



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:09 PM BST

PDB ID : 4EAH  
Title : Crystal structure of the formin homology 2 domain of FMNL3 bound to actin  
Authors : Thompson, M.E.; Heimsath, E.G.; Gauvin, T.J.; Higgs, H.N.; Kull, F.J.  
Deposited on : 2012-03-22  
Resolution : 3.40 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

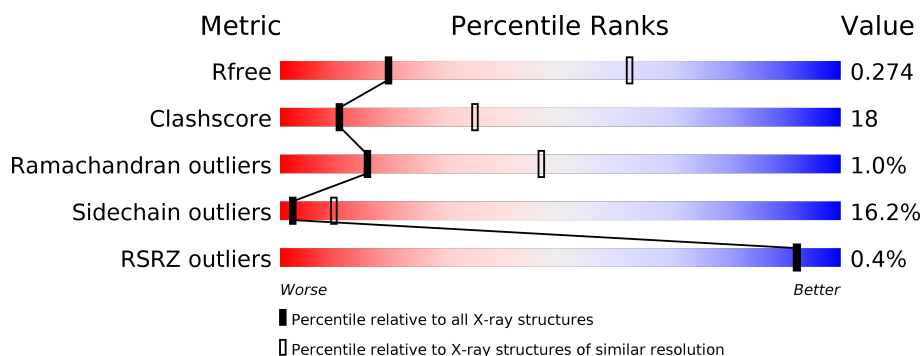
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	D	377	<div> <div></div> <div>55%33%6%6%</div> </div>
1	F	377	<div> <div>%</div> <div>55%34%6%6%</div> </div>
1	G	377	<div> <div></div> <div>54%35%5%6%</div> </div>
1	H	377	<div> <div>%</div> <div>52%37%5%6%</div> </div>
2	A	402	<div> <div></div> <div>51%30%7%11%</div> </div>
2	B	402	<div> <div></div> <div>50%30%8%11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	402	
2	E	402	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	1001	-	-	X	-
3	ACT	D	401	-	-	X	-
3	ACT	F	401	-	-	-	X
3	ACT	G	401	-	-	X	-
3	ACT	H	401	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22892 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	356	Total	C	N	O	S	121	0	0
			2785	1766	468	533	18			
1	H	356	Total	C	N	O	S	123	0	0
			2785	1766	468	533	18			
1	G	356	Total	C	N	O	S	132	0	0
			2785	1766	468	533	18			
1	F	356	Total	C	N	O	S	65	0	0
			2785	1766	468	533	18			

- Molecule 2 is a protein called Formin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	357	Total	C	N	O	S	265	0	0
			2895	1848	502	533	12			
2	E	357	Total	C	N	O	S	272	0	0
			2895	1848	502	533	12			
2	C	357	Total	C	N	O	S	252	0	0
			2895	1848	502	533	12			
2	B	357	Total	C	N	O	S	260	0	0
			2895	1848	502	533	12			

There are 8 discrepancies between the modelled and reference sequences:

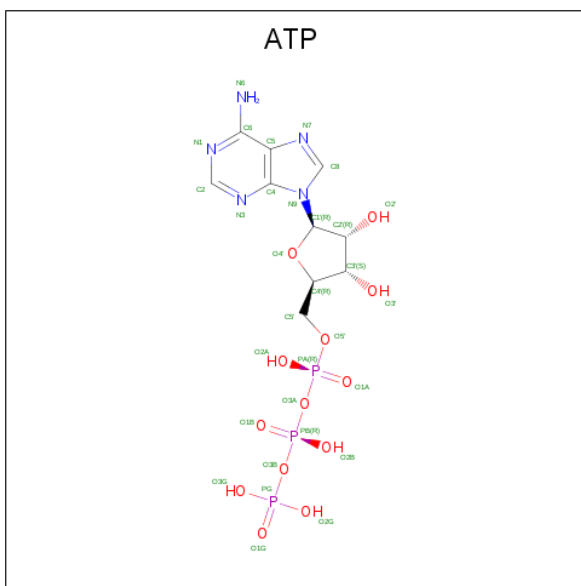
Chain	Residue	Modelled	Actual	Comment	Reference
A	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
A	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
E	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
E	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
C	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
C	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
B	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
B	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

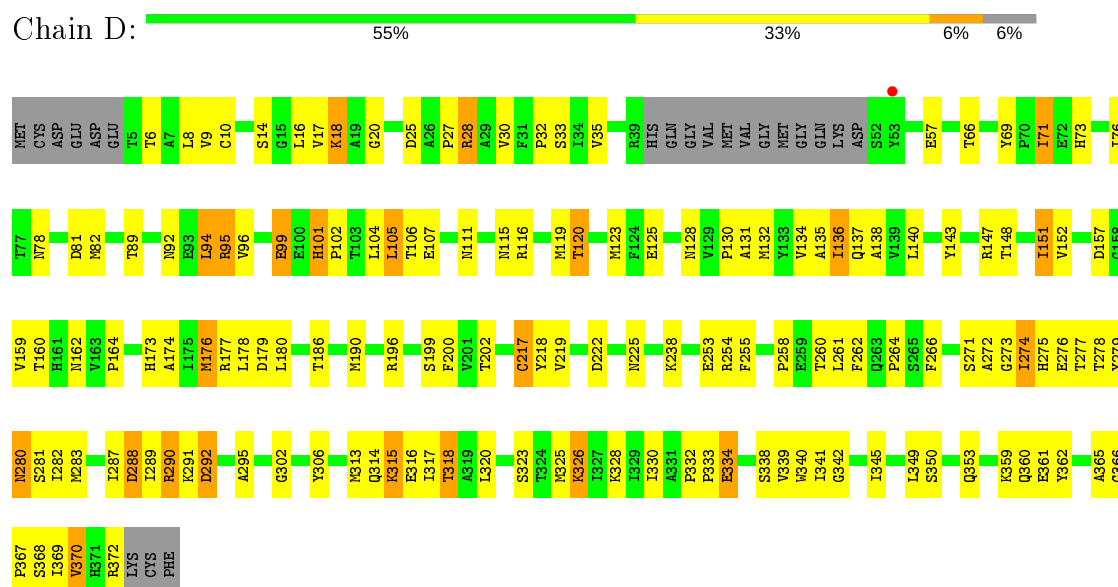
$$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3).$$


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

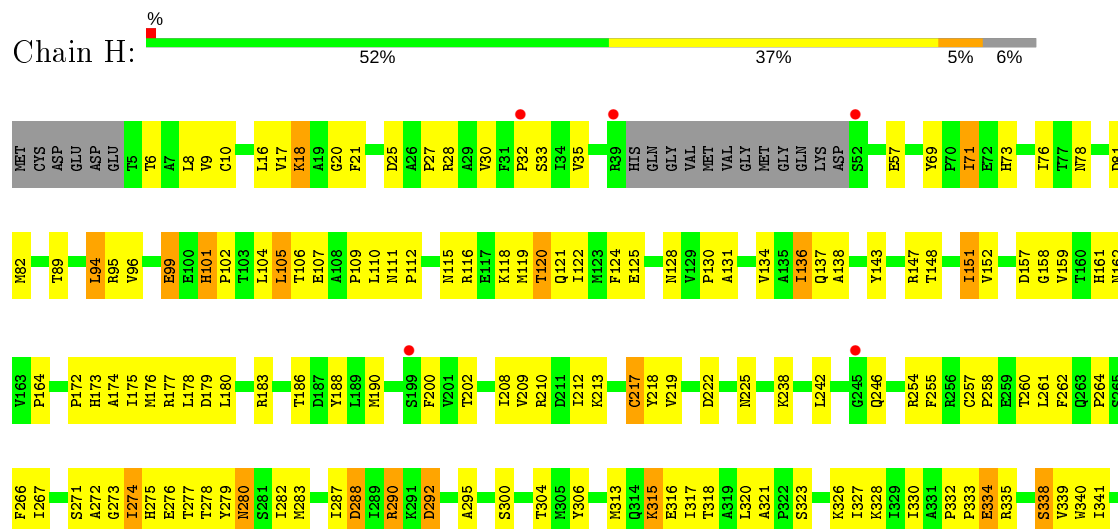
### 3 Residue-property plots

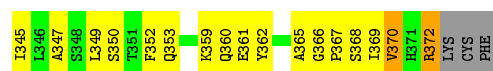
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Actin, alpha skeletal muscle



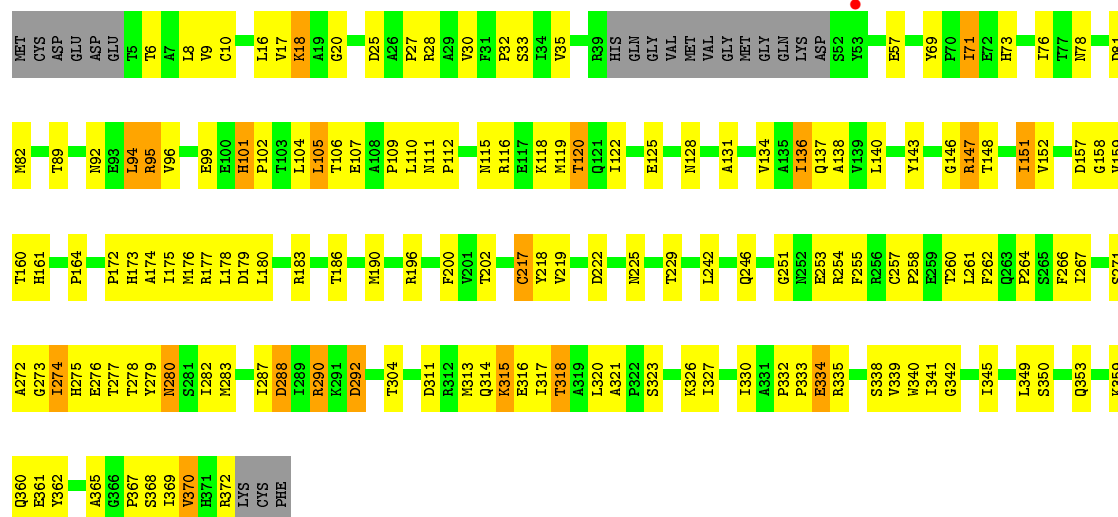
- Molecule 1: Actin, alpha skeletal muscle





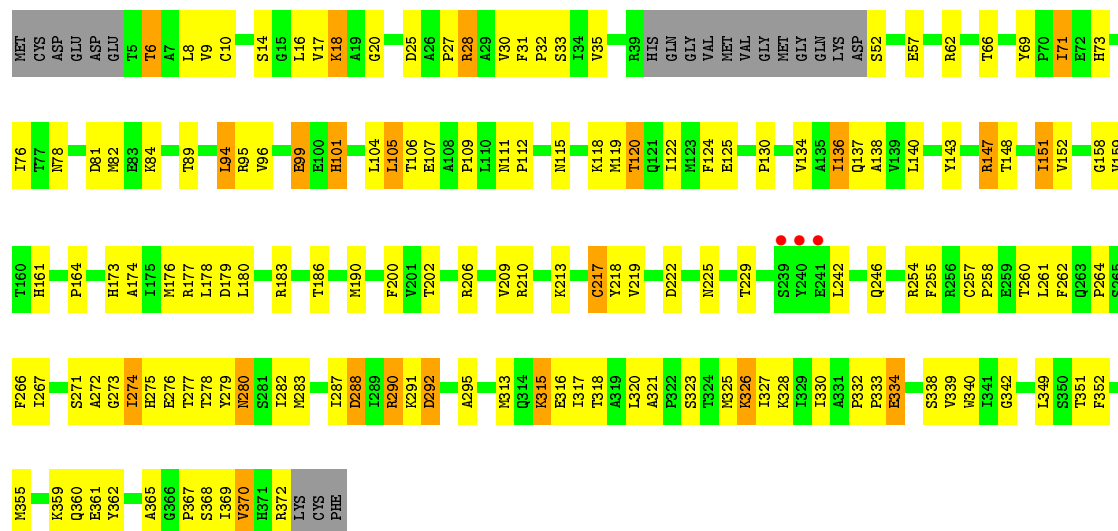
• Molecule 1: Actin, alpha skeletal muscle

Chain G: 54% 35% 5% 6%



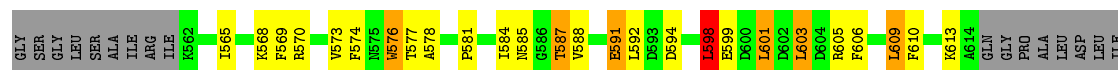
• Molecule 1: Actin, alpha skeletal muscle

Chain F: 55% 34% 6% 6%

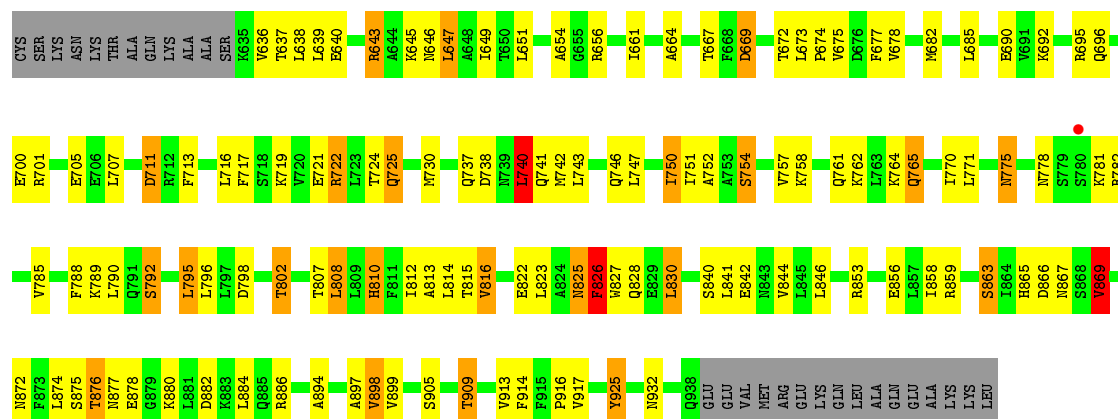


• Molecule 2: Formin-like protein 3

Chain A: 51% 30% 7% 11%

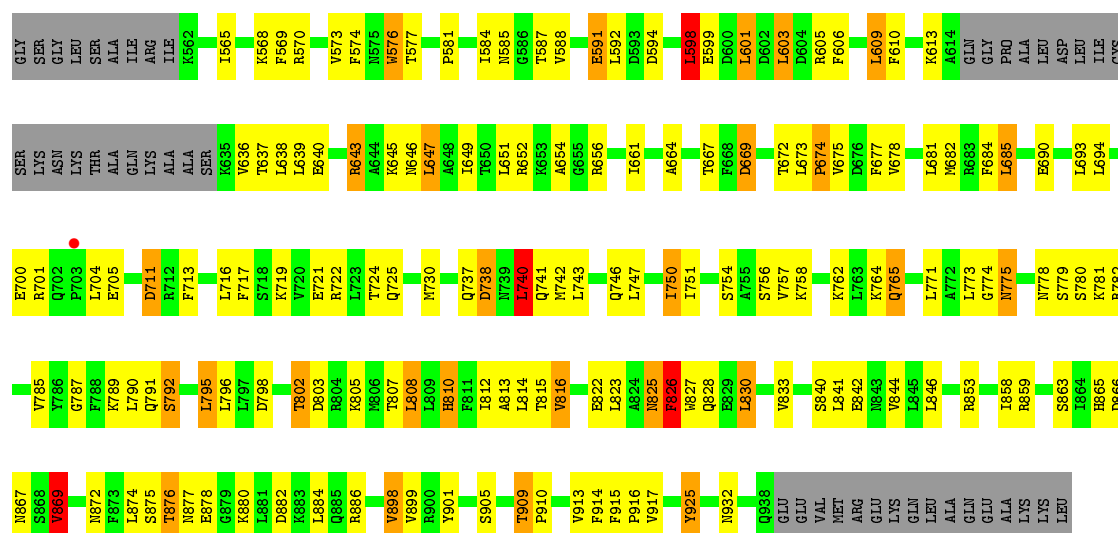






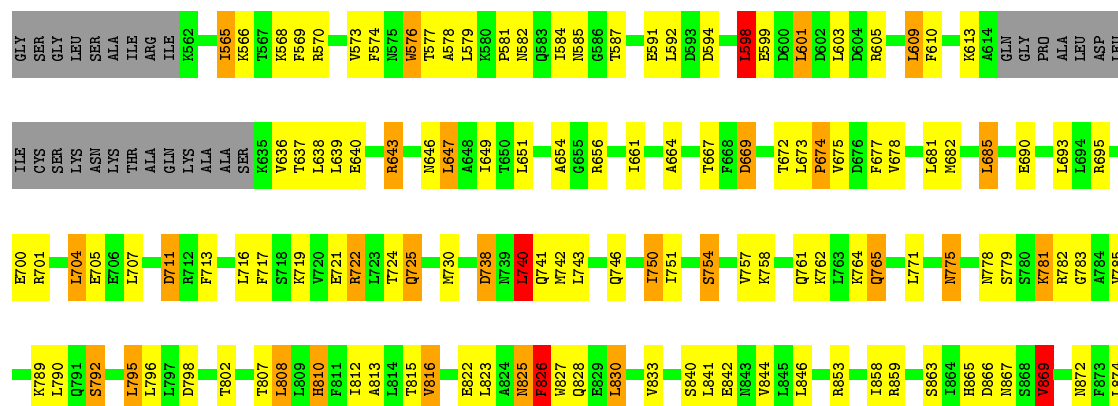
### • Molecule 2: Formin-like protein 3

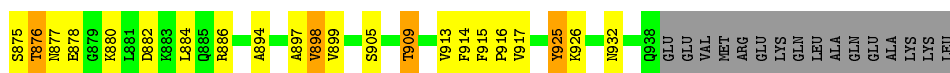
Chain E: 49% 32% 7% 11%



### • Molecule 2: Formin-like protein 3

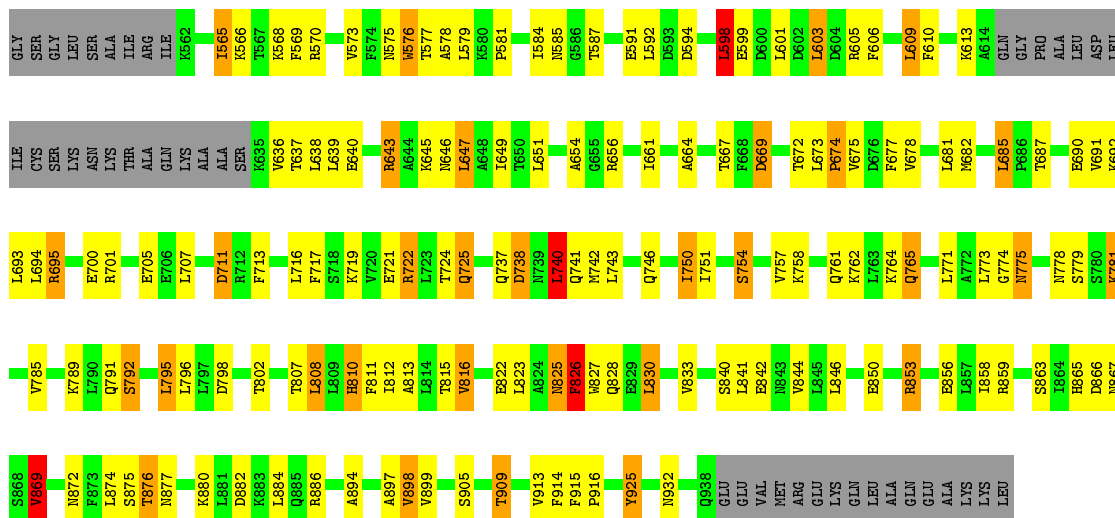
Chain C: 51% 29% 7% 11%





### • Molecule 2: Formin-like protein 3

Chain B: 50% 30% 8% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.98Å 126.05Å 129.62Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	19.82 – 3.40 19.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.82-3.40) 99.8 (19.82-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.230 , 0.277 0.225 , 0.274	Depositor DCC
$R_{free}$ test set	2894 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

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

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	D	0.51	0/2845	0.70	0/3858
1	F	0.48	0/2845	0.69	0/3858
1	G	0.48	0/2845	0.70	0/3858
1	H	0.48	0/2845	0.70	0/3858
2	A	0.48	0/2942	0.70	1/3956 (0.0%)
2	B	0.49	0/2942	0.69	1/3956 (0.0%)
2	C	0.49	0/2942	0.70	1/3956 (0.0%)
2	E	0.49	0/2942	0.70	1/3956 (0.0%)
All	All	0.49	0/23148	0.70	4/31256 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	740	LEU	CA-CB-CG	5.37	127.64	115.30
2	C	740	LEU	CA-CB-CG	5.25	127.37	115.30
2	A	740	LEU	CA-CB-CG	5.15	127.14	115.30
2	B	740	LEU	CA-CB-CG	5.07	126.96	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	D	2785	0	2758	100	1
1	F	2785	0	2758	97	1
1	G	2785	0	2758	105	0
1	H	2785	0	2758	111	0
2	A	2895	0	2971	101	0
2	B	2895	0	2971	104	0
2	C	2895	0	2971	99	0
2	E	2895	0	2971	105	0
3	A	12	0	9	1	0
3	B	4	0	3	2	0
3	C	8	0	6	2	0
3	D	4	0	3	2	0
3	E	4	0	3	1	0
3	F	8	0	6	1	0
3	G	4	0	3	2	0
3	H	4	0	3	2	0
4	D	31	0	12	5	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	H	31	0	12	2	0
All	All	22892	0	23000	776	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 18.

All (776) 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:H:147:ARG:HH12	1:H:330:ILE:HG12	1.29	0.94
1:H:261:LEU:HB3	1:H:274:ILE:HD11	1.54	0.90
1:D:261:LEU:HB3	1:D:274:ILE:HD11	1.55	0.89
1:D:147:ARG:HH12	1:D:330:ILE:HG12	1.36	0.88
1:G:261:LEU:HB3	1:G:274:ILE:HD11	1.55	0.88
1:G:137:GLN:NE2	4:G:402:ATP:O3G	2.08	0.87
1:G:147:ARG:HH12	1:G:330:ILE:HG12	1.39	0.86
1:F:147:ARG:HH12	1:F:330:ILE:HG12	1.41	0.85
1:F:261:LEU:HB3	1:F:274:ILE:HD11	1.58	0.85
1:H:137:GLN:NE2	4:H:402:ATP:O3G	2.11	0.83
2:B:746:GLN:HE22	1:H:323:SER:HB3	1.44	0.82
2:A:778:ASN:ND2	3:A:1003:ACT:O	2.14	0.81
2:A:758:LYS:HB2	2:A:898:VAL:HG13	1.62	0.81
2:E:789:LYS:O	2:E:792:SER:OG	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:789:LYS:O	2:C:792:SER:OG	2.00	0.79
2:B:807:THR:HG23	2:B:810:HIS:H	1.48	0.79
2:E:758:LYS:HB2	2:E:898:VAL:HG13	1.65	0.78
1:F:111:ASN:ND2	1:F:115:ASN:OD1	2.17	0.77
1:D:173:HIS:ND1	1:D:173:HIS:O	2.17	0.77
1:H:128:ASN:OD1	1:H:359:LYS:NZ	2.13	0.77
2:A:637:THR:HG22	2:A:639:LEU:H	1.50	0.77
2:A:789:LYS:O	2:A:792:SER:OG	2.03	0.76
2:B:789:LYS:O	2:B:792:SER:OG	2.01	0.76
2:C:758:LYS:HB2	2:C:898:VAL:HG13	1.68	0.75
1:F:173:HIS:ND1	1:F:173:HIS:O	2.19	0.75
1:H:173:HIS:O	1:H:173:HIS:ND1	2.20	0.74
2:E:765:GLN:HG2	2:E:823:LEU:HD11	1.69	0.74
1:G:173:HIS:O	1:G:173:HIS:ND1	2.19	0.74
2:B:758:LYS:HB2	2:B:898:VAL:HG13	1.70	0.74
1:G:164:PRO:HG2	1:G:174:ALA:HB1	1.69	0.73
1:D:164:PRO:HG2	1:D:174:ALA:HB1	1.69	0.73
2:C:637:THR:HG22	2:C:639:LEU:H	1.52	0.73
1:F:106:THR:HB	1:F:137:GLN:HG2	1.71	0.73
2:E:637:THR:HG22	2:E:639:LEU:H	1.54	0.73
2:E:807:THR:HG23	2:E:810:HIS:H	1.52	0.73
2:B:765:GLN:HG2	2:B:823:LEU:HD11	1.71	0.72
2:C:807:THR:HG23	2:C:810:HIS:H	1.53	0.72
2:A:765:GLN:HG2	2:A:823:LEU:HD11	1.71	0.72
1:D:106:THR:HB	1:D:137:GLN:HG2	1.71	0.72
1:G:106:THR:HB	1:G:137:GLN:HG2	1.71	0.72
2:B:637:THR:HG22	2:B:639:LEU:H	1.55	0.71
2:B:757:VAL:HA	2:B:830:LEU:HD23	1.72	0.71
2:E:598:LEU:HD12	2:E:599:GLU:H	1.55	0.71
1:F:20:GLY:HA2	1:F:94:LEU:HD21	1.70	0.71
2:C:598:LEU:HD12	2:C:599:GLU:H	1.55	0.71
1:H:164:PRO:HG2	1:H:174:ALA:HB1	1.72	0.71
2:A:807:THR:HG23	2:A:810:HIS:H	1.54	0.71
2:C:746:GLN:HE22	1:F:323:SER:HB3	1.55	0.71
1:H:106:THR:HB	1:H:137:GLN:HG2	1.71	0.71
1:G:20:GLY:HA2	1:G:94:LEU:HD21	1.73	0.71
2:B:598:LEU:HD12	2:B:599:GLU:H	1.57	0.70
1:H:20:GLY:HA2	1:H:94:LEU:HD21	1.73	0.70
2:C:757:VAL:HA	2:C:830:LEU:HD23	1.73	0.70
1:F:16:LEU:HD12	1:F:32:PRO:HA	1.73	0.70
1:H:111:ASN:ND2	1:H:115:ASN:OD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:SER:HB3	2:A:746:GLN:HE22	1.56	0.70
2:B:565:ILE:HD13	2:B:566:LYS:H	1.55	0.70
2:C:643:ARG:NH2	2:C:690:GLU:OE2	2.24	0.69
1:G:25:ASP:OD2	1:G:28:ARG:NH2	2.24	0.69
1:G:25:ASP:N	3:G:401:ACT:OXT	2.24	0.69
1:G:16:LEU:HD12	1:G:32:PRO:HA	1.74	0.69
1:G:260:THR:HG23	1:G:266:PHE:HB2	1.73	0.69
1:H:16:LEU:HD12	1:H:32:PRO:HA	1.74	0.69
2:A:598:LEU:HD12	2:A:599:GLU:H	1.55	0.69
2:B:643:ARG:NH2	2:B:690:GLU:OE2	2.26	0.69
1:D:20:GLY:HA2	1:D:94:LEU:HD21	1.73	0.69
2:E:746:GLN:HE22	1:G:323:SER:HB3	1.57	0.69
2:E:858:ILE:HG22	2:E:874:LEU:HD12	1.75	0.69
2:A:645:LYS:NZ	2:A:646:ASN:OD1	2.25	0.69
2:A:757:VAL:HA	2:A:830:LEU:HD23	1.74	0.69
1:F:260:THR:HG23	1:F:266:PHE:HB2	1.75	0.68
2:E:757:VAL:HA	2:E:830:LEU:HD23	1.73	0.68
1:F:164:PRO:HG2	1:F:174:ALA:HB1	1.75	0.68
1:D:278:THR:O	1:D:282:ILE:HD12	1.93	0.68
2:E:643:ARG:NH2	2:E:690:GLU:OE2	2.27	0.68
2:A:669:ASP:HB3	2:A:673:LEU:HB2	1.76	0.67
1:D:128:ASN:OD1	1:D:359:LYS:NZ	2.18	0.67
2:A:643:ARG:NH2	2:A:690:GLU:OE2	2.28	0.67
1:G:111:ASN:ND2	1:G:115:ASN:OD1	2.25	0.67
2:C:765:GLN:HG2	2:C:823:LEU:HD11	1.77	0.67
2:B:605:ARG:HG2	2:B:609:LEU:HD12	1.77	0.67
1:H:25:ASP:OD2	1:H:28:ARG:NH2	2.27	0.67
2:B:840:SER:N	1:H:323:SER:OG	2.20	0.67
1:D:136:ILE:H	1:D:136:ILE:HD12	1.60	0.67
1:G:128:ASN:OD1	1:G:359:LYS:NZ	2.17	0.67
1:H:217:CYS:HA	1:H:254:ARG:HG3	1.75	0.67
1:H:107:GLU:O	1:H:137:GLN:HG3	1.95	0.66
1:G:157:ASP:HB2	4:G:402:ATP:H5'1	1.77	0.66
2:A:605:ARG:HG2	2:A:609:LEU:HD12	1.77	0.66
1:G:217:CYS:HA	1:G:254:ARG:HG3	1.77	0.66
2:A:858:ILE:HG22	2:A:874:LEU:HD12	1.77	0.66
2:E:823:LEU:O	2:E:826:PHE:HB3	1.97	0.65
1:G:136:ILE:HD12	1:G:136:ILE:H	1.61	0.65
2:B:823:LEU:O	2:B:826:PHE:HB3	1.96	0.65
1:D:260:THR:HG23	1:D:266:PHE:HB2	1.79	0.64
1:D:111:ASN:ND2	1:D:115:ASN:OD1	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:HD12	1:D:32:PRO:HA	1.78	0.64
2:C:823:LEU:O	2:C:826:PHE:HB3	1.96	0.64
1:F:136:ILE:HD12	1:F:136:ILE:H	1.63	0.64
1:F:217:CYS:HA	1:F:254:ARG:HG3	1.78	0.64
1:F:25:ASP:OD2	1:F:28:ARG:NH2	2.30	0.64
1:H:136:ILE:HD12	1:H:136:ILE:H	1.62	0.64
2:C:858:ILE:HG22	2:C:874:LEU:HD12	1.79	0.64
2:E:605:ARG:HG2	2:E:609:LEU:HD12	1.79	0.64
2:C:669:ASP:HB3	2:C:673:LEU:HB2	1.79	0.64
2:C:866:ASP:N	2:C:867:ASN:OD1	2.31	0.64
1:D:25:ASP:OD2	1:D:28:ARG:NH2	2.31	0.64
2:A:823:LEU:O	2:A:826:PHE:HB3	1.98	0.64
1:H:260:THR:HG23	1:H:266:PHE:HB2	1.80	0.64
1:D:157:ASP:HB2	4:D:402:ATP:H5'1	1.79	0.63
1:H:96:VAL:HB	1:H:101:HIS:CE1	2.33	0.63
2:C:762:LYS:HB3	2:C:826:PHE:HB2	1.78	0.63
1:D:217:CYS:HA	1:D:254:ARG:HG3	1.79	0.63
2:A:654:ALA:HB2	2:A:677:PHE:CE1	2.34	0.63
2:A:762:LYS:HB3	2:A:826:PHE:HB2	1.80	0.63
1:D:25:ASP:N	3:D:401:ACT:OXT	2.32	0.63
2:E:654:ALA:HB2	2:E:677:PHE:CE1	2.33	0.63
2:E:669:ASP:HB3	2:E:673:LEU:HB2	1.81	0.63
2:A:866:ASP:N	2:A:867:ASN:OD1	2.31	0.63
2:B:866:ASP:N	2:B:867:ASN:OD1	2.32	0.63
1:D:107:GLU:O	1:D:137:GLN:HG3	1.99	0.63
2:B:858:ILE:HG22	2:B:874:LEU:HD12	1.80	0.62
2:B:638:LEU:N	2:B:711:ASP:OD2	2.18	0.62
2:B:762:LYS:HB3	2:B:826:PHE:HB2	1.81	0.62
2:C:654:ALA:HB2	2:C:677:PHE:CE1	2.34	0.62
2:C:789:LYS:HG3	2:B:579:LEU:HD21	1.80	0.62
1:H:18:LYS:HA	1:H:30:VAL:HG22	1.82	0.62
2:C:913:VAL:O	2:C:916:PRO:HD2	2.00	0.61
2:A:576:TRP:HB2	2:E:792:SER:HB3	1.82	0.61
2:A:782:ARG:NH1	2:E:573:VAL:HG23	2.15	0.61
2:B:654:ALA:HB2	2:B:677:PHE:CE1	2.35	0.61
1:F:138:ALA:O	1:F:152:VAL:HG21	1.99	0.61
2:E:771:LEU:O	2:E:775:ASN:HB2	2.01	0.61
2:A:672:THR:O	2:A:672:THR:OG1	2.15	0.61
1:D:367:PRO:HD3	2:A:573:VAL:HG11	1.83	0.61
2:C:779:SER:HB3	2:B:565:ILE:H	1.64	0.61
1:F:186:THR:O	1:F:190:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:743:LEU:HD22	2:C:844:VAL:HG13	1.81	0.61
1:G:18:LYS:HA	1:G:30:VAL:HG22	1.82	0.61
1:D:138:ALA:O	1:D:152:VAL:HG21	2.01	0.61
2:E:869:VAL:HA	2:E:872:ASN:HB3	1.83	0.61
2:A:913:VAL:O	2:A:916:PRO:HD2	2.01	0.60
2:B:645:LYS:NZ	2:B:646:ASN:OD1	2.34	0.60
2:B:669:ASP:HB3	2:B:673:LEU:HB2	1.83	0.60
2:E:866:ASP:N	2:E:867:ASN:OD1	2.35	0.60
2:A:573:VAL:HG23	2:E:782:ARG:NH1	2.16	0.60
2:E:743:LEU:HD22	2:E:844:VAL:HG13	1.83	0.60
1:D:137:GLN:NE2	4:D:402:ATP:O3G	2.35	0.60
1:G:272:ALA:HB1	1:G:276:GLU:HB2	1.82	0.60
1:G:96:VAL:HB	1:G:101:HIS:CE1	2.37	0.60
1:G:278:THR:O	1:G:282:ILE:HD12	2.02	0.60
2:C:579:LEU:HD21	2:B:789:LYS:HG3	1.84	0.60
2:E:762:LYS:HB3	2:E:826:PHE:HB2	1.83	0.60
1:G:280:ASN:HA	1:G:283:MET:HB2	1.84	0.60
2:C:605:ARG:HG2	2:C:609:LEU:HD12	1.83	0.59
2:C:638:LEU:N	2:C:711:ASP:OD2	2.21	0.59
1:G:107:GLU:O	1:G:137:GLN:HG3	2.01	0.59
2:A:578:ALA:HB1	2:E:785:VAL:HG21	1.83	0.59
2:A:743:LEU:HD22	2:A:844:VAL:HG13	1.83	0.59
1:F:18:LYS:HA	1:F:30:VAL:HG22	1.85	0.59
1:H:27:PRO:HD3	1:H:340:TRP:CE3	2.38	0.59
2:A:722:ARG:HA	2:A:722:ARG:NH1	2.18	0.59
2:A:875:SER:OG	2:A:876:THR:N	2.36	0.59
2:B:869:VAL:HA	2:B:872:ASN:HB3	1.84	0.58
2:C:869:VAL:HA	2:C:872:ASN:HB3	1.84	0.58
1:G:186:THR:O	1:G:190:MET:HG2	2.03	0.58
2:A:771:LEU:O	2:A:775:ASN:HB2	2.04	0.58
1:H:186:THR:O	1:H:190:MET:HG2	2.03	0.58
1:G:27:PRO:HD3	1:G:340:TRP:CE3	2.39	0.58
2:B:576:TRP:HD1	2:B:576:TRP:O	1.86	0.58
2:B:743:LEU:HD22	2:B:844:VAL:HG13	1.85	0.58
2:C:771:LEU:O	2:C:775:ASN:HB2	2.03	0.58
1:D:186:THR:O	1:D:190:MET:HG2	2.03	0.58
2:C:778:ASN:ND2	3:B:1001:ACT:O	2.37	0.57
2:B:913:VAL:O	2:B:916:PRO:HD2	2.03	0.57
1:H:222:ASP:HB3	1:H:225:ASN:HB2	1.86	0.57
2:A:869:VAL:HA	2:A:872:ASN:HB3	1.85	0.57
1:D:222:ASP:HB3	1:D:225:ASN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:VAL:HB	1:F:101:HIS:CE1	2.40	0.57
1:D:18:LYS:HA	1:D:30:VAL:HG22	1.86	0.57
1:F:222:ASP:HB3	1:F:225:ASN:HB2	1.87	0.57
1:D:96:VAL:HB	1:D:101:HIS:CE1	2.39	0.57
2:B:664:ALA:HA	2:B:667:THR:HG22	1.86	0.57
2:E:576:TRP:HD1	2:E:576:TRP:O	1.86	0.57
2:B:570:ARG:O	2:B:570:ARG:HG3	2.04	0.57
1:D:9:VAL:HG22	1:D:104:LEU:HB3	1.86	0.57
1:F:9:VAL:HG12	1:F:340:TRP:NE1	2.19	0.57
1:G:138:ALA:O	1:G:152:VAL:HG21	2.05	0.57
2:C:570:ARG:HG3	2:C:570:ARG:O	2.04	0.57
2:C:576:TRP:O	2:C:576:TRP:HD1	1.87	0.57
1:F:333:PRO:HG2	1:F:334:GLU:HG3	1.87	0.57
1:G:222:ASP:HB3	1:G:225:ASN:HB2	1.86	0.57
1:G:9:VAL:HG22	1:G:104:LEU:HB3	1.87	0.57
2:C:565:ILE:HD13	2:C:566:LYS:H	1.69	0.56
2:C:568:LYS:HB3	2:C:569:PHE:HD1	1.70	0.56
1:G:151:ILE:HD12	1:G:164:PRO:HG3	1.88	0.56
2:A:576:TRP:O	2:A:576:TRP:HD1	1.88	0.56
2:A:578:ALA:HB1	2:E:785:VAL:HG11	1.87	0.56
2:C:672:THR:OG1	2:C:672:THR:O	2.11	0.56
1:F:107:GLU:O	1:F:137:GLN:HG3	2.05	0.56
2:C:807:THR:OG1	2:C:808:LEU:N	2.38	0.56
2:B:740:LEU:HB2	2:B:884:LEU:HD13	1.87	0.56
2:A:568:LYS:HB3	2:A:569:PHE:HD1	1.70	0.56
2:E:638:LEU:N	2:E:711:ASP:OD2	2.23	0.56
2:C:875:SER:OG	2:C:876:THR:N	2.37	0.56
2:E:649:ILE:HD13	1:G:143:TYR:CE1	2.41	0.56
1:H:218:TYR:CZ	1:H:255:PHE:HB3	2.42	0.55
2:A:570:ARG:HG3	2:A:570:ARG:O	2.07	0.55
1:D:280:ASN:HA	1:D:283:MET:HB2	1.88	0.55
1:D:272:ALA:HB1	1:D:276:GLU:HB2	1.86	0.55
2:E:573:VAL:HG11	1:G:367:PRO:HD3	1.89	0.55
2:B:565:ILE:CD1	2:B:566:LYS:H	2.19	0.55
2:B:771:LEU:O	2:B:775:ASN:HB2	2.06	0.55
2:E:570:ARG:O	2:E:570:ARG:HG3	2.07	0.55
1:F:71:ILE:HG23	1:F:76:ILE:HG12	1.88	0.55
1:H:272:ALA:HB1	1:H:276:GLU:HB2	1.87	0.55
1:H:147:ARG:NH1	1:H:330:ILE:HG12	2.12	0.55
2:C:664:ALA:HA	2:C:667:THR:HG22	1.88	0.55
1:F:278:THR:O	1:F:282:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ASN:HA	1:F:283:MET:HB2	1.88	0.55
1:H:138:ALA:O	1:H:152:VAL:HG21	2.05	0.55
2:E:568:LYS:HB3	2:E:569:PHE:HD1	1.71	0.55
2:A:866:ASP:HB3	2:A:867:ASN:HA	1.89	0.55
1:D:14:SER:OG	4:D:402:ATP:O2B	2.25	0.55
1:D:71:ILE:HG23	1:D:76:ILE:HG12	1.89	0.54
2:E:913:VAL:O	2:E:916:PRO:HD2	2.07	0.54
2:C:905:SER:O	2:C:909:THR:HG23	2.08	0.54
1:H:71:ILE:HG23	1:H:76:ILE:HG12	1.88	0.54
2:E:645:LYS:NZ	2:E:646:ASN:OD1	2.41	0.54
1:F:14:SER:OG	4:F:403:ATP:O2B	2.23	0.54
1:D:151:ILE:HD12	1:D:164:PRO:HG3	1.89	0.54
1:H:278:THR:O	1:H:282:ILE:HD12	2.08	0.54
1:F:287:ILE:HG23	1:F:290:ARG:NH1	2.22	0.54
1:F:35:VAL:HG21	1:F:81:ASP:HB3	1.88	0.54
1:H:280:ASN:HA	1:H:283:MET:HB2	1.89	0.54
2:A:638:LEU:N	2:A:711:ASP:OD2	2.24	0.54
1:G:274:ILE:HG21	1:G:313:MET:HE1	1.89	0.54
2:A:792:SER:HB3	2:E:576:TRP:HB2	1.91	0.53
1:H:9:VAL:HG12	1:H:340:TRP:NE1	2.23	0.53
1:D:143:TYR:CE1	2:A:649:ILE:HD13	2.43	0.53
1:G:71:ILE:HG23	1:G:76:ILE:HG12	1.89	0.53
1:H:151:ILE:HD12	1:H:164:PRO:HG3	1.91	0.53
1:H:27:PRO:HD3	1:H:340:TRP:CD2	2.43	0.53
2:B:568:LYS:HB3	2:B:569:PHE:HD1	1.74	0.53
2:E:672:THR:OG1	2:E:672:THR:O	2.18	0.53
1:G:260:THR:HG21	1:G:267:ILE:HG23	1.90	0.53
1:G:287:ILE:HA	1:G:290:ARG:HD3	1.91	0.53
2:A:905:SER:O	2:A:909:THR:HG23	2.08	0.53
2:C:813:ALA:HB3	2:C:932:ASN:ND2	2.24	0.53
1:D:287:ILE:HA	1:D:290:ARG:HD3	1.90	0.53
2:A:827:TRP:CD1	2:A:828:GLN:HG3	2.43	0.53
1:F:151:ILE:HD12	1:F:164:PRO:HG3	1.91	0.53
1:G:178:LEU:HG	1:G:180:LEU:H	1.74	0.53
1:D:218:TYR:CZ	1:D:255:PHE:HB3	2.43	0.53
1:H:17:VAL:O	1:H:30:VAL:HA	2.09	0.53
2:B:905:SER:O	2:B:909:THR:HG23	2.08	0.53
2:C:785:VAL:HG21	2:B:578:ALA:HB1	1.91	0.53
2:C:827:TRP:CZ3	2:C:926:LYS:HG2	2.43	0.53
1:F:287:ILE:HA	1:F:290:ARG:HD3	1.91	0.53
1:G:196:ARG:HH21	1:G:251:GLY:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:866:ASP:HB3	2:C:867:ASN:HA	1.90	0.52
2:E:840:SER:N	1:G:323:SER:OG	2.33	0.52
2:B:713:PHE:O	2:B:717:PHE:HB2	2.08	0.52
2:E:664:ALA:HA	2:E:667:THR:HG22	1.91	0.52
2:C:573:VAL:HG11	1:F:367:PRO:HD3	1.91	0.52
2:B:813:ALA:HB3	2:B:932:ASN:ND2	2.25	0.52
1:G:264:PRO:HG2	1:G:271:SER:O	2.09	0.52
1:D:287:ILE:HG23	1:D:290:ARG:NH1	2.25	0.52
1:F:272:ALA:HB1	1:F:276:GLU:HB2	1.90	0.52
2:B:722:ARG:NH1	2:B:725:GLN:OE1	2.36	0.52
1:D:116:ARG:HG3	1:D:134:VAL:HG11	1.90	0.52
2:E:859:ARG:HB3	2:E:874:LEU:HD11	1.92	0.52
1:G:264:PRO:HG3	1:G:273:GLY:HA2	1.90	0.52
2:B:807:THR:OG1	2:B:808:LEU:N	2.43	0.52
2:B:866:ASP:HB3	2:B:867:ASN:HA	1.91	0.52
2:E:866:ASP:HB3	2:E:867:ASN:HA	1.91	0.52
1:G:218:TYR:CZ	1:G:255:PHE:HB3	2.45	0.52
1:G:333:PRO:HG2	1:G:334:GLU:HG3	1.92	0.52
2:B:692:LYS:HA	2:B:695:ARG:HG2	1.91	0.52
1:F:260:THR:HG21	1:F:267:ILE:HG23	1.91	0.52
2:C:565:ILE:H	2:B:779:SER:HB3	1.75	0.51
2:E:827:TRP:CD1	2:E:828:GLN:HG3	2.45	0.51
1:F:292:ASP:OD1	1:F:292:ASP:N	2.43	0.51
1:G:116:ARG:HG3	1:G:134:VAL:HG11	1.92	0.51
1:G:287:ILE:HG23	1:G:290:ARG:NH1	2.25	0.51
2:C:827:TRP:CD1	2:C:828:GLN:HG3	2.45	0.51
2:C:859:ARG:HB3	2:C:874:LEU:HD11	1.92	0.51
1:F:218:TYR:CZ	1:F:255:PHE:HB3	2.45	0.51
1:F:27:PRO:HD3	1:F:340:TRP:CE3	2.46	0.51
1:D:264:PRO:HG2	1:D:271:SER:O	2.11	0.51
1:H:9:VAL:HG22	1:H:104:LEU:HB3	1.92	0.51
2:E:905:SER:O	2:E:909:THR:HG23	2.10	0.51
1:H:287:ILE:HG23	1:H:290:ARG:NH1	2.25	0.51
2:A:664:ALA:HA	2:A:667:THR:HG22	1.91	0.51
2:E:737:GLN:O	2:E:741:GLN:HG2	2.11	0.51
2:B:722:ARG:HA	2:B:722:ARG:NH1	2.25	0.51
2:C:740:LEU:HB2	2:C:884:LEU:HD13	1.92	0.51
2:E:899:VAL:HG22	2:E:914:PHE:CD1	2.45	0.51
2:B:827:TRP:CD1	2:B:828:GLN:HG3	2.45	0.51
2:C:761:GLN:CD	2:C:761:GLN:H	2.14	0.51
1:F:9:VAL:HG12	1:F:340:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:HIS:HB3	1:H:177:ARG:HH22	1.75	0.51
1:F:264:PRO:HG2	1:F:271:SER:O	2.11	0.51
2:B:746:GLN:NE2	1:H:323:SER:HB3	2.19	0.51
2:A:750:ILE:O	2:A:754:SER:HB3	2.11	0.50
2:B:859:ARG:HB3	2:B:874:LEU:HD11	1.93	0.50
2:B:875:SER:OG	2:B:876:THR:N	2.43	0.50
1:D:9:VAL:HG12	1:D:340:TRP:NE1	2.26	0.50
1:D:125:GLU:OE1	3:E:1001:ACT:H2	2.10	0.50
1:H:313:MET:O	1:H:317:ILE:HG12	2.11	0.50
2:C:722:ARG:HA	2:C:722:ARG:NH1	2.26	0.50
1:D:17:VAL:O	1:D:30:VAL:HA	2.12	0.50
1:D:274:ILE:HG21	1:D:313:MET:HE1	1.93	0.50
1:H:157:ASP:OD2	1:H:183:ARG:NH1	2.44	0.50
1:H:9:VAL:HG12	1:H:340:TRP:CD1	2.46	0.50
2:A:775:ASN:ND2	2:A:785:VAL:O	2.36	0.50
2:A:859:ARG:HB3	2:A:874:LEU:HD11	1.94	0.50
2:B:825:ASN:O	2:B:827:TRP:N	2.44	0.50
2:E:813:ALA:HB3	2:E:932:ASN:ND2	2.27	0.50
1:G:9:VAL:HG12	1:G:340:TRP:NE1	2.27	0.50
1:D:315:LYS:HG3	1:D:316:GLU:N	2.25	0.50
2:E:827:TRP:CD1	2:E:828:GLN:N	2.80	0.50
1:G:8:LEU:HD11	1:G:94:LEU:CD1	2.42	0.50
1:H:287:ILE:HA	1:H:290:ARG:HD3	1.92	0.50
2:B:573:VAL:HG12	1:H:125:GLU:OE2	2.12	0.50
2:E:716:LEU:O	2:E:719:LYS:HB2	2.12	0.50
2:A:825:ASN:O	2:A:827:TRP:N	2.43	0.49
1:D:264:PRO:HG3	1:D:273:GLY:HA2	1.94	0.49
2:E:750:ILE:O	2:E:754:SER:HB3	2.12	0.49
1:H:315:LYS:HG3	1:H:316:GLU:N	2.27	0.49
1:F:291:LYS:HZ2	1:F:325:MET:HA	1.76	0.49
1:G:35:VAL:HG21	1:G:81:ASP:HB3	1.92	0.49
1:H:35:VAL:HG21	1:H:81:ASP:HB3	1.94	0.49
1:G:315:LYS:HG3	1:G:316:GLU:N	2.27	0.49
1:H:125:GLU:OE2	1:H:362:TYR:OH	2.31	0.49
1:H:178:LEU:HG	1:H:180:LEU:H	1.77	0.49
1:H:89:THR:O	1:H:94:LEU:HB2	2.13	0.49
2:A:761:GLN:CD	2:A:761:GLN:H	2.15	0.49
2:B:738:ASP:O	2:B:741:GLN:HB2	2.12	0.49
1:D:27:PRO:HD3	1:D:340:TRP:CE3	2.47	0.49
2:E:875:SER:OG	2:E:876:THR:N	2.46	0.49
1:H:333:PRO:HG2	1:H:334:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:722:ARG:NH1	2:C:725:GLN:OE1	2.38	0.49
1:H:264:PRO:HG2	1:H:271:SER:O	2.11	0.49
1:H:350:SER:O	1:H:353:GLN:HG2	2.13	0.49
2:B:716:LEU:O	2:B:719:LYS:HB2	2.13	0.49
1:G:196:ARG:HG3	1:G:253:GLU:HG3	1.94	0.49
1:G:17:VAL:O	1:G:30:VAL:HA	2.12	0.49
2:B:807:THR:HG22	2:B:810:HIS:ND1	2.28	0.49
1:F:313:MET:O	1:F:317:ILE:HG12	2.13	0.49
1:G:27:PRO:HD3	1:G:340:TRP:CD2	2.47	0.49
2:A:716:LEU:O	2:A:719:LYS:HB2	2.13	0.49
2:C:576:TRP:HB2	2:B:792:SER:HB3	1.93	0.49
3:C:1001:ACT:OXT	2:B:778:ASN:ND2	2.45	0.49
1:D:238:LYS:HB2	1:D:254:ARG:NH1	2.28	0.49
1:G:25:ASP:HB3	3:G:401:ACT:O	2.12	0.49
2:A:692:LYS:HA	2:A:695:ARG:HG2	1.93	0.49
2:B:833:VAL:HG23	2:B:915:PHE:HB3	1.95	0.49
2:C:913:VAL:HG23	2:C:914:PHE:N	2.28	0.49
2:C:833:VAL:HG23	2:C:915:PHE:HB3	1.95	0.49
2:E:790:LEU:HG	2:E:917:VAL:HG11	1.94	0.49
1:G:10:CYS:O	1:G:105:LEU:HA	2.13	0.49
1:G:173:HIS:CG	1:G:173:HIS:O	2.65	0.49
1:G:276:GLU:O	1:G:279:TYR:N	2.45	0.49
1:G:147:ARG:NH1	1:G:330:ILE:HG12	2.17	0.49
1:H:264:PRO:HG3	1:H:273:GLY:HA2	1.93	0.49
2:A:813:ALA:HB3	2:A:932:ASN:ND2	2.27	0.49
2:B:647:LEU:HD22	2:B:651:LEU:HG	1.95	0.48
2:E:808:LEU:O	2:E:812:ILE:HG13	2.13	0.48
1:F:17:VAL:HG23	1:F:33:SER:HB3	1.95	0.48
2:C:840:SER:N	1:F:323:SER:OG	2.34	0.48
2:A:722:ARG:HA	2:A:722:ARG:CZ	2.42	0.48
2:C:578:ALA:HB1	2:B:785:VAL:HG21	1.94	0.48
2:C:775:ASN:ND2	2:C:785:VAL:O	2.35	0.48
2:C:825:ASN:O	2:C:827:TRP:N	2.40	0.48
1:F:173:HIS:CG	1:F:173:HIS:O	2.64	0.48
1:H:25:ASP:N	3:H:401:ACT:OXT	2.46	0.48
1:D:73:HIS:HB3	1:D:177:ARG:HH22	1.79	0.48
2:E:795:LEU:H	2:E:795:LEU:HD23	1.78	0.48
1:F:330:ILE:HG22	1:F:332:PRO:HD3	1.95	0.48
1:G:89:THR:O	1:G:94:LEU:HB2	2.13	0.48
2:A:808:LEU:O	2:A:812:ILE:HG13	2.14	0.48
1:D:178:LEU:HG	1:D:180:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:722:ARG:NH1	2:A:725:GLN:OE1	2.39	0.48
2:C:649:ILE:HD13	1:F:143:TYR:CE1	2.49	0.48
1:F:276:GLU:O	1:F:279:TYR:N	2.47	0.48
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.95	0.48
1:G:157:ASP:OD2	1:G:183:ARG:NH1	2.47	0.48
2:C:877:ASN:O	2:C:880:LYS:N	2.45	0.48
1:D:196:ARG:HG3	1:D:253:GLU:HG3	1.95	0.48
1:F:262:PHE:HD1	1:F:275:HIS:ND1	2.12	0.48
1:F:8:LEU:HD11	1:F:94:LEU:CD1	2.43	0.48
2:B:575:ASN:HA	3:B:1001:ACT:H2	1.94	0.48
2:C:713:PHE:O	2:C:717:PHE:HB2	2.14	0.48
2:C:716:LEU:O	2:C:719:LYS:HB2	2.14	0.48
2:C:746:GLN:NE2	1:F:323:SER:HB3	2.27	0.48
2:A:574:PHE:CE2	2:A:576:TRP:HB3	2.49	0.48
2:A:807:THR:OG1	2:A:808:LEU:N	2.45	0.48
2:A:740:LEU:HB2	2:A:884:LEU:HD13	1.95	0.48
1:F:118:LYS:O	1:F:122:ILE:HG13	2.13	0.48
1:F:73:HIS:HB3	1:F:177:ARG:HH22	1.78	0.48
1:F:76:ILE:HD13	1:F:82:MET:HG2	1.96	0.48
1:H:10:CYS:O	1:H:105:LEU:HA	2.14	0.48
1:H:292:ASP:OD1	1:H:292:ASP:N	2.47	0.48
1:D:288:ASP:OD1	1:D:288:ASP:N	2.47	0.47
2:E:779:SER:O	2:E:780:SER:OG	2.26	0.47
1:G:292:ASP:N	1:G:292:ASP:OD1	2.47	0.47
1:H:173:HIS:O	1:H:173:HIS:CG	2.65	0.47
2:A:647:LEU:HD22	2:A:651:LEU:HG	1.96	0.47
2:A:827:TRP:NE1	2:A:828:GLN:HG3	2.29	0.47
2:B:795:LEU:H	2:B:795:LEU:HD23	1.79	0.47
1:D:313:MET:O	1:D:317:ILE:HG12	2.14	0.47
2:A:795:LEU:H	2:A:795:LEU:HD23	1.80	0.47
2:C:899:VAL:HG22	2:C:914:PHE:CD1	2.49	0.47
2:E:647:LEU:HD22	2:E:651:LEU:HG	1.96	0.47
2:E:713:PHE:O	2:E:717:PHE:HB2	2.14	0.47
2:B:913:VAL:HG23	2:B:914:PHE:N	2.30	0.47
2:C:808:LEU:O	2:C:812:ILE:HG13	2.15	0.47
1:D:323:SER:HB3	2:A:746:GLN:NE2	2.27	0.47
1:H:242:LEU:HD22	1:H:246:GLN:HG3	1.96	0.47
1:H:262:PHE:HD1	1:H:275:HIS:ND1	2.12	0.47
2:A:894:ALA:O	2:A:897:ALA:HB3	2.15	0.47
2:B:573:VAL:HG11	1:H:367:PRO:HD3	1.97	0.47
1:H:8:LEU:HD11	1:H:94:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:VAL:HG21	1:D:81:ASP:HB3	1.96	0.47
2:E:738:ASP:O	2:E:741:GLN:HB2	2.14	0.47
1:G:125:GLU:OE2	1:G:362:TYR:OH	2.33	0.47
2:B:750:ILE:O	2:B:754:SER:HB3	2.15	0.47
3:C:1002:ACT:OXT	1:H:121:GLN:NE2	2.47	0.47
2:C:565:ILE:CD1	2:C:566:LYS:H	2.27	0.47
1:D:173:HIS:O	1:D:173:HIS:CG	2.62	0.47
1:D:292:ASP:OD1	1:D:292:ASP:N	2.47	0.47
1:D:295:ALA:O	1:D:328:LYS:HB3	2.15	0.47
1:G:73:HIS:HB3	1:G:177:ARG:HH22	1.78	0.47
1:G:17:VAL:HG23	1:G:33:SER:HB3	1.97	0.47
1:F:9:VAL:HG22	1:F:104:LEU:HB3	1.97	0.47
1:G:361:GLU:H	1:G:361:GLU:HG2	1.49	0.47
1:H:238:LYS:HB2	1:H:254:ARG:NH1	2.29	0.47
1:H:260:THR:HG21	1:H:267:ILE:HG23	1.97	0.47
2:B:899:VAL:HG22	2:B:914:PHE:CD1	2.49	0.47
2:C:750:ILE:O	2:C:754:SER:HB3	2.14	0.47
2:E:807:THR:OG1	2:E:808:LEU:N	2.48	0.47
1:F:219:VAL:HG22	1:F:258:PRO:HB2	1.96	0.47
1:G:9:VAL:HG12	1:G:340:TRP:CD1	2.50	0.47
2:A:816:VAL:HG11	2:A:925:TYR:OH	2.15	0.46
2:A:827:TRP:CD1	2:A:828:GLN:N	2.83	0.46
2:C:827:TRP:CD1	2:C:828:GLN:N	2.83	0.46
2:E:656:ARG:HB3	2:E:661:ILE:HG13	1.97	0.46
2:E:796:LEU:HD23	2:E:796:LEU:HA	1.61	0.46
1:F:125:GLU:OE2	1:F:362:TYR:OH	2.33	0.46
1:F:17:VAL:O	1:F:30:VAL:HA	2.15	0.46
2:A:578:ALA:CB	2:E:785:VAL:HG11	2.45	0.46
2:B:808:LEU:O	2:B:812:ILE:HG13	2.15	0.46
1:G:242:LEU:HD22	1:G:246:GLN:HG3	1.97	0.46
2:B:609:LEU:C	2:B:610:PHE:HD1	2.19	0.46
1:F:140:LEU:O	1:F:342:GLY:HA3	2.16	0.46
1:H:73:HIS:HB3	1:H:177:ARG:NH2	2.30	0.46
1:H:276:GLU:O	1:H:279:TYR:N	2.49	0.46
1:D:89:THR:O	1:D:94:LEU:HB2	2.15	0.46
2:E:827:TRP:NE1	2:E:828:GLN:HG3	2.31	0.46
1:G:112:PRO:HD2	1:G:115:ASN:HB2	1.98	0.46
1:G:316:GLU:O	1:G:320:LEU:HD13	2.16	0.46
1:G:140:LEU:O	1:G:342:GLY:HA3	2.16	0.46
1:F:264:PRO:HG3	1:F:273:GLY:HA2	1.98	0.46
2:C:795:LEU:H	2:C:795:LEU:HD23	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:NH1	1:D:330:ILE:HG12	2.18	0.46
2:E:775:ASN:ND2	2:E:785:VAL:O	2.36	0.46
1:H:306:TYR:CE1	4:H:402:ATP:H2	2.32	0.46
2:A:713:PHE:O	2:A:717:PHE:HB2	2.14	0.46
2:B:827:TRP:NE1	2:B:828:GLN:HG3	2.31	0.46
2:B:877:ASN:O	2:B:880:LYS:N	2.48	0.46
1:D:262:PHE:HD1	1:D:275:HIS:ND1	2.14	0.46
2:E:825:ASN:O	2:E:827:TRP:N	2.42	0.46
1:D:330:ILE:HG22	1:D:332:PRO:HD3	1.97	0.46
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.97	0.46
1:G:160:THR:HB	1:G:178:LEU:HB3	1.98	0.46
1:G:262:PHE:HD1	1:G:275:HIS:ND1	2.14	0.46
1:H:275:HIS:CD2	1:H:276:GLU:HG3	2.51	0.46
2:C:646:ASN:HB3	1:F:148:THR:HG21	1.97	0.46
1:F:242:LEU:HD22	1:F:246:GLN:HG3	1.96	0.46
1:H:158:GLY:HA3	1:H:183:ARG:NH2	2.31	0.46
1:H:261:LEU:HB3	1:H:274:ILE:CD1	2.37	0.46
2:B:775:ASN:ND2	2:B:785:VAL:O	2.36	0.45
1:D:291:LYS:HZ2	1:D:325:MET:HA	1.81	0.45
1:D:9:VAL:HG12	1:D:340:TRP:CD1	2.51	0.45
1:F:10:CYS:O	1:F:105:LEU:HA	2.16	0.45
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.98	0.45
1:D:140:LEU:O	1:D:342:GLY:HA3	2.16	0.45
1:F:111:ASN:HA	1:F:112:PRO:HD3	1.67	0.45
1:H:219:VAL:HG22	1:H:258:PRO:HB2	1.98	0.45
2:B:827:TRP:CD1	2:B:828:GLN:N	2.85	0.45
1:D:306:TYR:CE1	4:D:402:ATP:H2	2.34	0.45
2:A:802:THR:HG23	2:E:609:LEU:O	2.16	0.45
1:G:330:ILE:HG22	1:G:332:PRO:HD3	1.98	0.45
1:H:330:ILE:HG22	1:H:332:PRO:HD3	1.97	0.45
2:C:656:ARG:HB3	2:C:661:ILE:HG13	1.99	0.45
1:D:125:GLU:OE2	1:D:362:TYR:OH	2.34	0.45
1:D:341:ILE:HG22	1:D:345:ILE:HD12	1.97	0.45
2:E:740:LEU:HB2	2:E:884:LEU:HD13	1.98	0.45
2:E:833:VAL:HG23	2:E:915:PHE:HB3	1.99	0.45
1:G:76:ILE:HD13	1:G:82:MET:HG2	1.99	0.45
2:A:609:LEU:C	2:A:610:PHE:HD1	2.20	0.45
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.98	0.45
1:H:295:ALA:O	1:H:328:LYS:HB3	2.16	0.45
2:A:737:GLN:O	2:A:741:GLN:HG2	2.17	0.45
2:B:825:ASN:HB2	2:B:828:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LYS:NZ	1:D:326:LYS:H	2.14	0.45
1:D:8:LEU:HD11	1:D:94:LEU:CD1	2.46	0.45
2:E:603:LEU:O	2:E:606:PHE:HB3	2.16	0.45
1:H:17:VAL:HG23	1:H:33:SER:HB3	1.98	0.45
2:B:761:GLN:CD	2:B:761:GLN:H	2.17	0.45
2:E:877:ASN:O	2:E:880:LYS:N	2.50	0.45
2:E:814:LEU:HG	2:E:932:ASN:ND2	2.32	0.45
1:G:158:GLY:HA3	1:G:183:ARG:NH2	2.32	0.45
1:G:18:LYS:HG3	1:G:30:VAL:HG22	1.98	0.45
1:H:116:ARG:HG3	1:H:134:VAL:HG11	1.99	0.45
2:B:656:ARG:HB3	2:B:661:ILE:HG13	1.98	0.45
2:B:722:ARG:HA	2:B:722:ARG:CZ	2.46	0.45
1:D:316:GLU:O	1:D:320:LEU:HD13	2.17	0.45
1:F:25:ASP:N	3:F:402:ACT:OXT	2.50	0.45
1:H:99:GLU:O	1:H:130:PRO:HD3	2.17	0.45
2:B:673:LEU:HA	2:B:674:PRO:HD3	1.75	0.45
1:D:10:CYS:O	1:D:105:LEU:HA	2.17	0.45
2:A:584:ILE:HD11	2:E:787:GLY:HA3	1.98	0.45
1:H:316:GLU:O	1:H:320:LEU:HD13	2.17	0.45
1:H:341:ILE:HG22	1:H:345:ILE:HD12	1.99	0.45
1:D:333:PRO:HG2	1:D:334:GLU:HG3	1.98	0.45
1:D:350:SER:O	1:D:353:GLN:HG2	2.17	0.45
2:E:599:GLU:O	2:E:601:LEU:HD12	2.17	0.45
1:G:304:THR:O	1:G:335:ARG:NH2	2.44	0.45
2:E:746:GLN:NE2	1:G:323:SER:HB3	2.29	0.45
1:H:288:ASP:OD1	1:H:288:ASP:N	2.50	0.45
2:C:738:ASP:O	2:C:741:GLN:HB2	2.16	0.44
2:C:827:TRP:NE1	2:C:828:GLN:HG3	2.32	0.44
2:E:682:MET:O	2:E:685:LEU:HD12	2.17	0.44
1:F:112:PRO:HD2	1:F:115:ASN:HB2	1.99	0.44
1:F:217:CYS:HB2	1:F:254:ARG:O	2.17	0.44
1:H:118:LYS:O	1:H:122:ILE:HG13	2.17	0.44
2:A:603:LEU:O	2:A:606:PHE:HB3	2.17	0.44
2:C:581:PRO:HA	2:C:584:ILE:HB	1.99	0.44
1:F:147:ARG:NH1	1:F:330:ILE:HG12	2.21	0.44
1:G:105:LEU:HD13	1:G:134:VAL:HG22	1.99	0.44
2:C:707:LEU:HA	2:C:707:LEU:HD23	1.82	0.44
2:C:669:ASP:HB2	2:C:730:MET:SD	2.57	0.44
1:D:362:TYR:O	1:D:366:GLY:N	2.40	0.44
1:F:288:ASP:OD1	1:F:288:ASP:N	2.50	0.44
1:G:172:PRO:O	1:G:175:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:LEU:HD23	2:B:707:LEU:HA	1.84	0.44
2:B:737:GLN:O	2:B:741:GLN:HG2	2.17	0.44
2:E:913:VAL:HG23	2:E:914:PHE:N	2.33	0.44
1:G:219:VAL:HG22	1:G:258:PRO:HB2	1.99	0.44
1:G:275:HIS:CD2	1:G:276:GLU:HG3	2.53	0.44
1:H:172:PRO:O	1:H:175:ILE:HG13	2.16	0.44
1:H:120:THR:HG21	1:H:370:VAL:HB	2.00	0.44
2:B:789:LYS:HB3	2:B:791:GLN:OE1	2.18	0.44
1:F:52:SER:OG	1:F:84:LYS:HD2	2.18	0.44
1:G:109:PRO:O	1:G:110:LEU:HB2	2.17	0.44
1:H:105:LEU:HD13	1:H:134:VAL:HG22	2.00	0.44
2:A:874:LEU:HD23	2:A:878:GLU:HG3	2.00	0.44
2:C:647:LEU:HD22	2:C:651:LEU:HG	1.99	0.44
1:D:365:ALA:HB3	1:D:369:ILE:HB	2.00	0.44
1:D:25:ASP:HB3	3:D:401:ACT:O	2.17	0.44
2:E:669:ASP:HB2	2:E:730:MET:SD	2.58	0.44
2:B:646:ASN:HB3	1:H:148:THR:HG21	1.99	0.44
1:H:124:PHE:HD1	1:H:359:LYS:HG3	1.83	0.44
2:A:599:GLU:O	2:A:601:LEU:HD12	2.17	0.44
1:H:76:ILE:HD13	1:H:82:MET:HG2	2.00	0.44
2:A:807:THR:HG22	2:A:810:HIS:ND1	2.33	0.44
2:B:649:ILE:HD13	1:H:143:TYR:CE1	2.53	0.44
2:C:677:PHE:CZ	2:C:681:LEU:HD13	2.53	0.44
2:A:790:LEU:HG	2:A:917:VAL:HG11	2.00	0.44
2:C:669:ASP:HB3	2:C:673:LEU:CB	2.47	0.44
2:C:722:ARG:CZ	2:C:722:ARG:HA	2.47	0.44
1:D:276:GLU:O	1:D:279:TYR:N	2.51	0.44
2:E:574:PHE:CE2	2:E:576:TRP:HB3	2.52	0.44
2:E:581:PRO:HA	2:E:584:ILE:HB	2.00	0.44
1:F:89:THR:O	1:F:94:LEU:HB2	2.17	0.44
2:B:581:PRO:HA	2:B:584:ILE:HB	2.01	0.43
1:F:73:HIS:HB3	1:F:177:ARG:NH2	2.32	0.43
1:F:99:GLU:O	1:F:130:PRO:HD3	2.18	0.43
2:A:669:ASP:HB3	2:A:673:LEU:CB	2.45	0.43
2:C:609:LEU:C	2:C:610:PHE:HD1	2.21	0.43
2:C:682:MET:O	2:C:685:LEU:HD12	2.18	0.43
1:D:105:LEU:O	1:D:134:VAL:HA	2.18	0.43
1:F:178:LEU:HG	1:F:180:LEU:H	1.82	0.43
1:F:352:PHE:HA	1:F:355:MET:HE2	2.00	0.43
2:A:695:ARG:HG3	2:A:696:GLN:H	1.83	0.43
1:F:6:THR:O	1:F:101:HIS:HB3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:HIS:CD2	1:F:276:GLU:HG3	2.53	0.43
2:B:682:MET:O	2:B:685:LEU:HD12	2.18	0.43
1:D:261:LEU:HB3	1:D:274:ILE:CD1	2.37	0.43
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.68	0.43
2:C:874:LEU:HD23	2:C:878:GLU:HG3	2.01	0.43
2:C:905:SER:O	2:C:909:THR:N	2.50	0.43
2:E:874:LEU:HD23	2:E:878:GLU:HG3	2.01	0.43
1:F:242:LEU:HB2	1:F:246:GLN:O	2.18	0.43
1:G:73:HIS:HB3	1:G:177:ARG:NH2	2.33	0.43
2:E:576:TRP:CD1	2:E:576:TRP:O	2.69	0.43
2:E:773:LEU:HA	2:E:773:LEU:HD12	1.82	0.43
1:G:341:ILE:HG22	1:G:345:ILE:HD12	2.00	0.43
2:B:576:TRP:CD1	2:B:576:TRP:O	2.68	0.43
2:C:599:GLU:O	2:C:601:LEU:HD12	2.18	0.43
1:D:73:HIS:HB3	1:D:177:ARG:NH2	2.33	0.43
2:E:606:PHE:HE1	2:E:610:PHE:CD2	2.37	0.43
2:A:840:SER:O	2:A:844:VAL:HG23	2.18	0.43
2:C:842:GLU:O	2:C:846:LEU:HG	2.18	0.43
1:H:300:SER:HB2	1:H:338:SER:HB2	2.01	0.43
1:D:148:THR:HG21	2:A:646:ASN:HB3	2.00	0.43
1:D:94:LEU:HD22	1:D:94:LEU:HA	1.76	0.43
2:E:678:VAL:O	2:E:682:MET:HG3	2.19	0.43
1:F:109:PRO:HG2	1:F:161:HIS:CG	2.54	0.43
1:H:111:ASN:HD21	1:H:115:ASN:CG	2.15	0.43
1:H:274:ILE:HG21	1:H:313:MET:HE1	2.00	0.43
2:A:656:ARG:HB3	2:A:661:ILE:HG13	2.00	0.43
2:B:894:ALA:O	2:B:897:ALA:HB3	2.19	0.43
1:D:264:PRO:CG	1:D:273:GLY:HA2	2.49	0.43
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.54	0.43
1:H:362:TYR:O	1:H:366:GLY:N	2.42	0.43
2:A:842:GLU:O	2:A:846:LEU:HG	2.19	0.42
2:B:690:GLU:O	2:B:694:LEU:HD23	2.18	0.42
2:E:645:LYS:HE3	2:E:645:LYS:HB3	1.74	0.42
1:H:112:PRO:HD2	1:H:115:ASN:HB2	2.01	0.42
2:A:637:THR:HG22	2:A:639:LEU:N	2.28	0.42
2:B:677:PHE:CZ	2:B:681:LEU:HD13	2.54	0.42
2:C:704:LEU:HA	2:C:704:LEU:HD13	1.77	0.42
2:C:779:SER:C	2:C:781:LYS:H	2.23	0.42
2:C:782:ARG:NH1	2:B:573:VAL:HG23	2.34	0.42
2:C:816:VAL:HG11	2:C:925:TYR:OH	2.18	0.42
2:E:690:GLU:O	2:E:694:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:LYS:NZ	1:F:326:LYS:H	2.17	0.42
1:F:316:GLU:O	1:F:320:LEU:HD13	2.19	0.42
1:H:188:TYR:HH	1:H:266:PHE:HD2	1.65	0.42
1:H:210:ARG:O	1:H:213:LYS:HB3	2.20	0.42
2:A:707:LEU:HD22	2:A:711:ASP:HB2	2.01	0.42
2:B:645:LYS:HB3	2:B:645:LYS:HE3	1.71	0.42
1:F:295:ALA:O	1:F:328:LYS:HB3	2.19	0.42
1:D:136:ILE:H	1:D:136:ILE:CD1	2.25	0.42
1:D:176:MET:HG3	1:D:281:SER:HB2	2.01	0.42
1:F:321:ALA:HB3	1:F:327:ILE:HD11	2.01	0.42
1:G:313:MET:O	1:G:317:ILE:HG12	2.19	0.42
1:G:350:SER:O	1:G:353:GLN:HG2	2.20	0.42
1:H:361:GLU:H	1:H:361:GLU:HG2	1.53	0.42
1:D:92:ASN:O	1:D:95:ARG:HD2	2.20	0.42
1:F:31:PHE:HZ	1:F:89:THR:HG1	1.66	0.42
1:H:109:PRO:O	1:H:110:LEU:HB2	2.20	0.42
2:A:678:VAL:O	2:A:682:MET:HG3	2.20	0.42
2:C:574:PHE:CE2	2:C:576:TRP:HB3	2.55	0.42
1:D:120:THR:HG21	1:D:370:VAL:HB	2.01	0.42
1:F:361:GLU:H	1:F:361:GLU:HG2	1.54	0.42
2:A:576:TRP:CD1	2:A:576:TRP:O	2.71	0.42
2:E:747:LEU:HD23	2:E:747:LEU:HA	1.79	0.42
1:F:274:ILE:HG21	1:F:313:MET:HE1	2.00	0.42
1:G:196:ARG:HH21	1:G:251:GLY:N	2.17	0.42
1:H:372:ARG:HG2	1:H:372:ARG:H	1.68	0.42
2:B:816:VAL:HG11	2:B:925:TYR:OH	2.20	0.42
2:C:576:TRP:O	2:C:576:TRP:CD1	2.70	0.42
2:C:894:ALA:O	2:C:897:ALA:HB3	2.20	0.42
1:D:219:VAL:HG22	1:D:258:PRO:HB2	2.00	0.42
1:D:275:HIS:CD2	1:D:276:GLU:HG3	2.54	0.42
2:E:646:ASN:HB3	2:E:684:PHE:HZ	1.83	0.42
2:E:673:LEU:HA	2:E:674:PRO:HD3	1.78	0.42
1:F:365:ALA:HB3	1:F:369:ILE:HB	2.02	0.42
1:G:264:PRO:CG	1:G:273:GLY:HA2	2.49	0.42
2:E:609:LEU:C	2:E:610:PHE:HD1	2.23	0.42
1:G:146:GLY:C	1:G:147:ARG:HG2	2.40	0.42
1:H:109:PRO:HG2	1:H:161:HIS:CG	2.54	0.42
2:A:645:LYS:HE3	2:A:645:LYS:HB3	1.72	0.42
2:A:863:SER:HB2	2:C:582:ASN:ND2	2.34	0.42
2:A:899:VAL:HG22	2:A:914:PHE:CD1	2.55	0.42
2:C:796:LEU:HD23	2:C:796:LEU:HA	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:ASN:HA	1:H:112:PRO:HD3	1.69	0.42
2:A:581:PRO:HA	2:A:584:ILE:HB	2.02	0.41
2:E:576:TRP:CD1	2:E:576:TRP:C	2.94	0.41
1:F:206:ARG:HA	1:F:209:VAL:HG23	2.02	0.41
1:F:315:LYS:HG3	1:F:316:GLU:N	2.35	0.41
1:F:120:THR:HG21	1:F:370:VAL:HB	2.02	0.41
1:G:365:ALA:HB3	1:G:369:ILE:HB	2.01	0.41
2:B:565:ILE:HG23	2:B:566:LYS:N	2.33	0.41
1:D:314:GLN:O	1:D:318:THR:OG1	2.38	0.41
1:D:99:GLU:O	1:D:130:PRO:HD3	2.20	0.41
2:E:646:ASN:HB3	1:G:148:THR:HG21	2.02	0.41
1:G:288:ASP:OD1	1:G:288:ASP:N	2.52	0.41
1:G:311:ASP:O	1:G:314:GLN:HB3	2.20	0.41
1:H:217:CYS:HB2	1:H:254:ARG:O	2.19	0.41
2:A:588:VAL:O	2:A:591:GLU:HB2	2.20	0.41
2:C:790:LEU:HD12	2:C:790:LEU:HA	1.90	0.41
2:E:789:LYS:HB3	2:E:791:GLN:OE1	2.20	0.41
1:F:158:GLY:HA3	1:F:183:ARG:NH2	2.34	0.41
1:H:151:ILE:HD11	1:H:162:ASN:HB3	2.01	0.41
1:H:94:LEU:HA	1:H:94:LEU:HD22	1.85	0.41
2:B:603:LEU:O	2:B:606:PHE:HB3	2.20	0.41
2:B:672:THR:O	2:B:672:THR:OG1	2.17	0.41
2:C:576:TRP:C	2:C:576:TRP:CD1	2.93	0.41
2:C:678:VAL:O	2:C:682:MET:HG3	2.20	0.41
2:C:779:SER:HA	2:C:783:GLY:O	2.21	0.41
2:E:588:VAL:O	2:E:591:GLU:HB2	2.20	0.41
2:E:677:PHE:CZ	2:E:681:LEU:HD13	2.56	0.41
2:E:812:ILE:HG13	2:E:812:ILE:H	1.67	0.41
2:E:910:PRO:HD2	2:E:913:VAL:HG22	2.03	0.41
1:F:173:HIS:H	1:F:173:HIS:CD2	2.35	0.41
1:G:120:THR:HG21	1:G:370:VAL:HB	2.00	0.41
1:G:92:ASN:O	1:G:95:ARG:HD2	2.21	0.41
2:A:584:ILE:O	2:A:587:THR:HG23	2.20	0.41
2:B:774:GLY:O	2:B:778:ASN:HB2	2.19	0.41
2:C:565:ILE:HG23	2:C:566:LYS:N	2.36	0.41
2:C:790:LEU:HG	2:C:917:VAL:HG11	2.03	0.41
1:D:302:GLY:O	4:D:402:ATP:C4	2.74	0.41
2:A:587:THR:HB	2:E:901:TYR:O	2.21	0.41
1:H:347:ALA:HA	1:H:352:PHE:CE2	2.56	0.41
2:A:747:LEU:HD23	2:A:747:LEU:HA	1.73	0.41
2:B:850:GLU:O	2:B:853:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:VAL:HG23	1:D:33:SER:HB3	2.02	0.41
2:E:704:LEU:HA	2:E:704:LEU:HD13	1.85	0.41
2:E:842:GLU:O	2:E:846:LEU:HG	2.20	0.41
1:G:321:ALA:HB3	1:G:327:ILE:HD11	2.03	0.41
2:A:606:PHE:HE1	2:A:610:PHE:CD2	2.38	0.41
2:A:913:VAL:HG23	2:A:914:PHE:N	2.35	0.41
2:B:651:LEU:O	2:B:654:ALA:HB3	2.20	0.41
1:D:173:HIS:H	1:D:173:HIS:CD2	2.35	0.41
2:E:757:VAL:HA	2:E:830:LEU:CD2	2.48	0.41
1:F:287:ILE:HG23	1:F:290:ARG:HH12	1.85	0.41
1:G:109:PRO:HG2	1:G:161:HIS:CG	2.55	0.41
1:G:261:LEU:HB3	1:G:274:ILE:CD1	2.38	0.41
1:G:314:GLN:O	1:G:318:THR:OG1	2.36	0.41
2:B:687:THR:O	2:B:691:VAL:HG23	2.21	0.41
2:B:807:THR:HG22	2:B:810:HIS:CG	2.56	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.03	0.41
1:G:118:LYS:O	1:G:122:ILE:HG13	2.20	0.41
1:H:321:ALA:HB3	1:H:327:ILE:HD11	2.02	0.41
2:B:842:GLU:O	2:B:846:LEU:HG	2.21	0.41
2:C:672:THR:O	2:C:674:PRO:HD3	2.21	0.41
1:F:18:LYS:HG3	1:F:30:VAL:HG22	2.01	0.41
1:G:242:LEU:HB2	1:G:246:GLN:O	2.20	0.41
2:E:652:ARG:NE	1:G:345:ILE:HG12	2.36	0.41
2:B:856:GLU:HA	2:B:859:ARG:HG2	2.03	0.41
2:E:672:THR:O	2:E:674:PRO:HD3	2.21	0.41
2:E:756:SER:HB2	2:E:830:LEU:HA	2.03	0.41
2:E:816:VAL:HG11	2:E:925:TYR:OH	2.21	0.41
1:H:21:PHE:HB2	3:H:401:ACT:H3	2.03	0.41
2:A:877:ASN:O	2:A:880:LYS:N	2.54	0.41
2:E:645:LYS:HG2	2:E:649:ILE:HD11	2.03	0.41
1:H:264:PRO:CG	1:H:273:GLY:HA2	2.51	0.41
2:C:673:LEU:HA	2:C:674:PRO:HD3	1.79	0.40
1:D:151:ILE:HD11	1:D:162:ASN:HB3	2.03	0.40
1:F:105:LEU:HD13	1:F:134:VAL:HG22	2.03	0.40
1:G:173:HIS:H	1:G:173:HIS:CD2	2.35	0.40
1:G:196:ARG:NH1	1:G:196:ARG:HB3	2.35	0.40
1:G:257:CYS:HB3	1:G:258:PRO:HD3	2.03	0.40
1:H:162:ASN:O	1:H:164:PRO:HD3	2.20	0.40
1:H:208:ILE:O	1:H:212:ILE:HD12	2.20	0.40
2:A:796:LEU:HD23	2:A:796:LEU:HA	1.65	0.40
2:A:814:LEU:HG	2:A:932:ASN:ND2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:856:GLU:HA	2:A:859:ARG:HG2	2.03	0.40
2:B:678:VAL:O	2:B:682:MET:HG3	2.22	0.40
2:C:610:PHE:CE2	2:B:808:LEU:HA	2.56	0.40
1:D:102:PRO:HB3	1:D:131:ALA:HB3	2.03	0.40
1:H:365:ALA:HB3	1:H:369:ILE:HB	2.03	0.40
2:A:770:ILE:HG22	2:A:788:PHE:CE2	2.57	0.40
2:B:584:ILE:HD13	2:B:584:ILE:HA	1.95	0.40
2:B:779:SER:C	2:B:781:LYS:H	2.24	0.40
1:D:160:THR:HB	1:D:178:LEU:HB3	2.03	0.40
1:F:124:PHE:HD1	1:F:359:LYS:HG3	1.86	0.40
1:F:287:ILE:H	1:F:287:ILE:HG12	1.65	0.40
2:A:609:LEU:O	2:E:802:THR:HG23	2.20	0.40
2:A:669:ASP:HB2	2:A:730:MET:SD	2.61	0.40
1:D:123:MET:HG3	1:D:132:MET:HE3	2.02	0.40
1:D:361:GLU:H	1:D:361:GLU:HG2	1.51	0.40
2:E:803:ASP:OD2	2:E:805:LYS:HB2	2.22	0.40
1:F:210:ARG:O	1:F:213:LYS:HB3	2.21	0.40
1:H:209:VAL:HA	1:H:212:ILE:HD13	2.03	0.40
1:H:257:CYS:HB3	1:H:258:PRO:HD3	2.04	0.40
2:A:913:VAL:C	2:A:916:PRO:HD2	2.42	0.40
2:B:773:LEU:HD21	2:B:811:PHE:CE2	2.56	0.40
1:D:106:THR:HA	1:D:135:ALA:O	2.21	0.40
2:E:774:GLY:O	2:E:778:ASN:HB2	2.22	0.40
1:H:304:THR:O	1:H:335:ARG:NH2	2.47	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:D:199:SER:OG	1:F:62:ARG:O[1_554]	2.11	0.09

## 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	D	352/377 (93%)	326 (93%)	25 (7%)	1 (0%)	41	72
1	F	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	41	72
1	G	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	41	72
1	H	352/377 (93%)	325 (92%)	26 (7%)	1 (0%)	41	72
2	A	353/402 (88%)	310 (88%)	37 (10%)	6 (2%)	9	34
2	B	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	9	34
2	C	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	9	34
2	E	353/402 (88%)	310 (88%)	38 (11%)	5 (1%)	11	37
All	All	2820/3116 (90%)	2545 (90%)	248 (9%)	27 (1%)	15	46

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	869	VAL
2	E	869	VAL
2	C	869	VAL
2	B	869	VAL
2	A	598	LEU
2	A	674	PRO
2	E	598	LEU
2	E	674	PRO
2	C	598	LEU
2	C	674	PRO
2	B	598	LEU
2	B	674	PRO
2	C	826	PHE
2	A	826	PHE
2	A	863	SER
2	E	826	PHE
2	E	863	SER
2	C	863	SER
2	B	695	ARG
2	B	826	PHE
2	B	863	SER
2	A	752	ALA
2	C	695	ARG
1	D	274	ILE
1	F	274	ILE

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Mol	Chain	Res	Type
1	G	274	ILE
1	H	274	ILE

### 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	D	302/320 (94%)	262 (87%)	40 (13%)	4	15
1	F	302/320 (94%)	260 (86%)	42 (14%)	3	13
1	G	302/320 (94%)	263 (87%)	39 (13%)	4	16
1	H	302/320 (94%)	265 (88%)	37 (12%)	4	17
2	A	316/351 (90%)	256 (81%)	60 (19%)	1	4
2	B	316/351 (90%)	255 (81%)	61 (19%)	1	4
2	C	316/351 (90%)	254 (80%)	62 (20%)	1	4
2	E	316/351 (90%)	256 (81%)	60 (19%)	1	4
All	All	2472/2684 (92%)	2071 (84%)	401 (16%)	2	9

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	18	LYS
1	D	28	ARG
1	D	57	GLU
1	D	66	THR
1	D	69	TYR
1	D	71	ILE
1	D	78	ASN
1	D	94	LEU
1	D	95	ARG
1	D	99	GLU
1	D	101	HIS
1	D	105	LEU

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Mol	Chain	Res	Type
1	D	119	MET
1	D	120	THR
1	D	136	ILE
1	D	151	ILE
1	D	159	VAL
1	D	176	MET
1	D	179	ASP
1	D	200	PHE
1	D	202	THR
1	D	217	CYS
1	D	277	THR
1	D	280	ASN
1	D	288	ASP
1	D	289	ILE
1	D	290	ARG
1	D	292	ASP
1	D	315	LYS
1	D	318	THR
1	D	326	LYS
1	D	334	GLU
1	D	338	SER
1	D	339	VAL
1	D	349	LEU
1	D	360	GLN
1	D	368	SER
1	D	370	VAL
1	D	372	ARG
2	A	565	ILE
2	A	576	TRP
2	A	577	THR
2	A	585	ASN
2	A	587	THR
2	A	591	GLU
2	A	592	LEU
2	A	594	ASP
2	A	598	LEU
2	A	601	LEU
2	A	603	LEU
2	A	609	LEU
2	A	613	LYS
2	A	636	VAL
2	A	640	GLU

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Mol	Chain	Res	Type
2	A	643	ARG
2	A	647	LEU
2	A	669	ASP
2	A	675	VAL
2	A	685	LEU
2	A	700	GLU
2	A	701	ARG
2	A	705	GLU
2	A	711	ASP
2	A	721	GLU
2	A	722	ARG
2	A	724	THR
2	A	725	GLN
2	A	738	ASP
2	A	740	LEU
2	A	742	MET
2	A	750	ILE
2	A	751	ILE
2	A	754	SER
2	A	764	LYS
2	A	765	GLN
2	A	775	ASN
2	A	781	LYS
2	A	792	SER
2	A	795	LEU
2	A	798	ASP
2	A	802	THR
2	A	808	LEU
2	A	810	HIS
2	A	815	THR
2	A	816	VAL
2	A	822	GLU
2	A	825	ASN
2	A	826	PHE
2	A	830	LEU
2	A	841	LEU
2	A	853	ARG
2	A	865	HIS
2	A	869	VAL
2	A	876	THR
2	A	882	ASP
2	A	886	ARG

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Mol	Chain	Res	Type
2	A	898	VAL
2	A	909	THR
2	A	925	TYR
2	E	565	ILE
2	E	576	TRP
2	E	577	THR
2	E	585	ASN
2	E	587	THR
2	E	591	GLU
2	E	592	LEU
2	E	594	ASP
2	E	598	LEU
2	E	601	LEU
2	E	603	LEU
2	E	609	LEU
2	E	613	LYS
2	E	636	VAL
2	E	640	GLU
2	E	643	ARG
2	E	647	LEU
2	E	669	ASP
2	E	675	VAL
2	E	685	LEU
2	E	693	LEU
2	E	700	GLU
2	E	701	ARG
2	E	705	GLU
2	E	711	ASP
2	E	721	GLU
2	E	722	ARG
2	E	724	THR
2	E	725	GLN
2	E	738	ASP
2	E	740	LEU
2	E	742	MET
2	E	750	ILE
2	E	751	ILE
2	E	764	LYS
2	E	765	GLN
2	E	775	ASN
2	E	781	LYS
2	E	792	SER

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Mol	Chain	Res	Type
2	E	795	LEU
2	E	798	ASP
2	E	802	THR
2	E	808	LEU
2	E	810	HIS
2	E	815	THR
2	E	816	VAL
2	E	822	GLU
2	E	825	ASN
2	E	826	PHE
2	E	830	LEU
2	E	841	LEU
2	E	853	ARG
2	E	865	HIS
2	E	869	VAL
2	E	876	THR
2	E	882	ASP
2	E	886	ARG
2	E	898	VAL
2	E	909	THR
2	E	925	TYR
2	C	565	ILE
2	C	576	TRP
2	C	577	THR
2	C	585	ASN
2	C	587	THR
2	C	591	GLU
2	C	592	LEU
2	C	594	ASP
2	C	598	LEU
2	C	601	LEU
2	C	603	LEU
2	C	609	LEU
2	C	613	LYS
2	C	636	VAL
2	C	640	GLU
2	C	643	ARG
2	C	647	LEU
2	C	669	ASP
2	C	675	VAL
2	C	685	LEU
2	C	693	LEU

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Mol	Chain	Res	Type
2	C	700	GLU
2	C	701	ARG
2	C	704	LEU
2	C	705	GLU
2	C	711	ASP
2	C	721	GLU
2	C	722	ARG
2	C	724	THR
2	C	725	GLN
2	C	738	ASP
2	C	740	LEU
2	C	742	MET
2	C	750	ILE
2	C	751	ILE
2	C	754	SER
2	C	764	LYS
2	C	765	GLN
2	C	775	ASN
2	C	781	LYS
2	C	792	SER
2	C	795	LEU
2	C	798	ASP
2	C	802	THR
2	C	808	LEU
2	C	810	HIS
2	C	815	THR
2	C	816	VAL
2	C	822	GLU
2	C	825	ASN
2	C	826	PHE
2	C	830	LEU
2	C	841	LEU
2	C	853	ARG
2	C	865	HIS
2	C	869	VAL
2	C	876	THR
2	C	882	ASP
2	C	886	ARG
2	C	898	VAL
2	C	909	THR
2	C	925	TYR
2	B	565	ILE

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Mol	Chain	Res	Type
2	B	576	TRP
2	B	577	THR
2	B	585	ASN
2	B	587	THR
2	B	591	GLU
2	B	592	LEU
2	B	594	ASP
2	B	598	LEU
2	B	601	LEU
2	B	603	LEU
2	B	609	LEU
2	B	613	LYS
2	B	636	VAL
2	B	640	GLU
2	B	643	ARG
2	B	647	LEU
2	B	669	ASP
2	B	675	VAL
2	B	685	LEU
2	B	693	LEU
2	B	700	GLU
2	B	701	ARG
2	B	705	GLU
2	B	711	ASP
2	B	721	GLU
2	B	722	ARG
2	B	724	THR
2	B	725	GLN
2	B	738	ASP
2	B	740	LEU
2	B	742	MET
2	B	750	ILE
2	B	751	ILE
2	B	754	SER
2	B	764	LYS
2	B	765	GLN
2	B	775	ASN
2	B	781	LYS
2	B	792	SER
2	B	795	LEU
2	B	798	ASP
2	B	802	THR

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Mol	Chain	Res	Type
2	B	808	LEU
2	B	810	HIS
2	B	815	THR
2	B	816	VAL
2	B	822	GLU
2	B	825	ASN
2	B	826	PHE
2	B	830	LEU
2	B	841	LEU
2	B	853	ARG
2	B	865	HIS
2	B	869	VAL
2	B	876	THR
2	B	882	ASP
2	B	886	ARG
2	B	898	VAL
2	B	909	THR
2	B	925	TYR
1	H	6	THR
1	H	18	LYS
1	H	57	GLU
1	H	69	TYR
1	H	71	ILE
1	H	78	ASN
1	H	94	LEU
1	H	95	ARG
1	H	99	GLU
1	H	101	HIS
1	H	105	LEU
1	H	119	MET
1	H	120	THR
1	H	136	ILE
1	H	151	ILE
1	H	159	VAL
1	H	176	MET
1	H	179	ASP
1	H	200	PHE
1	H	202	THR
1	H	217	CYS
1	H	277	THR
1	H	280	ASN
1	H	288	ASP

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Mol	Chain	Res	Type
1	H	290	ARG
1	H	292	ASP
1	H	315	LYS
1	H	318	THR
1	H	326	LYS
1	H	334	GLU
1	H	338	SER
1	H	339	VAL
1	H	349	LEU
1	H	360	GLN
1	H	368	SER
1	H	370	VAL
1	H	372	ARG
1	G	6	THR
1	G	18	LYS
1	G	57	GLU
1	G	69	TYR
1	G	71	ILE
1	G	78	ASN
1	G	94	LEU
1	G	95	ARG
1	G	99	GLU
1	G	101	HIS
1	G	105	LEU
1	G	119	MET
1	G	120	THR
1	G	136	ILE
1	G	147	ARG
1	G	151	ILE
1	G	159	VAL
1	G	176	MET
1	G	179	ASP
1	G	200	PHE
1	G	202	THR
1	G	217	CYS
1	G	229	THR
1	G	277	THR
1	G	280	ASN
1	G	288	ASP
1	G	290	ARG
1	G	292	ASP
1	G	315	LYS

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Mol	Chain	Res	Type
1	G	318	THR
1	G	326	LYS
1	G	334	GLU
1	G	338	SER
1	G	339	VAL
1	G	349	LEU
1	G	360	GLN
1	G	368	SER
1	G	370	VAL
1	G	372	ARG
1	F	6	THR
1	F	18	LYS
1	F	28	ARG
1	F	57	GLU
1	F	66	THR
1	F	69	TYR
1	F	71	ILE
1	F	78	ASN
1	F	94	LEU
1	F	95	ARG
1	F	99	GLU
1	F	101	HIS
1	F	105	LEU
1	F	119	MET
1	F	120	THR
1	F	136	ILE
1	F	147	ARG
1	F	151	ILE
1	F	159	VAL
1	F	176	MET
1	F	179	ASP
1	F	200	PHE
1	F	202	THR
1	F	217	CYS
1	F	229	THR
1	F	277	THR
1	F	280	ASN
1	F	288	ASP
1	F	290	ARG
1	F	292	ASP
1	F	315	LYS
1	F	318	THR

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Mol	Chain	Res	Type
1	F	326	LYS
1	F	334	GLU
1	F	338	SER
1	F	339	VAL
1	F	349	LEU
1	F	351	THR
1	F	360	GLN
1	F	368	SER
1	F	370	VAL
1	F	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	HIS
1	D	137	GLN
2	A	746	GLN
2	E	746	GLN
2	C	746	GLN
2	B	746	GLN
1	H	101	HIS
1	G	101	HIS
1	F	101	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	H	401	-	1,3,3	1.07	0	0,3,3	0.00	-
3	ACT	E	1001	-	1,3,3	2.08	1 (100%)	0,3,3	0.00	-
3	ACT	A	1002	-	1,3,3	1.85	0	0,3,3	0.00	-
3	ACT	C	1002	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
4	ATP	H	402	-	26,33,33	1.10	3 (11%)	31,52,52	1.27	5 (16%)
3	ACT	C	1001	-	1,3,3	0.83	0	0,3,3	0.00	-
3	ACT	B	1001	-	1,3,3	1.29	0	0,3,3	0.00	-
4	ATP	G	402	-	26,33,33	0.99	1 (3%)	31,52,52	1.37	6 (19%)
4	ATP	D	402	-	26,33,33	0.89	0	31,52,52	1.42	6 (19%)
3	ACT	F	402	-	1,3,3	1.47	0	0,3,3	0.00	-
4	ATP	F	403	-	26,33,33	0.88	1 (3%)	31,52,52	1.26	3 (9%)
3	ACT	G	401	-	1,3,3	0.63	0	0,3,3	0.00	-
3	ACT	F	401	-	1,3,3	1.84	0	0,3,3	0.00	-
3	ACT	D	401	-	1,3,3	0.75	0	0,3,3	0.00	-
3	ACT	A	1003	-	1,3,3	1.80	0	0,3,3	0.00	-
3	ACT	A	1001	-	1,3,3	0.45	0	0,3,3	0.00	-

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	D	402	-	-	7/18/38/38	0/3/3/3
4	ATP	H	402	-	-	4/18/38/38	0/3/3/3
4	ATP	G	402	-	-	0/18/38/38	0/3/3/3
4	ATP	F	403	-	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	402	ATP	C5-C4	2.91	1.48	1.40
4	G	402	ATP	C5-C4	2.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	ACT	CH3-C	2.40	1.51	1.48
4	H	402	ATP	C2-N3	2.30	1.35	1.32
4	F	403	ATP	C5-C4	2.14	1.46	1.40
4	H	402	ATP	O4'-C1'	2.09	1.44	1.41
3	E	1001	ACT	CH3-C	2.08	1.51	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	ATP	C4-C5-N7	-3.51	105.74	109.40
4	G	402	ATP	C4-C5-N7	-3.34	105.92	109.40
4	D	402	ATP	N3-C2-N1	-3.28	123.54	128.68
4	D	402	ATP	C1'-N9-C4	-3.13	121.14	126.64
4	F	403	ATP	N3-C2-N1	-2.81	124.29	128.68
4	G	402	ATP	N3-C2-N1	-2.68	124.49	128.68
4	H	402	ATP	O3'-C3'-C2'	-2.51	103.69	111.82
4	H	402	ATP	C2'-C3'-C4'	2.39	107.29	102.64
4	H	402	ATP	C4-C5-N7	-2.32	106.98	109.40
4	F	403	ATP	N6-C6-N1	2.25	123.24	118.57
4	G	402	ATP	PB-O3B-PG	-2.24	125.15	132.83
4	H	402	ATP	N3-C2-N1	-2.21	125.22	128.68
4	H	402	ATP	C3'-C2'-C1'	2.19	104.27	100.98
4	G	402	ATP	C5-C6-N6	2.17	123.65	120.35
4	D	402	ATP	C5-C6-N6	2.17	123.65	120.35
4	D	402	ATP	C2-N1-C6	2.11	122.36	118.75
4	F	403	ATP	C4-C5-N7	-2.06	107.25	109.40
4	G	402	ATP	PA-O3A-PB	-2.03	125.88	132.83
4	G	402	ATP	C2-N1-C6	2.02	122.21	118.75
4	D	402	ATP	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	402	ATP	C5'-O5'-PA-O1A
4	H	402	ATP	C5'-O5'-PA-O2A
4	D	402	ATP	PG-O3B-PB-O3A
4	H	402	ATP	C5'-O5'-PA-O3A
4	D	402	ATP	PA-O3A-PB-O1B
4	D	402	ATP	PB-O3A-PA-O2A
4	D	402	ATP	C3'-C4'-C5'-O5'
4	D	402	ATP	O4'-C4'-C5'-O5'

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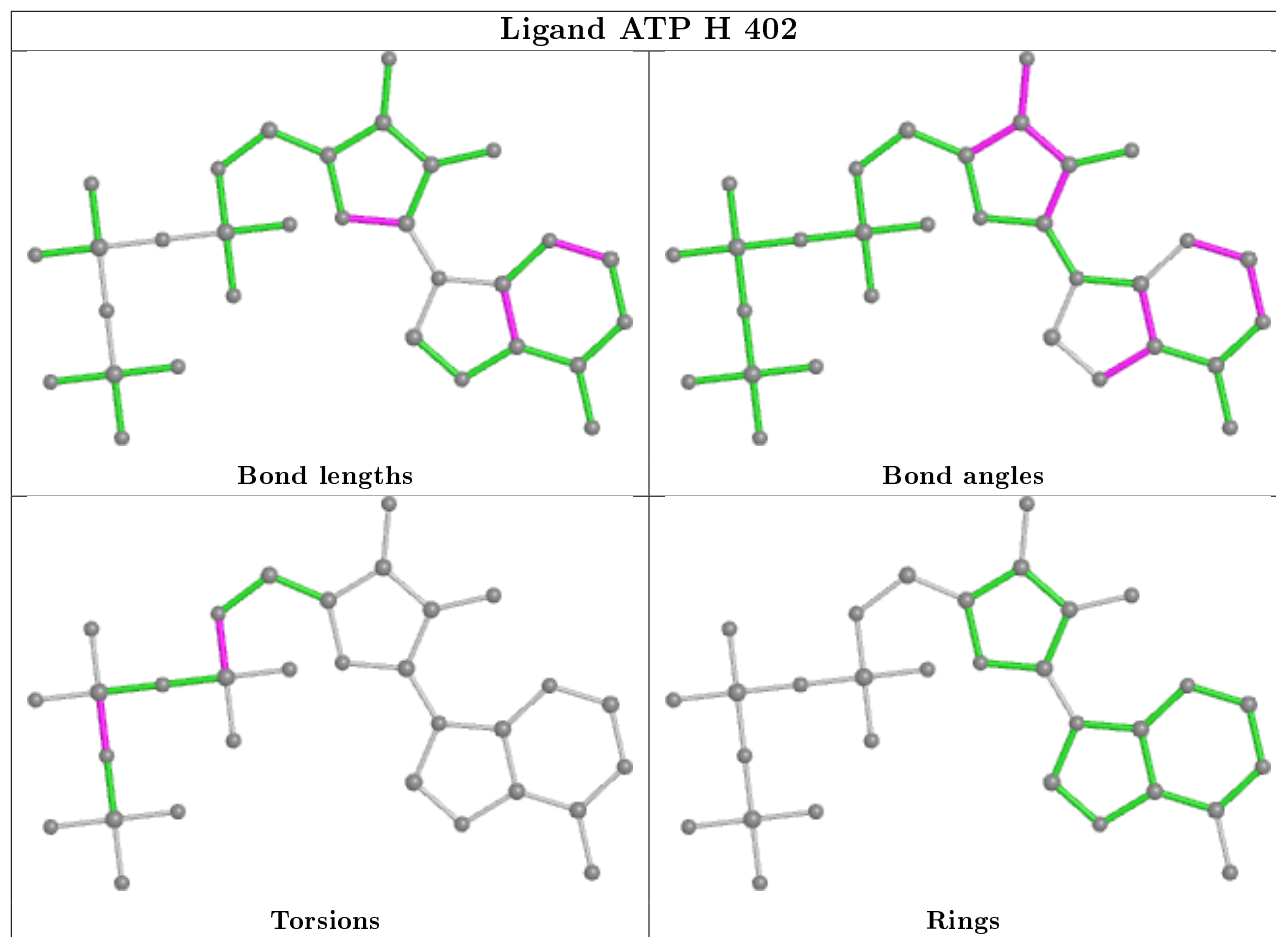
Mol	Chain	Res	Type	Atoms
4	H	402	ATP	PG-O3B-PB-O3A
4	D	402	ATP	PB-O3A-PA-O1A
4	D	402	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

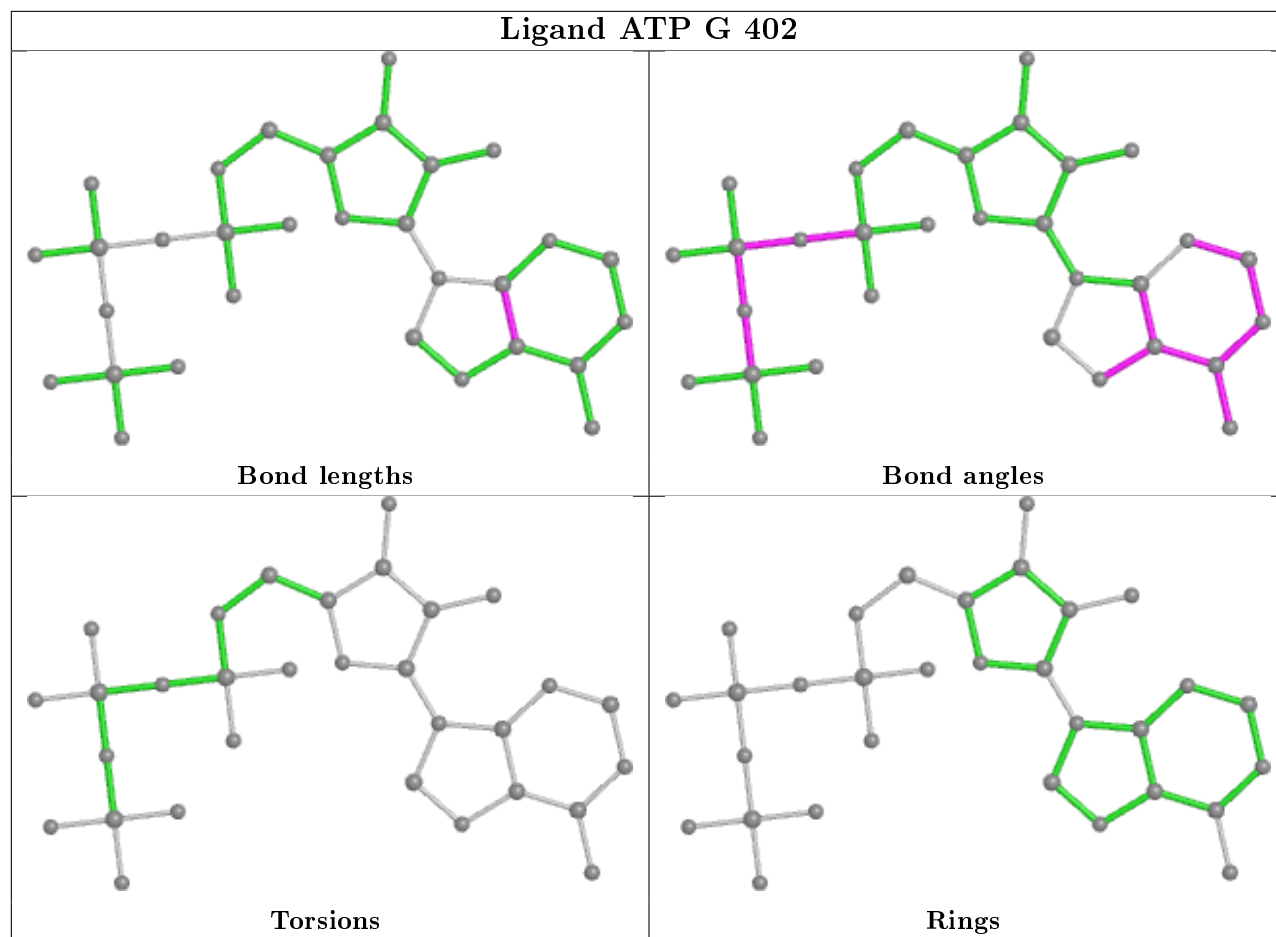
13 monomers are involved in 23 short contacts:

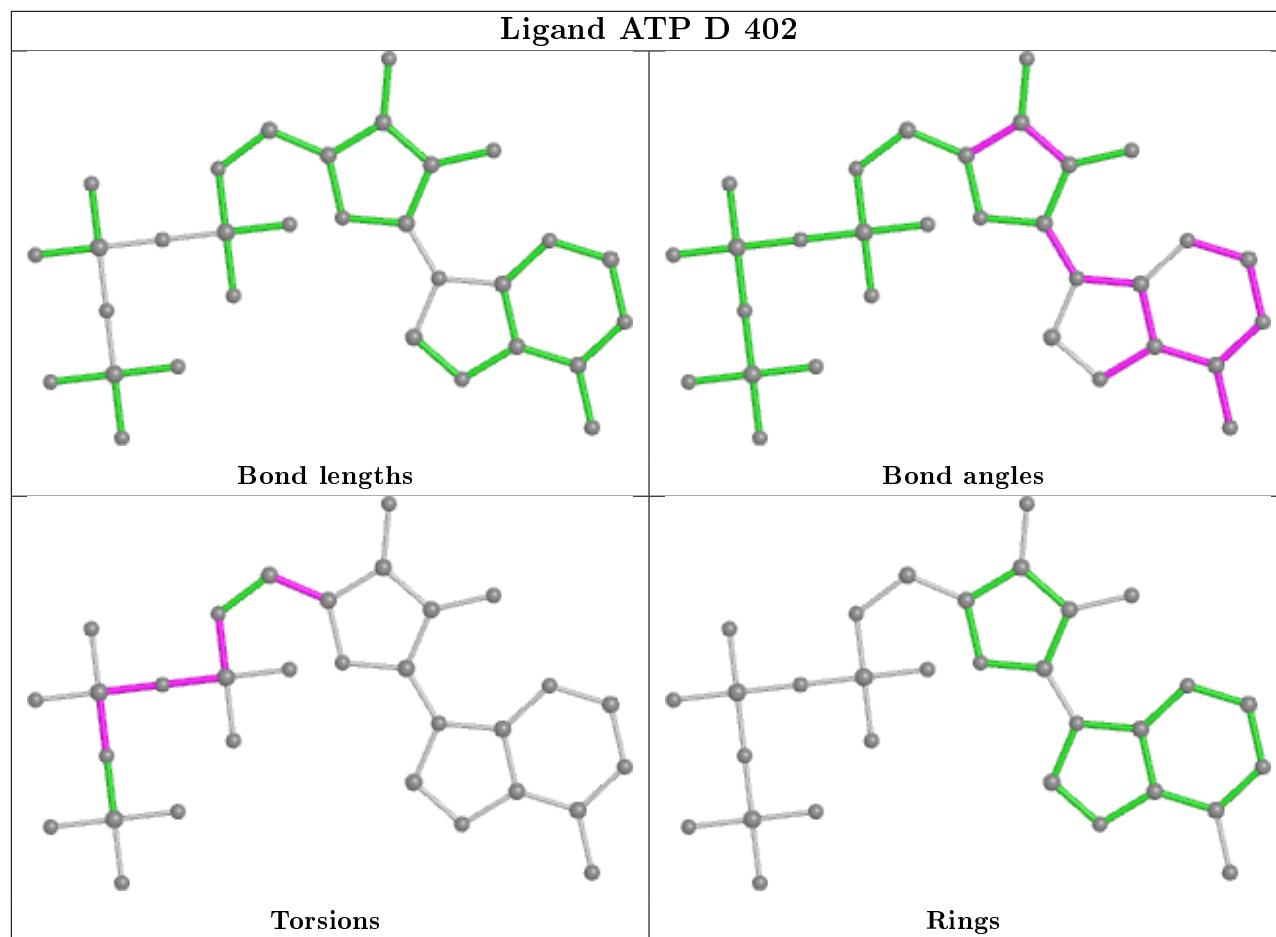
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	401	ACT	2	0
3	E	1001	ACT	1	0
3	C	1002	ACT	1	0
4	H	402	ATP	2	0
3	C	1001	ACT	1	0
3	B	1001	ACT	2	0
4	G	402	ATP	2	0
4	D	402	ATP	5	0
3	F	402	ACT	1	0
4	F	403	ATP	1	0
3	G	401	ACT	2	0
3	D	401	ACT	2	0
3	A	1003	ACT	1	0

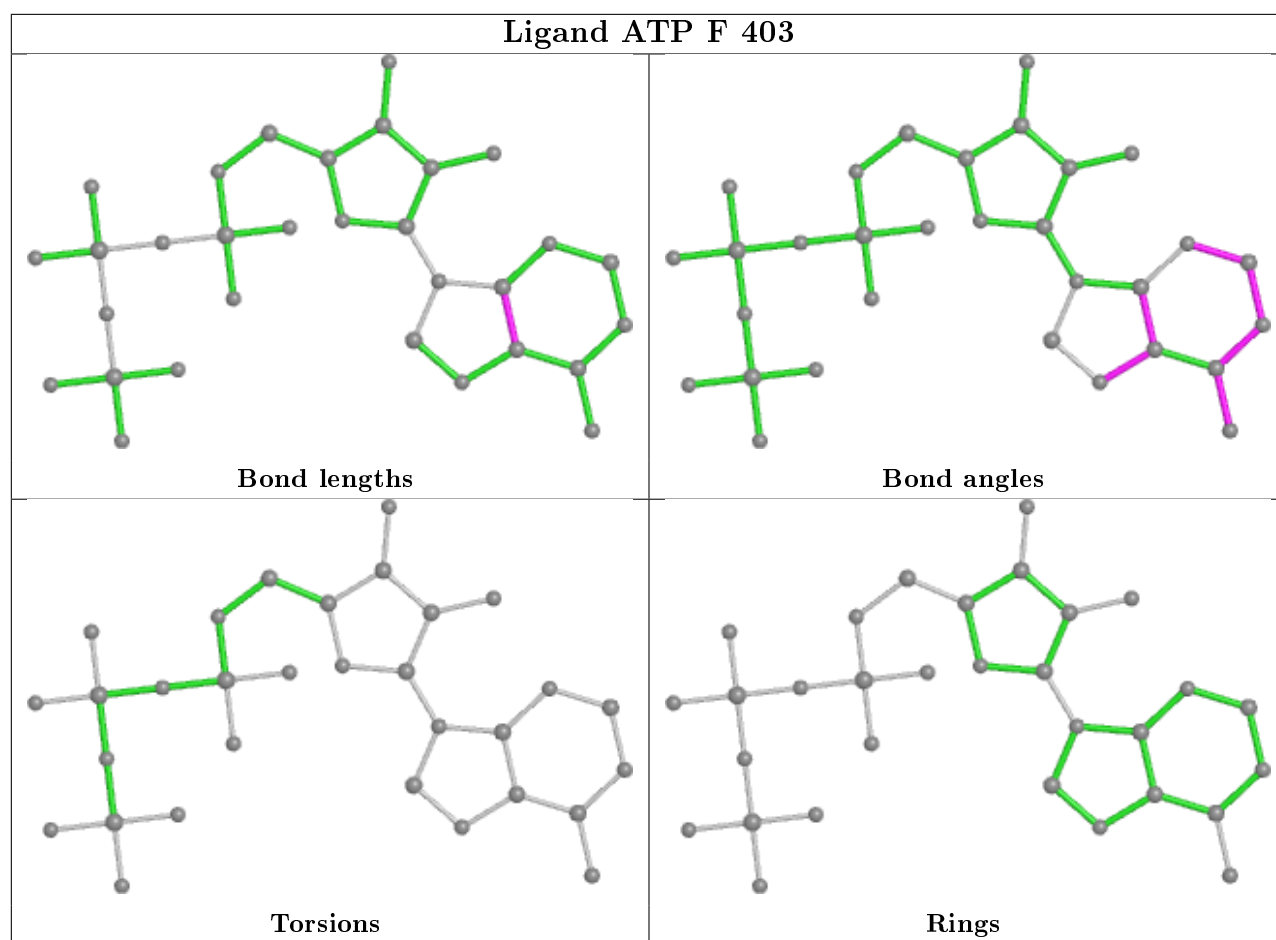
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	D	356/377 (94%)	0.00	1 (0%) 94 93	58, 95, 163, 191	33 (9%)
1	F	356/377 (94%)	0.03	3 (0%) 86 85	59, 95, 164, 190	15 (4%)
1	G	356/377 (94%)	-0.14	1 (0%) 94 93	61, 97, 165, 192	33 (9%)
1	H	356/377 (94%)	-0.03	5 (1%) 75 74	64, 97, 164, 194	28 (7%)
2	A	357/402 (88%)	-0.19	1 (0%) 94 93	64, 101, 144, 163	61 (17%)
2	B	357/402 (88%)	-0.24	0 100 100	64, 102, 144, 165	59 (16%)
2	C	357/402 (88%)	-0.16	0 100 100	65, 102, 144, 160	56 (15%)
2	E	357/402 (88%)	-0.26	1 (0%) 94 93	65, 102, 143, 161	62 (17%)
All	All	2852/3116 (91%)	-0.12	12 (0%) 92 92	58, 99, 156, 194	347 (12%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	52	SER	3.6
1	F	239	SER	3.0
2	A	780	SER	2.8
1	H	199	SER	2.8
1	H	245	GLY	2.6
2	E	703	PRO	2.3
1	G	53	TYR	2.3
1	D	53	TYR	2.2
1	H	39	ARG	2.2
1	F	240	TYR	2.1
1	H	32	PRO	2.1
1	F	241	GLU	2.1

## 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

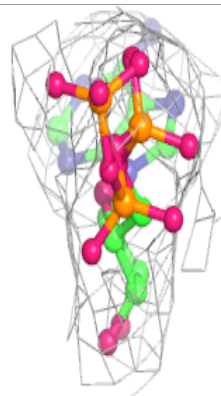
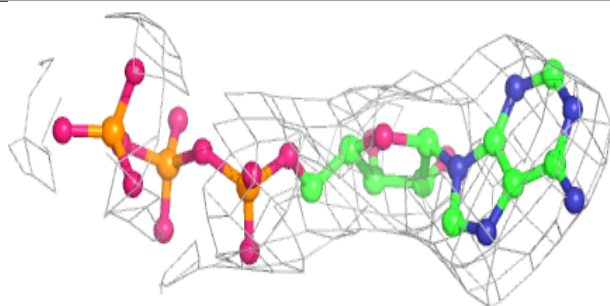
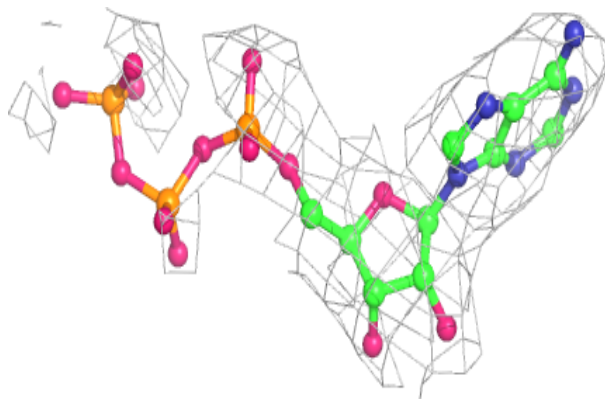
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	ACT	F	401	4/4	0.79	0.45	88,111,123,124	0
3	ACT	C	1002	4/4	0.89	0.21	69,89,92,102	0
3	ACT	F	402	4/4	0.90	0.27	78,80,106,107	0
3	ACT	A	1002	4/4	0.92	0.21	80,96,99,103	0
3	ACT	E	1001	4/4	0.92	0.54	73,103,103,103	0
3	ACT	C	1001	4/4	0.93	0.20	75,88,90,100	0
3	ACT	B	1001	4/4	0.93	0.17	75,94,95,97	0
3	ACT	H	401	4/4	0.94	0.34	70,89,100,122	0
3	ACT	A	1001	4/4	0.94	0.22	72,74,83,89	0
3	ACT	A	1003	4/4	0.95	0.18	81,83,97,104	0
4	ATP	H	402	31/31	0.95	0.17	85,109,122,133	0
4	ATP	G	402	31/31	0.96	0.19	73,104,119,122	0
3	ACT	D	401	4/4	0.97	0.26	62,66,91,110	0
3	ACT	G	401	4/4	0.97	0.26	84,88,105,122	0
4	ATP	F	403	31/31	0.97	0.18	70,91,110,116	0
4	ATP	D	402	31/31	0.98	0.21	53,86,104,106	0

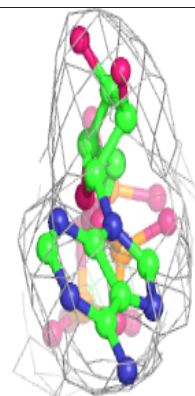
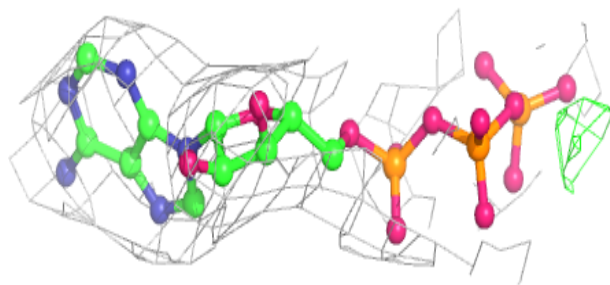
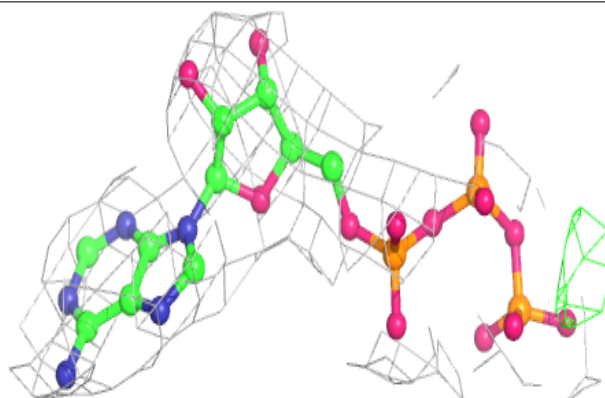
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP H 402:**

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

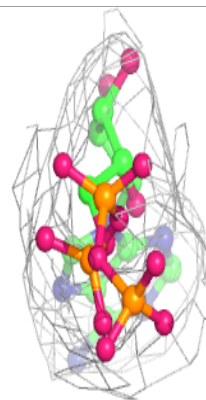
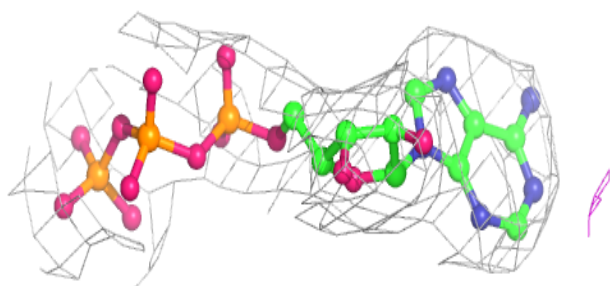
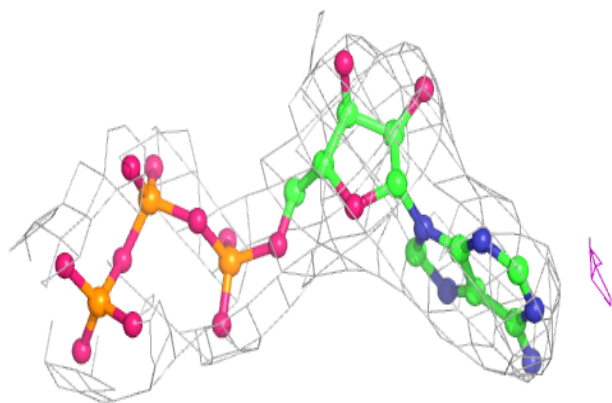
**Electron density around ATP G 402:**

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

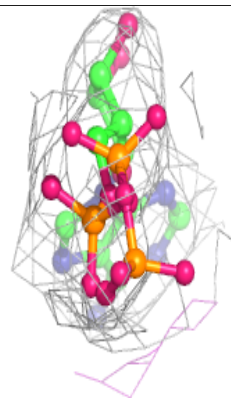
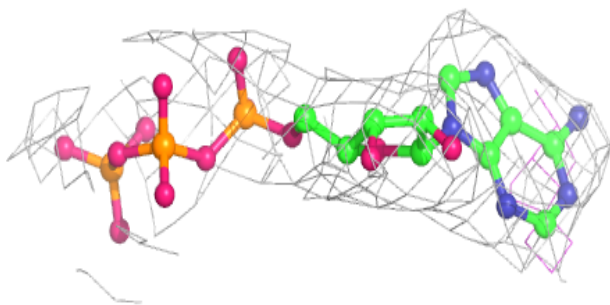
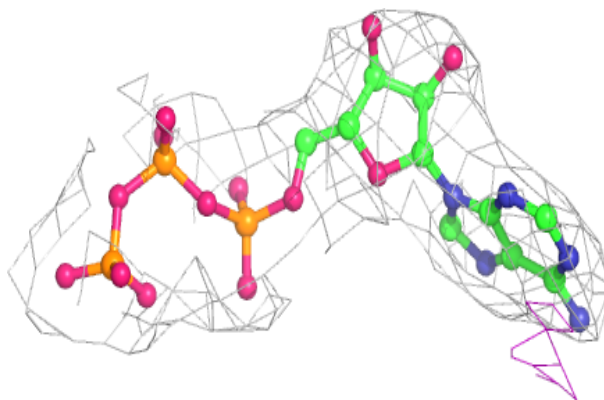


**Electron density around ATP F 403:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP D 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.