



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:54 PM BST

PDB ID : 5IT5  
Title : Thermus thermophilus PilB core ATPase region  
Authors : Mancl, J.; Robinson, H.; Black, W.; Yang, Z.; Schubot, F.  
Deposited on : 2016-03-16  
Resolution : 2.65 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

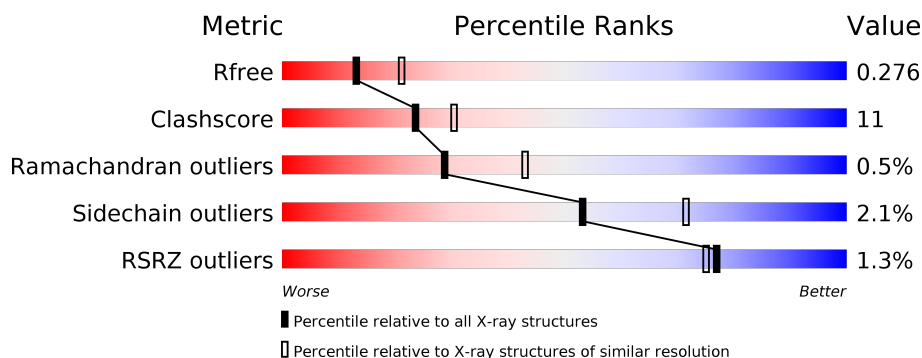
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	385	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>••</div> </div> </div>
1	B	385	<div> <div></div> <div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
1	C	385	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>•</div> </div> </div>
1	D	385	<div> <div></div> <div> <div></div> <div>78%</div> <div>21%</div> <div>•</div> </div> </div>
1	E	385	<div> <div></div> <div> <div></div> <div>74%</div> <div>25%</div> <div>•</div> </div> </div>
1	F	385	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>•</div> </div> </div>

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
5	MG	B	903	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18466 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 ATP binding motif-containing protein PilF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	385	Total	C	N	O	S	0	0	0
			2983	1879	536	558	10			
1	A	385	Total	C	N	O	S	0	0	0
			2984	1879	536	559	10			
1	B	385	Total	C	N	O	S	0	0	0
			2984	1879	536	559	10			
1	E	385	Total	C	N	O	S	0	0	0
			2984	1879	536	559	10			
1	C	385	Total	C	N	O	S	0	0	0
			2984	1879	536	559	10			
1	D	385	Total	C	N	O	S	0	0	0
			2984	1879	536	559	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

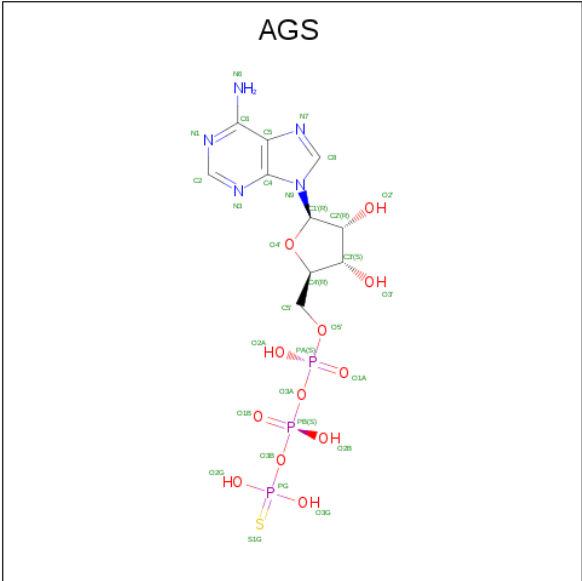
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	
			31	10	5	12	3	1	
4	C	1	Total	C	N	O	P	S	
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	
			31	10	5	12	3	1	

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg		
			1	1	0	0
5	E	1	Total	Mg		
			1	1	0	0

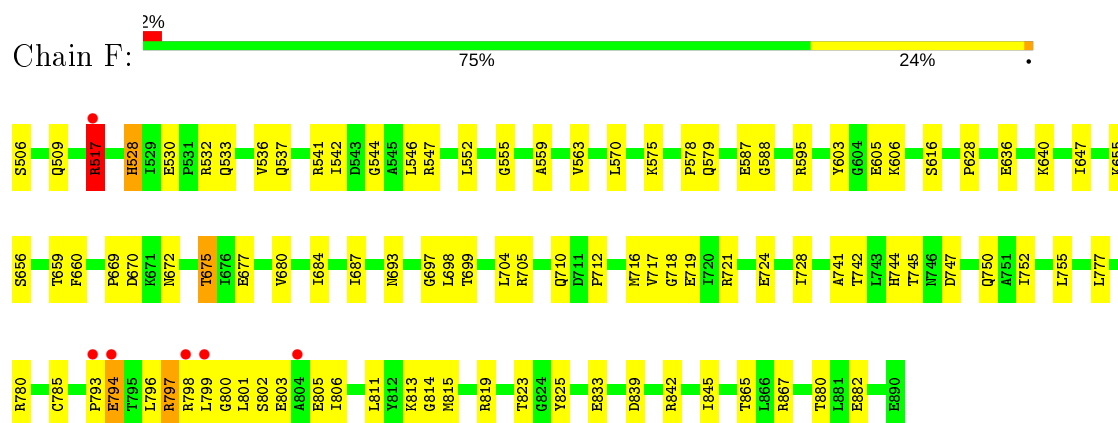
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	59	Total	O		
			59	59	0	0
6	A	69	Total	O		
			69	69	0	0
6	B	64	Total	O		
			64	64	0	0
6	E	55	Total	O		
			55	55	0	0
6	C	50	Total	O		
			50	50	0	0
6	D	72	Total	O		
			72	72	0	0

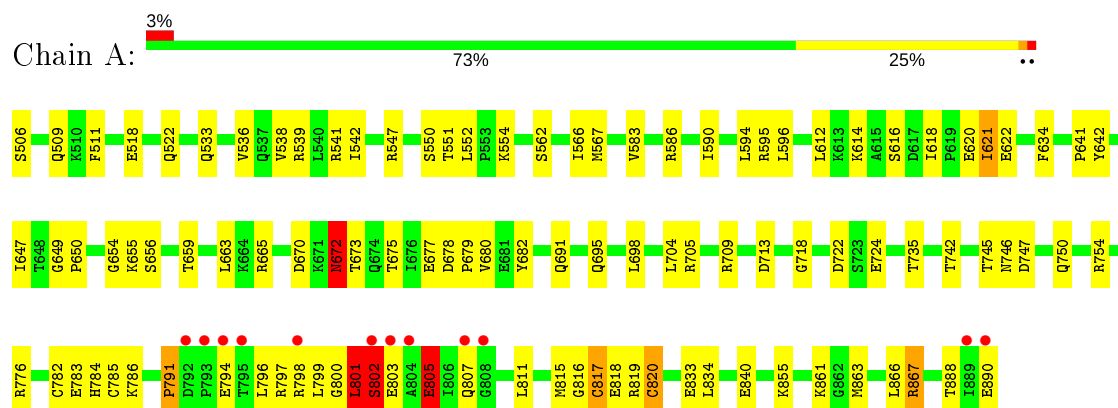
### 3 Residue-property plots

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.

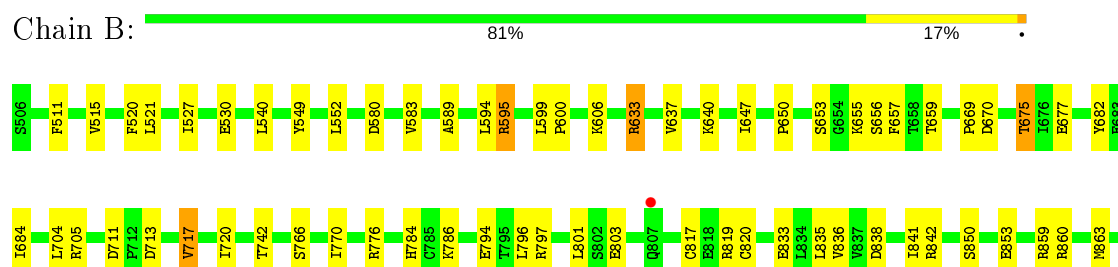
#### • Molecule 1: ATP binding motif-containing protein PilF



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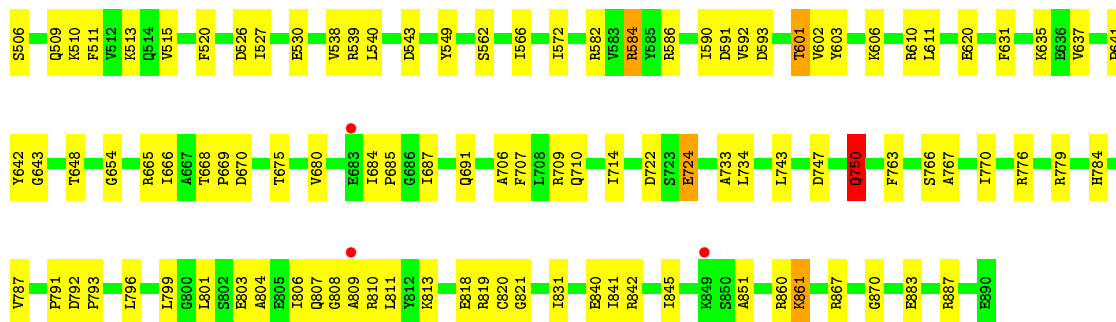
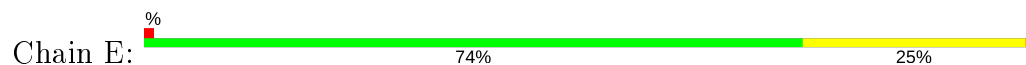


#### • Molecule 1: ATP binding motif-containing protein PilF

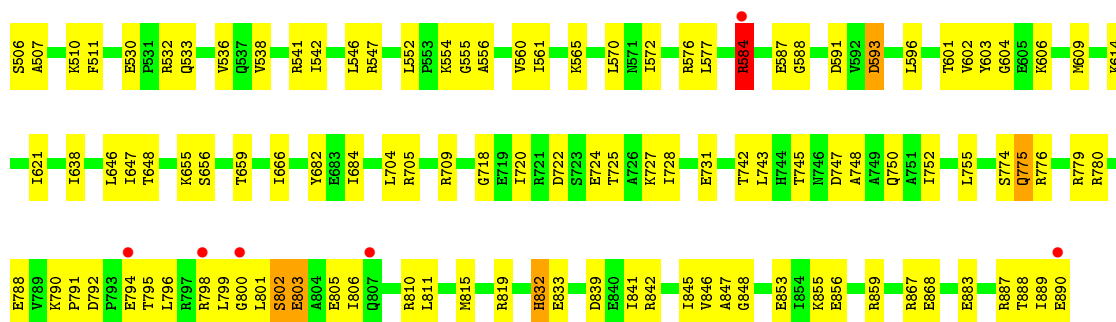




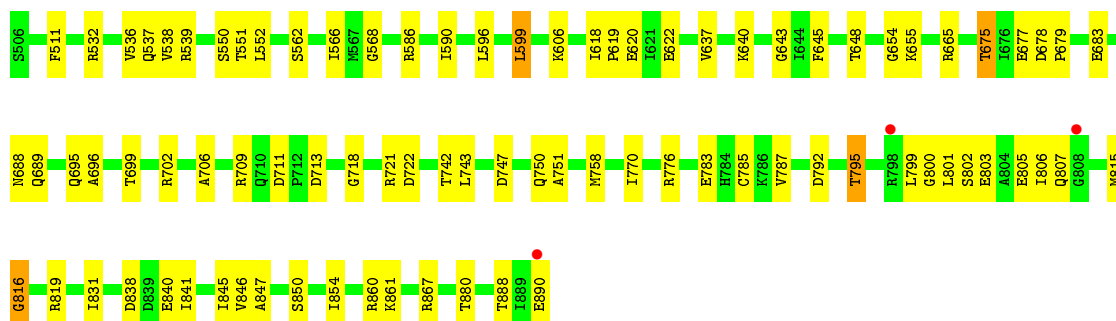
• Molecule 1: ATP binding motif-containing protein PilF



• Molecule 1: ATP binding motif-containing protein PilF



• Molecule 1: ATP binding motif-containing protein PilF





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.55Å 133.56Å 208.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.29 – 2.65 65.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.29-2.65) 91.0 (65.29-2.65)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.208 , 0.274 0.214 , 0.276	Depositor DCC
$R_{free}$ test set	2843 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.628	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7028e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, ZN, 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	0.53	2/3026 (0.1%)	0.68	2/4085 (0.0%)
1	B	0.50	0/3026	0.61	0/4085
1	C	0.52	1/3026 (0.0%)	0.68	2/4085 (0.0%)
1	D	0.49	0/3026	0.63	0/4085
1	E	0.51	0/3026	0.66	1/4085 (0.0%)
1	F	0.55	1/3025 (0.0%)	0.75	4/4084 (0.1%)
All	All	0.52	4/18155 (0.0%)	0.67	9/24509 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	794	GLU	CB-CG	-6.49	1.39	1.52
1	A	805	GLU	CG-CD	-5.77	1.43	1.51
1	C	775	GLN	CD-NE2	5.24	1.46	1.32
1	A	820	CYS	CB-SG	-5.08	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	797	ARG	NE-CZ-NH1	-10.49	115.05	120.30
1	A	801	LEU	CA-CB-CG	9.36	136.82	115.30
1	F	797	ARG	NE-CZ-NH2	9.27	124.94	120.30
1	E	750	GLN	CA-CB-CG	-7.82	96.20	113.40
1	F	517	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	584	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	672	ASN	CB-CA-C	-5.50	99.39	110.40
1	F	517	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	584	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	672	ASN	Sidechain
1	A	801	LEU	Peptide
1	C	832	HIS	Sidechain
1	E	750	GLN	Sidechain
1	F	528	HIS	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2984	0	3086	81	0
1	B	2984	0	3083	60	0
1	C	2984	0	3082	86	0
1	D	2984	0	3082	62	0
1	E	2984	0	3082	71	0
1	F	2983	0	3079	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	F	31	0	12	1	0
4	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	5	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
4	E	31	0	12	1	0
5	B	1	0	0	2	0
5	E	1	0	0	0	0
6	A	69	0	0	8	0
6	B	64	0	0	3	0
6	C	50	0	0	4	0
6	D	72	0	0	5	0
6	E	55	0	0	3	0
6	F	59	0	0	6	0
All	All	18466	0	18566	409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (409) 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:F:656:SER:CB	3:F:902:ATP:O2G	1.76	1.34
1:C:801:LEU:HG	1:C:805:GLU:HG3	1.35	1.05
1:B:595:ARG:NH2	4:B:901:AGS:S1G	2.34	1.01
1:F:880:THR:HG22	1:F:882:GLU:H	1.35	0.91
1:A:705:ARG:NH2	1:A:724:GLU:OE2	2.03	0.91
1:E:586:ARG:HG3	1:E:591:ASP:HB3	1.56	0.86
1:C:839:ASP:O	6:C:1001:HOH:O	1.93	0.85
4:B:901:AGS:H8	4:B:901:AGS:H5'1	1.59	0.85
1:C:792:ASP:OD1	1:C:794:GLU:HG2	1.75	0.84
1:E:601:THR:HG22	1:E:603:TYR:H	1.43	0.83
1:D:880:THR:OG1	6:D:1001:HOH:O	1.96	0.82
1:D:678:ASP:OD2	1:D:721:ARG:NH2	2.13	0.82
1:B:530:GLU:HG2	1:B:606:LYS:HE3	1.62	0.81
1:A:541:ARG:NH1	1:B:711:ASP:OD2	2.14	0.81
1:E:684:ILE:HD12	1:E:685:PRO:HD2	1.63	0.80
1:E:530:GLU:HG2	1:E:606:LYS:HE3	1.64	0.79
1:A:785:CYS:SG	1:A:815:MET:N	2.55	0.79
1:A:647:ILE:HG22	1:A:655:LYS:HG2	1.65	0.78
1:E:840:GLU:OE1	1:E:861:LYS:NZ	2.17	0.78
1:C:647:ILE:HD12	1:C:659:THR:HG22	1.66	0.77
1:F:797:ARG:HH11	1:F:806:ILE:HD12	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:CYS:SG	1:A:816:GLY:N	2.58	0.75
1:A:541:ARG:NH2	1:B:713:ASP:OD2	2.18	0.75
1:B:705:ARG:NH1	6:B:1001:HOH:O	2.18	0.75
4:B:901:AGS:O2G	4:B:901:AGS:O2B	2.04	0.75
1:F:541:ARG:NH2	1:A:713:ASP:OD2	2.19	0.74
1:F:796:LEU:HG	1:F:801:LEU:HD23	1.69	0.74
1:F:796:LEU:HD23	1:F:806:ILE:HG23	1.70	0.73
1:D:648:THR:HG22	1:D:743:LEU:HB3	1.70	0.72
1:C:541:ARG:NH2	1:D:713:ASP:OD2	2.23	0.72
1:D:622:GLU:OE1	1:D:665:ARG:NH2	2.20	0.71
1:C:656:SER:OG	4:C:901:AGS:S1G	2.48	0.71
1:D:675:THR:HG23	1:D:677:GLU:HG3	1.73	0.71
1:F:517:ARG:HH11	1:F:517:ARG:HG3	1.56	0.71
1:C:541:ARG:NH1	1:D:711:ASP:OD2	2.23	0.70
1:B:859:ARG:NH2	1:B:868:GLU:OE2	2.25	0.70
1:F:647:ILE:HD12	1:F:659:THR:HG22	1.71	0.70
1:E:509:GLN:NE2	6:E:1004:HOH:O	2.25	0.70
1:A:614:LYS:O	6:A:1001:HOH:O	2.11	0.69
1:B:650:PRO:O	1:B:653:SER:OG	2.11	0.69
1:B:655:LYS:HD2	1:B:742:THR:HG23	1.76	0.68
1:E:648:THR:HG22	1:E:743:LEU:HB2	1.76	0.68
1:E:543:ASP:OD1	6:E:1001:HOH:O	2.12	0.67
1:A:620:GLU:OE1	6:A:1002:HOH:O	2.13	0.67
1:A:672:ASN:HD22	1:A:673:THR:N	1.93	0.67
1:F:640:LYS:NZ	6:F:1003:HOH:O	2.27	0.67
1:A:695:GLN:OE1	6:A:1003:HOH:O	2.13	0.66
1:C:705:ARG:NH2	1:C:724:GLU:OE2	2.27	0.66
1:C:576:ARG:HH21	1:D:695:GLN:NE2	1.95	0.65
1:B:640:LYS:HG3	1:B:770:ILE:HG21	1.79	0.65
1:C:801:LEU:HB3	1:C:806:ILE:HD11	1.78	0.65
1:C:799:LEU:O	1:C:801:LEU:N	2.31	0.64
1:E:526:ASP:OD1	1:E:610:ARG:NE	2.22	0.64
1:E:766:SER:OG	1:E:842:ARG:HB2	1.98	0.63
1:C:803:GLU:HA	1:C:806:ILE:HG12	1.80	0.63
1:D:819:ARG:NH2	6:D:1002:HOH:O	2.10	0.63
1:E:620:GLU:HG3	1:E:665:ARG:HH21	1.64	0.63
1:F:530:GLU:HG2	1:F:606:LYS:HE3	1.80	0.62
1:B:801:LEU:HD11	1:B:875:LEU:HD11	1.81	0.62
1:C:888:THR:OG1	1:C:890:GLU:O	2.11	0.62
1:E:566:ILE:HD11	1:E:572:ILE:HD11	1.82	0.62
1:C:745:THR:HG22	1:C:747:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:710:GLN:HE21	1:D:606:LYS:HD3	1.65	0.61
1:E:806:ILE:O	1:E:809:ALA:HB2	2.00	0.61
1:E:799:LEU:HD22	1:E:867:ARG:HD3	1.83	0.61
1:F:528:HIS:HD2	1:F:546:LEU:HD21	1.65	0.61
1:A:518:GLU:OE1	1:A:522:GLN:NE2	2.32	0.61
1:B:656:SER:OG	5:B:903:MG:MG	1.42	0.61
1:C:747:ASP:OD1	1:C:748:ALA:N	2.33	0.61
1:C:752:ILE:HG21	1:C:845:ILE:HD12	1.82	0.61
1:A:784:HIS:CD2	1:A:819:ARG:HD2	2.35	0.61
1:A:622:GLU:OE1	1:A:665:ARG:NH2	2.29	0.60
1:C:747:ASP:OD1	6:C:1002:HOH:O	2.16	0.60
1:A:567:MET:HB3	1:A:583:VAL:HG11	1.82	0.60
1:C:648:THR:HG22	1:C:743:LEU:HB3	1.83	0.60
1:C:655:LYS:O	1:C:659:THR:HG23	2.02	0.59
1:C:565:LYS:HE3	1:C:572:ILE:HA	1.84	0.59
1:C:536:VAL:HB	1:C:552:LEU:HB2	1.83	0.59
4:B:901:AGS:C8	4:B:901:AGS:H5'1	2.32	0.59
1:C:591:ASP:O	1:C:614:LYS:NZ	2.24	0.59
1:B:595:ARG:CG	1:B:595:ARG:HH11	2.16	0.59
1:E:592:VAL:HG21	1:E:611:LEU:HD23	1.84	0.59
1:C:722:ASP:HB2	1:C:725:THR:H	1.66	0.59
1:E:722:ASP:HB3	1:E:724:GLU:HG3	1.85	0.59
1:A:796:LEU:O	1:A:801:LEU:HG	2.03	0.58
1:C:839:ASP:OD1	1:C:842:ARG:NH1	2.36	0.58
1:E:804:ALA:HA	1:E:807:GLN:HE22	1.67	0.58
1:F:570:LEU:HB3	1:F:579:GLN:HE21	1.67	0.58
1:C:532:ARG:O	1:C:554:LYS:NZ	2.37	0.58
1:E:527:ILE:HG12	1:E:540:LEU:HD22	1.83	0.58
1:B:883:GLU:OE1	1:B:887:ARG:NH2	2.37	0.58
1:C:601:THR:HB	1:C:604:GLY:O	2.04	0.58
1:A:745:THR:HG23	1:A:750:GLN:HB2	1.85	0.58
1:B:583:VAL:HG22	1:B:594:LEU:HB2	1.85	0.58
1:A:801:LEU:HB2	1:A:805:GLU:OE1	2.03	0.58
1:A:791:PRO:HB3	1:A:811:LEU:HD12	1.85	0.58
1:D:867:ARG:HB2	1:D:890:GLU:HA	1.86	0.58
1:A:672:ASN:HD22	1:A:672:ASN:C	2.08	0.57
1:F:647:ILE:HG22	1:F:655:LYS:HG2	1.85	0.57
1:A:745:THR:HG22	1:A:747:ASP:O	2.04	0.57
1:A:649:GLY:HA2	1:A:776:ARG:HH21	1.69	0.57
1:A:782:CYS:SG	1:A:820:CYS:SG	3.02	0.57
1:B:595:ARG:HG3	1:B:595:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:PRO:HB3	1:C:811:LEU:HD12	1.85	0.57
1:E:631:PHE:CE2	1:E:635:LYS:HD3	2.40	0.57
1:F:570:LEU:HB3	1:F:579:GLN:NE2	2.20	0.57
1:C:722:ASP:HB2	1:C:725:THR:HG23	1.85	0.57
1:F:542:ILE:HD12	1:F:547:ARG:HD2	1.86	0.57
1:B:838:ASP:O	1:B:842:ARG:HG3	2.05	0.56
1:B:656:SER:HG	5:B:903:MG:MG	1.13	0.56
1:C:638:ILE:O	1:C:666:ILE:HD11	2.06	0.56
1:C:796:LEU:HB3	1:C:806:ILE:HD12	1.88	0.56
1:C:530:GLU:HG2	1:C:606:LYS:HE3	1.87	0.56
1:C:682:TYR:HE1	1:C:684:ILE:HD11	1.71	0.56
1:D:840:GLU:OE2	1:D:861:LYS:NZ	2.34	0.56
1:E:669:PRO:O	1:D:539:ARG:NH1	2.39	0.56
1:D:840:GLU:OE1	1:D:860:ARG:NH2	2.39	0.55
1:D:620:GLU:HG3	1:D:665:ARG:HH21	1.70	0.55
1:F:672:ASN:HD22	1:F:712:PRO:HA	1.71	0.55
1:F:880:THR:HG22	1:F:882:GLU:N	2.13	0.55
1:C:511:PHE:HZ	1:C:538:VAL:HG21	1.72	0.55
1:E:750:GLN:HG2	1:E:851:ALA:CB	2.35	0.55
1:B:835:LEU:HB2	1:B:863:MET:HE3	1.87	0.55
1:C:606:LYS:HD2	1:D:688:ASN:ND2	2.22	0.55
1:C:532:ARG:NH1	1:D:688:ASN:OD1	2.36	0.55
1:E:818:GLU:CD	1:E:821:GLY:HA2	2.27	0.54
1:B:655:LYS:O	1:B:659:THR:HG23	2.07	0.54
1:C:888:THR:OG1	1:C:889:ILE:N	2.38	0.54
1:F:794:GLU:HG2	1:F:797:ARG:HG2	1.89	0.54
1:F:570:LEU:HD23	1:F:579:GLN:HB3	1.90	0.54
1:B:589:ALA:HB3	6:B:1063:HOH:O	2.06	0.54
1:C:506:SER:OG	1:C:507:ALA:N	2.40	0.54
1:C:646:LEU:HD11	1:C:755:LEU:HD11	1.89	0.54
1:C:555:GLY:O	6:C:1003:HOH:O	2.18	0.54
1:E:818:GLU:HG3	1:E:818:GLU:O	2.08	0.54
1:E:620:GLU:HG3	1:E:665:ARG:NH2	2.23	0.54
1:F:528:HIS:CD2	1:F:546:LEU:HD21	2.43	0.54
1:A:614:LYS:N	6:A:1001:HOH:O	2.37	0.54
1:B:889:ILE:HG21	1:C:731:GLU:HB2	1.89	0.54
1:B:520:PHE:HD2	1:B:521:LEU:HD12	1.72	0.53
1:A:595:ARG:HE	1:A:612:LEU:HD11	1.74	0.53
1:A:550:SER:OG	1:A:551:THR:N	2.41	0.53
1:C:779:ARG:H	1:C:883:GLU:HG2	1.72	0.53
1:A:797:ARG:HD3	1:A:803:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:THR:CG2	1:D:677:GLU:HG3	2.39	0.53
1:F:595:ARG:HH22	1:A:709:ARG:HG2	1.73	0.53
1:B:647:ILE:HG22	1:B:655:LYS:HG2	1.90	0.53
1:B:784:HIS:ND1	1:B:819:ARG:HG3	2.24	0.53
1:A:794:GLU:O	1:A:798:ARG:HG2	2.07	0.53
1:E:747:ASP:HB3	1:E:750:GLN:HB2	1.91	0.53
1:F:578:PRO:HD3	1:A:698:LEU:HD13	1.91	0.53
1:E:804:ALA:CA	1:E:807:GLN:HE22	2.22	0.53
1:B:670:ASP:OD1	1:B:670:ASP:N	2.41	0.53
1:E:641:PRO:HB2	1:E:642:TYR:CD1	2.44	0.53
1:E:648:THR:CG2	1:E:743:LEU:HB2	2.38	0.53
1:B:633:ARG:O	1:B:637:VAL:HG23	2.08	0.52
1:D:640:LYS:HD2	1:D:770:ILE:HG23	1.90	0.52
1:C:542:ILE:HD12	1:C:547:ARG:HD2	1.92	0.52
1:A:833:GLU:HB2	1:A:866:LEU:HG	1.91	0.52
1:D:792:ASP:O	1:D:795:THR:HG22	2.09	0.52
1:F:536:VAL:HB	1:F:552:LEU:HB2	1.90	0.52
1:E:509:GLN:O	1:E:513:LYS:HD3	2.09	0.52
1:A:641:PRO:HB2	1:A:642:TYR:CD2	2.45	0.52
1:A:785:CYS:HG	1:A:816:GLY:H	1.56	0.52
1:B:647:ILE:HD13	1:B:659:THR:HG22	1.92	0.51
1:F:587:GLU:HG2	1:F:588:GLY:N	2.13	0.51
1:C:775:GLN:HE21	1:C:832:HIS:CE1	2.28	0.51
1:F:669:PRO:O	1:E:539:ARG:NH1	2.44	0.51
1:A:622:GLU:CD	1:A:665:ARG:HH22	2.14	0.51
1:D:816:GLY:N	6:D:1015:HOH:O	2.44	0.51
1:E:582:ARG:NH2	6:E:1010:HOH:O	2.42	0.51
1:C:802:SER:O	1:C:805:GLU:HG2	2.11	0.51
1:C:792:ASP:CG	1:C:794:GLU:HG2	2.30	0.51
1:E:684:ILE:HG23	1:E:687:ILE:HD11	1.93	0.51
1:E:779:ARG:HD3	1:E:883:GLU:OE2	2.10	0.51
1:F:704:LEU:HB3	1:F:728:ILE:HG21	1.93	0.51
1:B:595:ARG:CG	1:B:595:ARG:NH1	2.74	0.51
1:B:675:THR:HG21	1:B:677:GLU:OE2	2.11	0.51
1:D:568:GLY:HA3	1:D:596:LEU:HD12	1.93	0.50
1:F:796:LEU:HG	1:F:801:LEU:CD2	2.38	0.50
1:A:562:SER:O	1:A:566:ILE:HG12	2.11	0.50
1:C:606:LYS:HD2	1:D:688:ASN:HD22	1.76	0.50
1:E:818:GLU:HA	1:E:821:GLY:H	1.75	0.50
1:D:721:ARG:NE	6:D:1014:HOH:O	2.44	0.50
1:D:785:CYS:HB3	1:D:815:MET:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:776:ARG:HG2	1:C:887:ARG:HB3	1.94	0.50
1:B:599:LEU:HD12	1:B:600:PRO:HD2	1.93	0.50
1:E:520:PHE:CD1	1:E:590:ILE:HG22	2.46	0.50
1:F:506:SER:HB3	1:F:509:GLN:H	1.75	0.50
1:A:805:GLU:HG2	1:A:805:GLU:O	2.12	0.50
1:C:561:ILE:HG22	1:C:565:LYS:HE2	1.94	0.49
1:E:515:VAL:HG22	1:E:549:TYR:CE2	2.47	0.49
1:B:647:ILE:CD1	1:B:659:THR:HG22	2.42	0.49
1:A:583:VAL:HG22	1:A:594:LEU:HB2	1.94	0.49
1:E:722:ASP:CB	1:E:724:GLU:HG3	2.42	0.49
1:A:817:CYS:SG	1:A:818:GLU:N	2.86	0.49
1:B:580:ASP:OD1	1:C:709:ARG:HD2	2.12	0.49
1:E:707:PHE:CE1	1:D:599:LEU:HD11	2.47	0.49
1:A:782:CYS:HA	6:A:1035:HOH:O	2.12	0.49
1:A:784:HIS:NE2	1:A:819:ARG:HD2	2.28	0.49
1:B:838:ASP:OD1	1:B:841:ILE:HG12	2.13	0.49
1:E:706:ALA:HA	1:E:709:ARG:NH1	2.28	0.49
1:F:541:ARG:NH1	1:F:544:GLY:O	2.45	0.49
1:E:883:GLU:OE2	1:E:887:ARG:NH2	2.45	0.49
1:F:785:CYS:HB2	1:F:815:MET:HB2	1.94	0.49
1:B:527:ILE:HG12	1:B:540:LEU:CD2	2.43	0.49
1:C:565:LYS:HA	1:C:570:LEU:HD12	1.95	0.49
1:E:841:ILE:O	1:E:845:ILE:HG13	2.13	0.49
1:B:794:GLU:HG3	1:C:847:ALA:HB2	1.94	0.48
1:C:795:THR:O	1:C:796:LEU:HB2	2.12	0.48
1:E:668:THR:OG1	1:E:670:ASP:OD1	2.22	0.48
1:C:792:ASP:C	1:C:792:ASP:OD1	2.52	0.48
1:F:745:THR:CG2	1:F:750:GLN:HB2	2.43	0.48
1:A:533:GLN:O	1:A:554:LYS:HD2	2.14	0.48
1:A:586:ARG:HA	1:A:590:ILE:O	2.14	0.48
1:A:680:VAL:H	1:A:691:GLN:HG3	1.78	0.48
1:E:776:ARG:HB3	1:E:887:ARG:HG2	1.96	0.48
1:A:799:LEU:O	1:A:801:LEU:N	2.47	0.48
1:A:656:SER:HB2	4:A:901:AGS:O2A	2.14	0.48
1:B:640:LYS:HG3	1:B:770:ILE:CG2	2.43	0.48
1:B:786:LYS:NZ	1:B:877:GLY:O	2.42	0.48
1:C:596:LEU:HD22	1:C:609:MET:HG2	1.94	0.48
1:C:774:SER:HB3	1:C:833:GLU:HB3	1.95	0.48
1:E:831:ILE:HD12	1:E:870:GLY:HA2	1.96	0.48
1:F:575:LYS:HG2	1:F:605:GLU:OE2	2.13	0.48
1:D:586:ARG:HA	1:D:590:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:GLU:OE1	6:A:1004:HOH:O	2.20	0.47
1:D:846:VAL:O	1:D:847:ALA:HB3	2.13	0.47
1:A:511:PHE:CZ	1:A:538:VAL:HG21	2.49	0.47
1:E:860:ARG:O	1:E:861:LYS:HB2	2.14	0.47
1:A:542:ILE:HD12	1:A:547:ARG:HD2	1.96	0.47
1:B:657:PHE:HB2	4:B:901:AGS:O2A	2.14	0.47
1:F:517:ARG:CG	1:F:517:ARG:HH11	2.27	0.47
1:C:867:ARG:HG3	1:C:868:GLU:N	2.29	0.47
1:F:595:ARG:NH2	1:A:709:ARG:HG2	2.30	0.47
1:F:839:ASP:OD1	1:F:842:ARG:NH1	2.47	0.47
1:C:601:THR:HG22	1:C:603:TYR:H	1.79	0.47
1:D:799:LEU:O	1:D:801:LEU:N	2.41	0.47
1:F:660:PHE:CD1	1:F:684:ILE:HD12	2.50	0.47
1:F:675:THR:HG23	1:F:677:GLU:HG3	1.97	0.47
1:D:550:SER:OG	1:D:551:THR:N	2.48	0.47
1:B:633:ARG:HD2	1:B:836:VAL:HG21	1.97	0.47
1:D:841:ILE:O	1:D:845:ILE:HG13	2.15	0.47
1:A:655:LYS:HB2	1:A:655:LYS:HE3	1.67	0.47
1:A:654:GLY:HA2	4:A:901:AGS:O1A	2.15	0.47
1:C:846:VAL:O	1:C:847:ALA:HB3	2.15	0.47
1:D:802:SER:O	1:D:806:ILE:HG13	2.14	0.47
1:E:506:SER:O	1:E:510:LYS:HG2	2.14	0.47
1:B:776:ARG:HB3	1:B:887:ARG:HG2	1.96	0.47
1:A:802:SER:OG	1:A:805:GLU:N	2.39	0.47
1:B:682:TYR:HB2	1:B:684:ILE:CD1	2.45	0.47
1:C:577:LEU:HD21	1:D:696:ALA:O	2.15	0.47
1:A:621:ILE:HG13	1:A:634:PHE:HE2	1.80	0.46
1:F:555:GLY:N	6:F:1004:HOH:O	2.28	0.46
1:B:675:THR:HG23	1:B:677:GLU:HG3	1.96	0.46
1:D:643:GLY:HA3	1:D:770:ILE:HD11	1.97	0.46
1:F:745:THR:HG22	1:F:747:ASP:H	1.79	0.46
1:C:846:VAL:C	1:C:848:GLY:H	2.18	0.46
1:D:850:SER:O	1:D:854:ILE:HG12	2.16	0.46
1:D:654:GLY:N	4:D:901:AGS:O1B	2.48	0.46
1:D:776:ARG:HB2	1:D:831:ILE:HD11	1.97	0.46
1:F:744:HIS:CD2	1:A:735:THR:HG22	2.50	0.46
1:F:797:ARG:O	1:F:800:GLY:N	2.46	0.46
1:D:706:ALA:HA	1:D:709:ARG:HE	1.79	0.46
1:D:803:GLU:O	1:D:807:GLN:HG3	2.16	0.46
1:E:784:HIS:ND1	1:E:819:ARG:HD3	2.31	0.46
1:A:583:VAL:HG13	1:A:596:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:GLU:HB2	1:B:866:LEU:HG	1.98	0.46
1:A:670:ASP:N	1:A:670:ASP:OD1	2.49	0.46
1:C:705:ARG:HG3	1:C:728:ILE:HD13	1.98	0.46
1:E:637:VAL:HG13	1:E:770:ILE:HG22	1.97	0.46
1:F:801:LEU:HG	1:F:805:GLU:HB3	1.98	0.46
1:F:802:SER:O	1:F:806:ILE:HG13	2.16	0.46
1:F:677:GLU:HB2	1:F:680:VAL:HG22	1.98	0.46
1:F:705:ARG:NH2	1:F:724:GLU:OE2	2.40	0.46
1:E:506:SER:HA	1:E:509:GLN:HB2	1.98	0.45
1:E:680:VAL:HG23	1:E:691:GLN:HB2	1.99	0.45
1:F:655:LYS:HE2	1:F:655:LYS:HB2	1.63	0.45
1:C:621:ILE:HG23	6:C:1021:HOH:O	2.15	0.45
1:A:867:ARG:HB2	1:A:890:GLU:HA	1.98	0.45
1:E:584:ARG:HD3	1:E:593:ASP:OD2	2.16	0.45
1:F:718:GLY:O	1:F:742:THR:OG1	2.35	0.45
1:C:682:TYR:CE1	1:C:684:ILE:HD11	2.50	0.45
1:C:788:GLU:OE2	1:C:810:ARG:NH1	2.50	0.45
1:D:655:LYS:HB2	1:D:655:LYS:HE2	1.45	0.45
1:F:744:HIS:HE1	6:F:1024:HOH:O	1.98	0.45
1:A:506:SER:HB3	1:A:509:GLN:HB2	1.99	0.45
1:A:536:VAL:HB	1:A:552:LEU:HB2	1.99	0.45
1:E:734:LEU:HD21	1:E:767:ALA:HB3	1.98	0.45
1:A:783:GLU:HA	1:A:786:LYS:HB2	1.98	0.44
1:F:823:THR:HG22	1:F:825:TYR:HD2	1.82	0.44
1:C:533:GLN:HA	1:C:603:TYR:CE1	2.52	0.44
1:C:718:GLY:O	1:C:742:THR:HB	2.18	0.44
1:D:637:VAL:HG13	1:D:770:ILE:HG22	1.99	0.44
1:F:517:ARG:NH1	1:F:587:GLU:OE1	2.49	0.44
1:F:780:ARG:NH2	6:F:1013:HOH:O	2.50	0.44
1:B:850:SER:OG	1:B:853:GLU:HG3	2.18	0.44
1:D:536:VAL:HB	1:D:552:LEU:HB2	1.98	0.44
1:D:618:ILE:HA	1:D:619:PRO:HD3	1.84	0.44
1:E:792:ASP:HA	1:E:793:PRO:HD2	1.86	0.44
1:A:649:GLY:HA2	1:A:776:ARG:NH2	2.31	0.44
1:B:530:GLU:HG2	1:B:606:LYS:CE	2.41	0.44
1:B:833:GLU:HG2	1:B:863:MET:CE	2.47	0.44
1:B:890:GLU:HG3	1:C:727:LYS:HD3	1.99	0.44
1:B:766:SER:HB2	1:B:842:ARG:HB3	1.99	0.44
1:A:539:ARG:NH1	1:B:669:PRO:O	2.50	0.44
1:C:794:GLU:O	1:C:798:ARG:HG3	2.18	0.44
1:E:707:PHE:HE1	1:D:599:LEU:HD11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:LEU:HB3	1:C:806:ILE:CD1	2.47	0.44
1:D:675:THR:HG21	1:D:689:GLN:HG2	1.99	0.44
1:C:790:LYS:N	1:C:790:LYS:HD2	2.33	0.43
1:E:803:GLU:O	1:E:804:ALA:HB3	2.17	0.43
1:A:621:ILE:HD12	1:A:621:ILE:HA	1.81	0.43
1:C:792:ASP:OD1	1:C:794:GLU:N	2.51	0.43
1:E:791:PRO:HB3	1:E:811:LEU:HD12	2.00	0.43
1:F:798:ARG:O	1:F:798:ARG:HG2	2.17	0.43
1:F:801:LEU:HA	1:F:801:LEU:HD12	1.64	0.43
1:A:834:LEU:O	1:A:863:MET:HG3	2.18	0.43
1:F:710:GLN:HE21	1:E:606:LYS:HD3	1.83	0.43
1:B:580:ASP:OD2	1:C:709:ARG:NH1	2.52	0.43
1:C:841:ILE:O	1:C:845:ILE:HG12	2.18	0.43
1:D:888:THR:C	1:D:890:GLU:H	2.21	0.43
1:E:666:ILE:HG13	1:E:714:ILE:HD13	2.01	0.43
1:D:718:GLY:O	1:D:742:THR:HB	2.18	0.43
1:B:717:VAL:HG21	1:B:720:ILE:HG13	2.00	0.43
1:B:860:ARG:HD3	6:B:1005:HOH:O	2.18	0.43
1:C:648:THR:CG2	1:C:743:LEU:HB3	2.47	0.43
1:C:752:ILE:HD13	1:C:845:ILE:CD1	2.49	0.43
1:D:655:LYS:HE3	1:D:742:THR:HG21	2.01	0.43
1:D:838:ASP:OD2	1:D:861:LYS:HE2	2.17	0.43
1:B:527:ILE:HG12	1:B:540:LEU:HD22	2.01	0.43
1:C:556:ALA:O	1:C:560:VAL:HG23	2.18	0.43
1:D:562:SER:O	1:D:566:ILE:HG12	2.19	0.43
1:D:678:ASP:HA	1:D:679:PRO:HA	1.84	0.43
1:F:693:ASN:HB3	1:F:698:LEU:HB3	2.01	0.43
1:A:805:GLU:HA	1:A:807:GLN:NE2	2.33	0.42
1:B:511:PHE:CE2	1:B:552:LEU:HD11	2.54	0.42
1:D:722:ASP:OD1	1:D:722:ASP:N	2.50	0.42
1:D:747:ASP:HB3	1:D:750:GLN:HG3	2.01	0.42
1:A:704:LEU:HD12	1:A:704:LEU:HA	1.78	0.42
1:A:783:GLU:HG3	1:A:786:LYS:HE2	2.00	0.42
1:B:511:PHE:O	1:B:515:VAL:HG23	2.18	0.42
1:D:802:SER:OG	1:D:805:GLU:HG3	2.19	0.42
1:D:880:THR:C	6:D:1001:HOH:O	2.57	0.42
1:F:559:ALA:O	1:F:563:VAL:HG23	2.20	0.42
1:B:796:LEU:HD22	1:B:801:LEU:HD12	2.02	0.42
1:E:515:VAL:HG12	1:E:527:ILE:HD13	2.02	0.42
1:A:718:GLY:O	1:A:742:THR:HB	2.19	0.42
1:C:745:THR:CG2	1:C:750:GLN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:511:PHE:HZ	1:E:538:VAL:HG21	1.85	0.42
1:F:636:GLU:OE2	6:F:1001:HOH:O	2.21	0.42
1:C:802:SER:O	1:C:806:ILE:HG12	2.19	0.42
1:E:808:GLY:O	1:E:810:ARG:HG3	2.19	0.42
1:B:797:ARG:NH1	1:B:803:GLU:OE1	2.52	0.42
1:B:817:CYS:HB3	1:B:820:CYS:SG	2.59	0.42
1:F:777:LEU:HA	1:F:777:LEU:HD12	1.82	0.42
1:A:840:GLU:OE1	1:A:861:LYS:HE2	2.20	0.42
1:E:654:GLY:HA2	4:E:901:AGS:O1A	2.19	0.42
1:A:675:THR:HG21	1:A:677:GLU:OE2	2.20	0.42
1:A:709:ARG:HD2	6:A:1056:HOH:O	2.20	0.42
1:D:511:PHE:HZ	1:D:538:VAL:HG21	1.85	0.42
1:F:752:ILE:HG21	1:F:845:ILE:HD12	2.02	0.42
1:E:750:GLN:HG2	1:E:851:ALA:HB2	2.02	0.42
1:A:618:ILE:HD11	1:A:682:TYR:CD2	2.55	0.41
1:A:678:ASP:HA	1:A:679:PRO:HA	1.83	0.41
1:D:637:VAL:HG11	1:D:645:PHE:CE1	2.54	0.41
1:E:643:GLY:HA2	1:E:733:ALA:HB1	2.02	0.41
1:F:704:LEU:HA	1:F:704:LEU:HD12	1.63	0.41
1:D:648:THR:HG21	1:D:751:ALA:HB2	2.01	0.41
1:F:537:GLN:HB2	6:F:1018:HOH:O	2.20	0.41
1:F:717:VAL:HG22	1:F:741:ALA:CB	2.50	0.41
1:A:867:ARG:NH1	1:A:888:THR:O	2.53	0.41
1:B:515:VAL:HG22	1:B:549:TYR:CE2	2.55	0.41
1:C:587:GLU:HG2	1:C:587:GLU:O	2.20	0.41
1:D:511:PHE:CZ	1:D:538:VAL:HG21	2.55	0.41
1:D:532:ARG:NH1	1:D:537:GLN:OE1	2.53	0.41
1:C:666:ILE:HD13	1:C:666:ILE:HG21	1.70	0.41
1:F:684:ILE:HB	1:F:687:ILE:HD11	2.02	0.41
1:E:584:ARG:HG3	1:E:593:ASP:OD1	2.20	0.41
1:D:699:THR:HB	1:D:702:ARG:H	1.85	0.41
1:C:704:LEU:HD23	1:C:704:LEU:HA	1.69	0.41
1:C:855:LYS:O	1:C:859:ARG:HG3	2.20	0.41
1:A:855:LYS:HG3	6:A:1040:HOH:O	2.19	0.41
1:B:704:LEU:HA	1:B:704:LEU:HD12	1.81	0.41
1:F:813:LYS:HG2	1:F:814:GLY:N	2.33	0.41
1:A:650:PRO:HD3	1:A:776:ARG:NH2	2.36	0.41
1:A:659:THR:O	1:A:663:LEU:HD13	2.20	0.41
1:A:722:ASP:OD1	1:A:722:ASP:N	2.54	0.41
1:E:796:LEU:HB3	1:E:801:LEU:HD23	2.01	0.41
1:F:533:GLN:HA	1:F:603:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:697:GLY:O	1:F:699:THR:N	2.54	0.41
1:F:797:ARG:HE	1:F:806:ILE:HD12	1.86	0.41
1:F:719:GLU:OE1	1:F:721:ARG:NE	2.55	0.40
1:A:745:THR:HG22	1:A:747:ASP:H	1.86	0.40
1:A:796:LEU:HB3	1:A:801:LEU:HD11	2.04	0.40
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.90	0.40
1:C:720:ILE:HB	1:C:743:LEU:HD13	2.04	0.40
1:E:562:SER:O	1:E:566:ILE:HG12	2.21	0.40
1:E:763:PHE:CE1	1:D:758:MET:HG2	2.56	0.40
1:F:799:LEU:CD2	1:F:867:ARG:HD2	2.51	0.40
1:C:584:ARG:HE	1:C:593:ASP:CG	2.23	0.40
1:C:853:GLU:O	1:C:856:GLU:HG2	2.22	0.40
1:E:641:PRO:HB2	1:E:642:TYR:HD1	1.85	0.40
1:F:755:LEU:HA	1:F:755:LEU:HD23	1.95	0.40
1:F:811:LEU:HD23	1:F:811:LEU:HA	1.92	0.40
1:F:833:GLU:HG3	1:F:865:THR:HA	2.02	0.40
1:F:595:ARG:HH21	1:A:709:ARG:NH1	2.19	0.40
1:E:787:VAL:HG22	1:E:813:LYS:O	2.22	0.40
1:F:670:ASP:N	1:F:670:ASP:OD1	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/385 (100%)	371 (97%)	9 (2%)	3 (1%)	19	28
1	B	383/385 (100%)	372 (97%)	11 (3%)	0	100	100
1	C	383/385 (100%)	371 (97%)	9 (2%)	3 (1%)	19	28
1	D	383/385 (100%)	376 (98%)	5 (1%)	2 (0%)	29	43
1	E	383/385 (100%)	371 (97%)	10 (3%)	2 (0%)	29	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	383/385 (100%)	373 (97%)	8 (2%)	2 (0%)	29	43
All	All	2298/2310 (100%)	2234 (97%)	52 (2%)	12 (0%)	29	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	SER
1	C	800	GLY
1	A	800	GLY
1	C	588	GLY
1	D	816	GLY
1	E	861	LYS
1	C	602	VAL
1	F	793	PRO
1	D	800	GLY
1	F	628	PRO
1	A	791	PRO
1	E	602	VAL

### 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	318/318 (100%)	309 (97%)	9 (3%)	43	61
1	B	318/318 (100%)	313 (98%)	5 (2%)	62	78
1	C	318/318 (100%)	310 (98%)	8 (2%)	47	66
1	D	318/318 (100%)	312 (98%)	6 (2%)	57	74
1	E	318/318 (100%)	312 (98%)	6 (2%)	57	74
1	F	317/318 (100%)	310 (98%)	7 (2%)	52	70
All	All	1907/1908 (100%)	1866 (98%)	41 (2%)	53	71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	517	ARG
1	F	532	ARG
1	F	616	SER
1	F	675	THR
1	F	716	MET
1	F	803	GLU
1	F	819	ARG
1	A	616	SER
1	A	621	ILE
1	A	672	ASN
1	A	746	ASN
1	A	754	ARG
1	A	802	SER
1	A	805	GLU
1	A	817	CYS
1	A	867	ARG
1	B	595	ARG
1	B	633	ARG
1	B	675	THR
1	B	717	VAL
1	B	890	GLU
1	E	584	ARG
1	E	601	THR
1	E	675	THR
1	E	724	GLU
1	E	750	GLN
1	E	820	CYS
1	C	510	LYS
1	C	584	ARG
1	C	593	ASP
1	C	780	ARG
1	C	802	SER
1	C	803	GLU
1	C	815	MET
1	C	819	ARG
1	D	599	LEU
1	D	675	THR
1	D	683	GLU
1	D	783	GLU
1	D	787	VAL
1	D	795	THR

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



Mol	Chain	Res	Type
1	F	579	GLN
1	F	672	ASN
1	F	688	ASN
1	E	528	HIS
1	E	750	GLN
1	E	807	GLN
1	C	832	HIS
1	D	695	GLN
1	D	775	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	AGS	A	901	-	26,33,33	0.90	1 (3%)	26,52,52	1.26	6 (23%)
3	ATP	F	902	-	26,33,33	1.79	8 (30%)	31,52,52	1.29	5 (16%)
4	AGS	E	901	5	26,33,33	1.96	9 (34%)	26,52,52	1.61	6 (23%)
4	AGS	B	901	5	26,33,33	1.85	10 (38%)	26,52,52	1.58	5 (19%)
4	AGS	D	901	-	26,33,33	0.96	1 (3%)	26,52,52	1.10	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	AGS	C	901	-	26,33,33	0.80	0	26,52,52	1.11	3 (11%)

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	AGS	A	901	-	-	2/17/38/38	0/3/3/3
3	ATP	F	902	-	-	9/18/38/38	0/3/3/3
4	AGS	E	901	5	-	6/17/38/38	0/3/3/3
4	AGS	B	901	5	-	5/17/38/38	0/3/3/3
4	AGS	D	901	-	-	0/17/38/38	0/3/3/3
4	AGS	C	901	-	-	9/17/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	901	AGS	PG-O3G	-4.16	1.41	1.54
4	E	901	AGS	C2'-C1'	-3.96	1.47	1.53
4	E	901	AGS	PG-S1G	3.85	1.99	1.90
3	F	902	ATP	C2'-C1'	-3.58	1.48	1.53
4	B	901	AGS	C2'-C1'	-3.37	1.48	1.53
4	D	901	AGS	PG-S1G	3.33	1.97	1.90
3	F	902	ATP	PA-O2A	-3.13	1.40	1.55
3	F	902	ATP	PB-O2B	-2.96	1.41	1.55
4	B	901	AGS	PG-O3G	-2.91	1.45	1.54
4	B	901	AGS	O4'-C4'	-2.85	1.38	1.45
4	B	901	AGS	PG-S1G	2.83	1.96	1.90
3	F	902	ATP	O4'-C4'	-2.74	1.38	1.45
4	B	901	AGS	C4-N3	-2.66	1.32	1.35
4	E	901	AGS	PB-O2B	-2.60	1.43	1.55
4	B	901	AGS	PA-O2A	-2.55	1.43	1.55
4	B	901	AGS	PB-O1B	-2.53	1.41	1.50
4	E	901	AGS	PA-O2A	-2.46	1.43	1.55
4	B	901	AGS	C5-N7	-2.42	1.31	1.39
4	A	901	AGS	PG-S1G	2.38	1.95	1.90
4	E	901	AGS	C4-N3	-2.30	1.32	1.35
3	F	902	ATP	C5-N7	-2.29	1.31	1.39
4	E	901	AGS	PA-O1A	-2.28	1.42	1.50
4	E	901	AGS	O4'-C4'	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	901	AGS	C5-N7	-2.17	1.31	1.39
3	F	902	ATP	PG-O3G	-2.16	1.46	1.54
3	F	902	ATP	PA-O1A	-2.07	1.43	1.50
4	B	901	AGS	PA-O1A	-2.04	1.43	1.50
3	F	902	ATP	C8-N7	-2.02	1.31	1.34
4	B	901	AGS	C3'-C4'	-2.00	1.47	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	AGS	C4-C5-N7	-3.77	105.47	109.40
4	D	901	AGS	O2G-PG-O3B	3.46	116.18	104.64
4	C	901	AGS	PA-O3A-PB	-3.42	121.09	132.83
3	F	902	ATP	N3-C2-N1	-3.40	123.37	128.68
4	B	901	AGS	O3G-PG-O3B	3.24	115.47	104.64
4	E	901	AGS	C4-C5-N7	-3.21	106.05	109.40
4	E	901	AGS	N3-C2-N1	-3.18	123.71	128.68
4	B	901	AGS	N3-C2-N1	-2.77	124.34	128.68
4	D	901	AGS	C5-C6-N6	2.73	124.50	120.35
4	E	901	AGS	O2G-PG-O3B	2.65	113.49	104.64
4	C	901	AGS	C5-C6-N6	2.53	124.19	120.35
3	F	902	ATP	C4-C5-N7	-2.52	106.77	109.40
4	A	901	AGS	O2G-PG-O3B	2.41	112.69	104.64
4	A	901	AGS	C5-C6-N6	2.35	123.93	120.35
4	E	901	AGS	C3'-C2'-C1'	2.25	104.37	100.98
4	C	901	AGS	O2G-PG-O3B	2.24	112.12	104.64
4	E	901	AGS	C2-N1-C6	2.24	122.58	118.75
4	B	901	AGS	C3'-C2'-C1'	2.23	104.33	100.98
4	B	901	AGS	O2B-PB-O1B	2.23	123.25	112.24
4	A	901	AGS	O3G-PG-O3B	2.21	112.00	104.64
4	A	901	AGS	O2'-C2'-C3'	-2.20	104.70	111.82
4	E	901	AGS	O2B-PB-O1B	2.20	123.12	112.24
3	F	902	ATP	C3'-C2'-C1'	2.13	104.19	100.98
4	A	901	AGS	C3'-C2'-C1'	2.13	104.18	100.98
3	F	902	ATP	O5'-C5'-C4'	2.12	116.29	108.99
4	A	901	AGS	O3'-C3'-C2'	-2.05	105.19	111.82
3	F	902	ATP	C2-N1-C6	2.04	122.24	118.75

There are no chirality outliers.

All (31) torsion outliers are listed below:

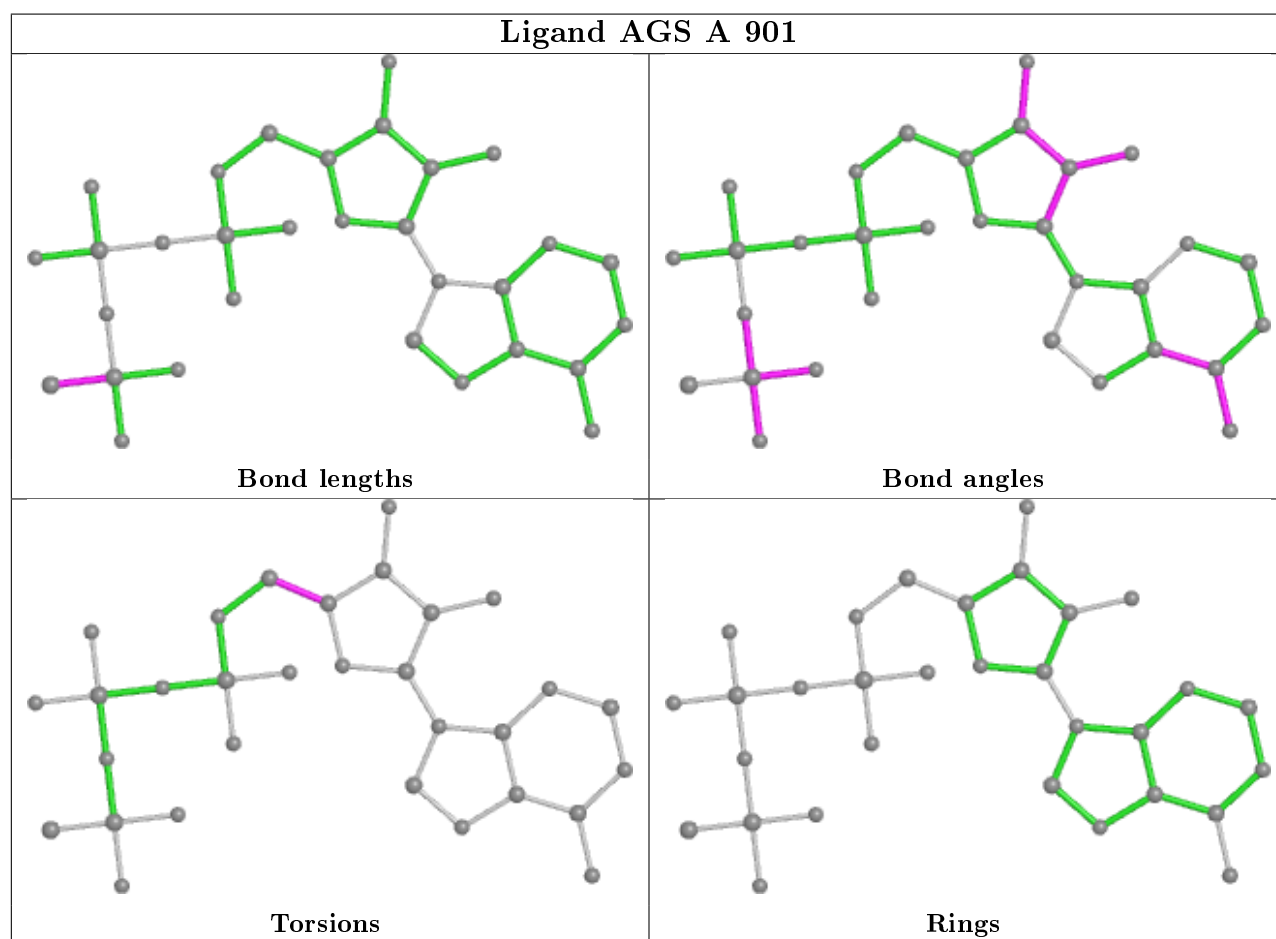
Mol	Chain	Res	Type	Atoms
3	F	902	ATP	PB-O3B-PG-O2G
3	F	902	ATP	PB-O3B-PG-O3G
3	F	902	ATP	C5'-O5'-PA-O1A
4	C	901	AGS	C5'-O5'-PA-O3A
4	A	901	AGS	O4'-C4'-C5'-O5'
4	E	901	AGS	O4'-C4'-C5'-O5'
4	C	901	AGS	O4'-C4'-C5'-O5'
4	A	901	AGS	C3'-C4'-C5'-O5'
4	C	901	AGS	C3'-C4'-C5'-O5'
4	E	901	AGS	C3'-C4'-C5'-O5'
3	F	902	ATP	O4'-C4'-C5'-O5'
3	F	902	ATP	C5'-O5'-PA-O3A
4	E	901	AGS	PA-O3A-PB-O1B
4	C	901	AGS	PA-O3A-PB-O1B
3	F	902	ATP	C5'-O5'-PA-O2A
4	C	901	AGS	C5'-O5'-PA-O1A
4	C	901	AGS	C5'-O5'-PA-O2A
4	B	901	AGS	PA-O3A-PB-O1B
4	E	901	AGS	PB-O3B-PG-O2G
4	E	901	AGS	PB-O3B-PG-O3G
4	B	901	AGS	PB-O3B-PG-O2G
4	B	901	AGS	PB-O3B-PG-O3G
4	B	901	AGS	PA-O3A-PB-O2B
4	C	901	AGS	PB-O3A-PA-O2A
3	F	902	ATP	C3'-C4'-C5'-O5'
3	F	902	ATP	PG-O3B-PB-O2B
4	C	901	AGS	PB-O3A-PA-O1A
4	E	901	AGS	C5'-O5'-PA-O1A
4	B	901	AGS	O4'-C4'-C5'-O5'
3	F	902	ATP	PB-O3B-PG-O1G
4	C	901	AGS	PA-O3A-PB-O3B

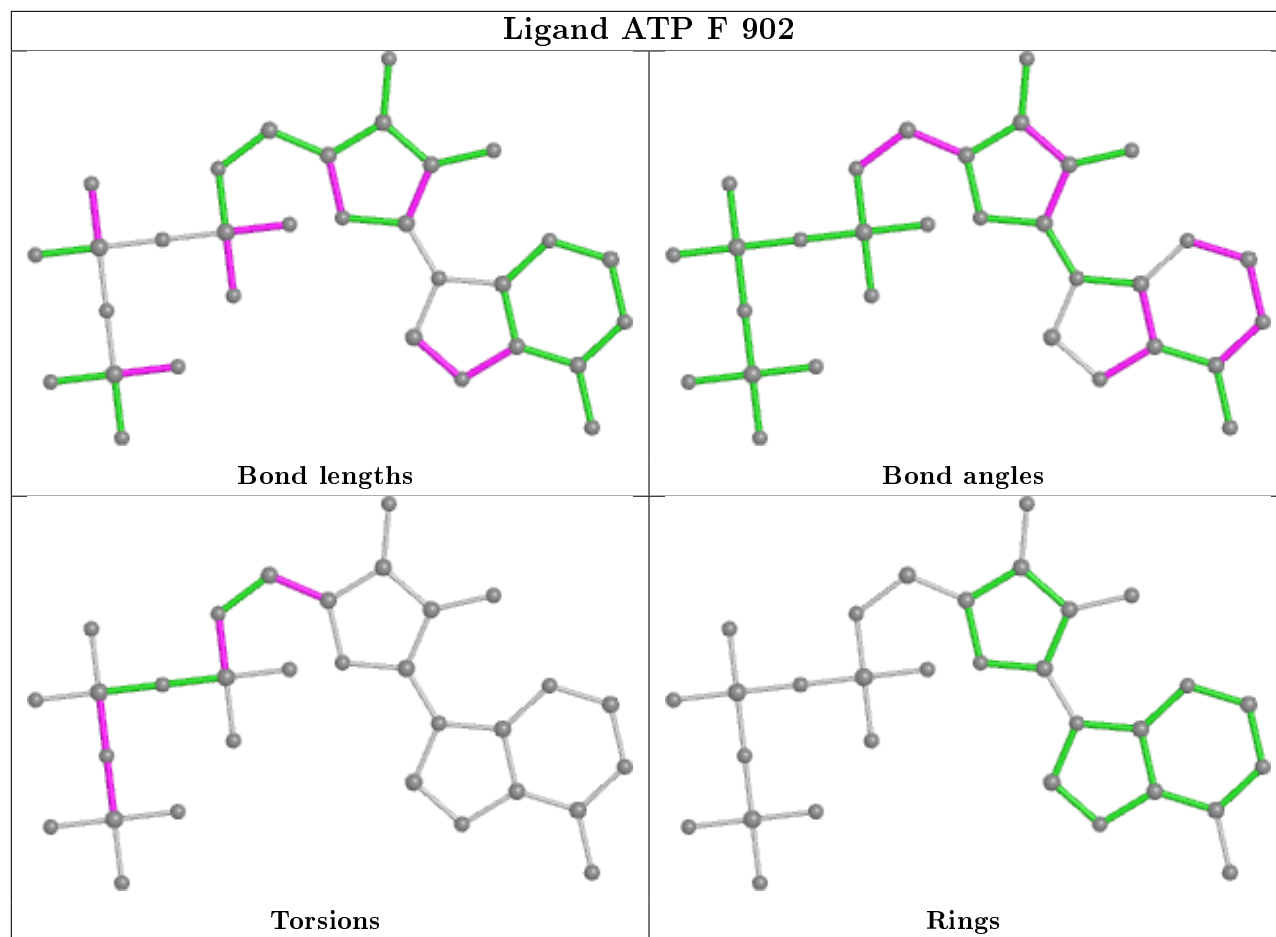
There are no ring outliers.

6 monomers are involved in 11 short contacts:

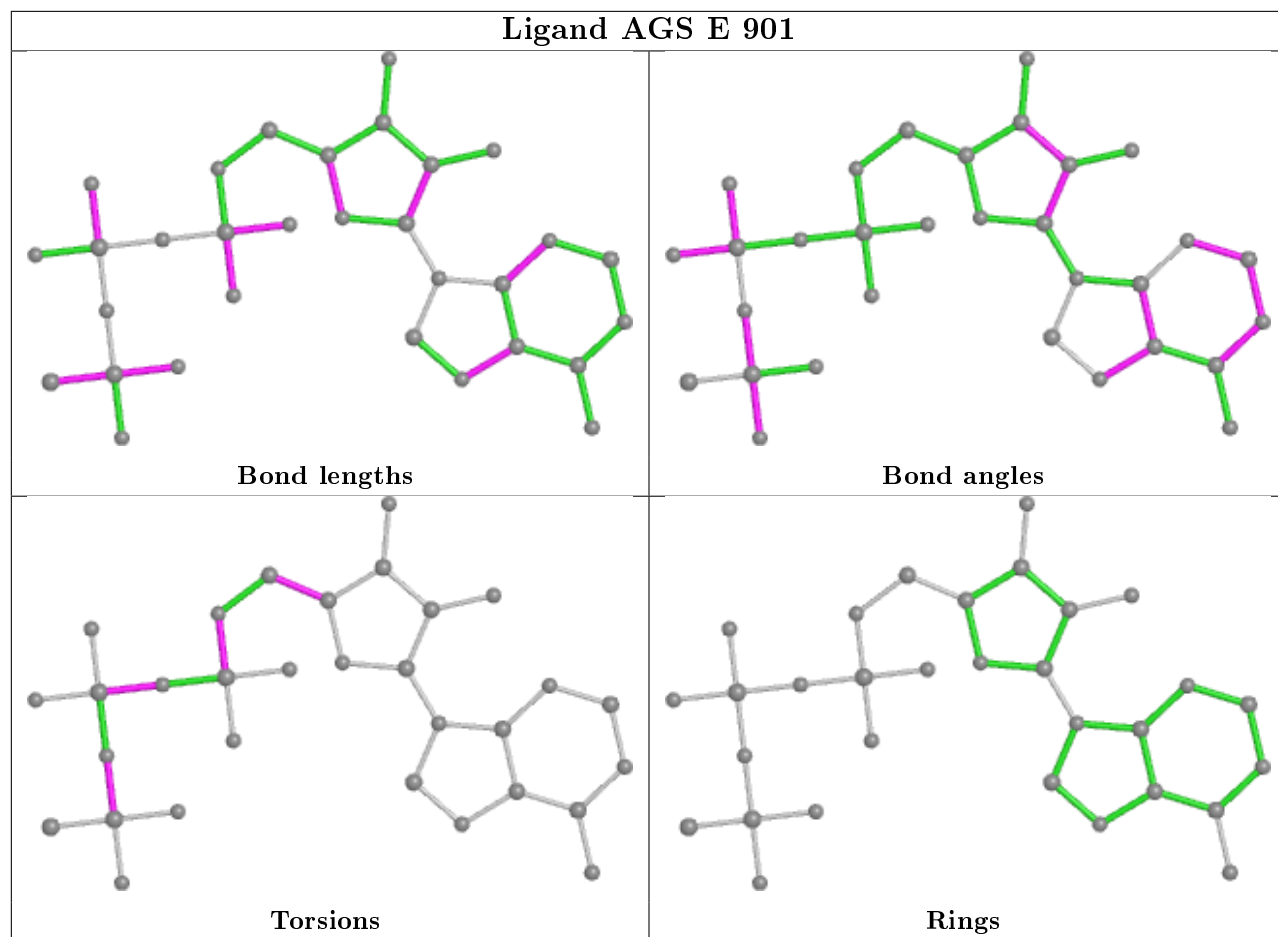
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	AGS	2	0
3	F	902	ATP	1	0
4	E	901	AGS	1	0
4	B	901	AGS	5	0
4	D	901	AGS	1	0
4	C	901	AGS	1	0

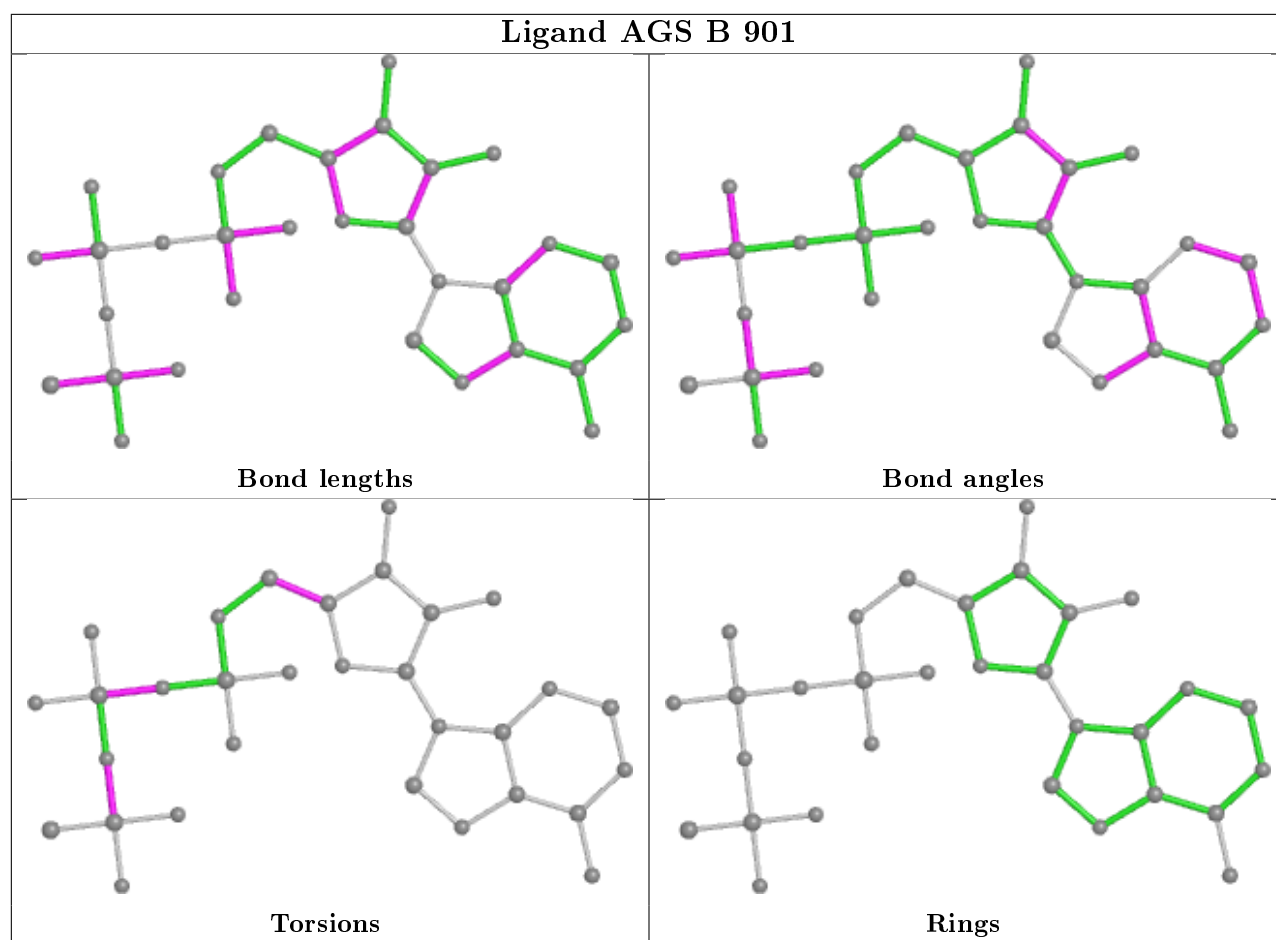
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



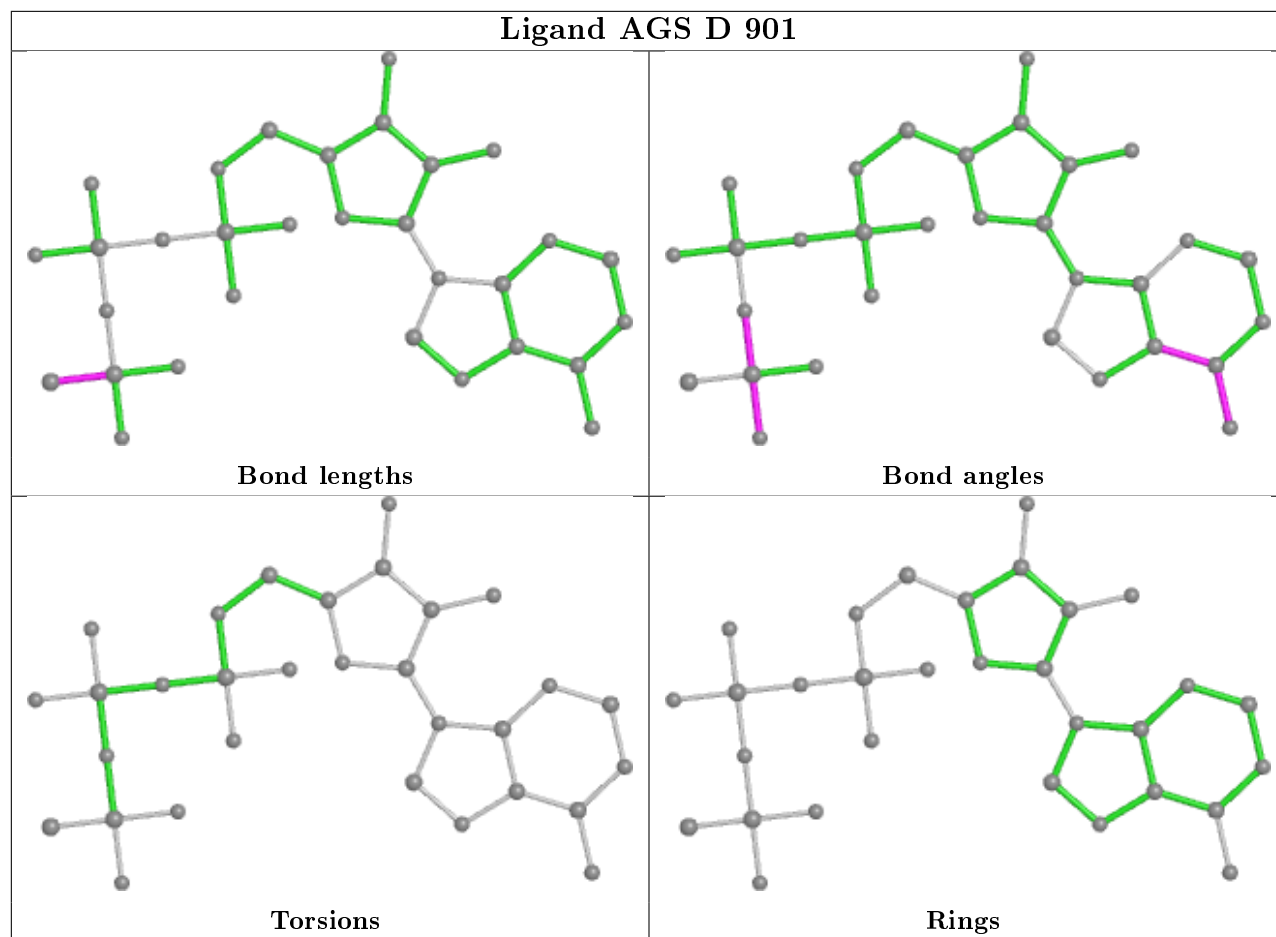


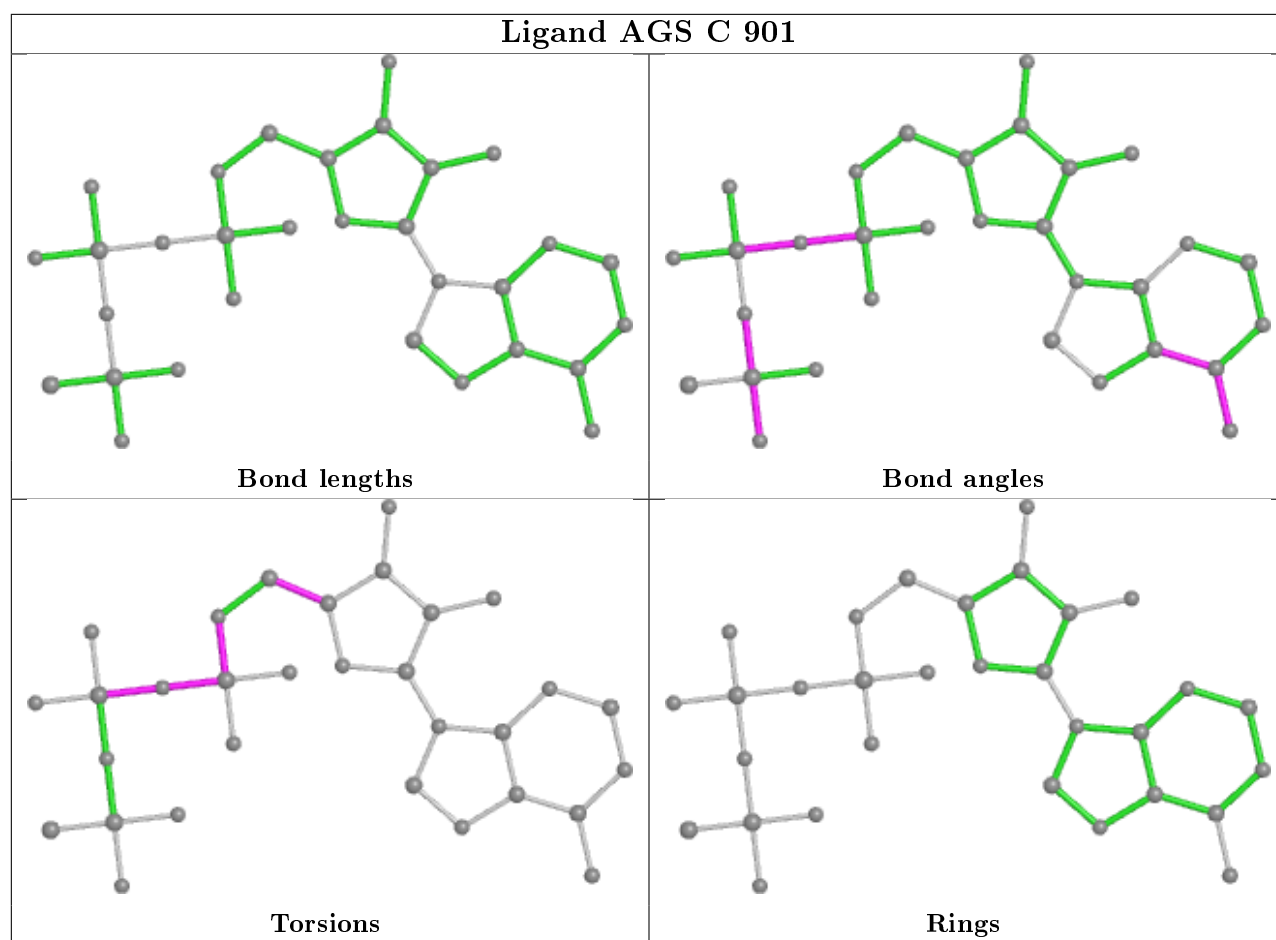
## Ligand AGS E 901











## 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	385/385 (100%)	-0.19	12 (3%)	49	45	24, 38, 73, 108	0
1	B	385/385 (100%)	-0.25	1 (0%)	94	95	25, 39, 57, 69	0
1	C	385/385 (100%)	-0.08	6 (1%)	72	69	22, 38, 71, 103	0
1	D	385/385 (100%)	-0.24	3 (0%)	86	85	25, 38, 60, 76	0
1	E	385/385 (100%)	-0.20	3 (0%)	86	85	26, 42, 64, 76	0
1	F	385/385 (100%)	-0.13	6 (1%)	72	69	24, 38, 71, 97	0
All	All	2310/2310 (100%)	-0.18	31 (1%)	77	75	22, 38, 65, 108	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	804	ALA	4.1
1	C	807	GLN	3.9
1	C	800	GLY	3.8
1	A	890	GLU	3.7
1	C	890	GLU	3.2
1	F	799	LEU	3.2
1	A	807	GLN	3.0
1	A	808	GLY	3.0
1	A	803	GLU	3.0
1	A	804	ALA	2.9
1	A	793	PRO	2.9
1	E	849	LYS	2.9
1	C	794	GLU	2.8
1	A	798	ARG	2.7
1	F	793	PRO	2.7
1	A	794	GLU	2.4
1	D	890	GLU	2.4
1	A	802	SER	2.4
1	F	798	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	794	GLU	2.3
1	F	517	ARG	2.3
1	D	798	ARG	2.2
1	A	792	ASP	2.1
1	E	809	ALA	2.1
1	A	795	THR	2.1
1	B	807	GLN	2.1
1	A	889	ILE	2.1
1	C	798	ARG	2.0
1	E	683	GLU	2.0
1	D	808	GLY	2.0
1	C	584	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

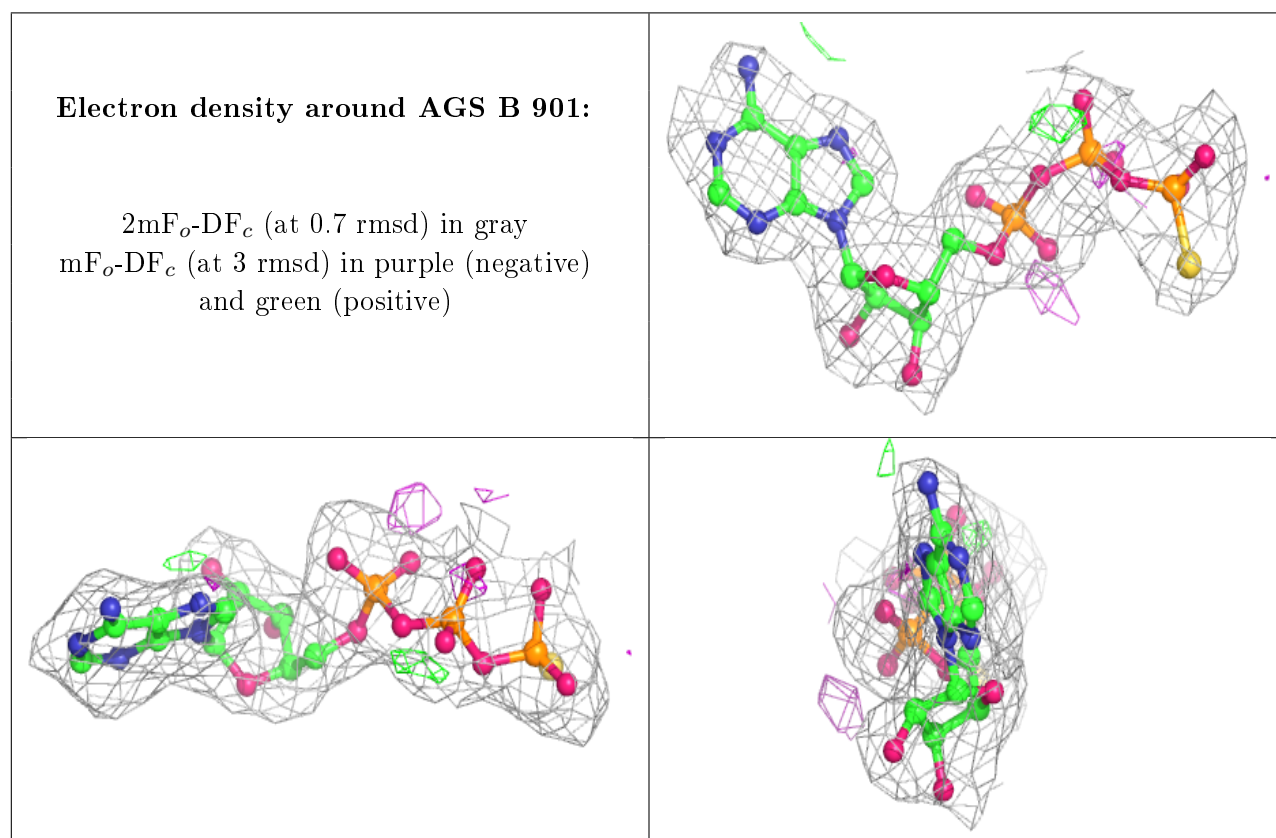
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	B	903	1/1	0.77	0.20	43,43,43,43	0
2	ZN	A	902	1/1	0.80	0.26	123,123,123,123	0
2	ZN	C	902	1/1	0.87	0.24	92,92,92,92	0
5	MG	E	903	1/1	0.91	0.15	41,41,41,41	0
4	AGS	B	901	31/31	0.95	0.14	34,40,54,59	0
4	AGS	D	901	31/31	0.96	0.15	28,34,60,73	0
4	AGS	C	901	31/31	0.96	0.16	26,31,44,62	0
3	ATP	F	902	31/31	0.96	0.14	22,32,41,80	0
4	AGS	A	901	31/31	0.96	0.15	27,33,55,72	0
4	AGS	E	901	31/31	0.97	0.12	30,37,43,47	0
2	ZN	B	902	1/1	0.97	0.06	63,63,63,63	0

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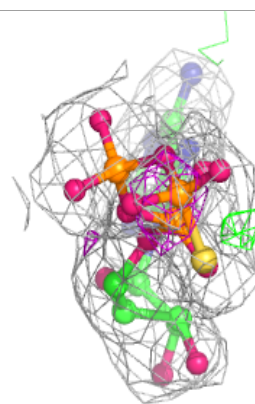
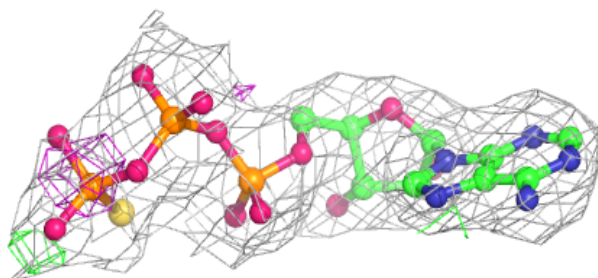
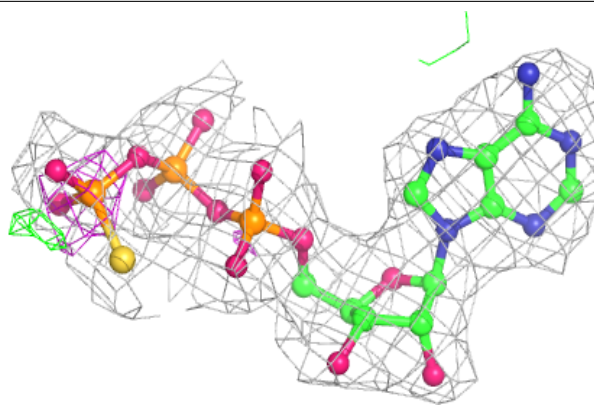
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	E	902	1/1	0.97	0.12	123,123,123,123	0
2	ZN	D	902	1/1	0.98	0.09	58,58,58,58	0
2	ZN	F	901	1/1	1.00	0.13	47,47,47,47	0

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.

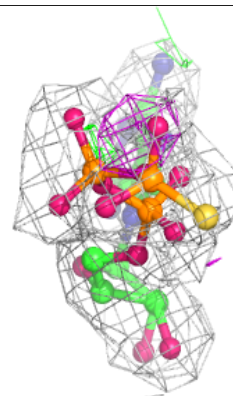
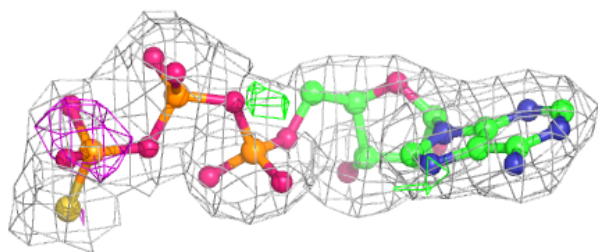
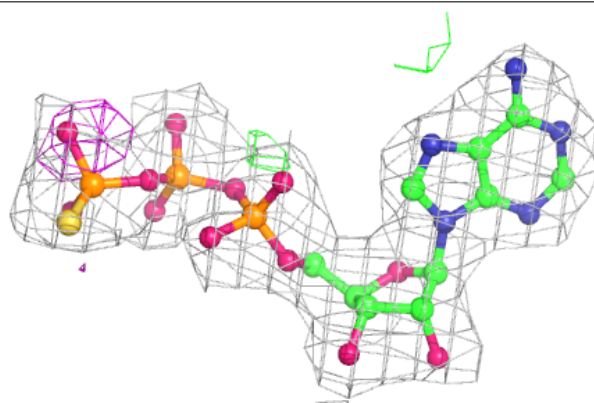


**Electron density around AGS D 901:**

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

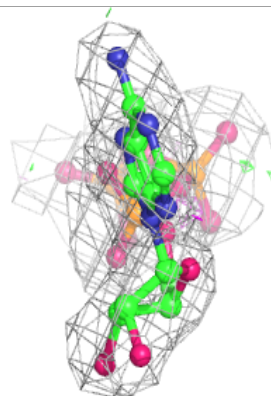
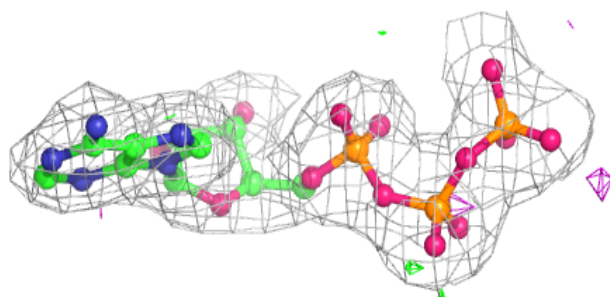
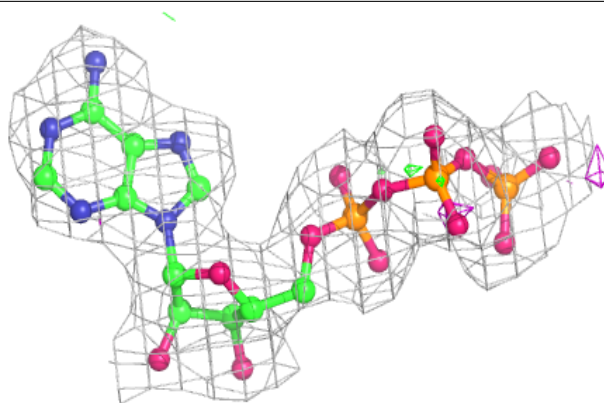
**Electron density around AGS C 901:**

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

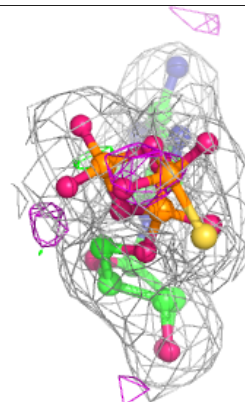
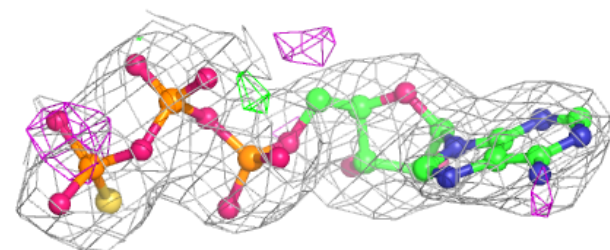
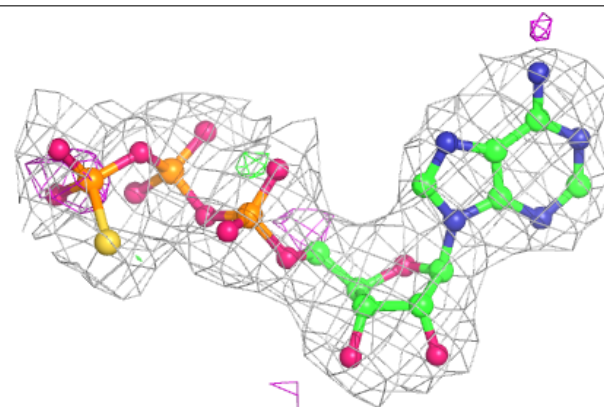


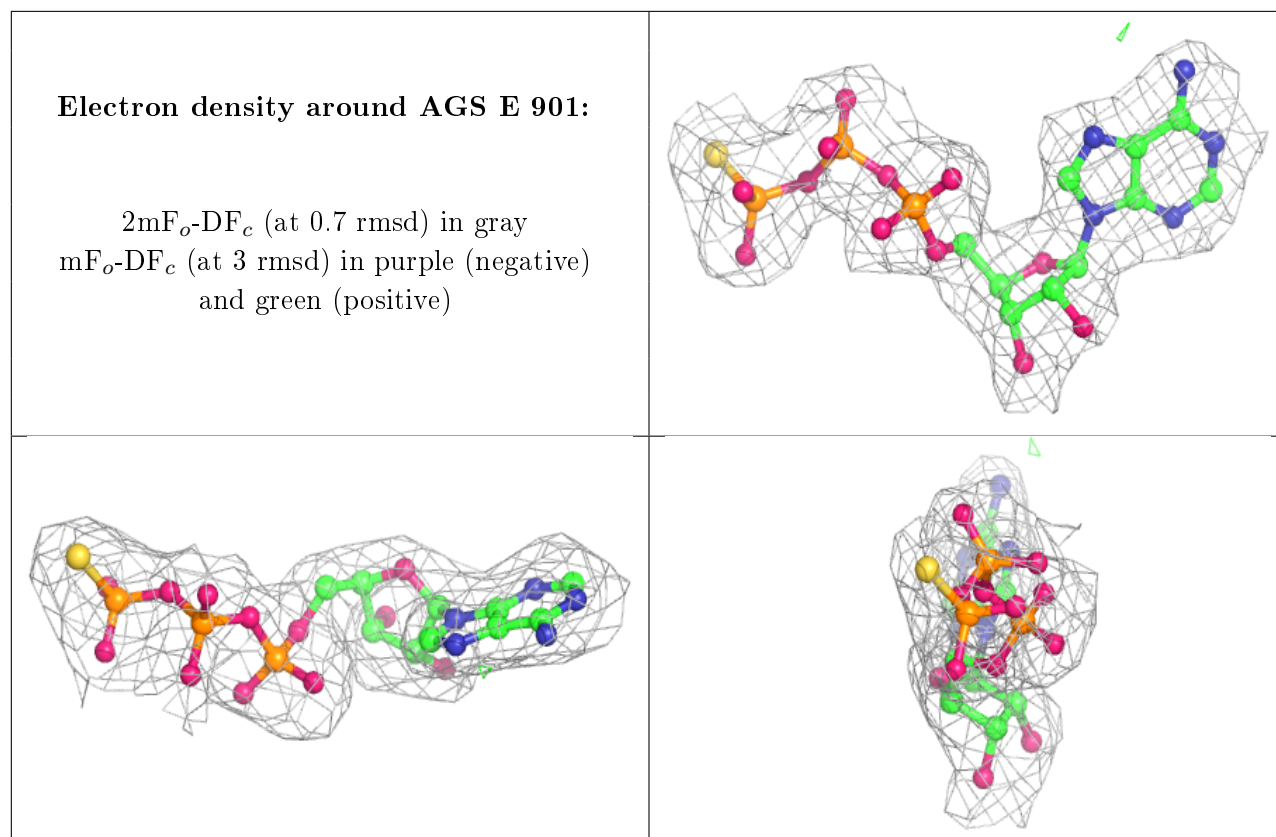
**Electron density around ATP F 902:**

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

**Electron density around AGS A 901:**

$2mF_o-DF_c$  (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.