



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 11:57 PM EDT

PDB ID : 1TIL  
Title : Crystal Structures of the ADP and ATP bound forms of the Bacillus Anti-sigma factor SpoIIAB in complex with the Anti-anti-sigma SpoIIAA:Poised for phosphorylation complex with ATP, crystal form II  
Authors : Masuda, S.; Murakami, K.S.; Wang, S.; Olson, C.A.; Donigan, J.; Leon, F.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2004-06-02  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

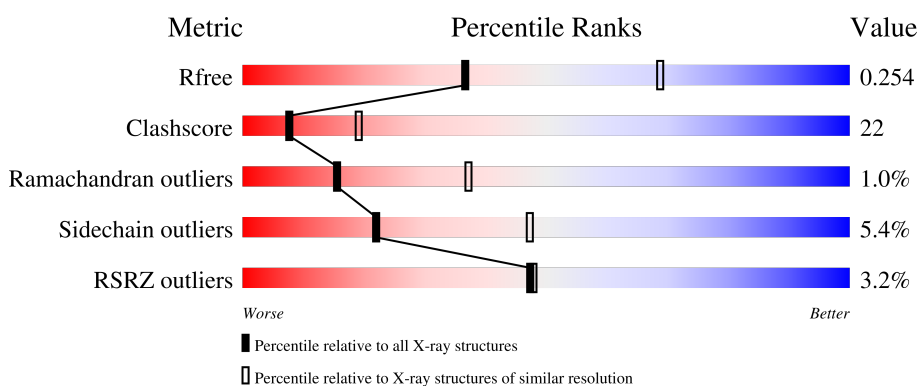
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	146	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">2%      63%      29%      . .</p>
1	C	146	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">3%      62%      32%      . .</p>
1	E	146	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">5%      54%      39%      . .</p>
2	B	119	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">3%      54%      41%      . .</p>
2	D	119	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">3%      66%      31%      . .</p>

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Mol	Chain	Length	Quality of chain
2	F	119	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a large green segment (51%), a large yellow segment (45%), and a very small grey segment (1%). The percentages are labeled below the bar.</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6248 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 Anti-sigma F factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1098	688	184	220	6	0	0	0
1	C	141	1097	688	184	219	6	0	0	0
1	E	140	1092	685	183	218	6	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	THR	SEE REMARK 999	UNP O32727
A	137	HIS	ALA	SEE REMARK 999	UNP O32727
A	138	ILE	TYR	SEE REMARK 999	UNP O32727
A	139	VAL	CYS	SEE REMARK 999	UNP O32727
A	140	LYS	GLU	SEE REMARK 999	UNP O32727
A	141	SER	LYS	SEE REMARK 999	UNP O32727
A	142	LYS	GLN	SEE REMARK 999	UNP O32727
A	143	ALA	THR	SEE REMARK 999	UNP O32727
A	145	SER	CYS	engineered mutation	UNP O32727
C	34	MET	THR	SEE REMARK 999	UNP O32727
C	137	HIS	ALA	SEE REMARK 999	UNP O32727
C	138	ILE	TYR	SEE REMARK 999	UNP O32727
C	139	VAL	CYS	SEE REMARK 999	UNP O32727
C	140	LYS	GLU	SEE REMARK 999	UNP O32727
C	141	SER	LYS	SEE REMARK 999	UNP O32727
C	142	LYS	GLN	SEE REMARK 999	UNP O32727
C	143	ALA	THR	SEE REMARK 999	UNP O32727
C	145	SER	CYS	engineered mutation	UNP O32727
E	34	MET	THR	SEE REMARK 999	UNP O32727
E	137	HIS	ALA	SEE REMARK 999	UNP O32727
E	138	ILE	TYR	SEE REMARK 999	UNP O32727
E	139	VAL	CYS	SEE REMARK 999	UNP O32727
E	140	LYS	GLU	SEE REMARK 999	UNP O32727

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	SER	LYS	SEE REMARK 999	UNP O32727
E	142	LYS	GLN	SEE REMARK 999	UNP O32727
E	143	ALA	THR	SEE REMARK 999	UNP O32727
E	145	SER	CYS	engineered mutation	UNP O32727

- Molecule 2 is a protein called Anti-sigma F factor antagonist.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	B	117	Total	C	N	O	S	0	0	0
			901	570	159	167	5			
2	D	118	Total	C	N	O	S	0	0	0
			903	571	160	168	4			
2	F	117	Total	C	N	O	S	0	0	0
			906	573	161	167	5			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	cloning artifact	UNP O32726
B	-1	SER	-	cloning artifact	UNP O32726
B	0	HIS	-	cloning artifact	UNP O32726
B	13	VAL	GLU	SEE REMARK 999	UNP O32726
B	29	GLU	ASN	SEE REMARK 999	UNP O32726
B	30	LEU	CYS	SEE REMARK 999	UNP O32726
B	31	ARG	MET	SEE REMARK 999	UNP O32726
B	32	GLU	ASN	SEE REMARK 999	UNP O32726
B	33	GLN	LYS	SEE REMARK 999	UNP O32726
B	34	VAL	CYS	SEE REMARK 999	UNP O32726
B	35	THR	ARG	SEE REMARK 999	UNP O32726
B	36	ASP	MET	SEE REMARK 999	UNP O32726
B	37	VAL	CYS	SEE REMARK 999	UNP O32726
B	40	ASN	LYS	SEE REMARK 999	UNP O32726
B	58	ALA	SER	engineered mutation	UNP O32726
D	-2	GLY	-	cloning artifact	UNP O32726
D	-1	SER	-	cloning artifact	UNP O32726
D	0	HIS	-	cloning artifact	UNP O32726
D	13	VAL	GLU	SEE REMARK 999	UNP O32726
D	29	GLU	ASN	SEE REMARK 999	UNP O32726
D	30	LEU	CYS	SEE REMARK 999	UNP O32726
D	31	ARG	MET	SEE REMARK 999	UNP O32726
D	32	GLU	ASN	SEE REMARK 999	UNP O32726
D	33	GLN	LYS	SEE REMARK 999	UNP O32726

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Chain	Residue	Modelled	Actual	Comment	Reference
D	34	VAL	CYS	SEE REMARK 999	UNP O32726
D	35	THR	ARG	SEE REMARK 999	UNP O32726
D	36	ASP	MET	SEE REMARK 999	UNP O32726
D	37	VAL	CYS	SEE REMARK 999	UNP O32726
D	40	ASN	LYS	SEE REMARK 999	UNP O32726
D	58	ALA	SER	engineered mutation	UNP O32726
F	-2	GLY	-	cloning artifact	UNP O32726
F	-1	SER	-	cloning artifact	UNP O32726
F	0	HIS	-	cloning artifact	UNP O32726
F	13	VAL	GLU	SEE REMARK 999	UNP O32726
F	29	GLU	ASN	SEE REMARK 999	UNP O32726
F	30	LEU	CYS	SEE REMARK 999	UNP O32726
F	31	ARG	MET	SEE REMARK 999	UNP O32726
F	32	GLU	ASN	SEE REMARK 999	UNP O32726
F	33	GLN	LYS	SEE REMARK 999	UNP O32726
F	34	VAL	CYS	SEE REMARK 999	UNP O32726
F	35	THR	ARG	SEE REMARK 999	UNP O32726
F	36	ASP	MET	SEE REMARK 999	UNP O32726
F	37	VAL	CYS	SEE REMARK 999	UNP O32726
F	40	ASN	LYS	SEE REMARK 999	UNP O32726
F	58	ALA	SER	engineered mutation	UNP O32726

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 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>).

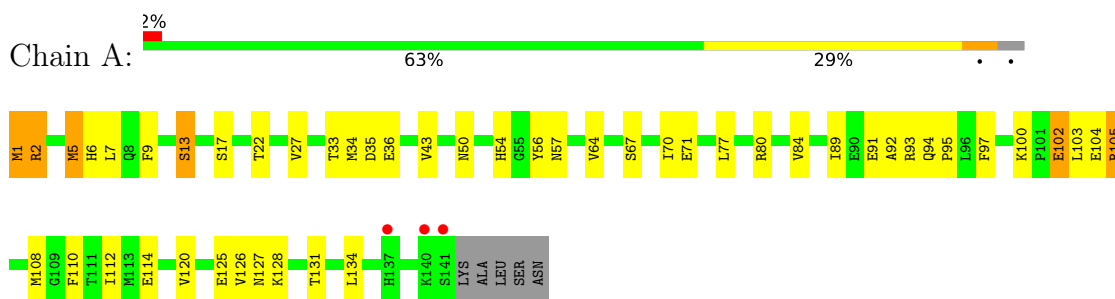




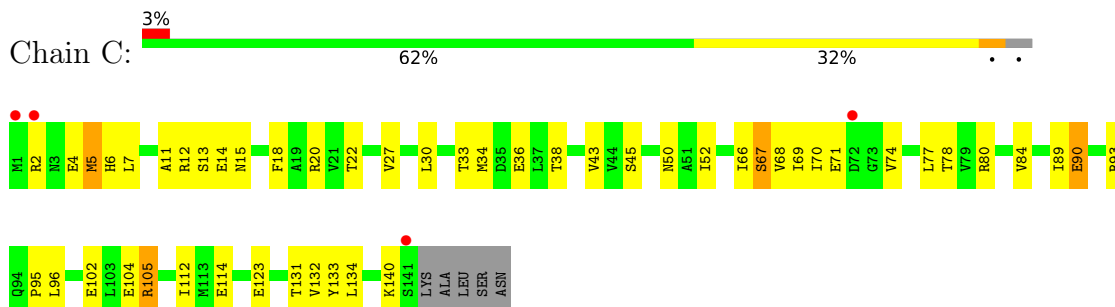
### 3 Residue-property plots [i](#)

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

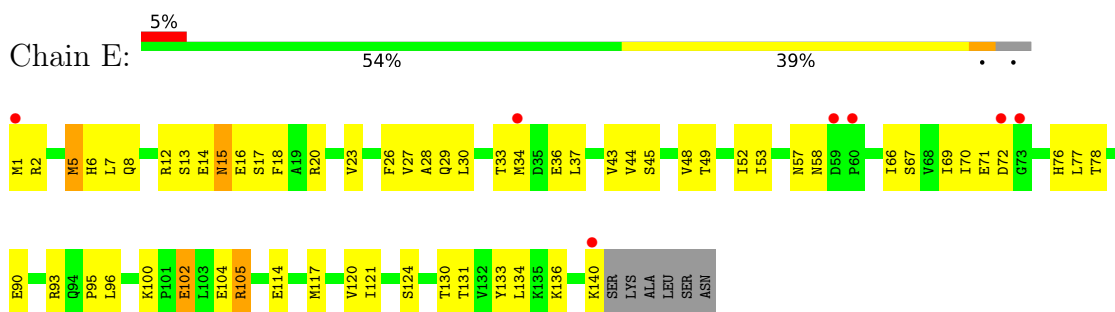
- Molecule 1: Anti-sigma F factor



- Molecule 1: Anti-sigma F factor



- Molecule 1: Anti-sigma F factor

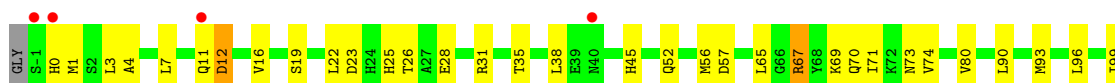


- Molecule 2: Anti-sigma F factor antagonist





- Molecule 2: Anti-sigma F factor antagonist



- Molecule 2: Anti-sigma F factor antagonist



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.13Å 115.13Å 256.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 97.7 (29.92-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.265 0.227 , 0.254	Depositor DCC
$R_{free}$ test set	5372 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.625	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.39	0/1114	0.66	0/1509
1	C	0.40	0/1113	0.63	0/1508
1	E	0.35	0/1108	0.60	0/1501
2	B	0.40	0/909	0.58	0/1223
2	D	0.40	0/911	0.60	2/1227 (0.2%)
2	F	0.40	0/915	0.63	0/1231
All	All	0.39	0/6070	0.62	2/8199 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MET	N-CA-C	-5.12	97.19	111.00
2	D	12	ASP	CB-CG-OD2	5.11	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1098	0	1091	43	0
1	C	1097	0	1088	47	0
1	E	1092	0	1086	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	901	0	937	48	0
2	D	903	0	932	42	0
2	F	906	0	942	49	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	31	0	12	1	0
4	C	31	0	12	2	0
4	E	31	0	12	2	0
5	A	42	0	0	0	0
5	B	18	0	0	2	0
5	C	35	0	0	0	0
5	D	17	0	0	0	0
5	E	20	0	0	0	0
5	F	23	0	0	0	0
All	All	6248	0	6112	267	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 22.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:LEU:HA	2:D:26:THR:HG21	1.32	1.07
2:F:23:ASP:H	2:F:26:THR:CG2	1.74	1.00
1:A:13:SER:HB2	2:B:25:HIS:HB2	1.46	0.94
1:A:33:THR:HB	1:A:36:GLU:HG3	1.49	0.91
2:B:23:ASP:H	2:B:26:THR:HG22	1.33	0.89
2:F:7:LEU:HD22	2:F:16:VAL:HG22	1.58	0.85
2:B:13:VAL:HG22	2:B:45:HIS:HB2	1.59	0.83
1:E:30:LEU:HB3	1:E:140:LYS:NZ	1.95	0.81
2:B:22:LEU:HA	2:B:26:THR:HG21	1.62	0.81
2:D:105:ASP:OD1	2:D:107:GLN:HG2	1.80	0.80
1:A:33:THR:HG22	1:A:35:ASP:H	1.46	0.79
2:D:23:ASP:H	2:D:26:THR:HG22	1.47	0.79
2:B:0:HIS:CB	2:B:29:GLU:HG2	2.13	0.79
2:D:22:LEU:HD12	2:D:26:THR:HG23	1.64	0.78
1:A:54:HIS:ND1	1:A:100:LYS:HE2	2.00	0.76
2:F:19:SER:HA	2:F:52:GLN:O	1.86	0.76
2:D:74:VAL:HG12	2:D:74:VAL:O	1.86	0.75
1:A:125:GLU:OE1	1:A:128:LYS:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ILE:HG22	1:E:58:ASN:OD1	1.86	0.75
1:E:120:VAL:HG22	1:E:134:LEU:HD23	1.69	0.75
2:D:22:LEU:HA	2:D:26:THR:CG2	2.14	0.73
2:B:74:VAL:HG12	2:B:74:VAL:O	1.89	0.72
1:C:80:ARG:HB3	1:C:131:THR:HG23	1.71	0.71
2:B:111:GLN:HA	2:B:116:ALA:O	1.89	0.71
1:C:2:ARG:HG3	1:C:2:ARG:O	1.91	0.70
2:B:22:LEU:HA	2:B:26:THR:CG2	2.20	0.70
1:A:1:MET:HG3	1:A:2:ARG:N	2.05	0.70
1:E:12:ARG:HG3	1:E:14:GLU:OE1	1.90	0.70
2:D:23:ASP:H	2:D:26:THR:CG2	2.05	0.70
2:B:6:ASP:HB3	2:B:17:ARG:HB2	1.74	0.69
2:D:69:LYS:HE3	2:D:73:ASN:HD21	1.56	0.68
1:C:7:LEU:HD22	1:C:22:THR:HG21	1.74	0.68
1:C:43:VAL:CG1	1:C:134:LEU:HD13	2.24	0.67
1:A:13:SER:HB2	2:B:25:HIS:CB	2.21	0.67
2:F:23:ASP:H	2:F:26:THR:HG23	1.58	0.67
2:D:23:ASP:N	2:D:26:THR:HG22	2.08	0.66
2:B:19:SER:HA	2:B:52:GLN:O	1.94	0.66
2:B:99:ILE:HA	5:B:126:HOH:O	1.95	0.66
2:D:7:LEU:HD23	2:D:16:VAL:HG22	1.78	0.66
2:F:50:LEU:HD22	2:F:53:LEU:HD22	1.77	0.65
1:A:95:PRO:HG2	2:F:108:PHE:HD2	1.60	0.65
2:B:77:GLN:HE21	2:B:113:LEU:HD23	1.61	0.64
2:B:66:GLY:HA3	2:B:67:ARG:HH21	1.62	0.64
2:F:67:ARG:HD3	2:F:70:GLN:OE1	1.97	0.64
2:D:96:LEU:O	2:D:99:ILE:HG12	1.97	0.64
1:E:23:VAL:O	1:E:27:VAL:HG23	1.95	0.64
1:E:12:ARG:HD2	1:E:13:SER:H	1.63	0.64
1:A:43:VAL:HG11	1:A:134:LEU:HD22	1.80	0.64
2:B:66:GLY:HA3	2:B:67:ARG:NH2	2.13	0.64
1:C:30:LEU:HD11	1:C:70:ILE:HG23	1.78	0.63
2:F:22:LEU:HD23	2:F:56:MET:HE3	1.78	0.63
2:F:22:LEU:HA	2:F:26:THR:HG21	1.80	0.63
2:D:35:THR:HG22	2:D:70:GLN:NE2	2.14	0.63
1:C:4:GLU:HB2	1:C:69:ILE:HG12	1.80	0.62
1:C:5:MET:HG2	1:C:6:HIS:N	2.14	0.62
1:E:53:ILE:O	1:E:57:ASN:HA	1.99	0.62
2:D:19:SER:HA	2:D:52:GLN:O	1.98	0.62
2:D:96:LEU:O	2:D:96:LEU:HD23	2.00	0.61
1:C:71:GLU:O	1:C:74:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:THR:HG22	2:D:70:GLN:HE22	1.66	0.60
1:E:16:GLU:OE2	2:F:24:HIS:HB3	2.02	0.60
1:C:123:GLU:HG3	1:C:133:TYR:HE1	1.65	0.60
2:F:74:VAL:HG12	2:F:74:VAL:O	2.00	0.60
1:E:13:SER:HB2	2:F:25:HIS:HB2	1.83	0.59
1:C:30:LEU:HD11	1:C:70:ILE:CG2	2.32	0.59
1:E:30:LEU:HD22	1:E:140:LYS:NZ	2.17	0.59
2:B:23:ASP:H	2:B:26:THR:CG2	2.10	0.59
2:B:22:LEU:HD12	2:B:26:THR:HG23	1.85	0.59
1:A:33:THR:HG22	1:A:34:MET:N	2.18	0.58
2:D:7:LEU:CD2	2:D:16:VAL:HG22	2.33	0.58
2:D:22:LEU:HD12	2:D:26:THR:CG2	2.31	0.58
1:A:104:GLU:OE1	2:B:67:ARG:NH2	2.36	0.58
1:A:43:VAL:CG1	1:A:134:LEU:HD22	2.33	0.57
1:C:95:PRO:O	1:C:96:LEU:HB2	2.03	0.57
1:A:89:ILE:O	1:A:93:ARG:HG3	2.04	0.57
1:A:33:THR:CB	1:A:36:GLU:HG3	2.30	0.57
2:F:23:ASP:N	2:F:26:THR:CG2	2.58	0.57
1:E:12:ARG:HG3	1:E:14:GLU:CD	2.25	0.57
1:E:48:VAL:O	1:E:52:ILE:HG13	2.04	0.56
1:E:105:ARG:HG3	4:E:202:ATP:O3G	2.05	0.56
1:E:30:LEU:HB3	1:E:140:LYS:HZ1	1.68	0.56
1:E:30:LEU:HD11	1:E:70:ILE:HG23	1.88	0.56
2:F:57:ASP:OD1	2:F:59:SER:N	2.38	0.56
1:C:133:TYR:O	1:C:134:LEU:HD23	2.06	0.55
1:E:26:PHE:CE2	1:E:70:ILE:HG12	2.42	0.55
2:F:23:ASP:H	2:F:26:THR:HG22	1.65	0.55
1:E:28:ALA:C	1:E:30:LEU:H	2.11	0.55
2:B:67:ARG:N	2:B:67:ARG:NE	2.55	0.55
2:B:101:ARG:NH2	2:B:112:ALA:HB1	2.23	0.54
2:D:4:ALA:HB3	2:D:19:SER:HB3	1.90	0.54
2:F:60:GLY:O	2:F:63:VAL:HG12	2.07	0.54
2:B:74:VAL:O	2:B:74:VAL:CG1	2.55	0.54
1:A:7:LEU:HD22	1:A:22:THR:HG21	1.89	0.54
2:B:10:LYS:O	2:B:11:GLN:C	2.46	0.54
1:E:120:VAL:HG22	1:E:134:LEU:CD2	2.35	0.54
2:B:23:ASP:N	2:B:26:THR:HG22	2.14	0.54
2:B:38:LEU:HD22	2:B:43:ILE:HB	1.90	0.54
2:D:22:LEU:CA	2:D:26:THR:HG21	2.22	0.53
1:E:66:ILE:HG22	1:E:67:SER:N	2.22	0.53
2:D:23:ASP:N	2:D:26:THR:CG2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ARG:HG3	2:F:67:ARG:CZ	2.38	0.53
1:A:91:GLU:O	1:A:94:GLN:HG3	2.08	0.53
1:A:6:HIS:ND1	1:A:67:SER:HB2	2.24	0.53
1:C:104:GLU:OE1	2:D:67:ARG:NH2	2.42	0.53
2:F:22:LEU:HD23	2:F:56:MET:CE	2.39	0.52
1:A:110:PHE:O	1:A:114:GLU:HG3	2.09	0.52
2:F:45:HIS:CD2	2:F:77:GLN:H	2.27	0.52
1:C:12:ARG:NH1	1:C:14:GLU:OE2	2.43	0.52
1:E:69:ILE:HG22	1:E:69:ILE:O	2.08	0.52
1:E:104:GLU:OE1	2:F:67:ARG:NH2	2.42	0.52
1:E:105:ARG:NH2	2:F:59:SER:OG	2.42	0.52
1:C:50:ASN:HB3	4:C:201:ATP:N7	2.25	0.52
1:E:33:THR:HG22	1:E:34:MET:N	2.25	0.52
1:E:77:LEU:HB3	1:E:134:LEU:HB2	1.91	0.52
1:E:100:LYS:HA	1:E:102:GLU:OE2	2.10	0.52
2:F:45:HIS:HD2	2:F:77:GLN:H	1.56	0.52
1:C:104:GLU:CD	2:D:67:ARG:HH22	2.13	0.52
2:B:110:LEU:HB2	2:B:116:ALA:HB3	1.91	0.51
1:E:7:LEU:HD12	1:E:8:GLN:H	1.74	0.51
1:A:104:GLU:OE2	2:B:31:ARG:HD2	2.09	0.51
1:C:13:SER:HB2	2:D:25:HIS:HB2	1.92	0.51
2:D:23:ASP:O	2:D:26:THR:HG22	2.10	0.51
2:B:38:LEU:CD2	2:B:43:ILE:HB	2.40	0.51
2:F:7:LEU:CD2	2:F:16:VAL:HG22	2.37	0.51
2:B:35:THR:O	2:B:39:GLU:HG3	2.11	0.51
2:D:90:LEU:HD23	2:D:93:MET:HE3	1.94	0.50
1:A:104:GLU:CD	2:B:67:ARG:HH22	2.15	0.50
1:E:67:SER:OG	1:E:78:THR:HB	2.12	0.50
2:F:31:ARG:HG3	2:F:67:ARG:NH2	2.27	0.50
1:E:5:MET:HG2	1:E:6:HIS:N	2.26	0.50
2:F:4:ALA:HB3	2:F:19:SER:HB3	1.93	0.50
2:F:22:LEU:HA	2:F:26:THR:CG2	2.42	0.50
1:C:71:GLU:O	1:C:71:GLU:HG3	2.12	0.50
1:E:20:ARG:HD3	1:E:45:SER:HB2	1.92	0.50
1:E:33:THR:HG22	1:E:34:MET:H	1.77	0.50
2:B:65:LEU:HD23	2:B:100:ILE:HD11	1.94	0.50
2:D:115:VAL:O	2:D:115:VAL:HG12	2.12	0.50
1:E:43:VAL:CG1	1:E:134:LEU:HD13	2.42	0.49
2:F:68:TYR:CE2	2:F:99:ILE:HD12	2.47	0.49
2:B:105:ASP:OD1	2:B:107:GLN:HB2	2.12	0.49
1:E:69:ILE:HB	1:E:76:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:VAL:O	2:D:74:VAL:CG1	2.58	0.49
1:E:95:PRO:O	1:E:96:LEU:HB2	2.12	0.49
1:A:80:ARG:HG3	1:A:131:THR:OG1	2.13	0.49
1:E:93:ARG:HH21	1:E:114:GLU:CD	2.15	0.49
1:E:120:VAL:O	1:E:121:ILE:HD13	2.13	0.48
1:C:33:THR:HB	1:C:36:GLU:H	1.79	0.48
1:C:33:THR:HG22	1:C:34:MET:N	2.29	0.48
1:A:50:ASN:HB3	4:A:200:ATP:N7	2.29	0.48
2:B:21:GLU:O	2:B:26:THR:HG21	2.14	0.48
2:F:36:ASP:OD1	2:F:40:ASN:ND2	2.47	0.48
1:C:15:ASN:HA	1:C:18:PHE:HB3	1.95	0.47
1:A:126:VAL:O	1:A:127:ASN:HB2	2.14	0.47
1:C:66:ILE:HG22	1:C:67:SER:N	2.28	0.47
2:F:44:ARG:O	2:F:76:GLY:HA3	2.14	0.47
1:E:43:VAL:HG12	1:E:134:LEU:HD13	1.95	0.47
2:B:3:LEU:HB3	2:B:26:THR:OG1	2.14	0.47
2:B:31:ARG:HB3	2:B:31:ARG:NH1	2.29	0.47
1:A:102:GLU:CD	1:A:102:GLU:H	2.18	0.47
1:E:117:MET:CE	1:E:136:LYS:HB2	2.44	0.47
1:E:124:SER:HB2	1:E:130:THR:HG23	1.97	0.47
2:B:110:LEU:CB	2:B:116:ALA:HB3	2.44	0.47
2:F:72:LYS:C	2:F:74:VAL:H	2.18	0.47
1:C:68:VAL:HG22	1:C:77:LEU:HD23	1.97	0.47
1:C:89:ILE:O	1:C:93:ARG:HG3	2.15	0.46
2:F:65:LEU:HD22	2:F:97:PHE:HE2	1.80	0.46
1:C:20:ARG:HD3	1:C:45:SER:HB2	1.97	0.46
1:A:33:THR:HG22	1:A:35:ASP:N	2.23	0.46
1:A:27:VAL:HG12	1:A:27:VAL:O	2.15	0.46
1:C:33:THR:HB	1:C:36:GLU:HG3	1.97	0.46
1:A:105:ARG:NH1	1:A:105:ARG:HG3	2.31	0.46
2:D:31:ARG:HG3	2:D:67:ARG:NH2	2.30	0.46
1:E:105:ARG:HG3	1:E:105:ARG:NH1	2.31	0.46
2:F:23:ASP:HB2	2:F:57:ASP:OD2	2.16	0.46
2:D:67:ARG:HD3	2:D:67:ARG:HA	1.73	0.45
1:E:44:VAL:HG22	1:E:77:LEU:HD21	1.98	0.45
1:A:102:GLU:C	1:A:103:LEU:HD23	2.37	0.45
2:B:68:TYR:HB2	2:B:78:MET:CE	2.47	0.45
1:E:15:ASN:HA	1:E:18:PHE:HB3	1.98	0.45
4:E:202:ATP:O1G	2:F:58:ALA:HB1	2.17	0.45
2:F:18:LEU:HD21	2:F:30:LEU:HD13	1.98	0.45
1:E:12:ARG:HD2	1:E:13:SER:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:CYS:O	2:F:82:ALA:HB3	2.17	0.45
1:C:2:ARG:O	1:C:2:ARG:CG	2.62	0.45
2:F:49:ASN:HD22	2:F:106:GLU:HB2	1.81	0.45
2:D:38:LEU:HD12	2:D:70:GLN:NE2	2.32	0.45
1:A:5:MET:HG2	1:A:6:HIS:N	2.31	0.45
1:C:14:GLU:HG3	2:D:25:HIS:CE1	2.52	0.45
2:F:67:ARG:HD3	2:F:67:ARG:HA	1.82	0.45
1:E:26:PHE:HE2	1:E:70:ILE:HG12	1.81	0.45
2:B:44:ARG:O	2:B:76:GLY:HA3	2.17	0.44
1:E:71:GLU:O	1:E:72:ASP:HB2	2.17	0.44
2:F:65:LEU:HD22	2:F:97:PHE:CE2	2.51	0.44
2:B:32:GLU:O	2:B:36:ASP:HB2	2.17	0.44
1:C:105:ARG:NH1	1:C:105:ARG:HG3	2.32	0.44
1:E:5:MET:HE2	1:E:7:LEU:HB2	1.98	0.44
2:B:50:LEU:HD22	2:B:53:LEU:HD22	1.99	0.44
1:C:43:VAL:HG11	1:C:134:LEU:HD13	1.97	0.44
2:F:7:LEU:HD13	2:F:37:VAL:HG21	1.99	0.44
1:C:112:ILE:HG12	2:D:93:MET:HE3	2.00	0.44
2:D:45:HIS:HB3	2:D:113:LEU:HD13	2.00	0.44
1:A:108:MET:O	1:A:112:ILE:HG13	2.17	0.44
1:A:126:VAL:HG12	1:A:127:ASN:ND2	2.33	0.44
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.82	0.44
1:C:33:THR:HG22	1:C:34:MET:H	1.83	0.43
1:C:68:VAL:HG22	1:C:77:LEU:CD2	2.47	0.43
1:C:90:GLU:HA	1:C:90:GLU:OE1	2.18	0.43
2:D:65:LEU:HD21	2:D:96:LEU:HD21	2.00	0.43
2:F:19:SER:OG	2:F:52:GLN:HB3	2.18	0.43
2:F:22:LEU:O	2:F:56:MET:HA	2.18	0.43
1:C:93:ARG:HH21	1:C:114:GLU:CD	2.21	0.43
1:C:123:GLU:HG3	1:C:133:TYR:CE1	2.51	0.43
2:F:34:VAL:O	2:F:38:LEU:HG	2.18	0.43
2:B:6:ASP:OD2	2:B:17:ARG:HD2	2.18	0.43
1:C:6:HIS:ND1	1:C:67:SER:HB2	2.33	0.43
1:C:132:VAL:CG1	1:C:134:LEU:HD21	2.48	0.43
2:F:10:LYS:O	2:F:11:GLN:C	2.57	0.43
2:B:68:TYR:HB2	2:B:78:MET:HE2	2.00	0.43
4:C:201:ATP:H5'1	4:C:201:ATP:H8	1.84	0.43
2:D:96:LEU:HD23	2:D:96:LEU:C	2.39	0.43
1:C:11:ALA:HB1	1:C:52:ILE:HG12	2.01	0.43
1:E:105:ARG:HG3	1:E:105:ARG:HH11	1.83	0.43
2:B:2:SER:N	5:B:118:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:THR:HG22	1:E:133:TYR:CE1	2.54	0.43
1:A:120:VAL:HG22	1:A:134:LEU:HD23	2.01	0.43
1:E:1:MET:HG2	1:E:2:ARG:N	2.34	0.43
1:A:33:THR:CG2	1:A:34:MET:N	2.82	0.42
2:B:34:VAL:C	2:B:36:ASP:N	2.73	0.42
2:D:35:THR:HG22	2:D:70:GLN:CD	2.40	0.42
1:A:9:PHE:CE1	1:A:64:VAL:HB	2.55	0.42
1:A:70:ILE:O	1:A:70:ILE:HG13	2.19	0.42
1:C:102:GLU:OE1	1:C:102:GLU:N	2.39	0.42
2:B:23:ASP:HA	2:B:57:ASP:OD1	2.20	0.42
1:E:1:MET:CG	1:E:2:ARG:H	2.33	0.42
1:A:54:HIS:CE1	1:A:100:LYS:HE2	2.55	0.42
1:A:92:ALA:HA	1:A:97:PHE:CD2	2.54	0.42
1:C:93:ARG:HH21	1:C:114:GLU:CG	2.33	0.42
1:E:33:THR:HB	1:E:36:GLU:HG3	2.00	0.42
2:D:23:ASP:HA	2:D:57:ASP:OD1	2.20	0.42
1:E:104:GLU:CD	2:F:67:ARG:HH22	2.23	0.42
2:B:46:ILE:HG13	2:B:71:ILE:HD11	2.02	0.42
1:C:140:LYS:H	1:C:140:LYS:HG2	1.67	0.42
1:E:28:ALA:C	1:E:30:LEU:N	2.73	0.42
1:A:56:TYR:O	1:A:57:ASN:C	2.58	0.42
1:C:66:ILE:CG2	1:C:67:SER:N	2.83	0.41
2:D:80:VAL:O	2:D:102:VAL:HA	2.21	0.41
2:F:65:LEU:HD21	2:F:96:LEU:HD21	2.02	0.41
1:E:30:LEU:CB	1:E:140:LYS:NZ	2.76	0.41
1:C:105:ARG:HG3	1:C:105:ARG:HH11	1.85	0.41
1:C:112:ILE:CD1	2:D:90:LEU:HD22	2.50	0.41
1:A:1:MET:O	1:A:71:GLU:HG3	2.21	0.41
1:A:77:LEU:HD23	1:A:134:LEU:HD13	2.02	0.41
2:D:22:LEU:HD23	2:D:56:MET:HE2	2.03	0.41
1:C:112:ILE:HD13	2:D:90:LEU:HD22	2.03	0.41
2:F:60:GLY:O	2:F:64:ILE:HG13	2.20	0.41
2:F:71:ILE:HG21	2:F:77:GLN:O	2.21	0.41
2:F:83:VAL:HG13	2:F:87:VAL:CG1	2.50	0.41
1:A:13:SER:CB	2:B:25:HIS:HB2	2.33	0.41
1:C:34:MET:CE	1:C:34:MET:HA	2.51	0.41
2:F:33:GLN:O	2:F:37:VAL:HG23	2.21	0.41
1:E:66:ILE:HA	1:E:78:THR:O	2.21	0.40
1:A:126:VAL:HG12	1:A:127:ASN:HD22	1.85	0.40
2:D:3:LEU:CB	2:D:26:THR:OG1	2.68	0.40
1:E:49:THR:O	1:E:53:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ASP:O	2:B:24:HIS:C	2.59	0.40
2:B:12:ASP:OD2	2:B:44:ARG:HB3	2.21	0.40
1:E:17:SER:HA	1:E:20:ARG:CZ	2.52	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	139/146 (95%)	129 (93%)	10 (7%)	0	100	100
1	C	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
1	E	138/146 (94%)	120 (87%)	16 (12%)	2 (1%)	11	28
2	B	115/119 (97%)	106 (92%)	7 (6%)	2 (2%)	9	23
2	D	116/119 (98%)	107 (92%)	6 (5%)	3 (3%)	5	13
2	F	115/119 (97%)	106 (92%)	8 (7%)	1 (1%)	17	40
All	All	762/795 (96%)	699 (92%)	55 (7%)	8 (1%)	15	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	104	ALA
2	B	11	GLN
2	D	11	GLN
1	E	29	GLN
2	F	11	GLN
2	B	115	VAL
1	E	15	ASN
2	D	0	HIS

### 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	125/129 (97%)	117 (94%)	8 (6%)	17	39
1	C	124/129 (96%)	116 (94%)	8 (6%)	17	38
1	E	124/129 (96%)	119 (96%)	5 (4%)	31	60
2	B	97/99 (98%)	93 (96%)	4 (4%)	30	59
2	D	96/99 (97%)	92 (96%)	4 (4%)	30	58
2	F	98/99 (99%)	91 (93%)	7 (7%)	14	34
All	All	664/684 (97%)	628 (95%)	36 (5%)	22	47

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	5	MET
1	A	13	SER
1	A	17	SER
1	A	84	VAL
1	A	102	GLU
1	A	105	ARG
2	B	1	MET
2	B	12	ASP
2	B	36	ASP
2	B	67	ARG
1	C	5	MET
1	C	27	VAL
1	C	38	THR
1	C	67	SER
1	C	78	THR
1	C	84	VAL
1	C	90	GLU
1	C	105	ARG
2	D	12	ASP
2	D	28	GLU

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Mol	Chain	Res	Type
2	D	67	ARG
2	D	71	ILE
1	E	5	MET
1	E	37	LEU
1	E	90	GLU
1	E	102	GLU
1	E	105	ARG
2	F	0	HIS
2	F	2	SER
2	F	12	ASP
2	F	65	LEU
2	F	67	ARG
2	F	93	MET
2	F	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
2	B	40	ASN
2	B	77	GLN
2	B	111	GLN
1	C	94	GLN
1	C	115	ASN
2	D	40	ASN
2	D	73	ASN
1	E	29	GLN
1	E	94	GLN
1	E	115	ASN
1	E	127	ASN
2	F	40	ASN
2	F	45	HIS
2	F	107	GLN
2	F	111	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	C	201	3	26,33,33	2.25	10 (38%)	31,52,52	3.20	12 (38%)
4	ATP	A	200	3	26,33,33	2.11	11 (42%)	31,52,52	3.25	10 (32%)
4	ATP	E	202	3	26,33,33	2.22	9 (34%)	31,52,52	3.25	9 (29%)

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	C	201	3	-	6/18/38/38	0/3/3/3
4	ATP	A	200	3	-	7/18/38/38	0/3/3/3
4	ATP	E	202	3	-	5/18/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	202	ATP	C4-N3	5.55	1.43	1.35
4	C	201	ATP	O4'-C1'	5.18	1.48	1.41
4	A	200	ATP	C4-N3	5.16	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	ATP	C4-N3	5.15	1.42	1.35
4	C	201	ATP	O5'-C5'	-4.56	1.27	1.44
4	E	202	ATP	O4'-C1'	4.38	1.47	1.41
4	E	202	ATP	O5'-C5'	-4.35	1.28	1.44
4	A	200	ATP	O5'-C5'	-4.23	1.28	1.44
4	A	200	ATP	O4'-C1'	4.08	1.46	1.41
4	A	200	ATP	PA-O5'	-3.26	1.46	1.59
4	C	201	ATP	PA-O5'	-3.24	1.46	1.59
4	E	202	ATP	PA-O5'	-3.15	1.46	1.59
4	E	202	ATP	C2-N3	2.87	1.36	1.32
4	C	201	ATP	C8-N7	-2.57	1.30	1.34
4	C	201	ATP	C2-N3	2.47	1.36	1.32
4	E	202	ATP	PB-O1B	-2.45	1.42	1.50
4	E	202	ATP	C8-N7	-2.44	1.30	1.34
4	C	201	ATP	PB-O2B	-2.40	1.44	1.55
4	E	202	ATP	PB-O2B	-2.38	1.44	1.55
4	C	201	ATP	PB-O1B	-2.38	1.42	1.50
4	A	200	ATP	C2-N3	2.31	1.35	1.32
4	A	200	ATP	PB-O2B	-2.24	1.44	1.55
4	A	200	ATP	PB-O1B	-2.20	1.43	1.50
4	A	200	ATP	C8-N7	-2.17	1.30	1.34
4	A	200	ATP	PA-O1A	-2.16	1.43	1.50
4	C	201	ATP	PA-O1A	-2.16	1.43	1.50
4	E	202	ATP	PA-O2A	-2.15	1.45	1.55
4	C	201	ATP	PA-O2A	-2.07	1.45	1.55
4	A	200	ATP	PA-O2A	-2.02	1.45	1.55
4	A	200	ATP	C2'-C1'	2.00	1.56	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	200	ATP	O5'-C5'-C4'	12.80	153.06	108.99
4	E	202	ATP	O5'-C5'-C4'	12.54	152.16	108.99
4	C	201	ATP	O5'-C5'-C4'	12.30	151.32	108.99
4	E	202	ATP	O5'-PA-O1A	-6.64	83.13	109.07
4	A	200	ATP	O5'-PA-O1A	-6.60	83.28	109.07
4	C	201	ATP	O5'-PA-O1A	-6.49	83.71	109.07
4	A	200	ATP	PA-O5'-C5'	5.99	156.79	121.68
4	E	202	ATP	PA-O5'-C5'	5.95	156.57	121.68
4	C	201	ATP	PA-O5'-C5'	5.90	156.30	121.68
4	E	202	ATP	C5'-C4'-C3'	-4.79	97.22	115.18
4	C	201	ATP	C5'-C4'-C3'	-4.59	97.99	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	200	ATP	C5'-C4'-C3'	-4.09	99.84	115.18
4	E	202	ATP	C3'-C2'-C1'	3.55	106.33	100.98
4	A	200	ATP	C3'-C2'-C1'	3.48	106.22	100.98
4	E	202	ATP	O4'-C4'-C5'	-3.10	99.18	109.37
4	C	201	ATP	C3'-C2'-C1'	2.91	105.36	100.98
4	E	202	ATP	O4'-C4'-C3'	2.83	110.72	105.11
4	C	201	ATP	O4'-C4'-C5'	-2.82	100.11	109.37
4	C	201	ATP	C4-C5-N7	2.80	112.32	109.40
4	A	200	ATP	C4-C5-N7	2.61	112.12	109.40
4	C	201	ATP	O4'-C4'-C3'	2.41	109.88	105.11
4	C	201	ATP	O4'-C1'-C2'	-2.36	103.47	106.93
4	E	202	ATP	C4-C5-N7	2.36	111.86	109.40
4	A	200	ATP	O4'-C4'-C3'	2.32	109.71	105.11
4	A	200	ATP	O4'-C4'-C5'	-2.29	101.83	109.37
4	C	201	ATP	O2B-PB-O1B	2.27	123.45	112.24
4	A	200	ATP	O3'-C3'-C4'	2.23	117.49	111.05
4	C	201	ATP	O3'-C3'-C4'	2.18	117.36	111.05
4	E	202	ATP	O2B-PB-O1B	2.13	122.78	112.24
4	C	201	ATP	O2A-PA-O1A	2.12	122.71	112.24
4	A	200	ATP	O2B-PB-O1B	2.11	122.66	112.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	200	ATP	C5'-O5'-PA-O2A
4	A	200	ATP	C5'-O5'-PA-O3A
4	A	200	ATP	C4'-C5'-O5'-PA
4	C	201	ATP	C5'-O5'-PA-O3A
4	C	201	ATP	C4'-C5'-O5'-PA
4	E	202	ATP	C5'-O5'-PA-O3A
4	E	202	ATP	C4'-C5'-O5'-PA
4	A	200	ATP	O4'-C4'-C5'-O5'
4	A	200	ATP	C3'-C4'-C5'-O5'
4	A	200	ATP	C5'-O5'-PA-O1A
4	C	201	ATP	C5'-O5'-PA-O1A
4	C	201	ATP	C5'-O5'-PA-O2A
4	E	202	ATP	C5'-O5'-PA-O1A
4	E	202	ATP	C5'-O5'-PA-O2A
4	C	201	ATP	O4'-C4'-C5'-O5'
4	E	202	ATP	O4'-C4'-C5'-O5'
4	A	200	ATP	PG-O3B-PB-O2B

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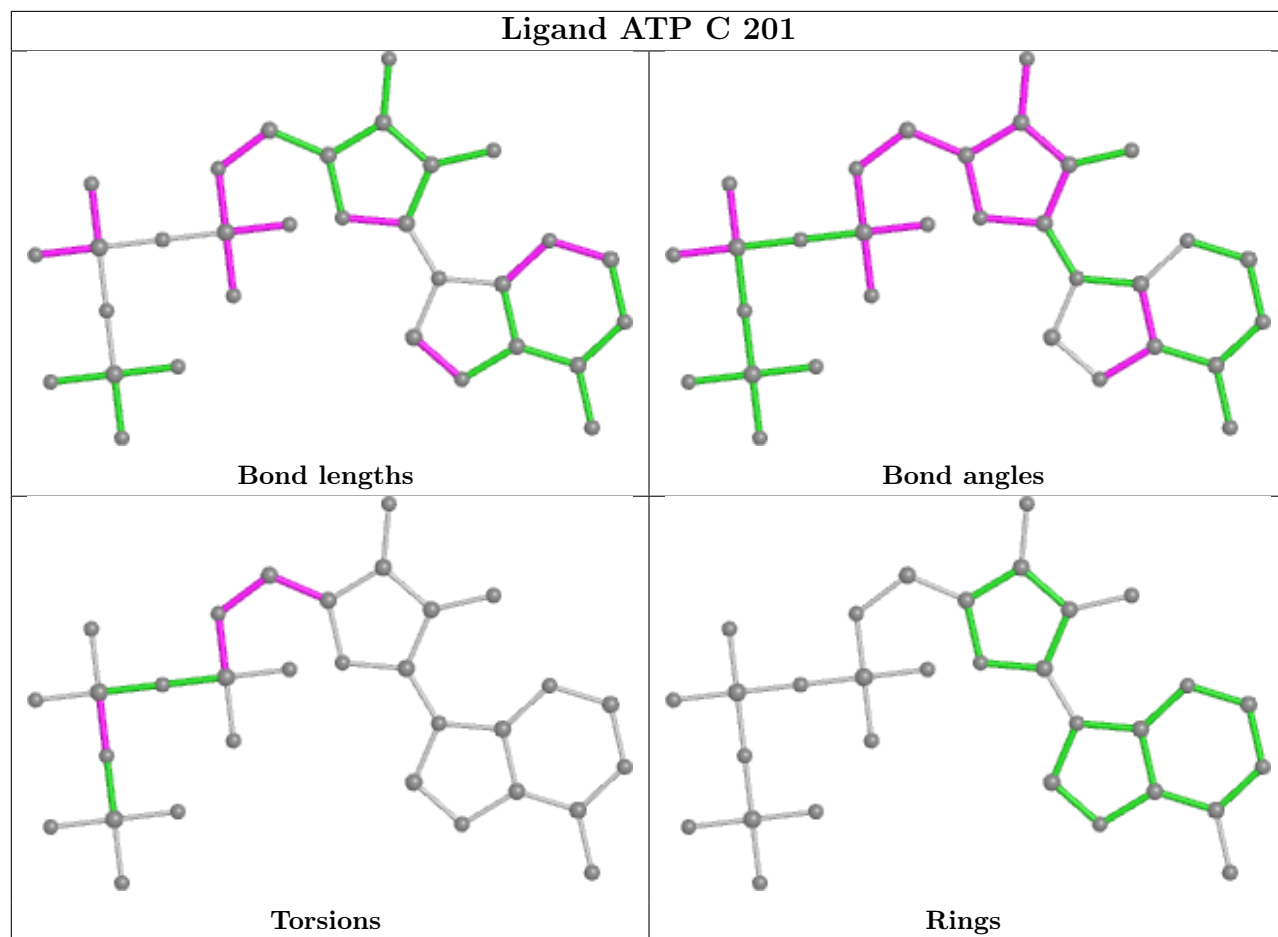
Mol	Chain	Res	Type	Atoms
4	C	201	ATP	PG-O3B-PB-O2B

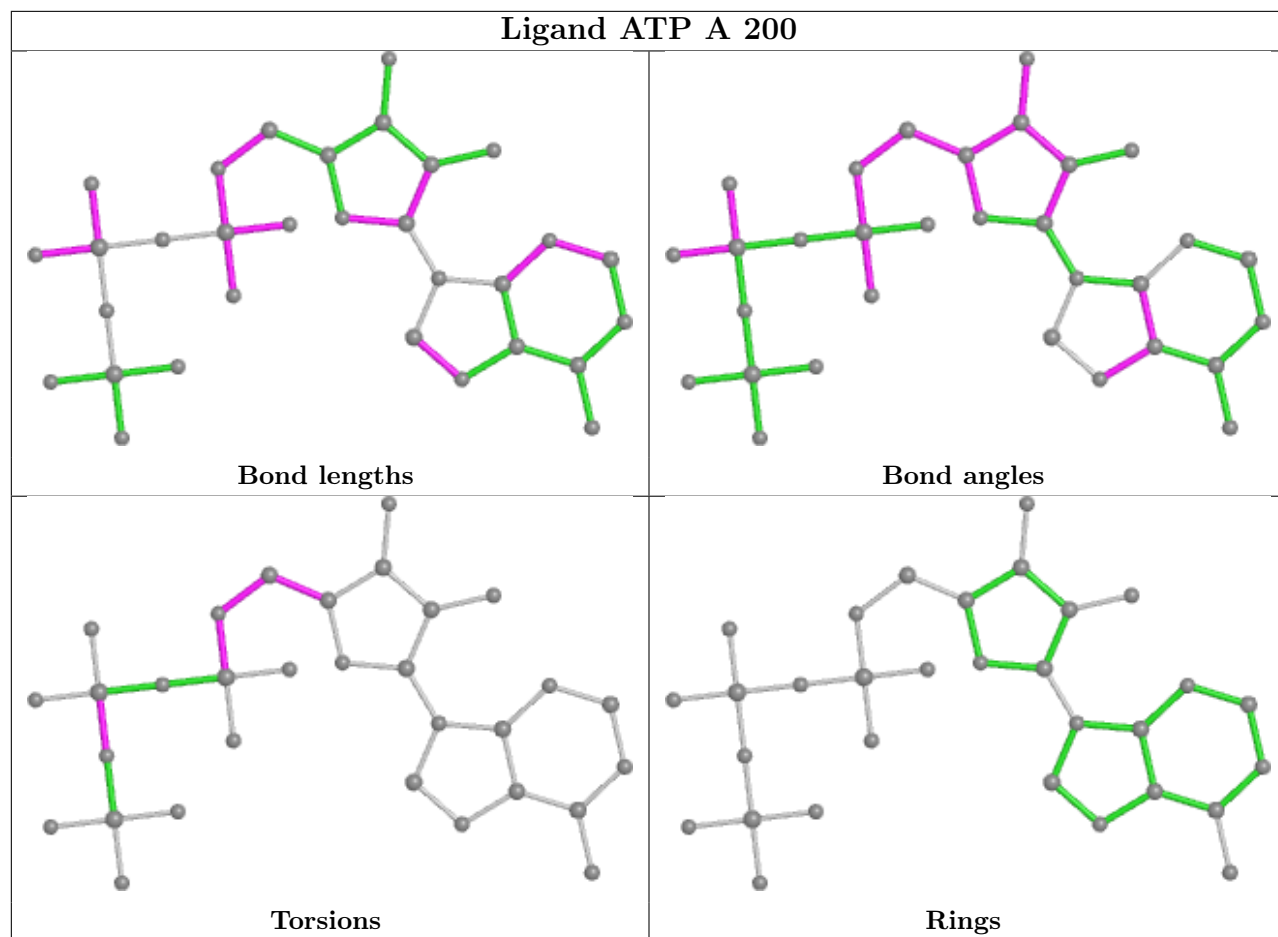
There are no ring outliers.

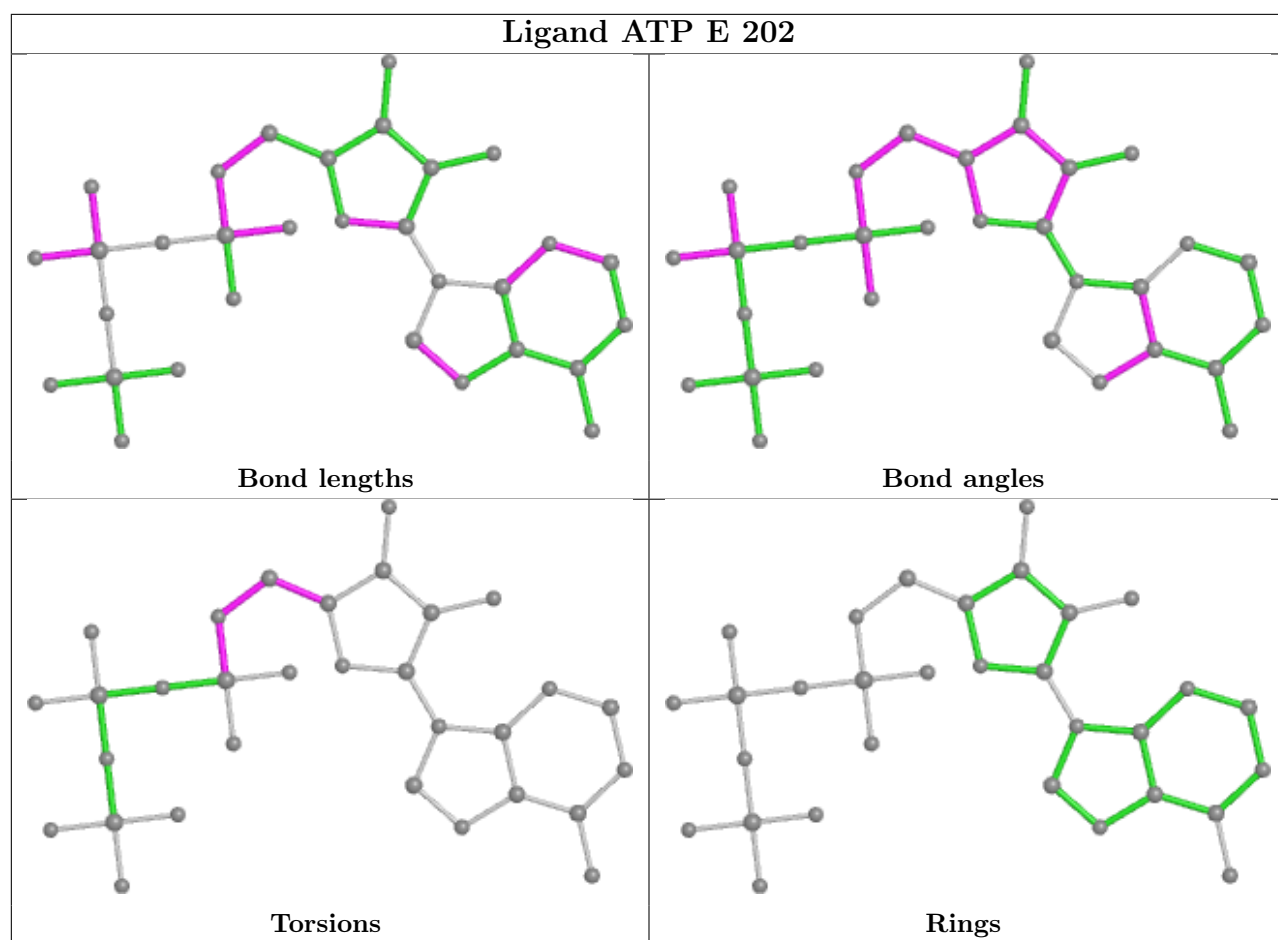
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	ATP	2	0
4	A	200	ATP	1	0
4	E	202	ATP	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	141/146 (96%)	-0.28	3 (2%) 63 65	19, 33, 54, 93	0
1	C	141/146 (96%)	-0.29	4 (2%) 53 54	21, 33, 67, 97	0
1	E	140/146 (95%)	0.05	7 (5%) 28 27	34, 52, 81, 98	0
2	B	117/119 (98%)	-0.11	4 (3%) 45 45	31, 47, 83, 109	0
2	D	118/119 (99%)	-0.28	4 (3%) 45 45	28, 47, 77, 89	0
2	F	117/119 (98%)	-0.27	3 (2%) 56 57	30, 46, 76, 100	0
All	All	774/795 (97%)	-0.19	25 (3%) 47 48	19, 43, 78, 109	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	0	HIS	5.9
1	C	141	SER	5.7
2	B	116	ALA	5.0
1	E	1	MET	4.6
1	A	141	SER	4.3
2	D	0	HIS	4.1
2	F	1	MET	4.0
2	B	11	GLN	3.9
1	E	140	LYS	3.3
2	D	-1	SER	3.2
1	C	1	MET	3.0
2	D	40	ASN	2.9
2	D	11	GLN	2.8
1	A	137	HIS	2.7
1	A	140	LYS	2.7
1	C	2	ARG	2.5
2	B	0	HIS	2.5
1	E	59	ASP	2.5
2	F	40	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	72	ASP	2.4
1	E	72	ASP	2.4
1	E	73	GLY	2.4
1	E	60	PRO	2.1
1	E	34	MET	2.1
2	B	99	ILE	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

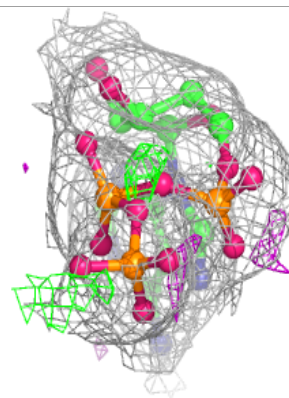
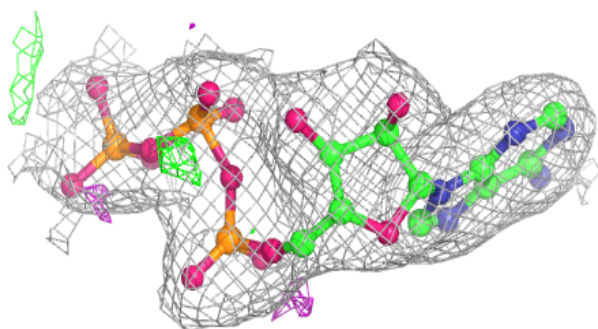
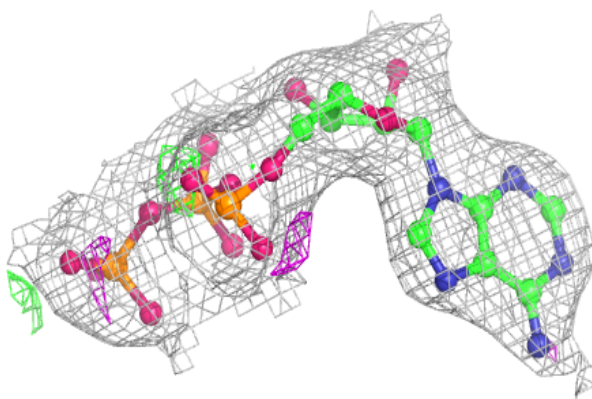
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	300	1/1	0.91	0.31	47,47,47,47	0
3	MG	E	302	1/1	0.93	0.20	35,35,35,35	0
3	MG	C	301	1/1	0.94	0.17	23,23,23,23	0
4	ATP	A	200	31/31	0.96	0.16	30,35,53,54	0
4	ATP	C	201	31/31	0.96	0.15	26,32,47,49	0
4	ATP	E	202	31/31	0.96	0.17	44,49,56,57	0

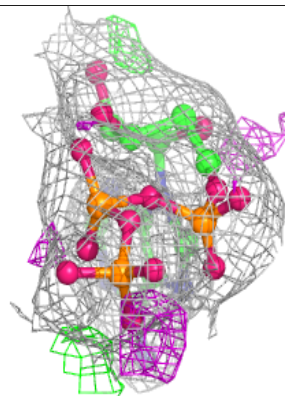
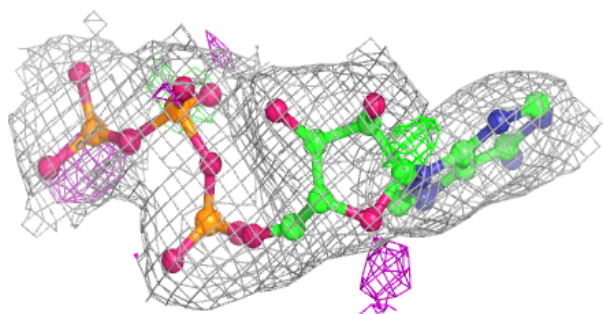
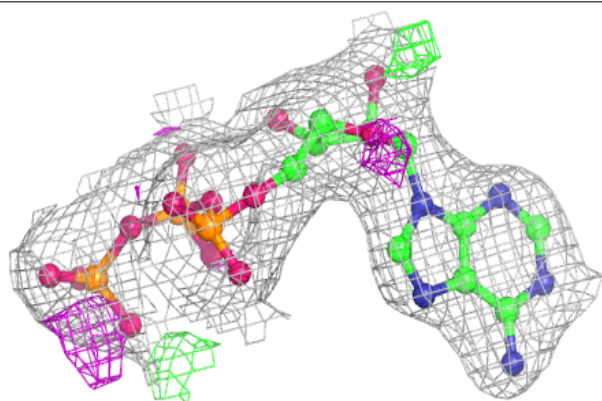
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP A 200:**

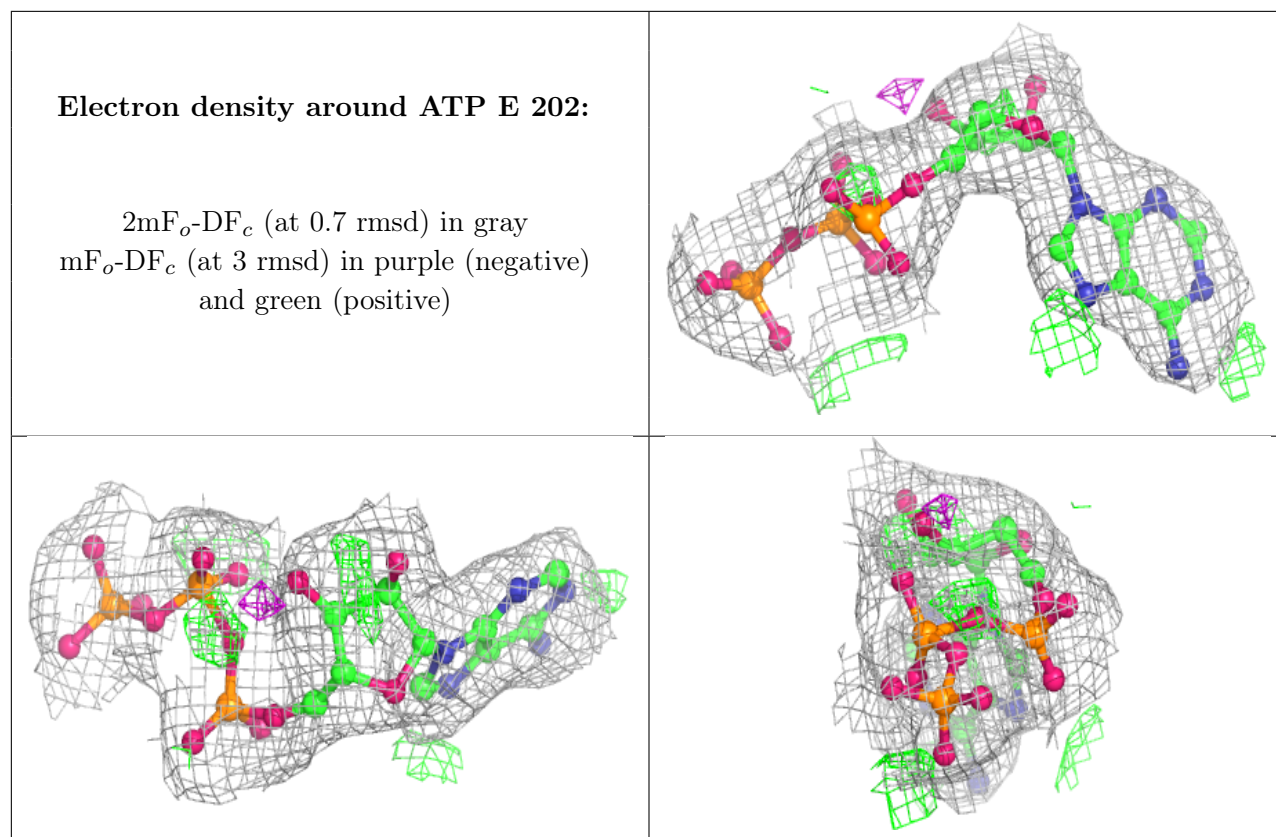
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP C 201:**

$2mF_o-DF_c$  (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.