Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:56 AM EDT

PDB ID	:	5D3M
Title	:	Folate ECF transporter: AMPPNP bound state
Authors	:	Guskov, A.; Swier, L.J.Y.M.; Slotboom, D.J.
Deposited on	:	2015-08-06
Resolution	:	3.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

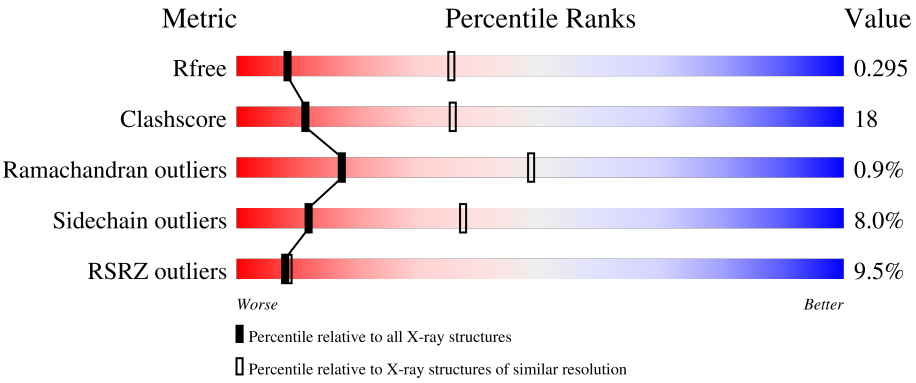
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	298	8% 62% 29% • 6%
1	E	298	9% 64% 27% • 6%
2	B	287	8% 70% 26% • •
2	F	287	10% 67% 28% • •
3	C	184	10% 46% 37% 8% 9%

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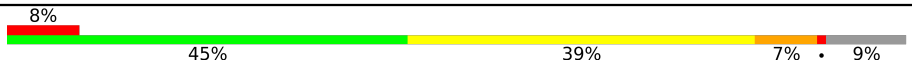
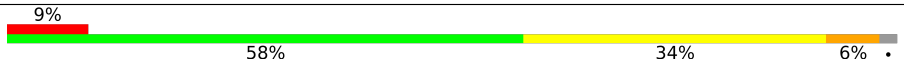
Mol	Chain	Length	Quality of chain
3	G	184	
4	D	265	
4	H	265	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15554 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 Energy-coupling factor transporter ATP-binding protein EcfA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2147	1354	359	430	4			
1	E	280	Total	C	N	O	S	0	0	0
			2147	1354	359	430	4			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q1GBJ0
A	-16	HIS	-	expression tag	UNP Q1GBJ0
A	-15	HIS	-	expression tag	UNP Q1GBJ0
A	-14	HIS	-	expression tag	UNP Q1GBJ0
A	-13	HIS	-	expression tag	UNP Q1GBJ0
A	-12	HIS	-	expression tag	UNP Q1GBJ0
A	-11	HIS	-	expression tag	UNP Q1GBJ0
A	-10	HIS	-	expression tag	UNP Q1GBJ0
A	-9	HIS	-	expression tag	UNP Q1GBJ0
A	-8	HIS	-	expression tag	UNP Q1GBJ0
A	-7	HIS	-	expression tag	UNP Q1GBJ0
A	-6	GLY	-	expression tag	UNP Q1GBJ0
A	-5	GLU	-	expression tag	UNP Q1GBJ0
A	-4	ASN	-	expression tag	UNP Q1GBJ0
A	-3	LEU	-	expression tag	UNP Q1GBJ0
A	-2	TYR	-	expression tag	UNP Q1GBJ0
A	-1	PHE	-	expression tag	UNP Q1GBJ0
A	0	GLN	-	expression tag	UNP Q1GBJ0
A	1	GLY	-	expression tag	UNP Q1GBJ0
E	-17	MET	-	initiating methionine	UNP Q1GBJ0
E	-16	HIS	-	expression tag	UNP Q1GBJ0
E	-15	HIS	-	expression tag	UNP Q1GBJ0
E	-14	HIS	-	expression tag	UNP Q1GBJ0
E	-13	HIS	-	expression tag	UNP Q1GBJ0
E	-12	HIS	-	expression tag	UNP Q1GBJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP Q1GBJ0
E	-10	HIS	-	expression tag	UNP Q1GBJ0
E	-9	HIS	-	expression tag	UNP Q1GBJ0
E	-8	HIS	-	expression tag	UNP Q1GBJ0
E	-7	HIS	-	expression tag	UNP Q1GBJ0
E	-6	GLY	-	expression tag	UNP Q1GBJ0
E	-5	GLU	-	expression tag	UNP Q1GBJ0
E	-4	ASN	-	expression tag	UNP Q1GBJ0
E	-3	LEU	-	expression tag	UNP Q1GBJ0
E	-2	TYR	-	expression tag	UNP Q1GBJ0
E	-1	PHE	-	expression tag	UNP Q1GBJ0
E	0	GLN	-	expression tag	UNP Q1GBJ0
E	1	GLY	-	expression tag	UNP Q1GBJ0

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total	C	N	O	S	0	0	0
			2183	1394	370	411	8			
2	F	281	Total	C	N	O	S	0	0	0
			2183	1394	370	411	8			

- Molecule 3 is a protein called S-component for folate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1302	876	206	210	10			
3	G	168	Total	C	N	O	S	0	0	0
			1302	876	206	210	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	177	TRP	-	expression tag	UNP Q1G929
C	178	SER	-	expression tag	UNP Q1G929
C	179	HIS	-	expression tag	UNP Q1G929
C	180	PRO	-	expression tag	UNP Q1G929
C	181	GLN	-	expression tag	UNP Q1G929
C	182	PHE	-	expression tag	UNP Q1G929
C	183	GLU	-	expression tag	UNP Q1G929
C	184	LYS	-	expression tag	UNP Q1G929
G	177	TRP	-	expression tag	UNP Q1G929

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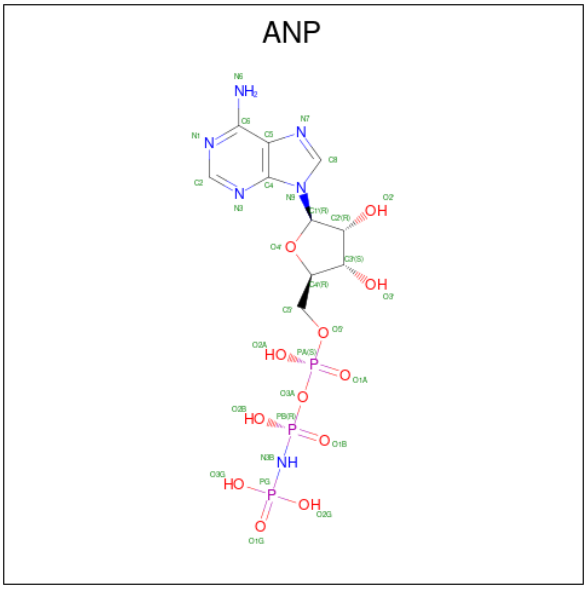
Chain	Residue	Modelled	Actual	Comment	Reference
G	178	SER	-	expression tag	UNP Q1G929
G	179	HIS	-	expression tag	UNP Q1G929
G	180	PRO	-	expression tag	UNP Q1G929
G	181	GLN	-	expression tag	UNP Q1G929
G	182	PHE	-	expression tag	UNP Q1G929
G	183	GLU	-	expression tag	UNP Q1G929
G	184	LYS	-	expression tag	UNP Q1G929

- Molecule 4 is a protein called Energy-coupling factor transporter transmembrane protein EcfT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	259	Total	C	N	O	S	0	0	0
			2083	1391	333	345	14			
4	H	259	Total	C	N	O	S	0	0	0
			2083	1391	333	345	14			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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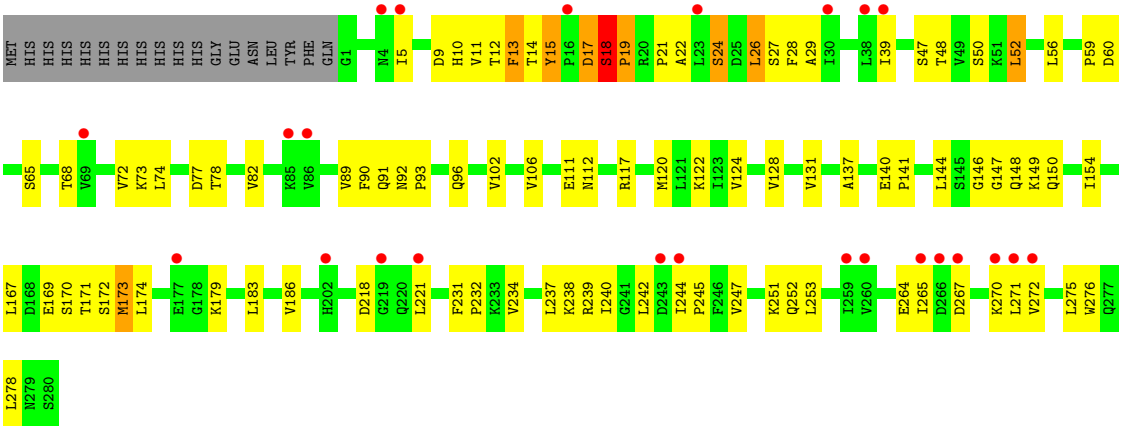
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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.

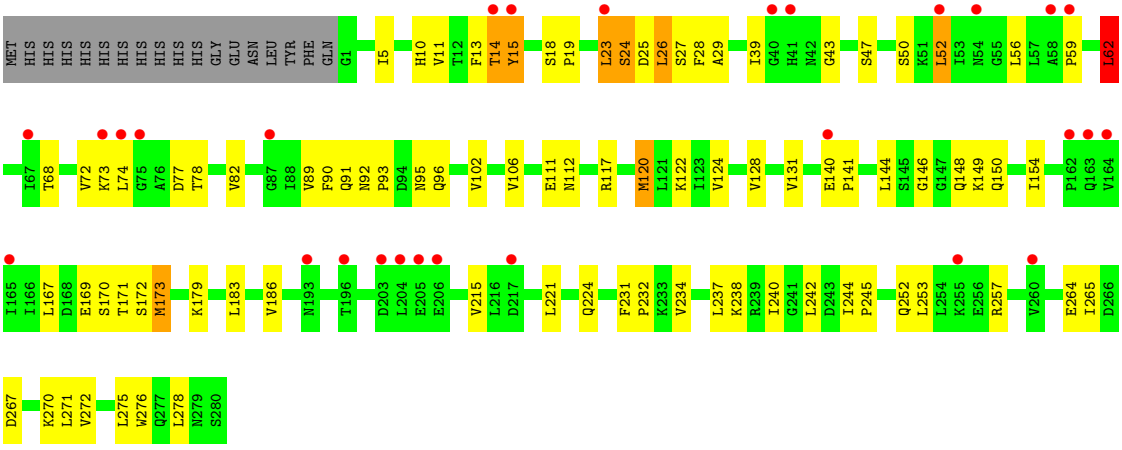
• Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1

Chain A:



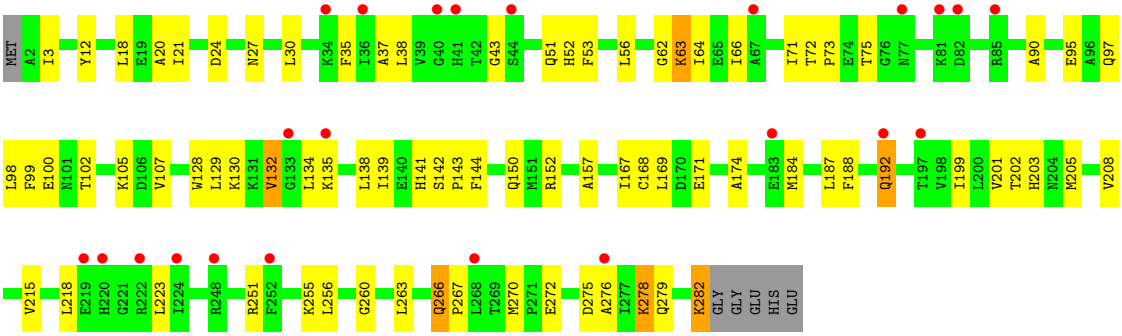
• Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1

Chain E:

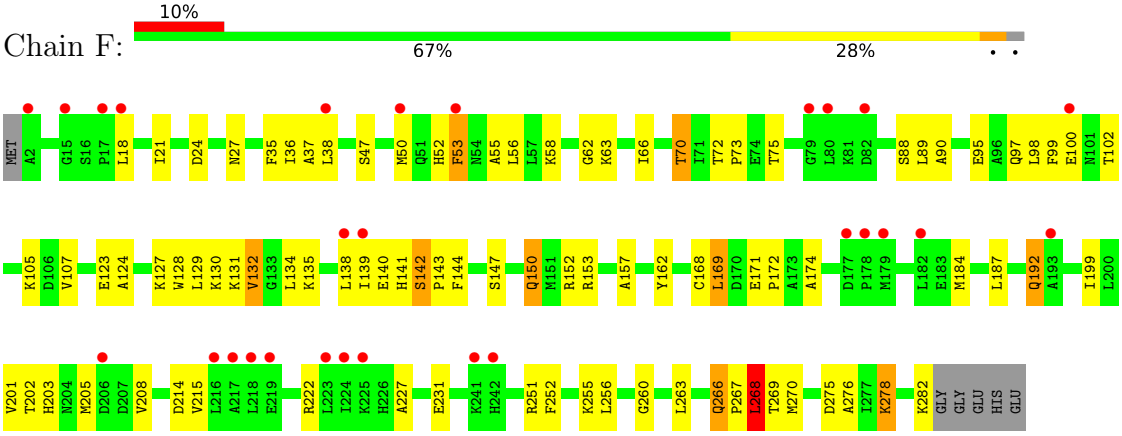


• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2

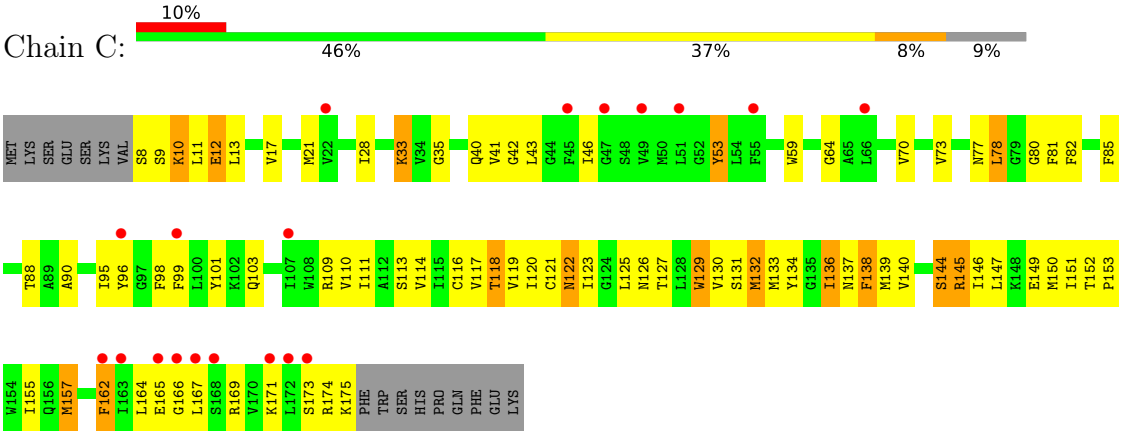
Chain B:



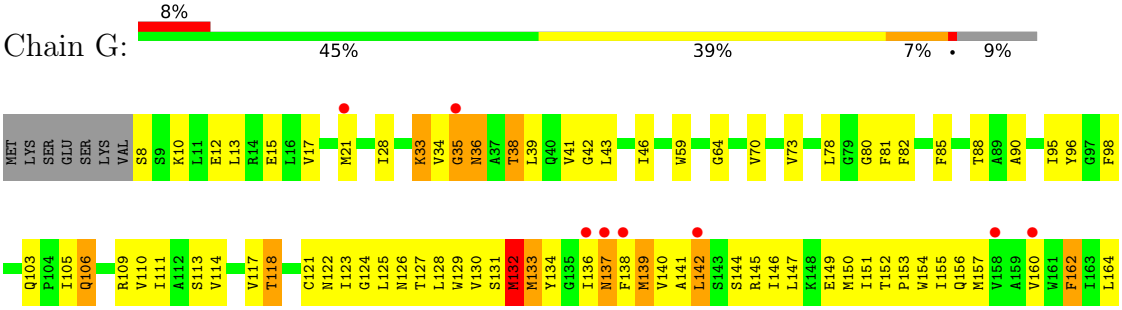
• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2

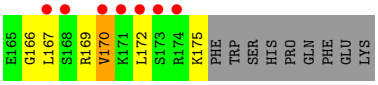


• Molecule 3: S-component for folate

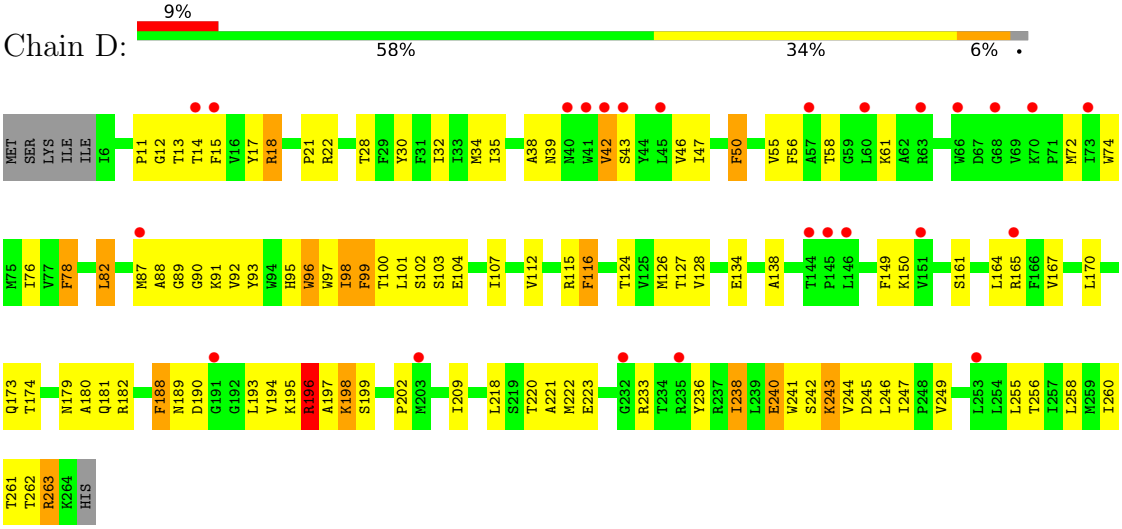


• Molecule 3: S-component for folate

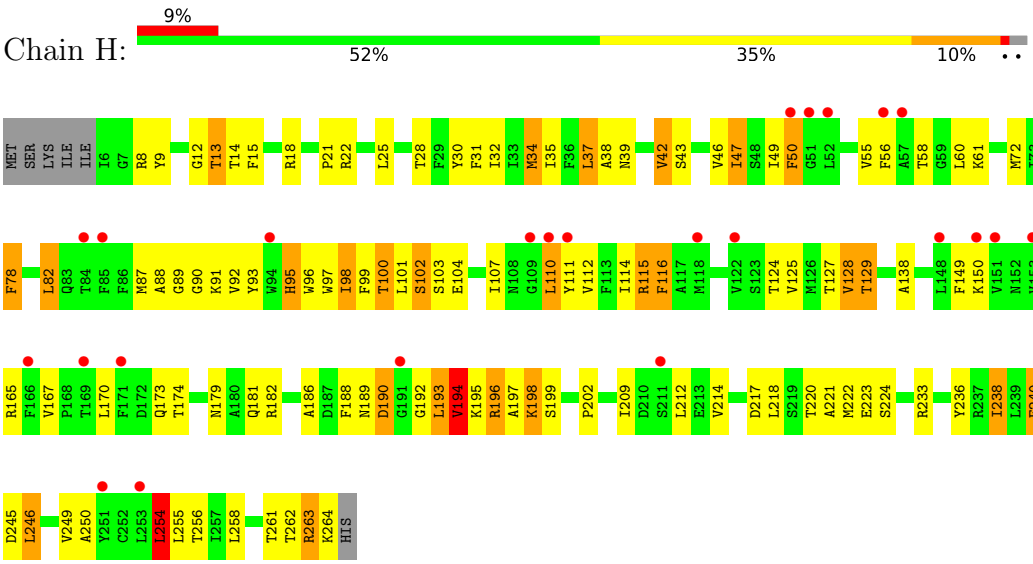




• Molecule 4: Energy-coupling factor transporter transmembrane protein EcfT



• Molecule 4: Energy-coupling factor transporter transmembrane protein EcfT



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.07Å 97.26Å 105.45Å 84.67° 64.78° 62.59°	Depositor
Resolution (Å)	43.86 – 3.30 43.86 – 3.30	Depositor EDS
% Data completeness (in resolution range)	78.8 (43.86-3.30) 78.5 (43.86-3.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.250 , 0.289 0.255 , 0.295	Depositor DCC
R_{free} test set	1709 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	132.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 84.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.368 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP

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	0.30	0/2180	0.57	0/2959
1	E	0.28	0/2180	0.59	1/2959 (0.0%)
2	B	0.26	0/2229	0.58	1/3009 (0.0%)
2	F	0.27	0/2229	0.60	1/3009 (0.0%)
3	C	0.41	0/1333	0.80	2/1806 (0.1%)
3	G	0.34	0/1333	0.78	1/1806 (0.1%)
4	D	0.30	0/2136	0.65	2/2901 (0.1%)
4	H	0.30	0/2136	0.72	6/2901 (0.2%)
All	All	0.30	0/15756	0.65	14/21350 (0.1%)

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	E	0	1
2	B	0	1
2	F	0	1
3	G	0	1
4	D	0	1
4	H	0	6
All	All	0	13

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	268	LEU	CA-CB-CG	9.88	138.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	110	LEU	CA-CB-CG	7.36	132.24	115.30
2	B	18	LEU	CA-CB-CG	7.17	131.78	115.30
4	H	193	LEU	CA-CB-CG	7.06	131.55	115.30
1	E	62	LEU	CA-CB-CG	6.81	130.96	115.30
4	H	98	ILE	C-N-CA	6.62	138.25	121.70
4	H	254	LEU	CA-CB-CG	6.04	129.18	115.30
3	G	35	GLY	N-CA-C	5.93	127.93	113.10
4	H	196	ARG	C-N-CA	5.88	136.40	121.70
3	C	129	TRP	N-CA-C	5.28	125.25	111.00
4	H	98	ILE	CA-C-N	5.28	128.81	117.20
4	D	98	ILE	C-N-CA	5.24	134.79	121.70
3	C	78	LEU	CA-CB-CG	5.16	127.16	115.30
4	D	196	ARG	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	SER	Peptide
1	A	26	LEU	Peptide
2	B	132	VAL	Peptide
4	D	196	ARG	Peptide
1	E	26	LEU	Peptide
2	F	132	VAL	Peptide
3	G	132	MET	Peptide
4	H	13	THR	Peptide
4	H	14	THR	Peptide
4	H	15	PHE	Peptide
4	H	192	GLY	Peptide
4	H	197	ALA	Peptide
4	H	97	TRP	Peptide

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	2147	0	2159	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2147	0	2159	63	0
2	B	2183	0	2187	63	0
2	F	2183	0	2187	67	0
3	C	1302	0	1380	87	0
3	G	1302	0	1380	93	0
4	D	2083	0	2185	87	0
4	H	2083	0	2185	98	0
5	A	31	0	13	4	0
5	B	31	0	13	1	0
5	E	31	0	13	5	0
5	F	31	0	13	1	0
All	All	15554	0	15874	558	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 18.

All (558) 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)
3:C:147:LEU:HG	3:G:147:LEU:H	1.34	0.92
1:E:43:GLY:HA2	5:E:301:ANP:H4'	1.53	0.91
4:D:98:ILE:HB	4:D:99:PHE:HB2	1.60	0.84
4:D:38:ALA:HB1	4:D:39:ASN:HB2	1.61	0.83
3:C:174:ARG:HG3	3:C:175:LYS:HB2	1.63	0.80
4:H:92:VAL:HG22	4:H:104:GLU:HB2	1.62	0.80
1:A:90:PHE:HB2	1:A:96:GLN:HG2	1.65	0.78
4:D:196:ARG:N	4:D:197:ALA:HB3	2.00	0.76
3:G:140:VAL:HG21	4:H:82:LEU:HD22	1.65	0.76
4:D:39:ASN:ND2	4:D:263:ARG:O	2.17	0.76
3:G:121:CYS:O	3:G:126:ASN:ND2	2.19	0.76
4:H:39:ASN:HD21	4:H:264:LYS:HE3	1.48	0.76
1:E:173:MET:SD	1:E:173:MET:N	2.59	0.75
1:A:141:PRO:O	1:A:149:LYS:NZ	2.20	0.75
3:C:121:CYS:HA	3:C:125:LEU:HD23	1.69	0.75
4:H:193:LEU:HA	4:H:196:ARG:HB2	1.69	0.75
3:G:125:LEU:HA	3:G:128:LEU:HG	1.68	0.74
3:G:150:MET:HE2	3:G:151:ILE:HG12	1.69	0.73
2:F:107:VAL:HG11	2:F:129:LEU:HD21	1.70	0.73
1:E:90:PHE:HB2	1:E:96:GLN:HG2	1.72	0.72
4:D:196:ARG:H	4:D:197:ALA:HB3	1.55	0.72
1:E:91:GLN:NE2	5:E:301:ANP:O3G	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:121:CYS:HA	3:G:125:LEU:HD23	1.71	0.71
4:D:100:THR:HG22	4:D:101:LEU:H	1.57	0.70
2:B:107:VAL:HG11	2:B:129:LEU:HD21	1.72	0.70
1:E:238:LYS:HE2	1:E:244:ILE:HD11	1.74	0.70
4:D:98:ILE:CB	4:D:99:PHE:HB2	2.22	0.70
3:C:116:CYS:HB2	3:C:120:ILE:HD11	1.74	0.69
4:H:89:GLY:O	4:H:91:LYS:NZ	2.23	0.69
1:A:238:LYS:HE2	1:A:244:ILE:HD11	1.74	0.69
1:E:141:PRO:O	1:E:149:LYS:NZ	2.26	0.68
3:G:140:VAL:HG11	4:H:82:LEU:HD13	1.74	0.68
1:A:106:VAL:HG23	1:A:124:VAL:HG23	1.73	0.68
4:D:39:ASN:N	4:D:43:SER:OG	2.27	0.68
2:F:171:GLU:HB3	2:F:174:ALA:HB2	1.76	0.68
1:E:106:VAL:HG23	1:E:124:VAL:HG23	1.74	0.67
4:H:39:ASN:N	4:H:43:SER:OG	2.26	0.67
4:D:88:ALA:HB2	4:D:98:ILE:HG23	1.78	0.66
3:C:132:MET:O	4:D:115:ARG:NH1	2.28	0.66
1:A:14:THR:HG22	5:A:301:ANP:HN61	1.61	0.66
2:B:171:GLU:HB3	2:B:174:ALA:HB2	1.78	0.66
3:C:88:THR:CG2	3:C:129:TRP:HE1	2.08	0.66
2:B:53:PHE:HB2	2:B:66:ILE:HD13	1.78	0.66
4:H:125:VAL:O	4:H:129:THR:OG1	2.14	0.66
3:C:131:SER:O	3:C:133:MET:HB2	1.95	0.66
3:G:154:TRP:HA	3:G:157:MET:HG3	1.78	0.65
4:H:263:ARG:HD2	4:H:264:LYS:HG2	1.78	0.65
2:F:134:LEU:HD12	2:F:135:LYS:HB2	1.77	0.65
1:A:14:THR:HG22	5:A:301:ANP:N6	2.11	0.65
5:E:301:ANP:O2A	5:E:301:ANP:N3B	2.29	0.65
3:C:118:THR:HG21	3:C:153:PRO:HG3	1.78	0.65
3:C:145:ARG:HA	3:G:147:LEU:HD21	1.79	0.65
4:D:92:VAL:HG22	4:D:104:GLU:HB2	1.79	0.65
4:H:190:ASP:O	4:H:196:ARG:NH1	2.30	0.64
4:H:193:LEU:C	4:H:195:LYS:H	2.00	0.64
2:B:63:LYS:HD3	2:F:70:THR:HG21	1.78	0.64
2:F:138:LEU:HA	2:F:141:HIS:CD2	2.31	0.64
3:G:128:LEU:HA	3:G:131:SER:HB3	1.78	0.64
3:G:139:MET:HA	3:G:142:LEU:HD23	1.78	0.64
3:G:164:LEU:O	3:G:169:ARG:HB3	1.98	0.64
2:B:138:LEU:HA	2:B:141:HIS:CD2	2.32	0.63
2:F:100:GLU:HA	3:G:167:LEU:HD13	1.80	0.63
1:A:17:ASP:OD2	1:A:17:ASP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HD12	2:B:135:LYS:HB2	1.79	0.63
3:G:155:ILE:HD13	4:H:193:LEU:HD11	1.78	0.63
3:C:147:LEU:HG	3:G:147:LEU:HB2	1.81	0.63
3:C:147:LEU:HB2	3:G:147:LEU:HB2	1.80	0.63
1:E:252:GLN:HG3	1:E:253:LEU:HD12	1.81	0.63
1:E:77:ASP:O	1:E:78:THR:HG22	1.98	0.63
1:A:112:ASN:OD1	4:D:233:ARG:NH1	2.32	0.63
1:A:252:GLN:HG3	1:A:253:LEU:HD12	1.81	0.63
2:B:90:ALA:HB3	2:B:169:LEU:HD22	1.81	0.63
1:A:11:VAL:HG22	1:A:59:PRO:HA	1.79	0.62
3:G:127:THR:O	3:G:138:PHE:HB2	1.99	0.62
1:A:77:ASP:O	1:A:78:THR:HG22	1.98	0.62
2:F:168:CYS:HB3	2:F:199:ILE:HB	1.80	0.62
1:A:11:VAL:O	1:A:22:ALA:HA	1.99	0.62
3:G:118:THR:HA	3:G:122:ASN:HB3	1.80	0.61
3:G:113:SER:O	3:G:117:VAL:HG23	2.00	0.61
3:G:162:PHE:O	3:G:166:GLY:HA3	2.01	0.61
4:H:39:ASN:ND2	4:H:263:ARG:O	2.32	0.61
3:C:162:PHE:O	3:C:166:GLY:HA3	2.01	0.61
2:B:168:CYS:HB3	2:B:199:ILE:HB	1.81	0.61
2:B:75:THR:HA	2:F:75:THR:HA	1.82	0.61
1:E:112:ASN:OD1	4:H:233:ARG:NH1	2.34	0.61
3:C:110:VAL:O	3:C:113:SER:OG	2.15	0.61
4:D:161:SER:O	4:D:165:ARG:NH1	2.34	0.61
4:H:92:VAL:HG23	4:H:93:TYR:CD1	2.35	0.61
1:A:171:THR:HB	1:A:179:LYS:HG3	1.81	0.60
1:E:272:VAL:HG21	2:F:255:LYS:HD2	1.83	0.60
4:H:38:ALA:HB1	4:H:39:ASN:HB2	1.83	0.60
3:C:147:LEU:HB2	3:G:147:LEU:HD12	1.82	0.60
4:H:50:PHE:HD2	4:H:255:LEU:HD13	1.65	0.60
4:D:194:VAL:O	4:D:195:LYS:HB3	2.02	0.60
1:A:74:LEU:HD12	1:A:82:VAL:HG11	1.84	0.60
4:H:112:VAL:HA	4:H:115:ARG:HG2	1.84	0.59
4:H:161:SER:O	4:H:165:ARG:NH1	2.35	0.59
1:E:74:LEU:HD12	1:E:82:VAL:HG11	1.85	0.59
2:F:98:LEU:HD13	2:F:143:PRO:HB2	1.84	0.59
4:H:190:ASP:O	4:H:196:ARG:HG3	2.02	0.59
2:F:53:PHE:HB2	2:F:66:ILE:HD13	1.83	0.59
1:A:26:LEU:HA	1:A:27:SER:HB2	1.85	0.59
4:H:195:LYS:HA	4:H:198:LYS:HB3	1.85	0.59
3:C:81:PHE:N	3:C:82:PHE:HA	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:PHE:N	3:G:82:PHE:HA	2.17	0.59
4:D:91:LYS:HB3	4:D:104:GLU:HB3	1.85	0.58
2:B:37:ALA:HB3	2:B:215:VAL:HG22	1.85	0.58
4:D:30:TYR:HE2	4:D:256:THR:HG21	1.68	0.58
4:H:34:MET:HA	4:H:37:LEU:HD23	1.84	0.58
4:H:96:TRP:HB3	4:H:100:THR:HB	1.85	0.58
1:E:144:LEU:HB3	1:E:148:GLN:HG3	1.85	0.58
2:B:128:TRP:O	2:B:132:VAL:HG12	2.04	0.58
2:B:97:GLN:O	4:D:181:GLN:NE2	2.37	0.58
4:D:95:HIS:N	4:D:96:TRP:HA	2.18	0.58
3:G:136:ILE:O	3:G:139:MET:HG3	2.03	0.58
3:C:96:TYR:CZ	3:C:117:VAL:HG21	2.38	0.57
3:G:136:ILE:HD12	3:G:139:MET:HG2	1.85	0.57
4:H:170:LEU:O	4:H:174:THR:OG1	2.21	0.57
4:H:189:ASN:HB3	4:H:196:ARG:HG2	1.86	0.57
2:B:167:ILE:HD11	2:B:169:LEU:HD21	1.87	0.57
3:C:130:VAL:HG22	3:C:138:PHE:CE1	2.40	0.57
3:G:167:LEU:HA	3:G:170:VAL:HG22	1.85	0.57
4:D:170:LEU:O	4:D:174:THR:OG1	2.21	0.57
2:F:268:LEU:HD13	2:F:269:THR:HG22	1.87	0.57
3:G:150:MET:CE	3:G:151:ILE:HG12	2.34	0.57
3:C:131:SER:O	3:C:133:MET:N	2.37	0.57
1:A:11:VAL:HG21	1:A:52:LEU:HD21	1.87	0.56
1:A:272:VAL:HG21	2:B:255:LYS:HD2	1.87	0.56
2:B:134:LEU:HD21	2:B:150:GLN:HB3	1.86	0.56
3:C:10:LYS:HE2	3:C:59:TRP:HE1	1.70	0.56
4:D:195:LYS:HA	4:D:198:LYS:HG2	1.87	0.56
4:D:28:THR:HG21	4:D:126:MET:HB2	1.87	0.56
4:D:96:TRP:HD1	4:D:97:TRP:CD1	2.24	0.56
3:G:127:THR:HG22	3:G:145:ARG:HH22	1.69	0.56
3:G:128:LEU:O	3:G:131:SER:OG	2.21	0.56
3:C:119:VAL:O	3:C:123:ILE:HB	2.05	0.56
3:G:126:ASN:O	3:G:130:VAL:HG23	2.06	0.56
1:A:169:GLU:HG2	1:A:172:SER:HB3	1.87	0.56
3:C:116:CYS:HB2	3:C:120:ILE:CD1	2.35	0.56
2:F:134:LEU:HD21	2:F:150:GLN:HB3	1.88	0.56
4:H:30:TYR:CE2	4:H:256:THR:HG21	2.41	0.56
4:H:124:THR:O	4:H:128:VAL:HG22	2.05	0.55
3:C:95:ILE:HD11	3:C:117:VAL:HG22	1.87	0.55
3:G:82:PHE:HB3	3:G:85:PHE:H	1.71	0.55
3:G:28:ILE:HD11	4:H:167:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:LEU:HD12	3:G:151:ILE:HD12	1.88	0.55
2:F:135:LYS:HB3	2:F:138:LEU:HG	1.89	0.55
3:G:36:ASN:N	3:G:36:ASN:HD22	2.03	0.55
1:A:102:VAL:O	1:A:106:VAL:HG22	2.07	0.55
3:C:53:TYR:HE1	3:C:169:ARG:HD3	1.71	0.55
3:G:126:ASN:ND2	3:G:126:ASN:H	2.04	0.55
3:G:95:ILE:HD11	3:G:117:VAL:HG22	1.89	0.55
3:G:172:LEU:O	3:G:175:LYS:N	2.31	0.55
4:H:91:LYS:HB3	4:H:104:GLU:HB3	1.88	0.55
4:H:21:PRO:HB2	4:H:138:ALA:HB2	1.89	0.55
1:A:231:PHE:N	1:A:232:PRO:HD2	2.22	0.55
2:F:37:ALA:HB3	2:F:215:VAL:HG22	1.89	0.55
3:C:99:PHE:O	3:C:109:ARG:HD3	2.06	0.55
4:D:88:ALA:CB	4:D:98:ILE:HG23	2.36	0.55
1:A:10:HIS:O	1:A:60:ASP:N	2.32	0.54
1:A:14:THR:O	1:A:14:THR:OG1	2.23	0.54
4:D:89:GLY:O	4:D:91:LYS:NZ	2.32	0.54
3:C:130:VAL:HG13	3:C:138:PHE:CZ	2.42	0.54
1:A:68:THR:HA	1:A:72:VAL:O	2.07	0.54
1:A:237:LEU:HA	1:A:240:ILE:HD12	1.90	0.54
1:E:167:LEU:HD11	1:E:186:VAL:HG21	1.90	0.54
3:G:34:VAL:HG13	3:G:35:GLY:HA2	1.89	0.54
1:E:26:LEU:HD12	1:E:221:LEU:HD23	1.90	0.54
1:E:231:PHE:N	1:E:232:PRO:HD2	2.22	0.54
5:A:301:ANP:N3B	5:A:301:ANP:O1A	2.40	0.54
2:B:98:LEU:HD13	2:B:143:PRO:HB2	1.90	0.54
4:H:115:ARG:HG3	4:H:116:PHE:N	2.23	0.54
4:H:149:PHE:CG	4:H:150:LYS:N	2.76	0.54
4:H:199:SER:O	4:H:202:PRO:HD2	2.08	0.54
1:A:167:LEU:HD11	1:A:186:VAL:HG21	1.89	0.53
3:C:130:VAL:HG13	3:C:138:PHE:HZ	1.73	0.53
3:C:126:ASN:O	3:C:138:PHE:CZ	2.62	0.53
4:H:196:ARG:O	4:H:199:SER:OG	2.19	0.53
1:A:144:LEU:HB3	1:A:148:GLN:HG3	1.90	0.53
3:C:118:THR:OG1	3:C:119:VAL:N	2.42	0.53
2:F:102:THR:HA	2:F:142:SER:HA	1.91	0.53
4:H:193:LEU:O	4:H:195:LYS:N	2.33	0.53
3:C:147:LEU:CG	3:G:147:LEU:HB2	2.39	0.53
2:B:134:LEU:HD12	2:B:135:LYS:HE3	1.90	0.53
4:D:21:PRO:HB2	4:D:138:ALA:HB2	1.91	0.53
1:E:172:SER:OG	1:E:173:MET:SD	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:VAL:O	1:E:106:VAL:HG22	2.09	0.53
1:E:237:LEU:HA	1:E:240:ILE:HD12	1.91	0.53
3:G:129:TRP:O	3:G:132:MET:HG3	2.09	0.53
3:C:118:THR:HA	3:C:122:ASN:HD22	1.75	0.52
4:D:72:MET:O	4:D:76:ILE:HG12	2.09	0.52
4:D:91:LYS:N	4:D:102:SER:OG	2.41	0.52
3:G:43:LEU:HB2	3:G:46:ILE:HD11	1.91	0.52
2:B:102:THR:HA	2:B:142:SER:HA	1.91	0.52
3:C:88:THR:HG21	3:C:129:TRP:HE1	1.74	0.52
3:C:150:MET:HE2	3:C:151:ILE:HG12	1.91	0.52
4:D:11:PRO:HD2	4:D:128:VAL:HG13	1.91	0.52
4:D:149:PHE:CG	4:D:150:LYS:N	2.78	0.52
3:G:126:ASN:H	3:G:126:ASN:HD22	1.57	0.52
3:C:28:ILE:HD11	4:D:167:VAL:HG13	1.90	0.52
4:D:12:GLY:HA2	4:D:18:ARG:NH1	2.24	0.52
4:D:30:TYR:CE2	4:D:256:THR:HG21	2.44	0.52
1:E:13:PHE:HB2	5:E:301:ANP:C2	2.39	0.52
1:E:89:VAL:HG21	1:E:154:ILE:HD13	1.90	0.52
2:B:100:GLU:HA	3:C:167:LEU:HD13	1.91	0.52
2:B:21:ILE:HD12	2:B:24:ASP:OD2	2.09	0.52
3:C:113:SER:O	3:C:117:VAL:HG23	2.10	0.52
4:D:190:ASP:O	4:D:196:ARG:NH1	2.42	0.52
2:B:99:PHE:HD1	2:B:100:GLU:HG3	1.75	0.52
2:B:279:GLN:HA	2:B:282:LYS:HB2	1.91	0.52
2:F:99:PHE:HD1	2:F:100:GLU:HG3	1.75	0.51
2:F:171:GLU:HA	2:F:202:THR:HG22	1.91	0.51
3:G:137:ASN:OD1	3:G:137:ASN:N	2.25	0.51
4:H:43:SER:O	4:H:47:ILE:HG23	2.09	0.51
3:G:96:TYR:CZ	3:G:117:VAL:HG21	2.46	0.51
4:H:28:THR:O	4:H:32:ILE:HG12	2.10	0.51
1:A:24:SER:OG	1:A:26:LEU:HD13	2.10	0.51
3:C:110:VAL:O	3:C:114:VAL:HG23	2.10	0.51
4:D:28:THR:O	4:D:32:ILE:HG12	2.10	0.51
4:H:30:TYR:HE2	4:H:256:THR:HG21	1.74	0.51
1:A:12:THR:HG22	1:A:21:PRO:O	2.10	0.51
3:C:144:SER:OG	3:G:150:MET:SD	2.53	0.51
3:G:141:ALA:O	3:G:144:SER:HB2	2.10	0.51
3:C:129:TRP:CE3	3:C:129:TRP:HA	2.45	0.51
1:A:89:VAL:HG21	1:A:154:ILE:HD13	1.91	0.51
3:C:132:MET:HB2	4:D:115:ARG:HH12	1.75	0.51
3:C:136:ILE:HD13	3:C:136:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:111:ILE:HG13	3:G:157:MET:SD	2.51	0.50
2:B:51:GLN:HB2	2:B:56:LEU:HB2	1.93	0.50
3:C:77:ASN:O	3:C:78:LEU:HG	2.11	0.50
4:D:92:VAL:HG23	4:D:93:TYR:CD1	2.46	0.50
4:H:263:ARG:HG3	4:H:264:LYS:N	2.26	0.50
4:D:38:ALA:HB1	4:D:39:ASN:CB	2.35	0.50
2:F:134:LEU:HD12	2:F:135:LYS:HE3	1.93	0.50
2:B:72:THR:H	2:B:75:THR:HG23	1.77	0.50
3:C:11:LEU:C	3:C:12:GLU:HG2	2.31	0.50
3:C:147:LEU:HD21	3:G:146:ILE:N	2.26	0.50
3:G:129:TRP:HA	3:G:129:TRP:CE3	2.47	0.50
2:B:152:ARG:O	2:B:152:ARG:HG2	2.11	0.50
2:B:266:GLN:N	2:B:267:PRO:HD3	2.27	0.50
1:E:267:ASP:HB2	1:E:270:LYS:HB2	1.93	0.50
2:B:38:LEU:HB3	2:B:201:VAL:HG22	1.92	0.50
1:E:171:THR:HB	1:E:179:LYS:HG3	1.93	0.50
2:F:256:LEU:O	2:F:260:GLY:HA3	2.10	0.50
1:A:147:GLY:HA2	1:A:174:LEU:HD22	1.94	0.50
3:C:43:LEU:HB2	3:C:46:ILE:HD11	1.93	0.50
1:E:68:THR:HA	1:E:72:VAL:O	2.12	0.50
4:H:38:ALA:HB1	4:H:39:ASN:CB	2.42	0.50
2:B:171:GLU:HA	2:B:202:THR:HG22	1.93	0.49
4:D:190:ASP:O	4:D:196:ARG:HG3	2.12	0.49
3:G:118:THR:HG21	3:G:153:PRO:HG3	1.94	0.49
3:C:70:VAL:HG13	4:D:164:LEU:HD23	1.93	0.49
2:F:152:ARG:HG2	2:F:152:ARG:O	2.12	0.49
2:F:169:LEU:HD13	2:F:172:PRO:HG3	1.94	0.49
2:F:275:ASP:O	2:F:278:LYS:HG3	2.12	0.49
1:E:96:GLN:HG3	4:H:221:ALA:HB2	1.94	0.49
2:F:278:LYS:HE3	2:F:282:LYS:HG3	1.93	0.49
2:B:256:LEU:O	2:B:260:GLY:HA3	2.11	0.49
2:F:50:MET:HE1	2:F:53:PHE:HZ	1.77	0.49
1:A:124:VAL:HG11	4:D:236:TYR:CE1	2.48	0.49
2:B:138:LEU:HA	2:B:141:HIS:CG	2.48	0.49
4:D:260:ILE:O	4:D:263:ARG:HB3	2.12	0.49
2:F:95:GLU:HG3	2:F:152:ARG:HB2	1.94	0.49
3:C:129:TRP:C	3:C:131:SER:H	2.14	0.49
2:F:88:SER:HG	2:F:162:TYR:HH	1.61	0.49
2:F:266:GLN:N	2:F:267:PRO:HD3	2.27	0.49
4:H:242:SER:O	4:H:244:VAL:N	2.41	0.49
2:F:97:GLN:O	4:H:181:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:70:VAL:HG13	4:H:164:LEU:HD23	1.93	0.49
2:B:134:LEU:CD2	2:B:150:GLN:HB3	2.42	0.49
3:C:145:ARG:HA	3:G:147:LEU:CD2	2.41	0.49
4:H:74:TRP:O	4:H:78:PHE:HB2	2.13	0.49
1:E:10:HIS:HE1	1:E:25:ASP:OD1	1.96	0.48
1:E:11:VAL:HG22	1:E:59:PRO:HA	1.95	0.48
2:F:138:LEU:HA	2:F:141:HIS:CG	2.48	0.48
3:G:103:GLN:HB3	3:G:109:ARG:CZ	2.43	0.48
4:D:74:TRP:HE1	3:G:150:MET:HE3	1.77	0.48
2:B:95:GLU:HG3	2:B:152:ARG:HB2	1.95	0.48
2:F:56:LEU:HD13	4:H:179:ASN:HB3	1.96	0.48
1:E:117:ARG:HD3	4:H:238:ILE:HG13	1.94	0.48
3:G:17:VAL:O	3:G:21:MET:HG2	2.14	0.48
1:E:5:ILE:HG13	1:E:29:ALA:HB2	1.96	0.48
2:F:144:PHE:CE2	4:H:209:ILE:HG21	2.48	0.48
3:G:152:THR:HA	3:G:155:ILE:HG22	1.94	0.48
1:A:150:GLN:O	1:A:154:ILE:HG12	2.13	0.48
4:D:198:LYS:O	4:D:198:LYS:NZ	2.45	0.48
3:C:17:VAL:O	3:C:21:MET:HG2	2.14	0.48
3:C:95:ILE:HA	3:C:98:PHE:HD2	1.79	0.48
3:C:131:SER:HB3	3:C:138:PHE:CD2	2.48	0.48
2:B:102:THR:HG23	2:B:105:LYS:H	1.78	0.48
2:B:132:VAL:HG11	2:B:157:ALA:HB2	1.96	0.48
2:B:135:LYS:HB3	2:B:138:LEU:HG	1.96	0.48
1:E:124:VAL:HG11	4:H:236:TYR:CE1	2.49	0.48
2:F:90:ALA:HB3	2:F:169:LEU:HB3	1.95	0.48
3:C:82:PHE:HB3	3:C:85:PHE:H	1.79	0.47
3:C:147:LEU:CB	3:G:147:LEU:HB2	2.43	0.47
3:C:33:LYS:HA	3:C:42:GLY:HA2	1.97	0.47
3:C:132:MET:HG3	4:D:115:ARG:HH22	1.79	0.47
4:D:188:PHE:HB2	4:D:189:ASN:HA	1.95	0.47
3:C:88:THR:HG21	3:C:129:TRP:NE1	2.30	0.47
2:F:47:SER:OG	5:F:301:ANP:O3G	2.32	0.47
2:B:168:CYS:O	2:B:169:LEU:HD23	2.14	0.47
3:C:121:CYS:O	3:C:125:LEU:HB2	2.14	0.47
1:E:91:GLN:HA	1:E:170:SER:HA	1.95	0.47
1:A:96:GLN:HG3	4:D:221:ALA:HB2	1.96	0.47
4:D:74:TRP:O	4:D:78:PHE:HB2	2.14	0.47
3:C:123:ILE:O	3:C:127:THR:HG23	2.15	0.47
3:C:147:LEU:HG	3:G:147:LEU:N	2.16	0.47
4:D:13:THR:O	4:D:14:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:GLN:O	1:E:154:ILE:HG12	2.14	0.47
2:F:129:LEU:HD13	2:F:139:ILE:HG13	1.96	0.47
3:C:147:LEU:HD21	3:G:146:ILE:H	1.80	0.47
4:D:246:LEU:O	4:D:249:VAL:HG22	2.15	0.47
3:G:153:PRO:O	3:G:156:GLN:HB2	2.14	0.47
4:H:93:TYR:HD2	4:H:95:HIS:CE1	2.33	0.47
2:B:99:PHE:CZ	4:D:202:PRO:HB3	2.50	0.47
4:H:88:ALA:HB2	4:H:98:ILE:O	2.15	0.47
4:H:46:VAL:O	4:H:49:ILE:HG13	2.14	0.47
1:A:117:ARG:HA	1:A:120:MET:HB2	1.97	0.47
3:G:46:ILE:HD12	3:G:46:ILE:H	1.80	0.47
1:A:117:ARG:HD3	4:D:238:ILE:HG13	1.96	0.46
3:C:127:THR:O	3:C:138:PHE:CD2	2.68	0.46
4:D:14:THR:HG23	4:D:15:PHE:HD2	1.78	0.46
3:G:110:VAL:O	3:G:113:SER:OG	2.26	0.46
2:B:144:PHE:CE2	4:D:209:ILE:HG21	2.50	0.46
4:D:90:GLY:HA3	4:D:91:LYS:HD2	1.96	0.46
2:F:35:PHE:HB2	2:F:192:GLN:HE21	1.80	0.46
1:A:267:ASP:HB2	1:A:270:LYS:HB2	1.97	0.46
4:D:38:ALA:HB2	4:D:263:ARG:HE	1.80	0.46
2:F:38:LEU:HB3	2:F:201:VAL:HG22	1.96	0.46
1:A:47:SER:O	1:A:50:SER:OG	2.30	0.46
3:C:122:ASN:O	3:C:126:ASN:ND2	2.48	0.46
4:D:258:LEU:O	4:D:262:THR:HG22	2.15	0.46
1:E:146:GLY:HA2	1:E:149:LYS:HD2	1.97	0.46
2:F:102:THR:HG23	2:F:105:LYS:H	1.79	0.46
3:G:36:ASN:HD22	3:G:36:ASN:H	1.62	0.46
3:C:111:ILE:HG23	3:C:157:MET:SD	2.56	0.46
2:F:72:THR:H	2:F:75:THR:HG23	1.79	0.46
1:E:39:ILE:HG12	1:E:242:LEU:HD22	1.98	0.46
2:F:99:PHE:CD1	2:F:100:GLU:HG3	2.51	0.46
3:G:36:ASN:OD1	3:G:38:THR:OG1	2.34	0.46
3:C:150:MET:CE	3:C:151:ILE:HG12	2.46	0.46
3:C:46:ILE:HD12	3:C:46:ILE:H	1.81	0.46
4:D:199:SER:O	4:D:202:PRO:HD2	2.16	0.46
4:H:246:LEU:O	4:H:249:VAL:HG22	2.16	0.46
2:B:169:LEU:HD12	2:B:188:PHE:CZ	2.50	0.46
1:E:271:LEU:O	1:E:275:LEU:HG	2.15	0.46
2:B:267:PRO:HA	2:B:272:GLU:OE1	2.17	0.45
4:D:96:TRP:CD1	4:D:100:THR:HG21	2.51	0.45
1:E:11:VAL:HG21	1:E:52:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:VAL:HB	3:G:152:THR:HG22	1.98	0.45
4:H:90:GLY:HA3	4:H:91:LYS:HD2	1.97	0.45
1:E:244:ILE:HG22	1:E:245:PRO:O	2.16	0.45
2:F:171:GLU:OE2	2:F:203:HIS:ND1	2.48	0.45
1:A:183:LEU:HA	1:A:186:VAL:HG22	1.99	0.45
3:G:121:CYS:SG	3:G:122:ASN:N	2.89	0.45
4:H:193:LEU:C	4:H:195:LYS:N	2.68	0.45
4:D:245:ASP:O	4:D:249:VAL:HG13	2.16	0.45
2:B:275:ASP:O	2:B:278:LYS:HG3	2.17	0.45
3:C:43:LEU:O	3:C:43:LEU:HD12	2.17	0.45
2:F:124:ALA:HA	2:F:127:LYS:HD2	1.98	0.45
2:F:128:TRP:O	2:F:132:VAL:HG12	2.15	0.45
1:A:146:GLY:HA2	1:A:149:LYS:HD2	1.99	0.45
3:C:8:SER:N	3:C:9:SER:HA	2.31	0.45
3:C:140:VAL:O	3:C:144:SER:HB3	2.16	0.45
3:C:174:ARG:CG	3:C:175:LYS:HB2	2.40	0.45
1:E:93:PRO:HB3	1:E:150:GLN:OE1	2.17	0.45
4:H:12:GLY:HA2	4:H:18:ARG:NH1	2.32	0.45
4:H:245:ASP:O	4:H:249:VAL:HG13	2.17	0.45
1:A:271:LEU:O	1:A:275:LEU:HG	2.16	0.45
3:C:116:CYS:O	3:C:120:ILE:HG13	2.17	0.45
4:D:50:PHE:CD2	4:D:255:LEU:HD13	2.51	0.45
2:B:184:MET:O	2:B:187:LEU:HG	2.17	0.44
4:D:104:GLU:O	4:D:107:ILE:HG13	2.16	0.44
1:A:111:GLU:HG3	4:D:233:ARG:NH2	2.32	0.44
1:A:244:ILE:HG22	1:A:245:PRO:O	2.17	0.44
2:B:64:ILE:HB	2:B:71:ILE:HB	1.98	0.44
3:C:88:THR:CG2	3:C:129:TRP:NE1	2.79	0.44
3:G:95:ILE:HA	3:G:98:PHE:HD2	1.81	0.44
2:B:99:PHE:CD1	2:B:100:GLU:HG3	2.52	0.44
3:C:70:VAL:O	3:C:73:VAL:HG22	2.18	0.44
1:E:117:ARG:HA	1:E:120:MET:HB2	1.99	0.44
2:F:267:PRO:O	2:F:268:LEU:HD12	2.17	0.44
3:G:33:LYS:HA	3:G:42:GLY:HA2	1.98	0.44
3:G:125:LEU:O	3:G:129:TRP:N	2.47	0.44
4:H:72:MET:O	4:H:76:ILE:HG12	2.17	0.44
3:C:80:GLY:HA3	3:C:81:PHE:HA	1.82	0.44
1:E:264:GLU:N	1:E:265:ILE:HB	2.33	0.44
4:H:31:PHE:O	4:H:35:ILE:HG13	2.17	0.44
1:A:11:VAL:HG21	1:A:52:LEU:HD11	1.99	0.44
1:A:26:LEU:HD11	1:A:221:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:N	1:A:265:ILE:HB	2.33	0.44
1:E:257:ARG:NH1	2:F:275:ASP:OD1	2.51	0.44
3:C:152:THR:HA	3:C:155:ILE:HG22	1.99	0.44
3:G:110:VAL:O	3:G:114:VAL:HG23	2.17	0.44
3:G:136:ILE:HD13	3:G:136:ILE:HA	1.83	0.44
4:H:91:LYS:N	4:H:102:SER:OG	2.39	0.44
1:A:5:ILE:HG13	1:A:29:ALA:HB2	2.00	0.44
4:D:55:VAL:O	4:D:58:THR:OG1	2.34	0.44
3:G:39:LEU:HD23	3:G:39:LEU:HA	1.86	0.44
3:G:80:GLY:HA3	3:G:81:PHE:HA	1.82	0.44
2:B:35:PHE:HB2	2:B:192:GLN:HE21	1.83	0.44
4:D:78:PHE:O	4:D:82:LEU:HB2	2.18	0.44
4:D:88:ALA:HA	4:D:89:GLY:HA3	1.55	0.44
1:E:62:LEU:HD22	1:E:62:LEU:O	2.18	0.44
1:E:95:ASN:ND2	4:H:214:VAL:HG12	2.32	0.44
2:F:134:LEU:HD22	2:F:153:ARG:CZ	2.48	0.44
3:G:124:GLY:O	3:G:127:THR:OG1	2.26	0.44
3:C:10:LYS:HE2	3:C:10:LYS:HB3	1.56	0.43
1:E:128:VAL:HA	1:E:131:VAL:HG22	2.00	0.43
3:G:88:THR:CG2	3:G:129:TRP:HE1	2.31	0.43
1:A:39:ILE:HG12	1:A:242:LEU:HD22	2.00	0.43
1:A:47:SER:HB3	5:A:301:ANP:O2G	2.18	0.43
3:C:131:SER:HB3	3:C:138:PHE:HD2	1.83	0.43
4:D:218:LEU:O	4:D:222:MET:HB2	2.17	0.43
3:G:123:ILE:O	3:G:127:THR:HG23	2.18	0.43
4:H:92:VAL:CG2	4:H:104:GLU:HB2	2.43	0.43
3:G:43:LEU:HD12	3:G:43:LEU:O	2.18	0.43
3:G:64:GLY:HA3	3:G:90:ALA:HA	2.01	0.43
3:C:101:TYR:O	3:C:103:GLN:HG2	2.18	0.43
4:D:242:SER:O	4:D:244:VAL:N	2.37	0.43
1:E:47:SER:O	1:E:50:SER:OG	2.33	0.43
2:F:62:GLY:O	2:F:73:PRO:HD3	2.18	0.43
4:H:55:VAL:O	4:H:58:THR:OG1	2.34	0.43
1:A:93:PRO:HB2	1:A:149:LYS:HB3	2.00	0.43
2:B:97:GLN:HG3	4:D:180:ALA:HB1	1.99	0.43
4:D:78:PHE:CZ	3:G:150:MET:HG2	2.53	0.43
2:F:139:ILE:HG23	2:F:140:GLU:HG3	2.01	0.43
4:H:50:PHE:CD2	4:H:255:LEU:HD13	2.50	0.43
3:C:64:GLY:HA3	3:C:90:ALA:HA	2.01	0.43
4:D:21:PRO:HG3	4:D:134:GLU:HB3	2.00	0.43
4:D:90:GLY:HA2	4:D:91:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:VAL:HG12	1:E:170:SER:HB3	1.99	0.43
2:F:21:ILE:HD12	2:F:24:ASP:OD2	2.19	0.43
3:G:118:THR:HA	3:G:122:ASN:CB	2.49	0.43
2:B:43:GLY:N	5:B:301:ANP:O1B	2.52	0.43
2:B:56:LEU:HD13	4:D:179:ASN:HB3	2.01	0.43
2:B:62:GLY:O	2:B:73:PRO:HD3	2.18	0.43
2:B:72:THR:OG1	2:B:75:THR:HG23	2.19	0.43
3:C:164:LEU:O	3:C:169:ARG:HB3	2.19	0.43
1:A:48:THR:HG22	1:A:52:LEU:HD13	2.01	0.43
2:B:129:LEU:HD13	2:B:139:ILE:HG13	2.00	0.43
1:E:13:PHE:CD1	1:E:14:THR:N	2.87	0.43
1:A:56:LEU:HD13	4:D:220:THR:HG23	2.00	0.42
1:E:56:LEU:HD11	4:H:224:SER:HB3	2.01	0.42
3:G:10:LYS:HB3	3:G:59:TRP:HE1	1.84	0.42
3:G:127:THR:CG2	3:G:145:ARG:HH22	2.32	0.42
3:G:133:MET:O	3:G:134:TYR:CG	2.71	0.42
1:E:96:GLN:HE22	4:H:217:ASP:HB3	1.84	0.42
1:E:140:GLU:HB3	1:E:141:PRO:HD2	2.01	0.42
2:F:263:LEU:HD13	2:F:276:ALA:HB1	2.01	0.42
3:G:36:ASN:HB3	4:H:196:ARG:CZ	2.49	0.42
4:H:43:SER:HA	4:H:46:VAL:HG22	2.02	0.42
1:A:173:MET:SD	1:A:173:MET:N	2.90	0.42
3:C:146:ILE:HG22	3:G:146:ILE:HG22	2.00	0.42
4:D:103:SER:O	4:D:107:ILE:HG23	2.18	0.42
1:E:183:LEU:HA	1:E:186:VAL:HG22	2.01	0.42
2:F:24:ASP:HB2	2:F:222:ARG:HD2	2.00	0.42
2:F:131:LYS:HB2	2:F:131:LYS:HE3	1.72	0.42
3:G:157:MET:HA	3:G:160:VAL:HG12	2.00	0.42
4:H:218:LEU:O	4:H:222:MET:HB2	2.19	0.42
3:C:136:ILE:O	3:C:140:VAL:HG22	2.20	0.42
4:D:242:SER:C	4:D:244:VAL:H	2.22	0.42
4:D:258:LEU:O	4:D:261:THR:HG22	2.19	0.42
1:E:56:LEU:HD13	4:H:220:THR:HG23	2.02	0.42
3:G:133:MET:H	4:H:115:ARG:CZ	2.32	0.42
4:H:50:PHE:CE2	4:H:255:LEU:HB2	2.54	0.42
4:H:98:ILE:HB	4:H:99:PHE:HB2	2.01	0.42
4:H:250:ALA:O	4:H:254:LEU:HB3	2.19	0.42
4:D:17:TYR:OH	4:D:247:ILE:HD13	2.20	0.42
1:E:215:VAL:HG13	1:E:242:LEU:HD21	2.02	0.42
2:F:99:PHE:CZ	4:H:202:PRO:HB3	2.54	0.42
2:F:135:LYS:HB2	2:F:135:LYS:HE3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:SER:H	2:F:150:GLN:NE2	2.17	0.42
3:G:128:LEU:HA	3:G:131:SER:CB	2.47	0.42
4:H:243:LYS:HE2	4:H:243:LYS:HB3	1.85	0.42
1:A:9:ASP:HB3	1:A:65:SER:HA	2.01	0.42
4:D:35:ILE:HG12	4:D:47:ILE:HG21	2.02	0.42
2:F:55:ALA:O	2:F:58:LYS:NZ	2.53	0.42
4:H:195:LYS:C	4:H:198:LYS:H	2.23	0.42
2:B:72:THR:HG22	2:F:70:THR:HG23	2.00	0.42
4:D:240:GLU:HG3	4:D:241:TRP:N	2.34	0.42
4:H:90:GLY:HA2	4:H:91:LYS:HA	1.73	0.42
4:H:104:GLU:O	4:H:107:ILE:HG13	2.19	0.42
1:A:91:GLN:HA	1:A:170:SER:HA	2.02	0.42
3:C:130:VAL:C	3:C:132:MET:HG2	2.40	0.42
3:G:43:LEU:HB2	3:G:46:ILE:CD1	2.49	0.42
4:D:100:THR:HG22	4:D:101:LEU:N	2.29	0.41
1:E:26:LEU:HA	1:E:27:SER:HB2	2.01	0.41
2:F:89:LEU:HA	2:F:168:CYS:O	2.20	0.41
2:F:205:MET:O	2:F:208:VAL:HG12	2.20	0.41
4:H:124:THR:HA	4:H:127:THR:HG22	2.01	0.41
2:B:171:GLU:OE2	2:B:203:HIS:ND1	2.50	0.41
4:D:22:ARG:HB3	4:D:138:ALA:HA	2.01	0.41
2:F:184:MET:O	2:F:187:LEU:HG	2.20	0.41
3:G:106:GLN:HB3	3:G:109:ARG:HG3	2.01	0.41
4:H:193:LEU:HD23	4:H:194:VAL:H	1.84	0.41
2:B:218:LEU:HD23	2:B:223:LEU:HA	2.02	0.41
4:D:124:THR:HA	4:D:127:THR:HG22	2.01	0.41
2:B:3:ILE:HB	2:B:30:LEU:HB2	2.01	0.41
2:B:72:THR:H	2:B:75:THR:CG2	2.33	0.41
2:B:205:MET:O	2:B:208:VAL:HG12	2.21	0.41
2:B:278:LYS:HE3	2:B:278:LYS:HB2	1.84	0.41
2:B:263:LEU:HD13	2:B:276:ALA:HB1	2.02	0.41
3:C:121:CYS:SG	3:C:122:ASN:N	2.93	0.41
4:D:42:VAL:O	4:D:46:VAL:HG13	2.19	0.41
4:D:182:ARG:HE	4:D:188:PHE:HE1	1.68	0.41
1:E:253:LEU:HD22	2:F:270:MET:HB3	2.02	0.41
4:H:240:GLU:HG3	4:H:241:TRP:N	2.35	0.41
1:A:173:MET:O	1:A:174:LEU:HD23	2.21	0.41
3:C:134:TYR:N	3:C:134:TYR:CD1	2.88	0.41
1:E:169:GLU:OE1	1:E:172:SER:HB3	2.21	0.41
3:G:70:VAL:O	3:G:73:VAL:HG22	2.21	0.41
4:H:22:ARG:HB3	4:H:138:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:MET:HE2	2:B:205:MET:HA	2.02	0.41
4:D:112:VAL:O	4:D:116:PHE:HB2	2.20	0.41
1:E:111:GLU:HG3	4:H:233:ARG:NH2	2.35	0.41
3:C:147:LEU:HD11	3:G:145:ARG:C	2.40	0.41
1:E:96:GLN:OE1	1:E:96:GLN:N	2.54	0.41
1:A:13:PHE:HE2	1:A:48:THR:HG1	1.64	0.41
1:A:18:SER:C	1:A:19:PRO:O	2.59	0.41
1:A:128:VAL:HA	1:A:131:VAL:HG22	2.03	0.41
1:A:140:GLU:HB3	1:A:141:PRO:HD2	2.02	0.41
2:B:12:TYR:N	2:B:20:ALA:O	2.45	0.41
3:C:13:LEU:HD23	4:D:223:GLU:HG3	2.03	0.41
3:C:173:SER:HA	3:C:174:ARG:HA	1.84	0.41
2:F:205:MET:HE2	2:F:205:MET:HA	2.02	0.41
4:H:258:LEU:O	4:H:261:THR:HG22	2.20	0.41
2:F:36:ILE:HA	2:F:214:ASP:HB2	2.03	0.41
2:F:147:SER:N	2:F:150:GLN:HG3	2.36	0.41
2:F:227:ALA:HB1	2:F:231:GLU:OE1	2.21	0.41
3:G:13:LEU:HD23	4:H:223:GLU:HG3	2.03	0.41
4:H:111:TYR:HA	4:H:114:ILE:HG12	2.03	0.41
4:H:182:ARG:HA	4:H:186:ALA:O	2.21	0.41
1:E:23:LEU:HB2	1:E:24:SER:H	1.78	0.40
3:G:12:GLU:HB3	3:G:15:GLU:OE1	2.20	0.40
4:H:8:ARG:HA	4:H:9:TYR:HA	1.85	0.40
4:H:101:LEU:HD22	4:H:102:SER:H	1.86	0.40
4:H:258:LEU:O	4:H:262:THR:HG22	2.21	0.40
1:A:92:ASN:HA	1:A:93:PRO:HD2	1.79	0.40
3:C:35:GLY:HA2	3:C:40:GLN:HA	2.03	0.40
1:E:124:VAL:HG11	4:H:236:TYR:HE1	1.86	0.40
4:H:101:LEU:HD22	4:H:102:SER:N	2.35	0.40
1:A:102:VAL:CG2	1:A:137:ALA:HA	2.52	0.40
1:A:124:VAL:HG11	4:D:236:TYR:HE1	1.86	0.40
1:A:247:VAL:O	1:A:251:LYS:HG2	2.20	0.40
1:E:13:PHE:CD1	5:E:301:ANP:C5	3.05	0.40
2:F:123:GLU:HB2	2:F:127:LYS:NZ	2.37	0.40
4:H:42:VAL:O	4:H:46:VAL:HG13	2.21	0.40
4:H:103:SER:O	4:H:107:ILE:HG23	2.21	0.40
2:B:134:LEU:HG	2:B:138:LEU:HD21	2.03	0.40
1:E:92:ASN:HA	1:E:93:PRO:HD2	1.84	0.40
4:H:88:ALA:HA	4:H:89:GLY:HA3	1.63	0.40
4:H:91:LYS:HB3	4:H:104:GLU:CB	2.51	0.40
1:A:253:LEU:HD22	2:B:270:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:VAL:O	1:E:221:LEU:HA	2.21	0.40
2:F:153:ARG:O	2:F:157:ALA:N	2.53	0.40
4:H:112:VAL:O	4:H:116:PHE:HB2	2.21	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	278/298 (93%)	243 (87%)	30 (11%)	5 (2%)	8 35
1	E	278/298 (93%)	242 (87%)	32 (12%)	4 (1%)	11 38
2	B	279/287 (97%)	264 (95%)	15 (5%)	0	100 100
2	F	279/287 (97%)	261 (94%)	18 (6%)	0	100 100
3	C	166/184 (90%)	149 (90%)	15 (9%)	2 (1%)	13 42
3	G	166/184 (90%)	150 (90%)	16 (10%)	0	100 100
4	D	257/265 (97%)	231 (90%)	23 (9%)	3 (1%)	13 42
4	H	257/265 (97%)	230 (90%)	24 (9%)	3 (1%)	13 42
All	All	1960/2068 (95%)	1770 (90%)	173 (9%)	17 (1%)	17 48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
4	H	194	VAL
3	C	132	MET
4	D	42	VAL
1	A	18	SER
1	A	234	VAL
1	E	234	VAL

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Mol	Chain	Res	Type
1	A	15	TYR
1	A	24	SER
4	D	243	LYS
1	E	24	SER
4	H	95	HIS
4	D	238	ILE
4	H	238	ILE
1	E	15	TYR
3	C	41	VAL
1	E	19	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	240/257 (93%)	228 (95%)	12 (5%)	24 55
1	E	240/257 (93%)	226 (94%)	14 (6%)	20 50
2	B	230/234 (98%)	221 (96%)	9 (4%)	32 62
2	F	230/234 (98%)	214 (93%)	16 (7%)	15 43
3	C	139/155 (90%)	122 (88%)	17 (12%)	5 20
3	G	139/155 (90%)	123 (88%)	16 (12%)	5 22
4	D	227/233 (97%)	209 (92%)	18 (8%)	12 37
4	H	227/233 (97%)	196 (86%)	31 (14%)	3 16
All	All	1672/1758 (95%)	1539 (92%)	133 (8%)	12 37

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	15	TYR
1	A	17	ASP
1	A	28	PHE
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	122	LYS
1	A	173	MET
1	A	218	ASP
1	A	239	ARG
1	A	276	TRP
1	A	278	LEU
2	B	27	ASN
2	B	52	HIS
2	B	63	LYS
2	B	130	LYS
2	B	192	GLN
2	B	251	ARG
2	B	266	GLN
2	B	278	LYS
2	B	282	LYS
3	C	10	LYS
3	C	12	GLU
3	C	33	LYS
3	C	53	TYR
3	C	118	THR
3	C	122	ASN
3	C	136	ILE
3	C	137	ASN
3	C	138	PHE
3	C	139	MET
3	C	144	SER
3	C	145	ARG
3	C	149	GLU
3	C	157	MET
3	C	162	PHE
3	C	165	GLU
3	C	171	LYS
4	D	18	ARG
4	D	34	MET
4	D	50	PHE
4	D	56	PHE
4	D	61	LYS
4	D	78	PHE
4	D	82	LEU
4	D	87	MET
4	D	96	TRP

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Mol	Chain	Res	Type
4	D	99	PHE
4	D	116	PHE
4	D	173	GLN
4	D	188	PHE
4	D	193	LEU
4	D	198	LYS
4	D	240	GLU
4	D	243	LYS
4	D	263	ARG
1	E	14	THR
1	E	15	TYR
1	E	18	SER
1	E	23	LEU
1	E	28	PHE
1	E	52	LEU
1	E	62	LEU
1	E	73	LYS
1	E	120	MET
1	E	122	LYS
1	E	173	MET
1	E	224	GLN
1	E	276	TRP
1	E	278	LEU
2	F	18	LEU
2	F	27	ASN
2	F	52	HIS
2	F	53	PHE
2	F	63	LYS
2	F	70	THR
2	F	130	LYS
2	F	142	SER
2	F	150	GLN
2	F	169	LEU
2	F	192	GLN
2	F	251	ARG
2	F	252	PHE
2	F	266	GLN
2	F	268	LEU
2	F	278	LYS
3	G	8	SER
3	G	33	LYS
3	G	36	ASN

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Mol	Chain	Res	Type
3	G	38	THR
3	G	78	LEU
3	G	105	ILE
3	G	106	GLN
3	G	118	THR
3	G	132	MET
3	G	133	MET
3	G	137	ASN
3	G	139	MET
3	G	142	LEU
3	G	149	GLU
3	G	162	PHE
3	G	170	VAL
4	H	13	THR
4	H	25	LEU
4	H	34	MET
4	H	37	LEU
4	H	42	VAL
4	H	47	ILE
4	H	50	PHE
4	H	56	PHE
4	H	60	LEU
4	H	61	LYS
4	H	78	PHE
4	H	82	LEU
4	H	87	MET
4	H	100	THR
4	H	102	SER
4	H	110	LEU
4	H	115	ARG
4	H	116	PHE
4	H	128	VAL
4	H	129	THR
4	H	173	GLN
4	H	188	PHE
4	H	190	ASP
4	H	194	VAL
4	H	198	LYS
4	H	212	LEU
4	H	240	GLU
4	H	243	LYS
4	H	246	LEU

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Mol	Chain	Res	Type
4	H	254	LEU
4	H	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	122	ASN
3	C	126	ASN
2	F	141	HIS
2	F	150	GLN
3	G	126	ASN
4	H	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ANP	B	301	-	29,33,33	2.12	6 (20%)	31,52,52	1.10	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ANP	A	301	-	29,33,33	2.18	6 (20%)	31,52,52	1.21	3 (9%)
5	ANP	E	301	-	29,33,33	1.07	4 (13%)	31,52,52	1.10	2 (6%)
5	ANP	F	301	-	29,33,33	1.11	4 (13%)	31,52,52	1.01	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	B	301	-	-	6/14/38/38	0/3/3/3
5	ANP	A	301	-	-	5/14/38/38	0/3/3/3
5	ANP	E	301	-	-	10/14/38/38	0/3/3/3
5	ANP	F	301	-	-	6/14/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	ANP	PG-O1G	7.88	1.58	1.46
5	B	301	ANP	PG-O1G	7.55	1.58	1.46
5	A	301	ANP	PB-O1B	6.23	1.56	1.46
5	B	301	ANP	PB-O1B	6.15	1.55	1.46
5	A	301	ANP	PG-N3B	2.63	1.70	1.63
5	B	301	ANP	PB-O2B	-2.58	1.49	1.56
5	A	301	ANP	PB-O2B	-2.56	1.49	1.56
5	E	301	ANP	PG-N3B	2.56	1.70	1.63
5	A	301	ANP	PG-O3G	-2.53	1.49	1.56
5	B	301	ANP	PG-O2G	-2.51	1.50	1.56
5	F	301	ANP	PG-N3B	2.47	1.69	1.63
5	F	301	ANP	PG-O1G	2.46	1.50	1.46
5	B	301	ANP	PG-N3B	2.46	1.69	1.63
5	E	301	ANP	PG-O1G	2.41	1.50	1.46
5	F	301	ANP	PB-O1B	2.35	1.49	1.46
5	E	301	ANP	PB-O1B	2.22	1.49	1.46
5	B	301	ANP	PB-O3A	-2.18	1.56	1.59
5	F	301	ANP	PB-O3A	-2.07	1.56	1.59
5	E	301	ANP	PB-O3A	-2.03	1.56	1.59
5	A	301	ANP	PB-N3B	2.01	1.68	1.63

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	ANP	PB-O3A-PA	-3.43	120.52	132.62
5	F	301	ANP	PB-O3A-PA	-3.28	121.07	132.62
5	B	301	ANP	PB-O3A-PA	-3.25	121.18	132.62
5	E	301	ANP	PB-O3A-PA	-3.12	121.64	132.62
5	B	301	ANP	O1B-PB-N3B	-2.43	108.19	111.77
5	E	301	ANP	C5-C6-N6	2.33	123.90	120.35
5	F	301	ANP	C5-C6-N6	2.27	123.80	120.35
5	A	301	ANP	C5-C6-N6	2.24	123.75	120.35
5	A	301	ANP	O1B-PB-N3B	-2.18	108.56	111.77
5	B	301	ANP	C5-C6-N6	2.08	123.51	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	ANP	PB-N3B-PG-O1G
5	A	301	ANP	PA-O3A-PB-O1B
5	A	301	ANP	PA-O3A-PB-O2B
5	B	301	ANP	PB-N3B-PG-O1G
5	B	301	ANP	PG-N3B-PB-O1B
5	E	301	ANP	PB-N3B-PG-O1G
5	E	301	ANP	PG-N3B-PB-O3A
5	E	301	ANP	PA-O3A-PB-O1B
5	E	301	ANP	PA-O3A-PB-O2B
5	E	301	ANP	C5'-O5'-PA-O1A
5	E	301	ANP	C5'-O5'-PA-O2A
5	E	301	ANP	O4'-C4'-C5'-O5'
5	E	301	ANP	C3'-C4'-C5'-O5'
5	F	301	ANP	PB-N3B-PG-O1G
5	F	301	ANP	PG-N3B-PB-O3A
5	B	301	ANP	O4'-C4'-C5'-O5'
5	B	301	ANP	C3'-C4'-C5'-O5'
5	F	301	ANP	O4'-C4'-C5'-O5'
5	F	301	ANP	C3'-C4'-C5'-O5'
5	F	301	ANP	PB-O3A-PA-O1A
5	A	301	ANP	PG-N3B-PB-O3A
5	B	301	ANP	PG-N3B-PB-O3A
5	B	301	ANP	PB-O3A-PA-O2A
5	A	301	ANP	O4'-C4'-C5'-O5'
5	E	301	ANP	PB-O3A-PA-O1A
5	F	301	ANP	PB-O3A-PA-O2A
5	E	301	ANP	C5'-O5'-PA-O3A

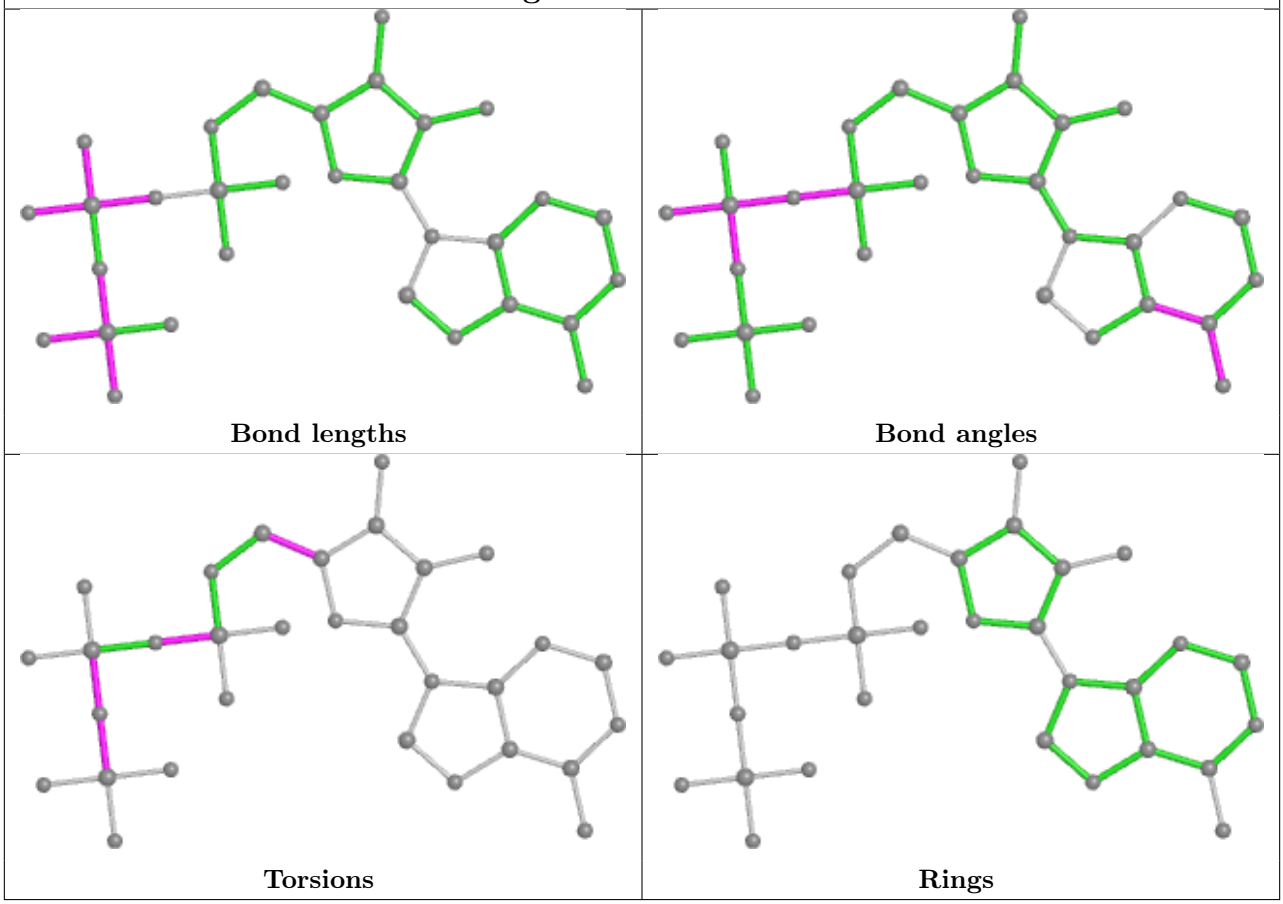
There are no ring outliers.

4 monomers are involved in 11 short contacts:

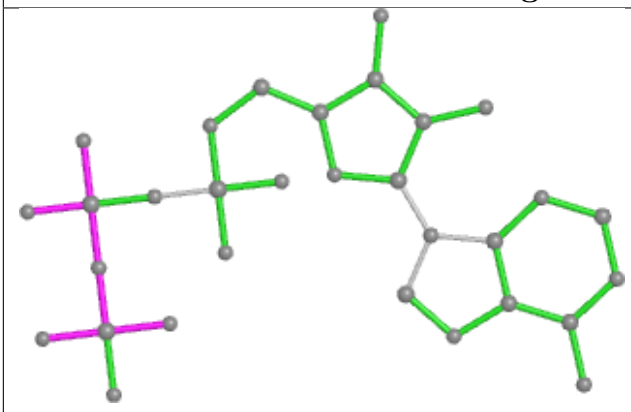
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	ANP	1	0
5	A	301	ANP	4	0
5	E	301	ANP	5	0
5	F	301	ANP	1	0

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 then 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.

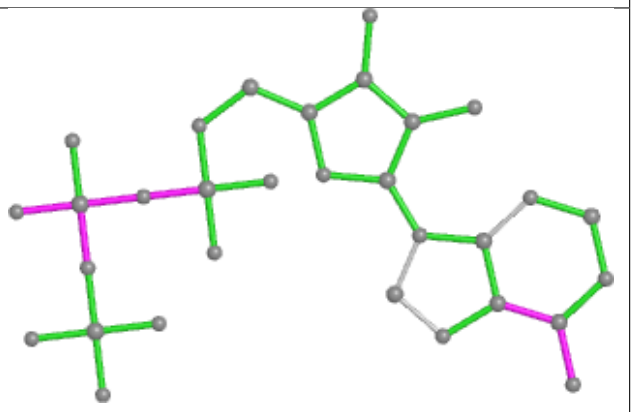
Ligand ANP B 301



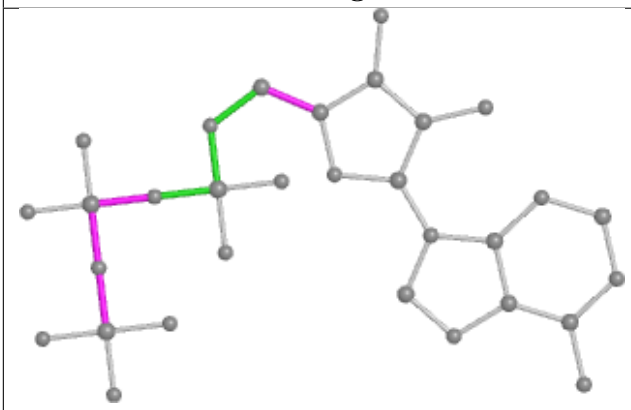
Ligand ANP A 301



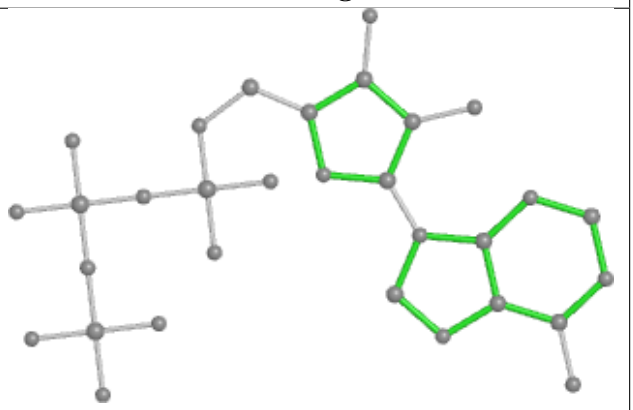
Bond lengths



Bond angles

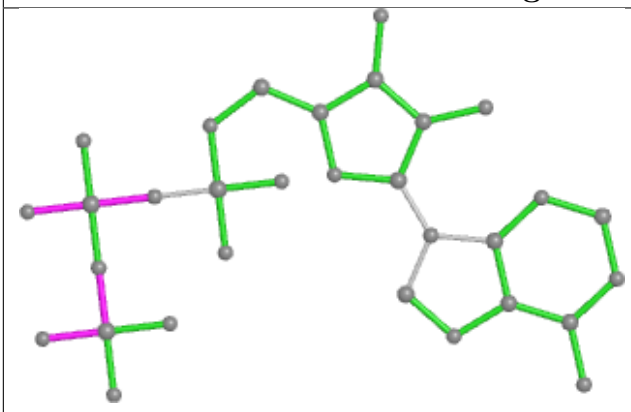


Torsions

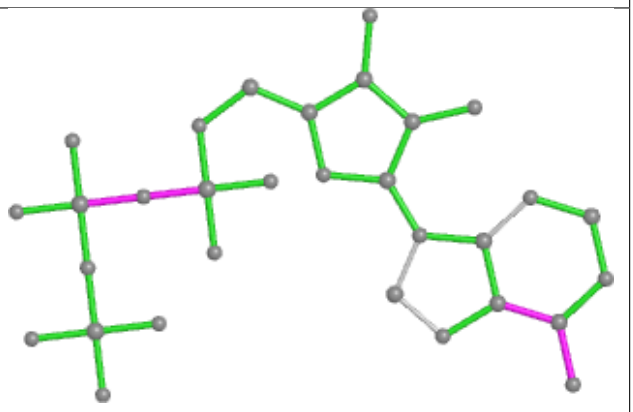


Rings

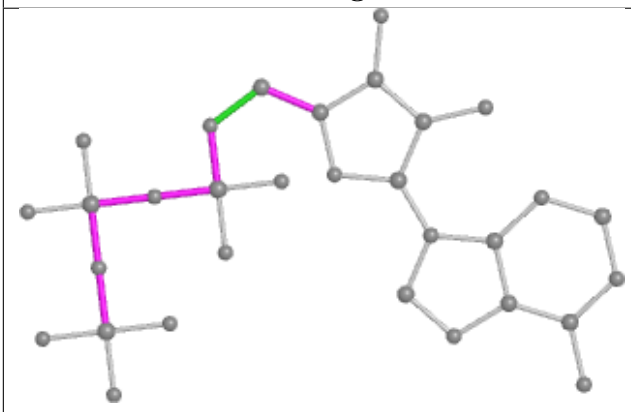
Ligand ANP E 301



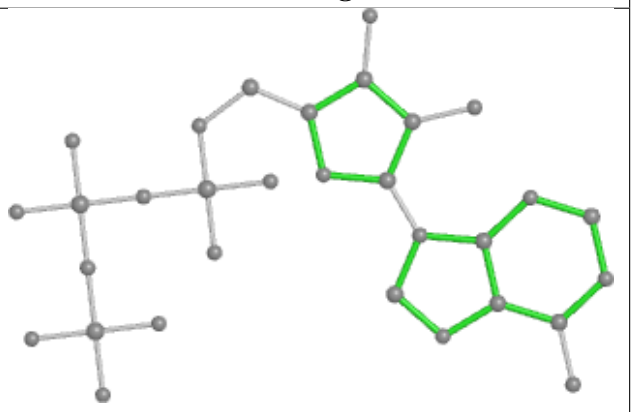
Bond lengths



Bond angles

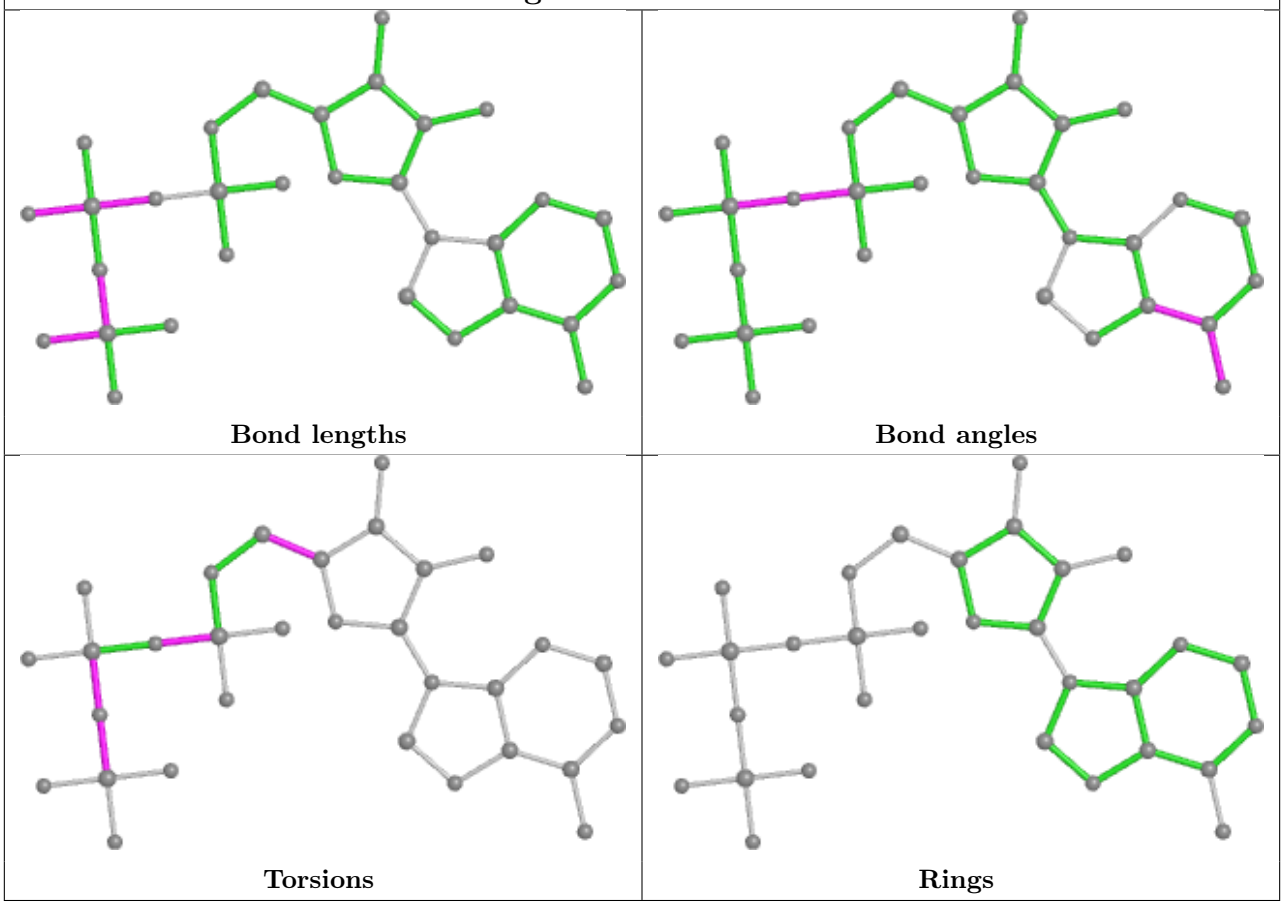


Torsions



Rings

Ligand ANP F 301



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^{th} 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^2)	Q<0.9
1	A	280/298 (93%)	0.24	24 (8%) 10 10	69, 140, 260, 421	0
1	E	280/298 (93%)	0.35	28 (10%) 7 7	77, 144, 262, 320	0
2	B	281/287 (97%)	0.08	23 (8%) 11 11	90, 137, 219, 281	0
2	F	281/287 (97%)	0.13	28 (9%) 7 7	92, 139, 211, 257	0
3	C	168/184 (91%)	0.41	19 (11%) 5 5	85, 163, 255, 338	0
3	G	168/184 (91%)	0.20	15 (8%) 9 10	90, 163, 296, 349	0
4	D	259/265 (97%)	0.17	25 (9%) 7 8	89, 162, 252, 414	0
4	H	259/265 (97%)	0.21	25 (9%) 7 8	90, 155, 243, 368	0
All	All	1976/2068 (95%)	0.21	187 (9%) 8 8	69, 148, 250, 421	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	165	GLU	15.5
4	D	14	THR	11.3
1	E	205	GLU	8.0
3	G	171	LYS	6.8
1	E	204	LEU	6.6
3	G	170	VAL	6.5
3	C	163	ILE	6.4
2	F	223	LEU	6.4
3	G	173	SER	6.4
2	B	219	GLU	6.3
3	G	172	LEU	6.2
4	H	111	TYR	6.2
1	E	163	GLN	6.0
1	E	203	ASP	6.0
1	A	177	GLU	5.9
4	D	41	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	59	PRO	5.7
3	C	166	GLY	5.7
3	G	174	ARG	5.5
1	A	202	HIS	5.5
1	E	193	ASN	5.5
3	G	137	ASN	5.5
3	C	162	PHE	5.2
4	D	203	MET	5.2
3	G	136	ILE	5.0
2	F	224	ILE	5.0
4	H	151	VAL	5.0
3	C	22	VAL	5.0
4	D	66	TRP	4.9
2	F	218	LEU	4.9
1	A	243	ASP	4.9
1	A	221	LEU	4.9
4	H	150	LYS	4.8
1	E	67	ILE	4.7
1	A	86	VAL	4.7
4	D	73	ILE	4.6
4	H	211	SER	4.6
1	E	74	LEU	4.6
3	C	168	SER	4.5
3	G	35	GLY	4.4
4	H	85	PHE	4.4
4	D	40	ASN	4.3
1	A	266	ASP	4.3
2	F	38	LEU	4.3
4	D	68	GLY	4.2
4	H	171	PHE	4.2
1	E	15	TYR	4.1
3	C	47	GLY	4.1
1	A	16	PRO	4.1
2	F	177	ASP	4.0
4	H	94	TRP	4.0
1	A	244	ILE	4.0
1	A	265	ILE	4.0
2	B	252	PHE	4.0
2	F	139	ILE	4.0
2	B	85	ARG	3.8
1	E	206	GLU	3.8
3	C	167	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	H	110	LEU	3.8
4	D	232	GLY	3.8
1	A	23	LEU	3.8
3	C	51	LEU	3.6
4	H	118	MET	3.6
2	F	241	LYS	3.6
4	D	145	PRO	3.6
1	A	272	VAL	3.6
1	A	85	LYS	3.5
2	F	2	ALA	3.5
4	D	43	SER	3.5
4	D	146	LEU	3.5
1	E	54	ASN	3.5
1	A	4	ASN	3.4
3	G	142	LEU	3.4
1	A	39	ILE	3.4
4	H	57	ALA	3.4
1	E	41	HIS	3.4
1	E	14	THR	3.4
4	D	191	GLY	3.4
2	B	82	ASP	3.3
1	A	5	ILE	3.3
2	B	41	HIS	3.3
4	H	169	THR	3.3
4	D	42	VAL	3.3
4	D	235	ARG	3.2
2	F	182	LEU	3.2
1	A	270	LYS	3.2
2	B	36	ILE	3.2
3	G	167	LEU	3.2
4	H	109	GLY	3.2
3	G	21	MET	3.2
3	C	107	ILE	3.1
4	H	166	PHE	3.1
4	H	52	LEU	3.1
1	E	58	ALA	3.1
4	H	56	PHE	3.1
4	H	84	THR	3.1
1	E	23	LEU	3.1
3	C	49	VAL	3.1
3	G	138	PHE	3.1
1	E	255	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	52	LEU	3.1
2	F	17	PRO	3.1
2	F	225	LYS	3.1
1	E	165	ILE	3.0
1	E	164	VAL	3.0
2	B	192	GLN	3.0
2	F	242	HIS	3.0
4	D	70	LYS	2.9
1	E	260	VAL	2.9
4	D	15	PHE	2.9
1	A	260	VAL	2.9
1	E	73	LYS	2.9
1	A	267	ASP	2.9
1	A	30	ILE	2.9
4	H	253	LEU	2.9
4	D	87	MET	2.9
2	F	138	LEU	2.9
2	F	18	LEU	2.8
4	H	251	TYR	2.8
1	E	75	GLY	2.8
1	A	271	LEU	2.8
2	F	50	MET	2.8
4	H	51	GLY	2.7
2	F	178	PRO	2.7
2	B	248	ARG	2.7
2	F	216	LEU	2.7
3	C	172	LEU	2.7
3	C	66	LEU	2.7
3	C	171	LYS	2.7
1	E	217	ASP	2.6
2	F	15	GLY	2.6
2	F	100	GLU	2.6
3	C	55	PHE	2.6
1	E	140	GLU	2.6
2	B	44	SER	2.6
2	F	82	ASP	2.6
1	E	162	PRO	2.6
1	A	38	LEU	2.5
4	D	57	ALA	2.5
2	F	206	ASP	2.5
4	H	191	GLY	2.5
4	H	164	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	197	THR	2.5
2	B	220	HIS	2.5
2	B	224	ILE	2.5
2	F	79	GLY	2.5
2	B	135	LYS	2.4
2	B	268	LEU	2.4
2	B	222	ARG	2.4
4	D	144	THR	2.4
2	F	217	ALA	2.4
2	F	219	GLU	2.4
4	D	151	VAL	2.4
1	A	259	ILE	2.4
4	H	153	VAL	2.4
2	B	183	GLU	2.4
1	A	69	VAL	2.4
3	C	96	TYR	2.4
4	D	253	LEU	2.4
1	E	87	GLY	2.3
2	B	81	LYS	2.3
2	B	133	GLY	2.3
2	F	179	MET	2.3
4	D	165	ARG	2.3
1	E	40	GLY	2.3
2	B	276	ALA	2.3
4	D	60	LEU	2.2
3	C	45	PHE	2.2
4	D	63	ARG	2.2
3	G	168	SER	2.2
1	E	196	THR	2.2
3	C	99	PHE	2.2
4	H	50	PHE	2.2
4	H	148	LEU	2.1
2	F	193	ALA	2.1
2	F	80	LEU	2.1
4	H	122	VAL	2.1
2	B	40	GLY	2.1
3	G	158	VAL	2.1
2	B	67	ALA	2.0
3	C	173	SER	2.0
3	G	160	VAL	2.0
1	A	219	GLY	2.0
2	F	53	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	34	LYS	2.0
2	B	77	ASN	2.0
4	D	45	LEU	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)

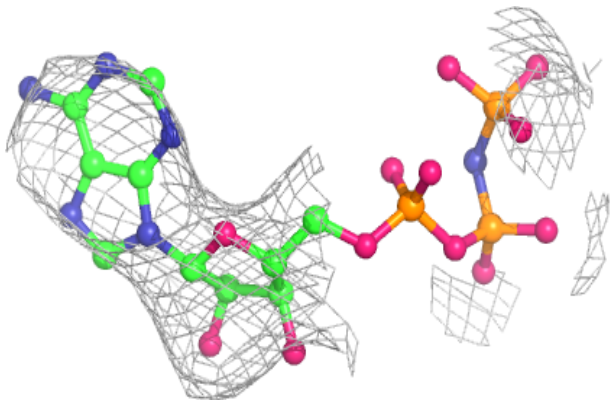
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

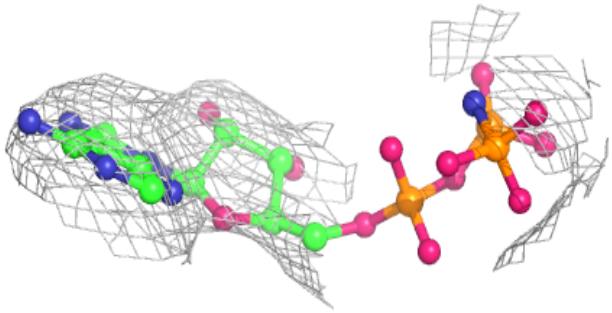
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ANP	A	301	31/31	0.89	0.18	133,177,206,207	0
5	ANP	F	301	31/31	0.89	0.24	78,130,178,273	0
5	ANP	E	301	31/31	0.90	0.14	126,173,203,246	0
5	ANP	B	301	31/31	0.93	0.16	133,136,164,222	0

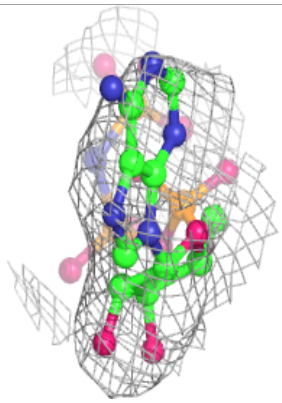
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 301:

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

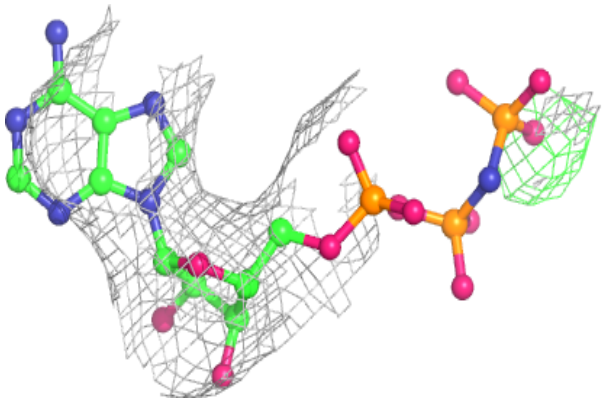


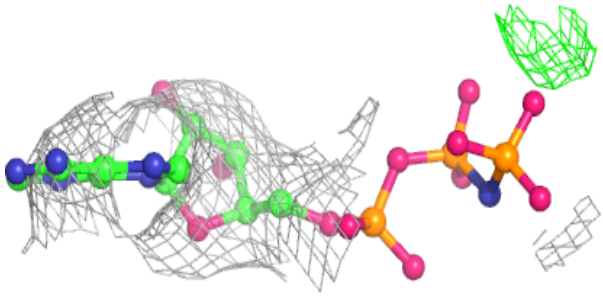


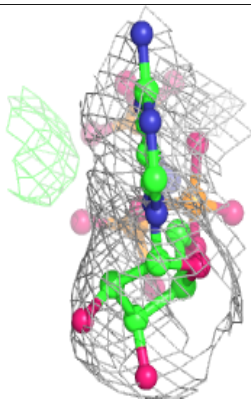


Electron density around ANP F 301:

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

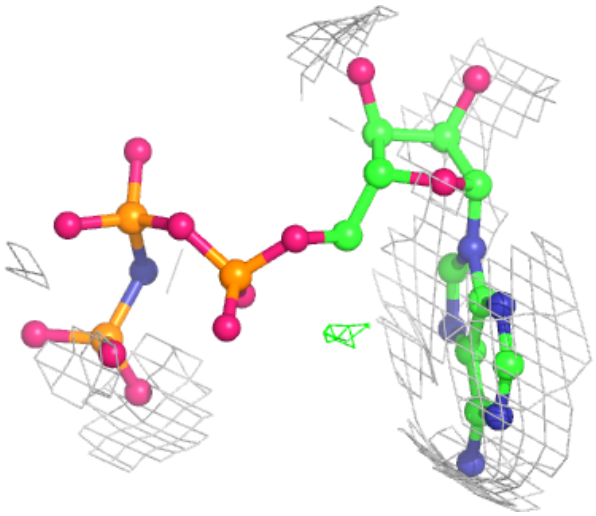


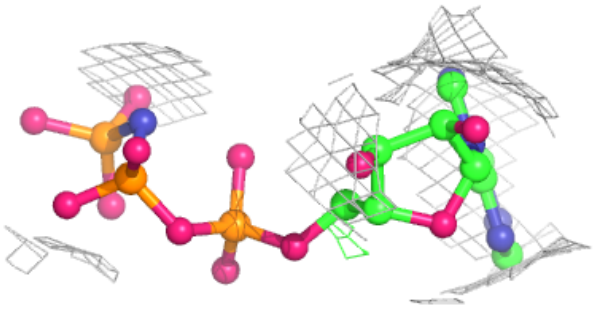


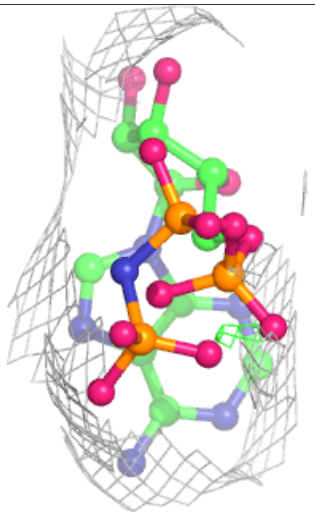


Electron density around ANP E 301:

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

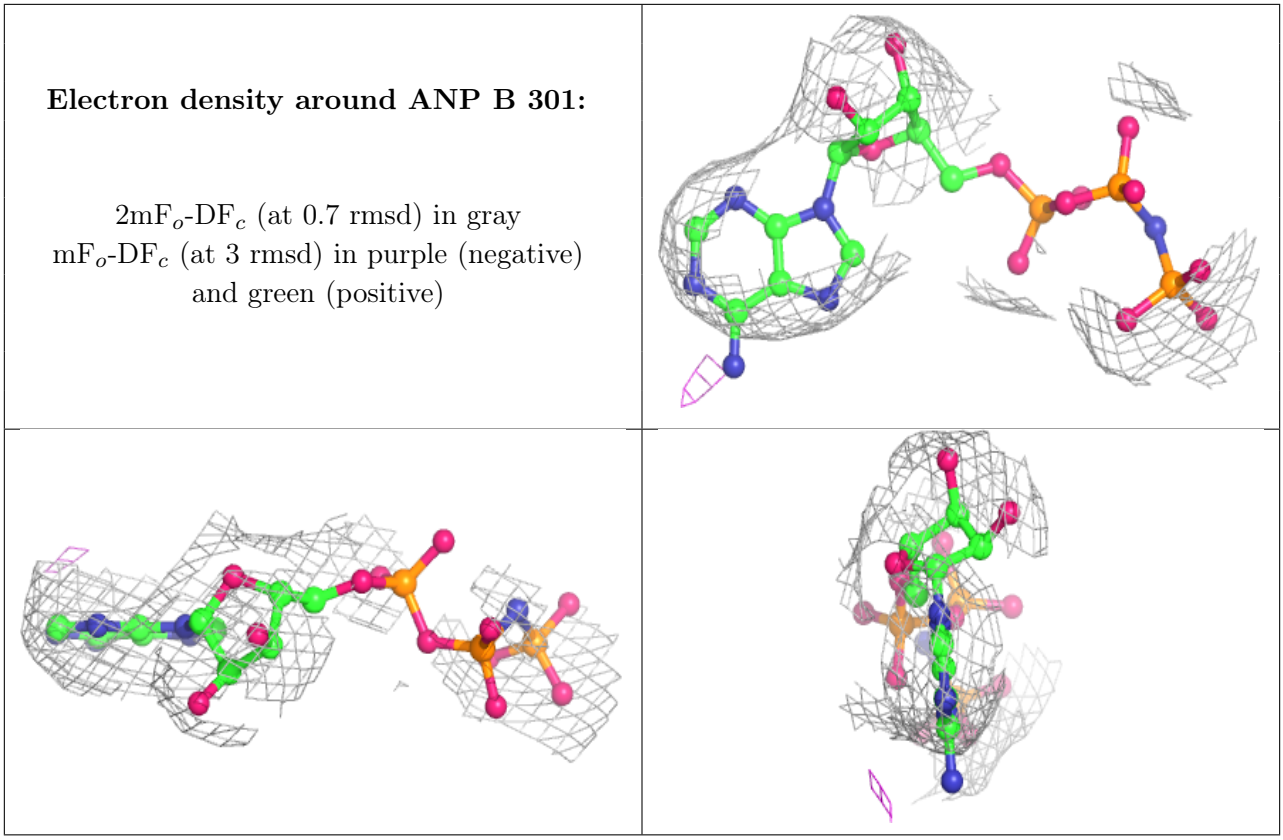






Electron density around ANP B 301:

$2mF_o$-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.