:O	2.33	0.52
1:F:46:LEU:HD13	1:F:75:PRO:HA	1.91	0.52
1:D:25:ARG:NH1	1:E:72:ARG:HH22	2.08	0.51
1:F:195:LEU:HD23	1:F:196:PRO:HD2	1.91	0.51
1:D:225:ARG:NH1	1:D:265:GLY:O	2.44	0.51
1:D:294:ALA:O	1:D:298:VAL:HG23	2.10	0.51
1:B:28:ARG:NH1	1:C:72:ARG:HH22	2.08	0.51
1:E:28:ARG:NH2	1:F:72:ARG:HB3	2.25	0.51
2:G:253:ILE:HD12	2:G:263:ILE:HG13	1.91	0.51
1:D:42:ILE:O	1:D:46:LEU:HG	2.10	0.51
2:G:158:SER:H	2:G:266:VAL:HG11	1.74	0.51
1:F:17:PHE:HB3	1:F:96:ASP:HA	1.93	0.51
1:A:106:ILE:HG12	1:A:152:ALA:HB3	1.92	0.51
4:D:401:ATP:O2G	4:D:401:ATP:O1B	2.27	0.51
1:A:165:GLN:HB3	1:A:172:MSE:HE1	1.93	0.51
1:A:73:ARG:HH12	1:F:281:LEU:HD11	1.76	0.51
1:B:12:GLU:CD	1:C:189:ARG:HH22	2.15	0.51
1:D:88:THR:OG1	4:D:401:ATP:O3G	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:LEU:HD22	1:F:32:LEU:HD12	1.93	0.51
1:F:50:TYR:HD1	1:F:50:TYR:H	1.57	0.51
2:G:114:GLN:HE22	2:G:119:THR:HG1	1.58	0.50
1:C:184:ILE:HD11	1:C:213:VAL:HG22	1.94	0.50
1:C:275:LEU:HD11	1:C:298:VAL:HG22	1.93	0.50
1:A:288:ALA:HB2	1:B:59:TYR:CD1	2.46	0.50
3:H:76:GLU:OE1	3:H:169:ARG:NH1	2.45	0.50
1:A:173:HIS:CD2	1:A:175:GLU:H	2.27	0.50
1:B:242:LEU:HD22	1:B:289:VAL:HG21	1.93	0.50
1:F:74:PRO:HB2	1:F:216:ARG:O	2.12	0.50
1:B:54:GLU:HA	1:B:57:LYS:HE3	1.94	0.50
2:G:241:ARG:HD2	2:G:253:ILE:HD13	1.94	0.50
1:B:280:ILE:HD11	1:C:66:ALA:HB1	1.93	0.50
1:C:119:GLY:HA2	1:D:121:VAL:HG22	1.94	0.50
1:C:122:GLY:O	1:C:126:GLN:HG2	2.12	0.50
1:C:173:HIS:HD2	1:C:175:GLU:HG2	1.77	0.49
2:G:300:TYR:CE2	3:H:31:ARG:HD2	2.47	0.49
1:D:19:ASP:OD1	1:D:20:PHE:N	2.45	0.49
1:A:74:PRO:O	1:A:218:ALA:HB2	2.12	0.49
1:E:249:VAL:O	1:E:253:VAL:HG23	2.13	0.49
1:D:89:GLU:OE2	1:E:72:ARG:NH1	2.45	0.49
1:E:280:ILE:HD11	1:F:66:ALA:HB1	1.93	0.49
1:B:19:ASP:HB3	1:B:22:PRO:HD2	1.94	0.49
1:D:120:ARG:HB2	1:D:123:GLU:HB2	1.94	0.49
1:D:273:GLN:OE1	1:E:215:ARG:NH1	2.45	0.49
1:F:16:ASN:O	1:F:19:ASP:HB2	2.11	0.49
1:D:249:VAL:O	1:D:253:VAL:HG23	2.11	0.49
1:A:88:THR:HG23	1:A:158:ASP:OD1	2.12	0.49
1:A:246:SER:O	1:A:250:GLU:HG2	2.12	0.49
1:B:77:VAL:HB	1:B:200:LEU:HD23	1.93	0.49
1:F:19:ASP:HB3	1:F:22:PRO:CD	2.43	0.49
1:A:182:ALA:HA	1:A:185:ARG:HE	1.78	0.49
1:C:76:LEU:CD1	1:C:201:MSE:HE3	2.42	0.49
1:F:206:LEU:O	1:F:209:LEU:HD22	2.13	0.49
1:D:25:ARG:HB2	1:D:93:THR:HG21	1.93	0.48
1:F:205:ARG:NE	1:F:207:LYS:HE3	2.26	0.48
1:C:26:LEU:HD12	1:C:93:THR:O	2.13	0.48
1:A:82:ASP:OD2	1:A:224:SER:HA	2.13	0.48
1:D:84:GLY:N	4:D:401:ATP:O1B	2.43	0.48
1:E:5:PRO:O	1:E:134:TYR:OH	2.18	0.48
1:F:252:LEU:HD23	1:F:298:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:NH2	1:D:175:GLU:OE2	2.45	0.48
1:C:173:HIS:HD2	1:C:175:GLU:H	1.61	0.48
1:B:6:SER:HB2	1:B:9:GLU:HG3	1.95	0.48
1:B:76:LEU:HD22	1:B:187:ILE:HD13	1.96	0.48
1:D:87:LYS:HG2	1:D:223:PHE:CD1	2.48	0.48
1:D:113:LEU:HD12	1:E:182:ALA:HB2	1.95	0.48
1:E:184:ILE:HG23	1:E:216:ARG:CZ	2.43	0.48
1:E:260:ASP:HB2	1:E:261:PRO:HD2	1.94	0.48
1:F:19:ASP:C	1:F:22:PRO:HD2	2.34	0.48
1:F:249:VAL:HA	1:F:252:LEU:HD12	1.95	0.48
1:D:226:PRO:HB3	1:D:268:PHE:CZ	2.49	0.48
1:D:82:ASP:N	1:D:82:ASP:OD1	2.46	0.48
1:C:236:HIS:O	1:C:240:THR:HG23	2.13	0.48
1:E:25:ARG:NH1	1:E:89:GLU:OE2	2.46	0.48
1:F:81:GLY:HA3	1:F:223:PHE:HB2	1.96	0.48
3:H:18:HIS:CD2	3:H:159:GLY:H	2.32	0.48
1:B:96:ASP:O	1:B:100:ARG:HG3	2.14	0.47
1:F:252:LEU:CD2	1:F:298:VAL:HG21	2.44	0.47
1:C:69:THR:O	1:C:73:ARG:HG3	2.13	0.47
2:G:260:VAL:HB	2:G:273:ALA:HB1	1.96	0.47
1:A:180:VAL:O	1:A:184:ILE:HG12	2.14	0.47
1:B:82:ASP:O	1:B:87:LYS:NZ	2.48	0.47
1:B:39:LEU:HD13	1:B:94:ILE:HG12	1.97	0.47
1:D:108:LEU:HD11	1:D:156:LEU:HB2	1.96	0.47
1:F:226:PRO:HA	1:F:230:GLN:OE1	2.14	0.47
1:B:246:SER:O	1:B:250:GLU:HG3	2.15	0.47
1:E:154:LEU:HA	1:E:154:LEU:HD23	1.74	0.47
1:D:180:VAL:O	1:D:184:ILE:HG12	2.15	0.47
1:F:48:ASN:HD21	1:F:50:TYR:HB2	1.79	0.47
1:D:69:THR:O	1:D:73:ARG:HG3	2.14	0.47
3:H:23:ALA:HA	3:H:52:LEU:HD23	1.96	0.47
2:G:201:LYS:HZ3	4:G:401:ATP:HN61	1.63	0.47
3:H:74:TRP:HB3	3:H:78:THR:HG21	1.96	0.47
1:D:142:LEU:HD22	1:D:151:GLY:HA3	1.96	0.47
1:A:84:GLY:HA3	1:A:269:SER:HB3	1.97	0.47
1:F:189:ARG:NH2	2:G:17:ASP:OD1	2.43	0.47
1:A:294:ALA:O	1:A:298:VAL:HG23	2.14	0.46
1:B:111:LEU:HD11	1:B:115:THR:HG21	1.96	0.46
1:E:203:THR:HG22	1:E:205:ARG:H	1.80	0.46
1:D:288:ALA:HB2	1:E:59:TYR:CD2	2.51	0.46
1:A:193:GLN:HB2	1:A:195:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:ALA:O	1:F:298:VAL:HG23	2.16	0.46
2:G:241:ARG:HD3	2:G:261:GLN:OE1	2.15	0.46
3:H:55:PHE:CE2	3:H:115:TYR:HE1	2.33	0.46
1:D:296:GLN:HE21	1:D:300:LYS:CE	2.28	0.46
1:D:280:ILE:HG22	1:E:52:ILE:HD11	1.97	0.46
1:E:236:HIS:CD2	1:E:249:VAL:HG11	2.51	0.46
1:A:236:HIS:CE1	1:A:249:VAL:HG21	2.50	0.46
1:E:29:LEU:HD11	1:E:89:GLU:HB3	1.97	0.46
1:D:183:PHE:HZ	1:D:201:MSE:HE1	1.79	0.46
1:D:266:PHE:HZ	1:D:301:MSE:HG2	1.81	0.46
1:A:59:TYR:CD1	1:F:288:ALA:HB2	2.51	0.46
2:G:236:THR:HG23	2:G:240:GLU:HB3	1.98	0.46
1:F:17:PHE:CD1	1:F:96:ASP:HB2	2.51	0.46
1:D:296:GLN:HE21	1:D:300:LYS:HE3	1.81	0.46
1:B:120:ARG:HA	3:H:8:VAL:O	2.16	0.45
1:C:29:LEU:HD13	1:C:32:LEU:HD12	1.97	0.45
1:D:29:LEU:HD21	1:D:89:GLU:HG2	1.98	0.45
1:B:116:ARG:HH22	1:C:175:GLU:CD	2.20	0.45
1:C:277:PRO:CG	1:D:73:ARG:HD3	2.33	0.45
1:F:82:ASP:OD1	1:F:82:ASP:N	2.49	0.45
1:A:29:LEU:HD13	1:A:32:LEU:HD12	1.98	0.45
1:C:155:LEU:HB3	1:C:199:VAL:HG22	1.98	0.45
1:D:293:SER:O	1:D:297:VAL:HG12	2.16	0.45
1:F:249:VAL:O	1:F:253:VAL:HG23	2.17	0.45
1:E:77:VAL:HG23	1:E:200:LEU:HD23	1.99	0.45
1:C:136:ILE:HG23	1:C:195:LEU:HD11	1.97	0.45
2:G:59:GLY:HA3	2:G:74:ASP:HB2	1.99	0.45
3:H:60:TYR:CG	3:H:119:TYR:HD1	2.35	0.45
1:E:292:HIS:O	1:E:296:GLN:HG2	2.17	0.45
1:C:274:ARG:HH21	1:C:301:MSE:HG3	1.82	0.45
1:C:171:GLN:NE2	1:D:172:MSE:O	2.50	0.45
1:F:43:LEU:O	1:F:47:VAL:HG22	2.17	0.45
1:E:20:PHE:CE1	2:G:68:ARG:HG3	2.52	0.45
1:B:119:GLY:HA2	1:C:121:VAL:HG12	1.99	0.44
1:C:173:HIS:CD2	1:C:175:GLU:HG2	2.52	0.44
1:C:304:THR:HG21	1:D:215:ARG:HB3	1.98	0.44
2:G:248:TYR:CE2	2:G:268:PRO:HB3	2.52	0.44
1:C:79:LEU:HD12	1:C:91:ALA:HB2	1.99	0.44
2:G:249:PRO:HD2	2:G:252:LYS:HD2	2.00	0.44
3:H:80:ARG:O	3:H:165:ARG:HA	2.17	0.44
3:H:81:TYR:CD2	3:H:165:ARG:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:HA	1:A:195:LEU:HD22	2.00	0.44
2:G:133:PRO:HG2	2:G:147:ILE:HG13	2.00	0.44
1:C:288:ALA:HB2	1:D:59:TYR:HD1	1.81	0.44
1:B:53:GLN:O	1:B:57:LYS:HG3	2.18	0.44
1:A:252:LEU:HD22	1:A:298:VAL:HG21	1.99	0.44
1:B:293:SER:O	1:B:297:VAL:HG12	2.16	0.44
1:C:276:ILE:HB	1:C:277:PRO:HD3	2.00	0.44
1:D:12:GLU:HG3	1:D:112:SER:HB3	1.99	0.44
1:C:65:ALA:O	1:C:69:THR:HG23	2.18	0.44
1:D:193:GLN:HB2	1:D:195:LEU:HG	1.99	0.44
1:A:24:GLU:O	1:A:28:ARG:HG3	2.17	0.44
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.86	0.44
1:B:204:ASN:HD22	1:C:167:ARG:HH22	1.66	0.44
1:F:41:LYS:O	1:F:45:LEU:HG	2.18	0.44
1:C:24:GLU:HG3	1:C:28:ARG:HE	1.82	0.44
1:D:29:LEU:HA	4:D:401:ATP:C2	2.53	0.44
1:A:76:LEU:O	1:A:218:ALA:N	2.48	0.43
1:C:226:PRO:HB3	1:C:268:PHE:CE1	2.52	0.43
1:A:19:ASP:HB3	1:A:22:PRO:HD2	1.99	0.43
1:C:270:ASP:OD2	1:C:304:THR:HG23	2.18	0.43
1:E:6:SER:HB2	1:E:9:GLU:HG3	2.00	0.43
2:G:29:PHE:HB2	2:G:61:LEU:HD21	2.00	0.43
3:H:32:ARG:HB2	3:H:98:ILE:HD12	2.00	0.43
1:B:14:ARG:HD3	1:B:14:ARG:N	2.33	0.43
1:C:10:LEU:HD12	1:C:134:TYR:HE2	1.83	0.43
1:F:19:ASP:HB3	1:F:22:PRO:HD2	1.99	0.43
1:D:106:ILE:HG12	1:D:152:ALA:HB3	2.00	0.43
1:E:235:LEU:HD12	1:E:253:VAL:HG22	2.00	0.43
1:F:12:GLU:CD	1:F:109:TYR:HB3	2.39	0.43
1:F:205:ARG:HD2	1:F:205:ARG:HA	1.87	0.43
1:F:158:ASP:O	1:F:202:CYS:HB2	2.18	0.43
1:F:209:LEU:HD21	1:F:214:GLN:OE1	2.19	0.43
3:H:105:SER:OG	3:H:106:GLY:N	2.49	0.43
1:E:203:THR:HG22	1:E:205:ARG:N	2.33	0.43
2:G:150:GLU:OE2	2:G:201:LYS:HE3	2.19	0.43
1:C:249:VAL:O	1:C:253:VAL:HG23	2.18	0.43
1:A:10:LEU:HD21	1:A:127:LEU:HD22	2.01	0.43
1:C:157:ILE:HD13	1:C:183:PHE:CZ	2.54	0.43
1:F:76:LEU:HB3	1:F:217:ALA:HA	2.00	0.43
1:E:150:ARG:HH12	2:G:197:ASN:N	2.08	0.43
1:C:77:VAL:HG22	1:C:200:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD21	1:A:89:GLU:HG2	2.01	0.42
1:D:116:ARG:HD3	1:E:125:THR:HG21	2.00	0.42
1:D:201:MSE:HE2	1:D:201:MSE:HB3	1.82	0.42
1:E:166:SER:HA	1:E:210:ASP:HB2	2.00	0.42
1:E:87:LYS:NZ	1:E:203:THR:O	2.52	0.42
1:A:227:ASN:O	1:A:231:ARG:HG3	2.19	0.42
1:B:28:ARG:CZ	1:C:72:ARG:HH22	2.31	0.42
1:C:76:LEU:O	1:C:218:ALA:N	2.52	0.42
1:F:13:ARG:O	1:F:110:PRO:HD2	2.18	0.42
1:E:284:TYR:HE2	1:F:52:ILE:HA	1.83	0.42
2:G:29:PHE:CB	2:G:61:LEU:HD21	2.49	0.42
1:C:173:HIS:CE1	3:H:4:TYR:HA	2.54	0.42
1:F:112:SER:OG	1:F:113:LEU:N	2.53	0.42
1:F:12:GLU:HB3	1:F:110:PRO:O	2.20	0.42
1:B:25:ARG:HA	1:B:28:ARG:HD2	2.00	0.42
1:D:19:ASP:HB3	1:D:22:PRO:HD2	2.00	0.42
1:F:234:LEU:HD11	1:F:268:PHE:HE1	1.85	0.42
3:H:70:LYS:HE3	3:H:75:ILE:HD13	2.02	0.42
1:E:133:ASP:OD1	1:E:189:ARG:NH2	2.51	0.42
1:F:154:LEU:HD23	1:F:154:LEU:HA	1.86	0.42
1:F:76:LEU:O	1:F:218:ALA:N	2.48	0.42
1:F:99:ALA:O	1:F:103:ASP:N	2.53	0.42
1:B:266:PHE:HA	1:B:303:PRO:HB3	2.01	0.42
1:B:29:LEU:HD13	1:B:32:LEU:HD12	2.02	0.42
1:B:89:GLU:HB2	4:B:402:ATP:O2A	2.19	0.42
1:C:120:ARG:HG3	3:H:6:TYR:CZ	2.54	0.42
1:C:39:LEU:HG	1:C:94:ILE:HG12	2.01	0.42
1:A:19:ASP:HB3	1:A:22:PRO:CD	2.50	0.42
1:B:281:LEU:HD11	1:C:73:ARG:HH12	1.85	0.42
1:D:47:VAL:CG2	1:D:102:GLU:HG3	2.50	0.42
1:D:50:TYR:HD1	1:D:53:GLN:OE1	2.03	0.42
2:G:114:GLN:HE21	2:G:114:GLN:HB2	1.61	0.42
2:G:262:ILE:HD12	2:G:273:ALA:HB2	2.01	0.42
1:A:12:GLU:HG3	1:A:112:SER:HB2	2.01	0.41
1:A:284:TYR:HA	1:A:285:PRO:HA	1.81	0.41
1:E:76:LEU:O	1:E:218:ALA:N	2.52	0.41
1:B:194:LYS:HA	1:B:194:LYS:HD3	1.93	0.41
1:C:116:ARG:HB3	1:C:116:ARG:HE	1.34	0.41
1:D:238:LYS:HB3	1:D:276:ILE:HD13	2.02	0.41
2:G:143:ARG:HD3	2:G:156:GLU:OE1	2.19	0.41
2:G:2:SER:N	2:G:5:HIS:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:ASN:OD1	2:G:71:ASN:N	2.51	0.41
1:A:87:LYS:HG2	1:A:223:PHE:CD1	2.55	0.41
1:E:19:ASP:O	1:E:22:PRO:HD2	2.21	0.41
3:H:78:THR:OG1	3:H:168:VAL:HB	2.20	0.41
1:C:121:VAL:HG23	1:C:175:GLU:OE2	2.20	0.41
1:C:162:ALA:HB2	1:D:181:ASN:HD22	1.85	0.41
1:D:206:LEU:HD12	1:D:209:LEU:HD12	2.03	0.41
1:F:242:LEU:HB3	1:F:289:VAL:HG21	2.01	0.41
2:G:227:GLN:HG2	3:H:35:ARG:CZ	2.51	0.41
1:C:288:ALA:HB2	1:D:59:TYR:CD1	2.55	0.41
1:D:288:ALA:HB2	1:E:59:TYR:HD2	1.85	0.41
1:A:60:HIS:CE1	1:F:289:VAL:HG22	2.55	0.41
1:F:91:ALA:O	1:F:94:ILE:HG22	2.20	0.41
2:G:236:THR:HG22	2:G:238:LEU:H	1.85	0.41
1:B:193:GLN:HB2	1:B:195:LEU:HG	2.02	0.41
1:B:238:LYS:HB3	1:B:276:ILE:HD13	2.03	0.41
1:D:21:GLU:HB2	1:D:22:PRO:HD3	2.01	0.41
1:A:116:ARG:HA	1:A:124:MSE:SE	2.71	0.41
1:A:225:ARG:NH1	1:A:264:PRO:HB2	2.36	0.41
1:C:215:ARG:HG3	1:C:216:ARG:N	2.34	0.41
1:C:291:VAL:O	1:C:295:LEU:HG	2.20	0.41
1:C:32:LEU:HD22	1:C:35:HIS:HD2	1.84	0.41
1:D:142:LEU:HD13	1:D:151:GLY:HA3	2.02	0.41
1:F:209:LEU:HD11	1:F:214:GLN:HB2	2.03	0.41
2:G:119:THR:CG2	2:G:128:ASP:HB3	2.50	0.41
3:H:40:PRO:HB3	3:H:109:PHE:CE2	2.56	0.41
1:B:25:ARG:HD2	1:B:89:GLU:OE2	2.20	0.41
1:B:284:TYR:CE2	1:B:285:PRO:HB3	2.56	0.41
4:B:401:ATP:O2G	4:B:401:ATP:O1B	2.38	0.41
1:E:209:LEU:HA	1:E:209:LEU:HD23	1.93	0.41
1:E:273:GLN:O	1:F:73:ARG:NH2	2.53	0.41
2:G:167:LYS:O	2:G:171:ARG:HG3	2.21	0.41
1:B:173:HIS:HD2	1:B:175:GLU:HB2	1.85	0.41
1:B:89:GLU:N	4:B:402:ATP:O2A	2.53	0.41
1:C:159:GLN:H	1:D:185:ARG:HH21	1.68	0.41
1:D:80:ALA:O	1:D:222:THR:HA	2.21	0.41
1:F:54:GLU:HG3	1:F:57:LYS:HE2	2.03	0.41
3:H:153:ASP:N	3:H:153:ASP:OD1	2.54	0.41
1:C:32:LEU:HD13	1:C:90:LEU:HD22	2.03	0.41
1:A:226:PRO:HB3	1:A:268:PHE:CZ	2.56	0.40
1:B:120:ARG:HG3	1:B:123:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ILE:HG12	1:D:297:VAL:HG11	2.03	0.40
1:F:26:LEU:HA	1:F:26:LEU:HD23	1.94	0.40
1:A:89:GLU:N	4:B:401:ATP:O2A	2.55	0.40
1:C:284:TYR:O	1:D:41:LYS:NZ	2.37	0.40
1:E:43:LEU:HA	1:E:43:LEU:HD23	1.92	0.40
1:F:43:LEU:HA	1:F:43:LEU:HD23	1.89	0.40
1:F:50:TYR:N	1:F:50:TYR:CD1	2.90	0.40
2:G:96:ALA:O	2:G:100:ARG:HG3	2.21	0.40
3:H:0:ASN:HB3	3:H:1:ALA:H	1.46	0.40
1:A:22:PRO:HA	1:A:93:THR:HG22	2.04	0.40
1:D:284:TYR:HA	1:D:285:PRO:HA	1.90	0.40
1:E:118:GLN:HB2	1:E:123:GLU:OE2	2.21	0.40
1:E:284:TYR:O	1:F:41:LYS:NZ	2.39	0.40
1:B:290:SER:HB3	1:B:293:SER:HB2	2.04	0.40
1:C:284:TYR:HA	1:C:285:PRO:HA	1.90	0.40
1:E:284:TYR:HA	1:E:285:PRO:HA	1.83	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:260:ASP:OD2	2:G:252:LYS:NZ[2_555]	2.14	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/311 (95%)	290 (98%)	4 (1%)	1 (0%)	41	56
1	B	298/311 (96%)	293 (98%)	5 (2%)	0	100	100
1	C	299/311 (96%)	294 (98%)	5 (2%)	0	100	100
1	D	299/311 (96%)	294 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	292/311 (94%)	287 (98%)	5 (2%)	0	100	100
1	F	262/311 (84%)	257 (98%)	5 (2%)	0	100	100
2	G	318/321 (99%)	314 (99%)	4 (1%)	0	100	100
3	H	166/174 (95%)	158 (95%)	8 (5%)	0	100	100
All	All	2229/2361 (94%)	2187 (98%)	41 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PRO

### 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	248/253 (98%)	244 (98%)	4 (2%)	62	78
1	B	249/253 (98%)	239 (96%)	10 (4%)	31	47
1	C	250/253 (99%)	244 (98%)	6 (2%)	49	67
1	D	250/253 (99%)	246 (98%)	4 (2%)	62	78
1	E	245/253 (97%)	237 (97%)	8 (3%)	38	55
1	F	224/253 (88%)	211 (94%)	13 (6%)	20	31
2	G	276/272 (102%)	272 (99%)	4 (1%)	67	80
3	H	141/141 (100%)	136 (96%)	5 (4%)	36	53
All	All	1883/1931 (98%)	1829 (97%)	54 (3%)	42	60

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	121	VAL
1	A	158	ASP

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Mol	Chain	Res	Type
1	A	269	SER
1	B	14	ARG
1	B	33	ASP
1	B	69	THR
1	B	72	ARG
1	B	104	ILE
1	B	115	THR
1	B	150	ARG
1	B	161	ASP
1	B	215	ARG
1	B	228	ASP
1	C	14	ARG
1	C	33	ASP
1	C	82	ASP
1	C	140	ASP
1	C	193	GLN
1	C	205	ARG
1	D	14	ARG
1	D	26	LEU
1	D	82	ASP
1	D	260	ASP
1	E	10	LEU
1	E	14	ARG
1	E	33	ASP
1	E	85	SER
1	E	144	ASN
1	E	150	ARG
1	E	168	GLU
1	E	293	SER
1	F	12	GLU
1	F	37	ASP
1	F	38	ARG
1	F	50	TYR
1	F	82	ASP
1	F	112	SER
1	F	177	ARG
1	F	209	LEU
1	F	214	GLN
1	F	228	ASP
1	F	260	ASP
1	F	267	THR
1	F	290	SER

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Mol	Chain	Res	Type
2	G	3	THR
2	G	114	GLN
2	G	200	PHE
2	G	220	SER
3	H	71	ASN
3	H	78	THR
3	H	143	SER
3	H	151	GLU
3	H	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	204	ASN
1	A	236	HIS
1	B	48	ASN
1	B	60	HIS
1	B	171	GLN
1	B	173	HIS
1	B	181	ASN
1	B	204	ASN
1	C	60	HIS
1	C	171	GLN
1	C	173	HIS
1	C	181	ASN
1	C	204	ASN
1	D	23	GLN
1	D	171	GLN
1	D	173	HIS
1	D	287	ASN
1	D	296	GLN
1	E	101	GLN
1	E	165	GLN
1	E	236	HIS
1	E	299	ASN
1	F	48	ASN
1	F	101	GLN
1	F	181	ASN
1	F	232	HIS
2	G	5	HIS
2	G	114	GLN

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Mol	Chain	Res	Type
2	G	193	GLN
2	G	197	ASN

### 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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ATP	B	401	-	26,33,33	0.95	1 (3%)	31,52,52	1.71	6 (19%)
4	ATP	G	401	5	26,33,33	0.93	1 (3%)	31,52,52	1.50	5 (16%)
4	ATP	D	401	-	26,33,33	0.95	1 (3%)	31,52,52	1.49	5 (16%)
4	ATP	B	402	-	26,33,33	0.94	1 (3%)	31,52,52	1.56	5 (16%)
4	ATP	C	401	-	26,33,33	0.98	1 (3%)	31,52,52	1.53	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
4	ATP	B	401	-	-	5/18/38/38	0/3/3/3
4	ATP	G	401	5	-	5/18/38/38	0/3/3/3
4	ATP	D	401	-	-	3/18/38/38	0/3/3/3
4	ATP	B	402	-	-	4/18/38/38	0/3/3/3
4	ATP	C	401	-	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ATP	C5-C4	2.54	1.47	1.40
4	G	401	ATP	C5-C4	2.53	1.47	1.40
4	C	401	ATP	C5-C4	2.52	1.47	1.40
4	B	402	ATP	C5-C4	2.45	1.47	1.40
4	B	401	ATP	C5-C4	2.45	1.47	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ATP	PB-O3B-PG	-4.70	116.70	132.83
4	D	401	ATP	PB-O3B-PG	-3.91	119.41	132.83
4	B	402	ATP	PB-O3B-PG	-3.85	119.60	132.83
4	B	401	ATP	C3'-C2'-C1'	3.66	106.49	100.98
4	G	401	ATP	C3'-C2'-C1'	3.55	106.33	100.98
4	C	401	ATP	PB-O3B-PG	-3.47	120.91	132.83
4	C	401	ATP	PA-O3A-PB	-3.39	121.19	132.83
4	B	402	ATP	C3'-C2'-C1'	3.26	105.88	100.98
4	C	401	ATP	N3-C2-N1	-3.17	123.73	128.68
4	D	401	ATP	N3-C2-N1	-3.11	123.82	128.68
4	G	401	ATP	N3-C2-N1	-3.07	123.88	128.68
4	C	401	ATP	C4-C5-N7	-3.06	106.21	109.40
4	B	401	ATP	N3-C2-N1	-3.05	123.92	128.68
4	G	401	ATP	PB-O3B-PG	-3.02	122.47	132.83
4	B	402	ATP	PA-O3A-PB	-3.00	122.53	132.83
4	B	402	ATP	N3-C2-N1	-2.93	124.09	128.68
4	C	401	ATP	C3'-C2'-C1'	2.81	105.21	100.98
4	G	401	ATP	PA-O3A-PB	-2.79	123.25	132.83
4	B	401	ATP	PA-O3A-PB	-2.78	123.29	132.83
4	D	401	ATP	C3'-C2'-C1'	2.76	105.13	100.98
4	B	401	ATP	O3G-PG-O2G	2.70	117.96	107.64
4	B	402	ATP	C4-C5-N7	-2.70	106.58	109.40
4	G	401	ATP	C4-C5-N7	-2.70	106.59	109.40
4	D	401	ATP	PA-O3A-PB	-2.64	123.75	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ATP	C4-C5-N7	-2.62	106.67	109.40
4	B	401	ATP	C4-C5-N7	-2.38	106.92	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	ATP	C5'-O5'-PA-O2A
4	B	402	ATP	PB-O3B-PG-O2G
4	B	402	ATP	PB-O3B-PG-O3G
4	B	402	ATP	C5'-O5'-PA-O2A
4	B	402	ATP	C5'-O5'-PA-O3A
4	B	401	ATP	PB-O3B-PG-O2G
4	B	401	ATP	C5'-O5'-PA-O2A
4	B	401	ATP	C5'-O5'-PA-O3A
4	D	401	ATP	C5'-O5'-PA-O1A
4	D	401	ATP	C5'-O5'-PA-O2A
4	C	401	ATP	C5'-O5'-PA-O1A
4	G	401	ATP	C5'-O5'-PA-O3A
4	C	401	ATP	C5'-O5'-PA-O2A
4	C	401	ATP	O4'-C4'-C5'-O5'
4	G	401	ATP	PG-O3B-PB-O2B
4	B	401	ATP	PB-O3B-PG-O3G
4	D	401	ATP	C5'-O5'-PA-O3A
4	C	401	ATP	C5'-O5'-PA-O3A
4	G	401	ATP	PG-O3B-PB-O1B
4	G	401	ATP	C5'-O5'-PA-O1A
4	B	401	ATP	PB-O3B-PG-O1G

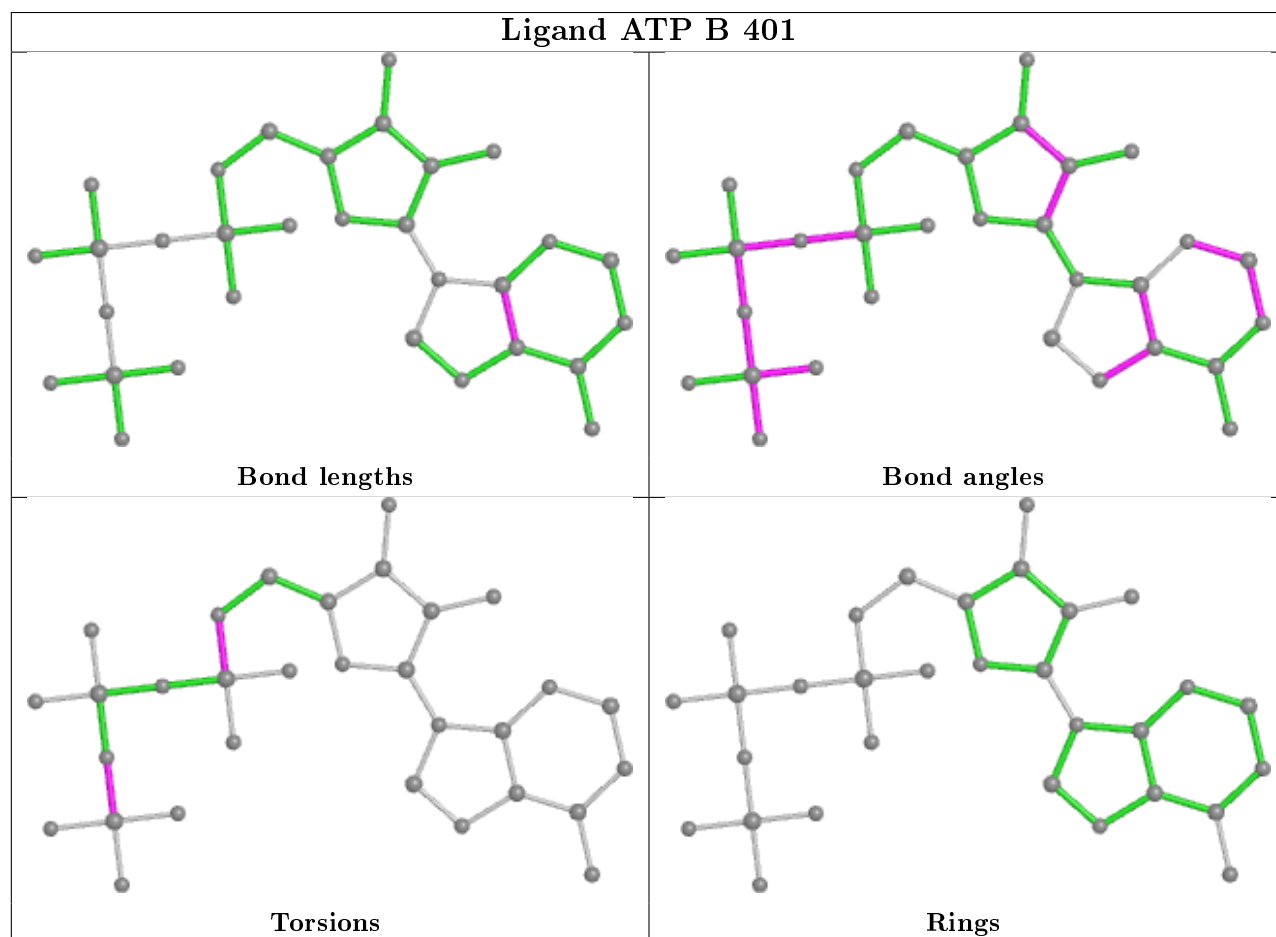
There are no ring outliers.

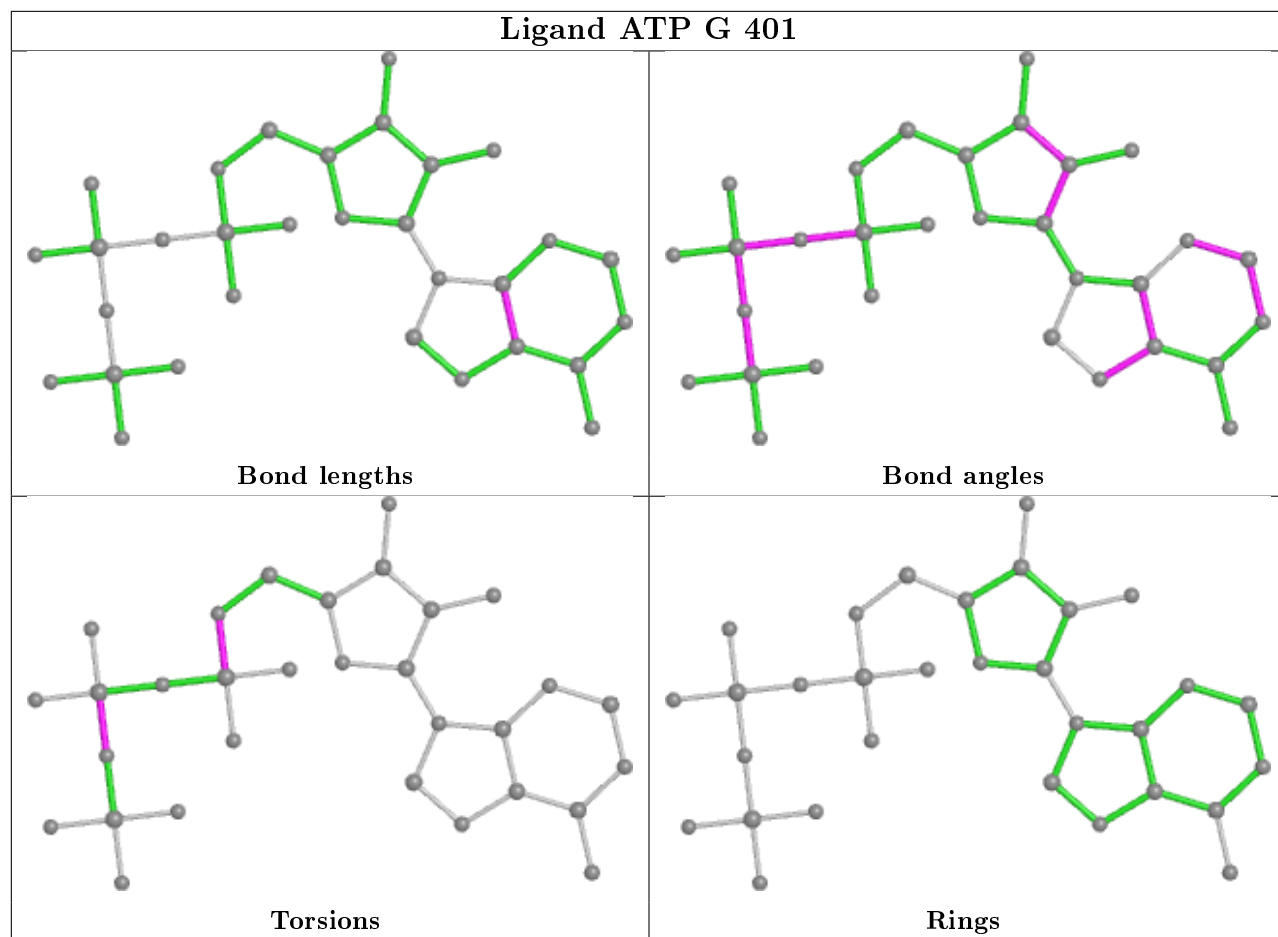
4 monomers are involved in 11 short contacts:

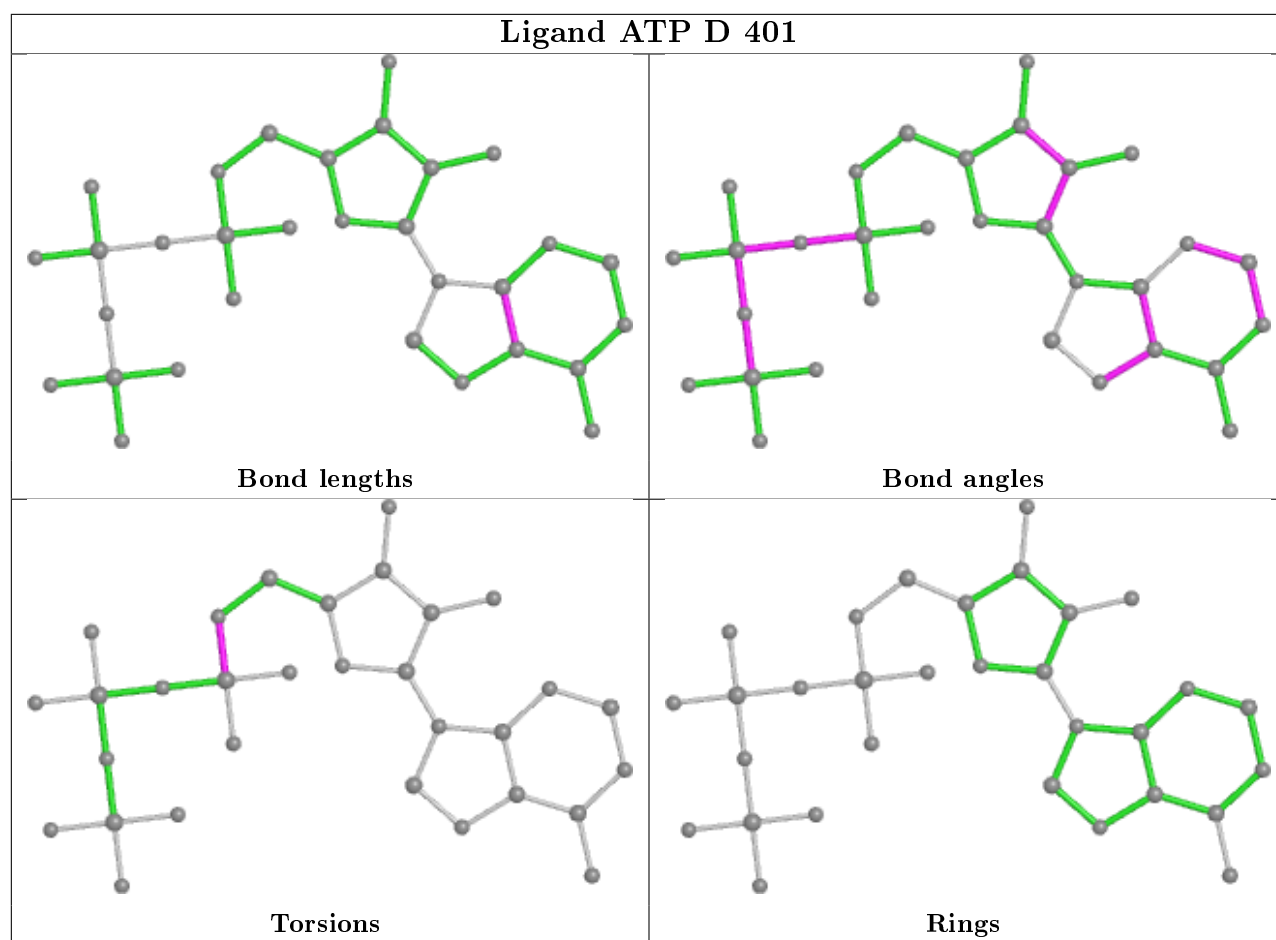
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ATP	2	0
4	G	401	ATP	2	0
4	D	401	ATP	4	0
4	B	402	ATP	3	0

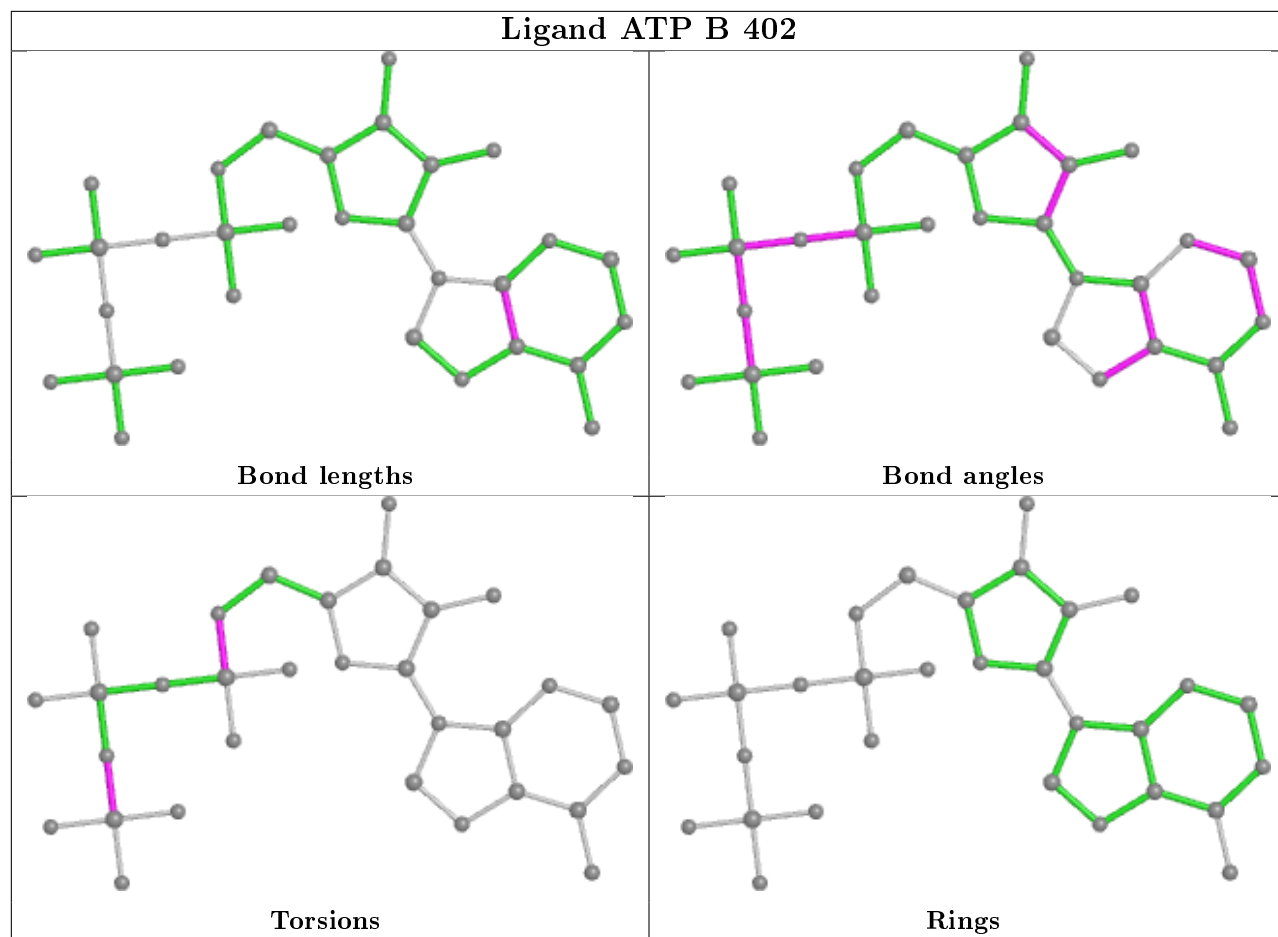
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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

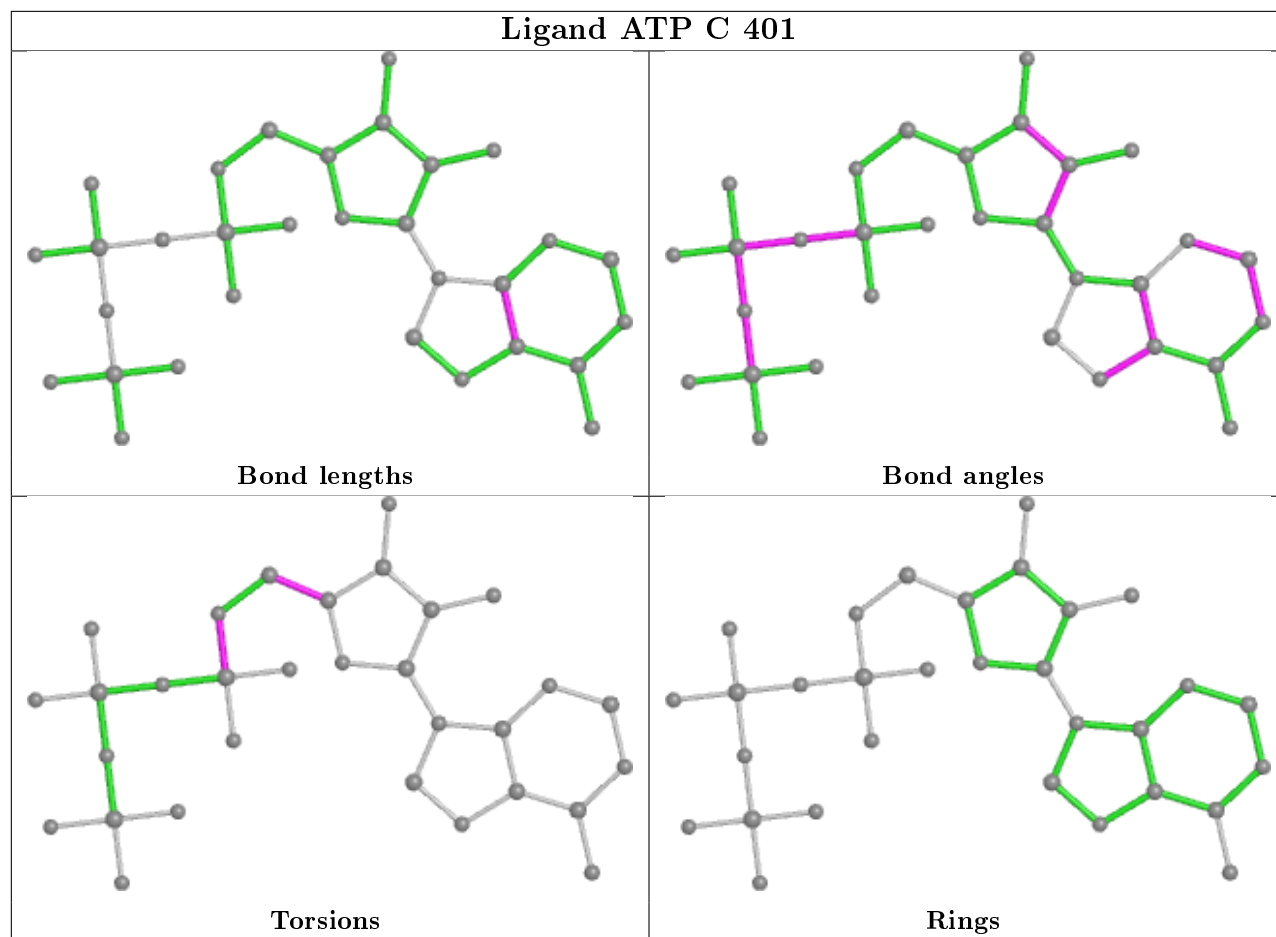












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	295/311 (94%)	0.11	1 (0%) 94 95	49, 67, 90, 111	0
1	B	298/311 (95%)	0.04	1 (0%) 94 95	43, 60, 85, 98	0
1	C	299/311 (96%)	0.15	5 (1%) 70 67	49, 69, 94, 109	0
1	D	299/311 (96%)	0.10	8 (2%) 54 50	48, 64, 94, 131	0
1	E	294/311 (94%)	0.22	12 (4%) 37 33	45, 69, 96, 117	0
1	F	267/311 (85%)	0.49	23 (8%) 10 8	56, 89, 118, 125	0
2	G	316/321 (98%)	-0.11	1 (0%) 94 95	43, 60, 83, 111	0
3	H	167/174 (95%)	0.11	4 (2%) 59 55	50, 71, 99, 115	0
All	All	2235/2361 (94%)	0.14	55 (2%) 57 53	43, 67, 101, 131	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	ALA	6.1
1	D	50	TYR	5.1
1	F	142	LEU	4.3
3	H	172	VAL	4.2
1	F	178	ALA	4.1
1	F	144	ASN	4.0
1	F	233	TYR	4.0
3	H	85	ASP	3.8
1	E	52	ILE	3.7
1	C	50	TYR	3.6
1	E	208	ALA	3.2
1	E	85	SER	3.1
3	H	120	LEU	3.1
1	D	309	ASP	3.0
1	C	197	ALA	3.0
1	E	86	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	194	LYS	2.9
1	F	154	LEU	2.9
1	F	176	ASP	2.9
1	F	80	ALA	2.8
1	F	191	ALA	2.8
1	F	206	LEU	2.7
1	C	148	LYS	2.7
1	D	294	ALA	2.7
1	F	139	ALA	2.6
1	F	126	GLN	2.6
1	E	239	LEU	2.6
1	F	152	ALA	2.6
1	F	10	LEU	2.6
1	A	160	ALA	2.5
1	E	177	ARG	2.5
1	D	151	GLY	2.5
1	D	58	LYS	2.4
2	G	125	SER	2.4
1	C	75	PRO	2.4
1	F	190	ILE	2.4
1	F	64	ARG	2.3
1	F	106	ILE	2.3
3	H	110	TYR	2.3
1	D	46	LEU	2.2
1	E	114	ALA	2.2
1	E	295	LEU	2.2
1	D	57	LYS	2.2
1	F	183	PHE	2.2
1	B	72	ARG	2.2
1	E	171	GLN	2.1
1	F	179	GLY	2.1
1	E	32	LEU	2.1
1	C	250	GLU	2.1
1	D	307	PHE	2.1
1	E	37	ASP	2.1
1	F	104	ILE	2.1
1	F	17	PHE	2.1
1	F	21	GLU	2.0
1	E	57	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

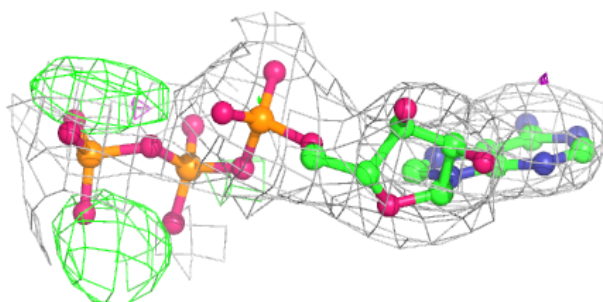
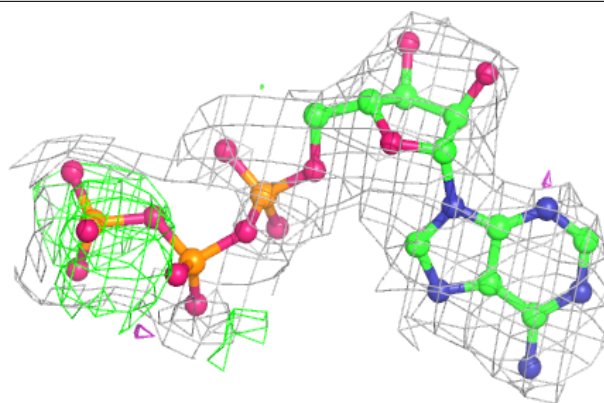
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	ATP	C	401	31/31	0.90	0.18	44,63,96,105	0
4	ATP	B	401	31/31	0.93	0.18	44,55,75,80	0
4	ATP	D	401	31/31	0.94	0.15	44,61,93,101	0
4	ATP	B	402	31/31	0.95	0.15	44,57,75,91	0
5	MG	G	402	1/1	0.96	0.20	53,53,53,53	0
4	ATP	G	401	31/31	0.96	0.14	44,56,65,70	0

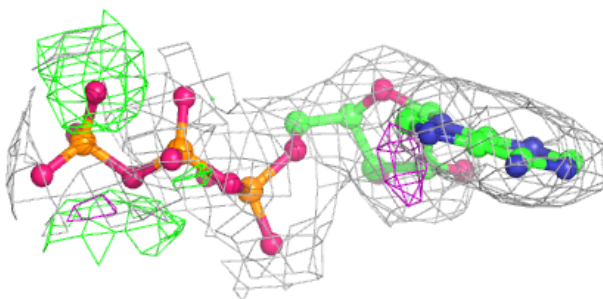
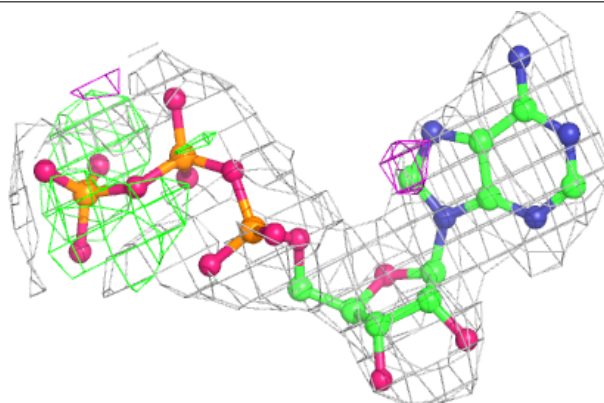
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP C 401:**

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

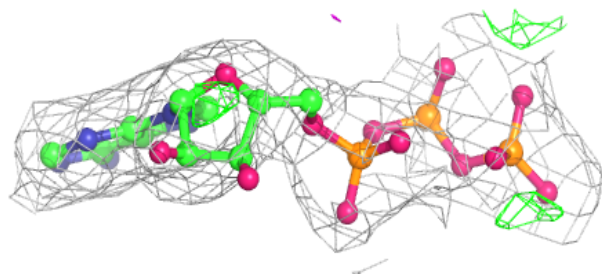
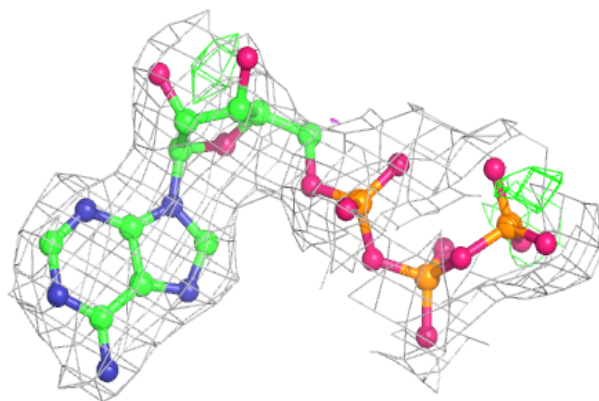
**Electron density around ATP B 401:**

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

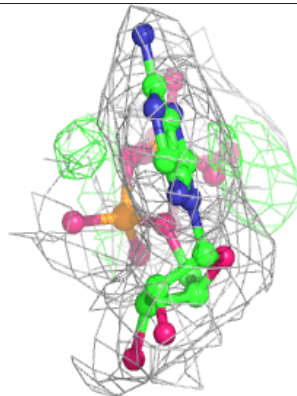
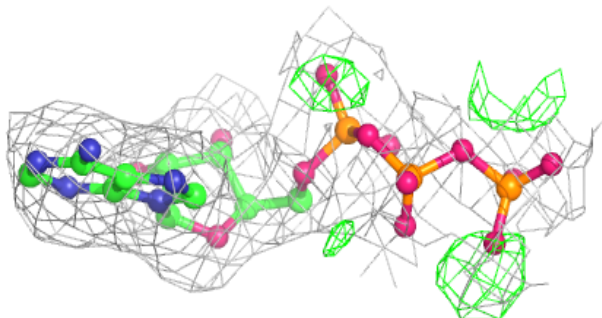
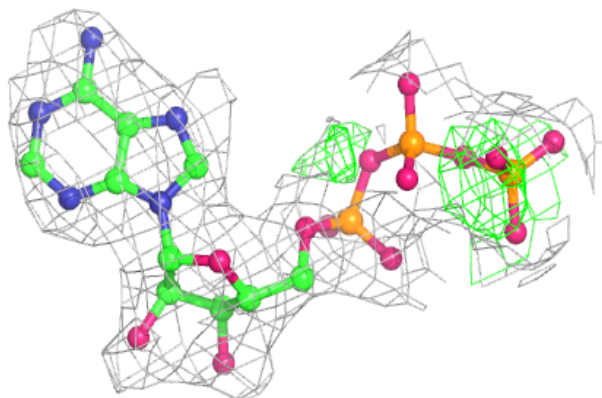


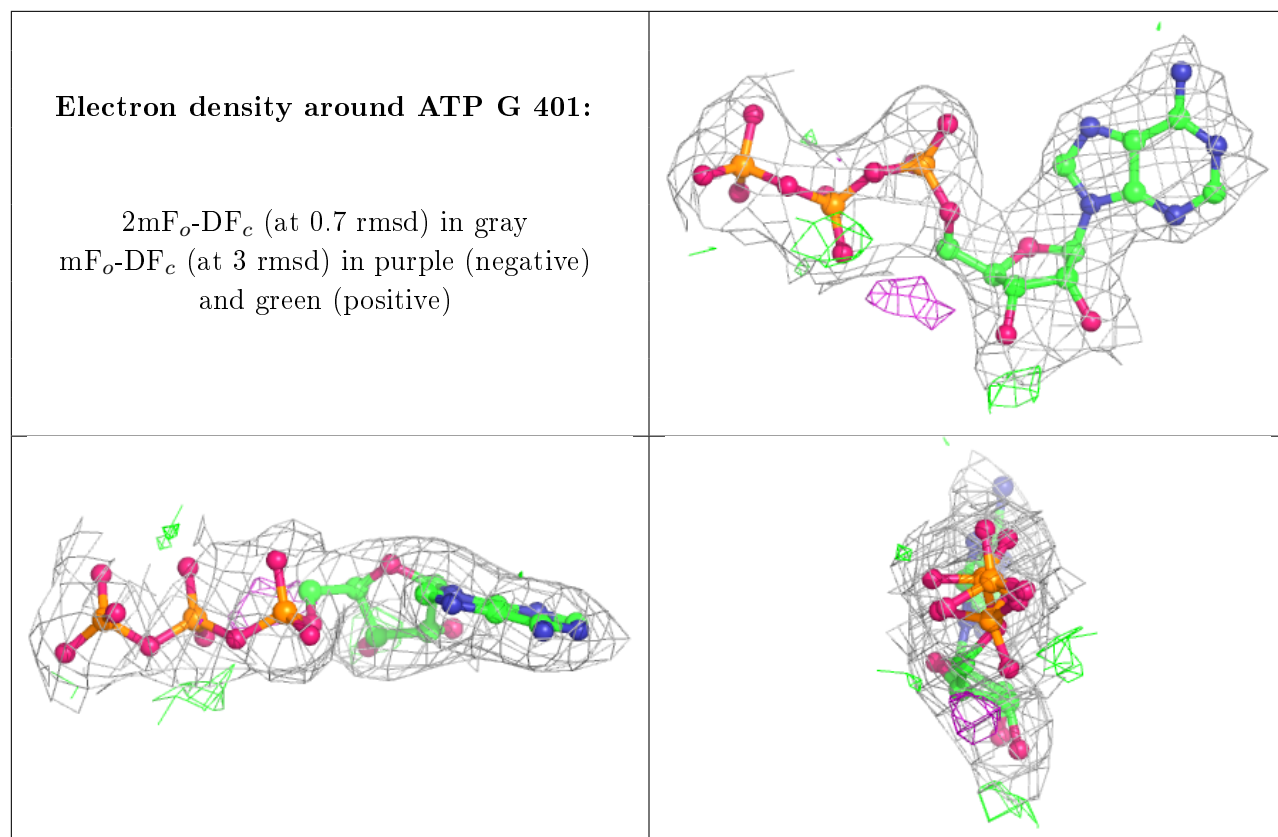
**Electron density around ATP D 401:**

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

**Electron density around ATP B 402:**

$2mF_o-DF_c$  (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.