Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 11:39 AM EST

PDB ID	:	3SE7
Title	:	ancient VanA
Authors	:	Wright, G.D.; Morar, M.
Deposited on	:	2011-06-10
Resolution	:	3.07 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:

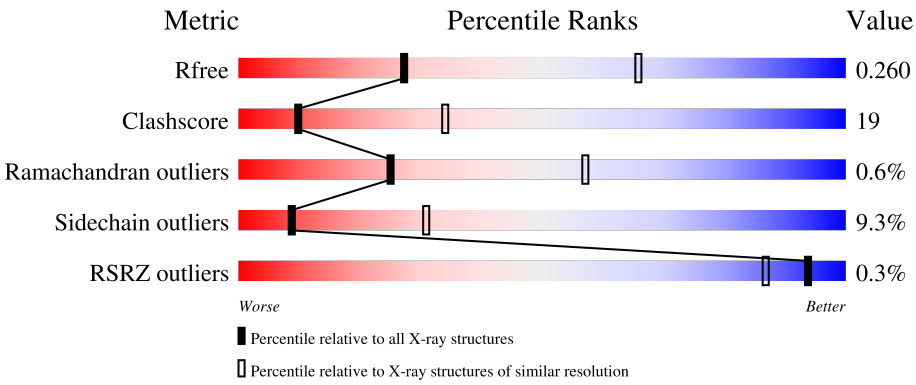
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	346	65% 26% • 5%
1	B	346	65% 24% 6% 5%
1	C	346	65% 25% 5% •
1	D	346	.% 60% 28% 6% 5%
1	E	346	72% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	346	% 63% 25% 6% 5%

2 Entry composition (i)

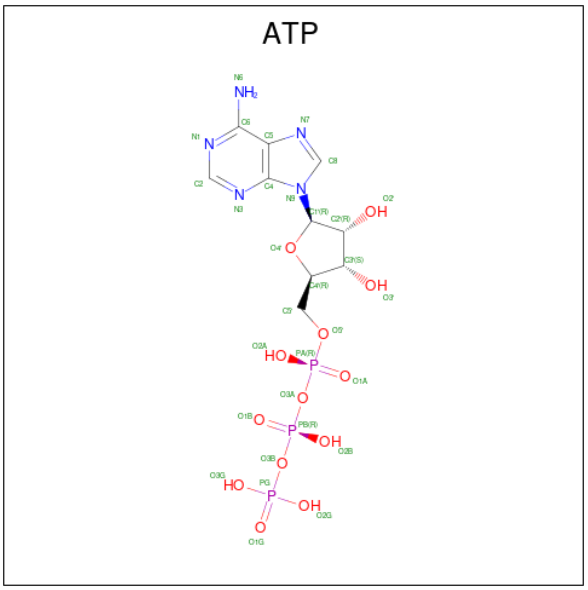
There are 4 unique types of molecules in this entry. The entry contains 14925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VanA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2406	1513	410	471	12	0	0	0
1	B	329	2418	1520	411	475	12	0	0	0
1	C	331	2432	1530	413	477	12	0	0	0
1	D	327	2406	1512	407	475	12	0	0	0
1	E	331	2433	1531	414	476	12	0	0	0
1	F	327	2397	1507	407	471	12	0	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
2	B	1	31	10	5	13	3	0	0
2	C	1	31	10	5	13	3	0	0
2	D	1	31	10	5	13	3	0	0
2	E	1	31	10	5	13	3	0	0
2	F	1	31	10	5	13	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0
3	F	2	2	2	0	0

- Molecule 4 is water.

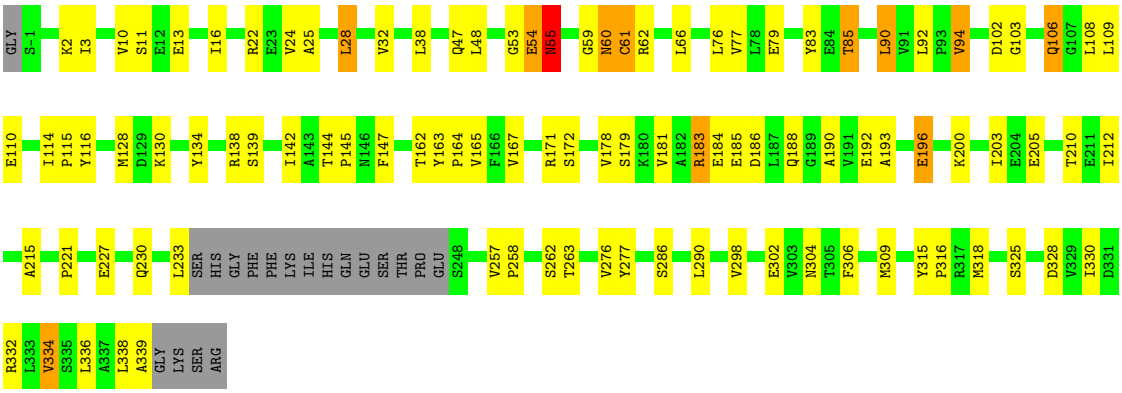
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	42	42	42	0	0
4	B	51	51	51	0	0
4	C	39	39	39	0	0
4	D	35	35	35	0	0
4	E	40	40	40	0	0
4	F	28	28	28	0	0

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.

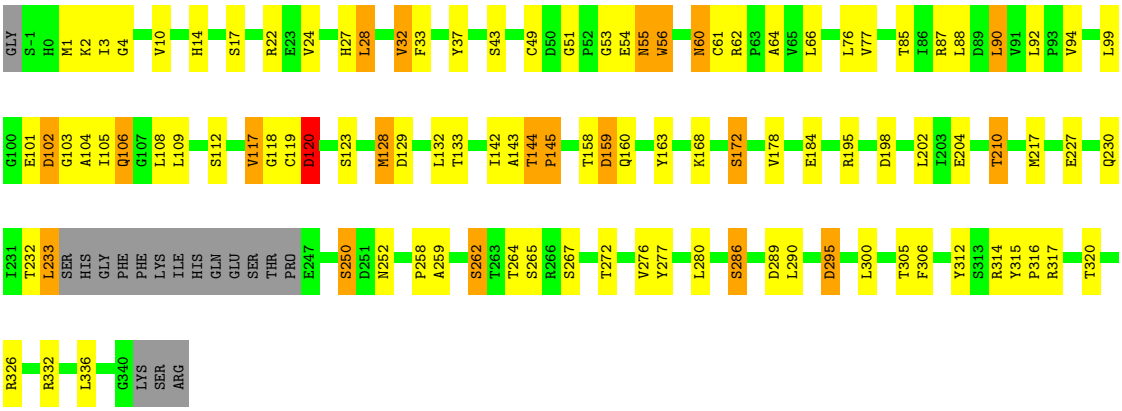
- Molecule 1: VanA

Chain A: 65% 26% • 5%



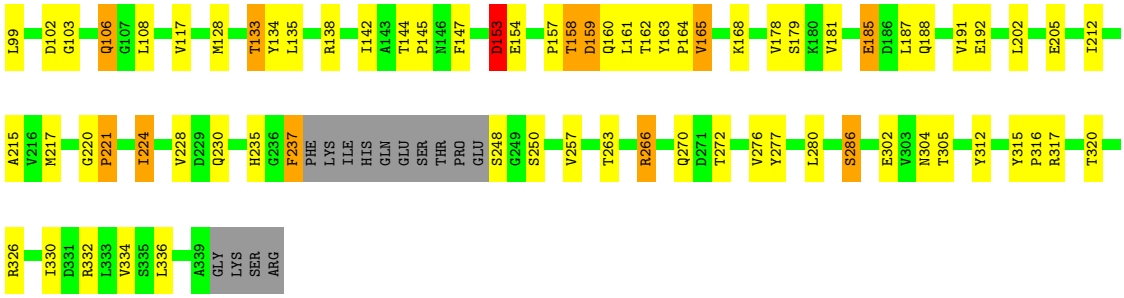
- Molecule 1: VanA

Chain B: 65% 24% 6% 5%



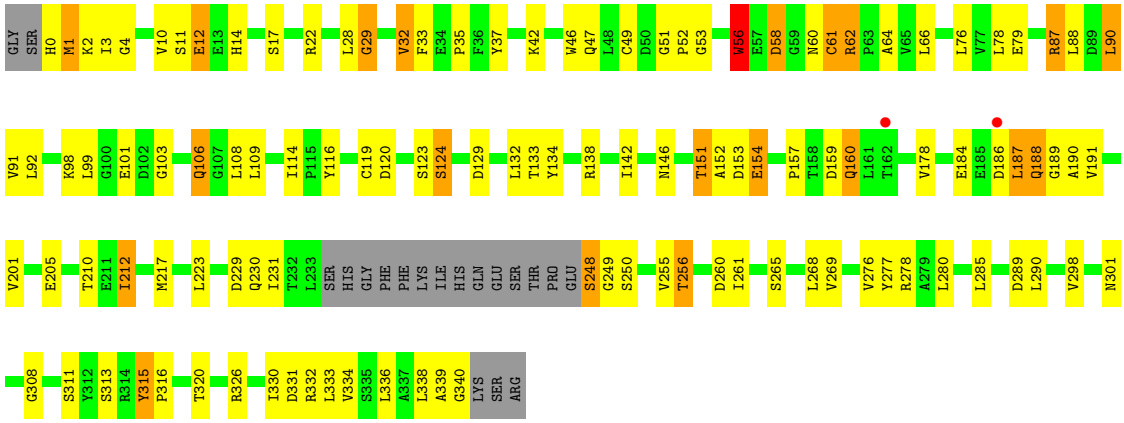
- Molecule 1: VanA

Chain C: 65% 25% 5% •



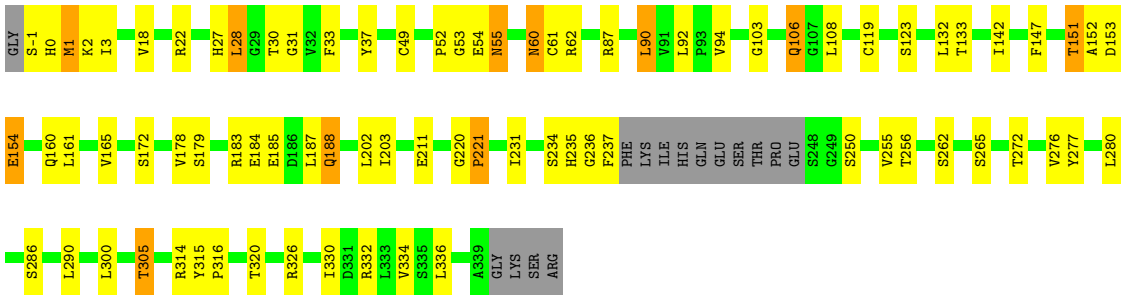
• Molecule 1: VanA

Chain D:



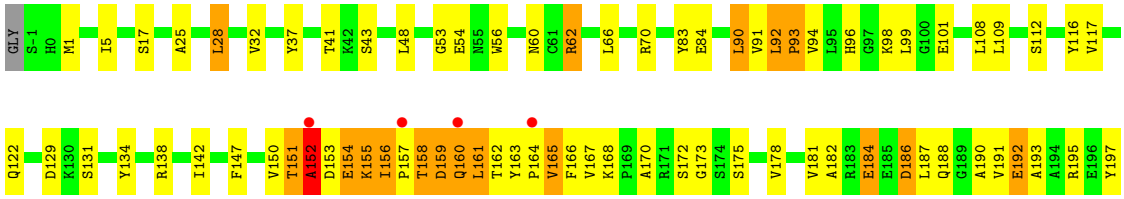
• Molecule 1: VanA

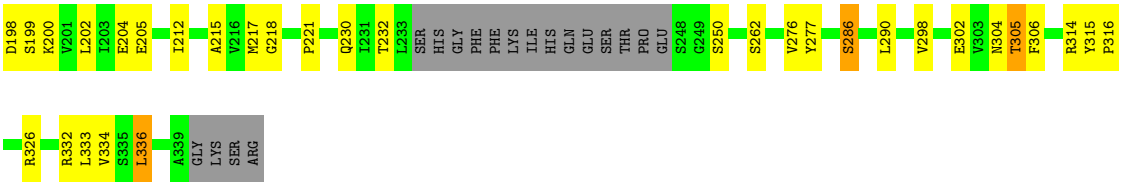
Chain E:



• Molecule 1: VanA

Chain F:




D198
S199
K200
V201
L202
I203
E204
E205
I212
A215
V216
M217
G218
P221
Q230
I231
T232
L233
SER
HIS
GLY
PHE
PHE
LYS
ILE
HIS
GLN
GLU
SER
THR
PRO
GLU
S248
G249
S250
S262
V276
Y277
S286
L290
V298
E302
V303
N304
T305
F306
R314
Y315
P316
R326
R332
L333
V334
S335
L336
A339
GLY
LYS
SER
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.13Å 136.03Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.10 – 3.07 45.69 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (108.10-3.07) 99.8 (45.69-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.193 , 0.263 0.199 , 0.260	Depositor DCC
R_{free} test set	1963 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14925	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.38% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.93	5/2446 (0.2%)	0.76	3/3327 (0.1%)
1	B	0.88	5/2458 (0.2%)	0.82	7/3342 (0.2%)
1	C	0.69	1/2474 (0.0%)	0.76	4/3365 (0.1%)
1	D	0.87	4/2446 (0.2%)	0.73	5/3327 (0.2%)
1	E	0.65	0/2475	0.68	3/3366 (0.1%)
1	F	0.65	0/2437	0.90	10/3316 (0.3%)
All	All	0.79	15/14736 (0.1%)	0.78	32/20043 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	CYS	CB-SG	-7.31	1.69	1.82
1	A	277	TYR	CE1-CZ	-6.68	1.29	1.38
1	B	101	GLU	CG-CD	-6.61	1.42	1.51
1	A	277	TYR	CE2-CZ	-5.60	1.31	1.38
1	B	120	ASP	CB-CG	-5.59	1.40	1.51
1	D	315	TYR	CE1-CZ	-5.55	1.31	1.38
1	B	117	VAL	CB-CG1	-5.41	1.41	1.52
1	B	101	GLU	CD-OE1	-5.37	1.19	1.25
1	D	315	TYR	CE2-CZ	-5.27	1.31	1.38
1	B	102	ASP	CB-CG	-5.25	1.40	1.51
1	A	306	PHE	CD1-CE1	-5.23	1.28	1.39
1	A	334	VAL	CB-CG1	-5.16	1.42	1.52
1	C	61	CYS	CB-SG	-5.13	1.73	1.81
1	D	315	TYR	CD2-CE2	-5.08	1.31	1.39
1	D	101	GLU	CD-OE1	-5.01	1.20	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	155	LYS	CB-CA-C	-17.85	74.70	110.40
1	C	53	GLY	N-CA-C	-13.51	79.33	113.10
1	F	153	ASP	CB-CA-C	-12.16	86.08	110.40
1	F	152	ALA	CB-CA-C	-10.92	93.72	110.10
1	B	56	TRP	N-CA-CB	-10.86	91.05	110.60
1	B	102	ASP	CB-CA-C	-9.71	90.99	110.40
1	F	156	ILE	N-CA-CB	-9.69	88.50	110.80
1	A	59	GLY	N-CA-C	8.53	134.42	113.10
1	F	154	GLU	N-CA-CB	-8.49	95.32	110.60
1	F	154	GLU	N-CA-C	8.34	133.51	111.00
1	C	58	ASP	CB-CA-C	8.29	126.99	110.40
1	C	153	ASP	CB-CA-C	-7.66	95.08	110.40
1	B	120	ASP	N-CA-CB	-7.58	96.97	110.60
1	F	154	GLU	CB-CA-C	-7.38	95.63	110.40
1	F	152	ALA	N-CA-C	7.07	130.10	111.00
1	E	202	LEU	CA-CB-CG	6.80	130.94	115.30
1	E	160	GLN	CB-CA-C	6.63	123.66	110.40
1	A	306	PHE	N-CA-C	-6.62	93.14	111.00
1	A	55	ASN	N-CA-C	-6.49	93.47	111.00
1	D	153	ASP	CB-CA-C	6.26	122.93	110.40
1	F	152	ALA	N-CA-CB	-6.04	101.65	110.10
1	D	154	GLU	CB-CA-C	-5.89	98.61	110.40
1	B	120	ASP	CB-CA-C	-5.86	98.67	110.40
1	E	161	LEU	N-CA-C	5.57	126.03	111.00
1	B	119	CYS	CB-CA-C	5.45	121.30	110.40
1	B	120	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	C	153	ASP	N-CA-C	5.26	125.21	111.00
1	D	56	TRP	N-CA-C	-5.22	96.90	111.00
1	D	188	GLN	N-CA-C	-5.19	96.98	111.00
1	B	101	GLU	C-N-CA	5.12	134.51	121.70
1	D	190	ALA	CB-CA-C	-5.07	102.49	110.10
1	F	155	LYS	N-CA-C	5.01	124.52	111.00

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	2406	0	2367	79	0
1	B	2418	0	2381	95	0
1	C	2432	0	2383	97	0
1	D	2406	0	2363	104	0
1	E	2433	0	2387	68	0
1	F	2397	0	2347	109	0
2	A	31	0	12	3	0
2	B	31	0	12	5	0
2	C	31	0	12	3	0
2	D	31	0	12	3	0
2	E	31	0	12	3	0
2	F	31	0	12	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	42	0	0	1	0
4	B	51	0	0	3	0
4	C	39	0	0	2	0
4	D	35	0	0	2	0
4	E	40	0	0	6	0
4	F	28	0	0	2	0
All	All	14925	0	14300	557	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 19.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HE2	1:D:33:PHE:CE1	1.72	1.24
1:D:28:LEU:CD2	1:D:330:ILE:HG21	1.71	1.20
1:F:157:PRO:CB	1:F:160:GLN:HB2	1.75	1.15
1:D:1:MET:CE	1:D:33:PHE:HE1	1.60	1.14
1:E:108:LEU:HD13	1:F:108:LEU:HD13	1.17	1.12
1:D:28:LEU:HD21	1:D:330:ILE:HG21	1.12	1.12
1:D:1:MET:CE	1:D:33:PHE:CE1	2.31	1.11
1:C:108:LEU:HD13	1:D:108:LEU:HD13	1.29	1.11
1:A:22:ARG:HH21	1:A:53:GLY:HA2	1.16	1.10
1:A:54:GLU:OE1	1:A:54:GLU:HA	1.37	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:HD23	1:D:188:GLN:N	1.66	1.09
2:D:400:ATP:H5'1	2:D:400:ATP:H8	1.17	1.09
1:F:157:PRO:HB2	1:F:160:GLN:HB2	1.33	1.08
1:D:10:VAL:O	1:D:10:VAL:HG12	1.54	1.07
1:D:142:ILE:HD13	1:D:276:VAL:HG22	1.36	1.03
1:D:1:MET:HE2	1:D:33:PHE:CD1	1.95	1.01
1:E:142:ILE:HD13	1:E:276:VAL:HG22	1.43	1.00
1:A:183:ARG:HH21	1:A:185:GLU:HB2	1.26	0.99
1:F:195:ARG:HA	1:F:198:ASP:O	1.64	0.96
1:C:54:GLU:OE2	1:C:54:GLU:HA	1.63	0.94
1:D:1:MET:HE1	1:D:33:PHE:HE1	1.30	0.94
1:C:60:ASN:C	1:C:60:ASN:HD22	1.71	0.94
1:A:103:GLY:HA2	1:A:106:GLN:NE2	1.86	0.90
2:D:400:ATP:H5'1	2:D:400:ATP:C8	2.05	0.90
1:D:256:THR:O	1:D:256:THR:HG22	1.70	0.90
1:F:157:PRO:HB3	1:F:160:GLN:HB2	1.51	0.90
2:B:400:ATP:H5'1	2:B:400:ATP:H8	1.36	0.90
1:D:53:GLY:O	1:D:56:TRP:HD1	1.55	0.89
1:E:119:CYS:SG	1:E:305:THR:HG22	2.13	0.89
2:E:400:ATP:H5'1	2:E:400:ATP:H8	1.38	0.89
1:D:278:ARG:HD2	4:D:357:HOH:O	1.71	0.88
1:E:151:THR:H	1:E:154:GLU:HG3	1.36	0.88
1:D:28:LEU:HD21	1:D:330:ILE:CG2	2.02	0.88
1:F:157:PRO:HB2	1:F:160:GLN:CB	2.04	0.88
1:B:103:GLY:HA2	1:B:106:GLN:HG3	1.58	0.86
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.39	0.86
2:A:400:ATP:H5'1	2:A:400:ATP:H8	1.39	0.85
1:A:212:ILE:HG22	1:A:290:LEU:HB2	1.59	0.85
1:F:150:VAL:HA	1:F:154:GLU:OE1	1.77	0.85
1:F:142:ILE:HD13	1:F:276:VAL:HG22	1.58	0.84
1:B:27:HIS:CE1	1:B:326:ARG:HD3	2.11	0.84
2:A:400:ATP:H5'1	2:A:400:ATP:C8	2.13	0.83
1:E:0:HIS:CD2	1:E:31:GLY:O	2.31	0.83
1:F:152:ALA:HA	1:F:195:ARG:HH12	1.44	0.83
2:B:400:ATP:H5'1	2:B:400:ATP:C8	2.13	0.83
1:F:159:ASP:OD2	1:F:160:GLN:NE2	2.10	0.83
1:D:210:THR:HG21	1:D:230:GLN:HE21	1.43	0.82
1:B:232:THR:HG22	1:B:233:LEU:N	1.94	0.82
1:F:152:ALA:CA	1:F:195:ARG:HH12	1.93	0.81
1:C:60:ASN:C	1:C:60:ASN:ND2	2.30	0.81
1:C:217:MET:HE3	1:C:332:ARG:HD3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:CA	1:A:106:GLN:NE2	2.44	0.80
1:A:90:LEU:CD1	1:A:334:VAL:HG13	2.12	0.80
1:C:54:GLU:OE2	1:C:54:GLU:CA	2.30	0.80
1:D:187:LEU:HD23	1:D:188:GLN:H	1.46	0.80
1:B:53:GLY:O	1:B:56:TRP:HD1	1.66	0.78
1:D:290:LEU:HD13	1:D:298:VAL:CG1	2.14	0.78
1:C:312:TYR:HD2	1:C:312:TYR:O	1.68	0.77
1:B:87:ARG:HD3	4:B:357:HOH:O	1.84	0.77
1:F:151:THR:HG23	1:F:154:GLU:CD	2.06	0.76
1:A:190:ALA:O	1:A:193:ALA:HB3	1.85	0.76
1:F:152:ALA:HA	1:F:195:ARG:NH1	2.01	0.76
1:D:142:ILE:HD13	1:D:276:VAL:CG2	2.15	0.75
1:A:22:ARG:HH21	1:A:53:GLY:CA	1.98	0.75
1:C:20:SER:O	1:C:24:VAL:HG23	1.85	0.75
1:A:162:THR:HB	1:A:205:GLU:OE2	1.86	0.74
1:B:159:ASP:OD2	1:B:160:GLN:HB2	1.87	0.74
1:B:232:THR:CG2	1:B:233:LEU:N	2.50	0.74
1:F:90:LEU:HD23	1:F:91:VAL:H	1.53	0.74
1:C:312:TYR:C	1:C:312:TYR:CD2	2.60	0.73
1:D:265:SER:O	1:D:269:VAL:HG23	1.88	0.73
1:A:183:ARG:HH21	1:A:185:GLU:CB	2.00	0.73
1:F:53:GLY:O	1:F:56:TRP:HD1	1.71	0.73
1:A:162:THR:O	1:A:165:VAL:HG23	1.87	0.73
1:D:134:TYR:O	1:D:138:ARG:HG3	1.88	0.73
1:B:159:ASP:OD2	1:B:160:GLN:N	2.22	0.73
1:A:90:LEU:HD11	1:A:334:VAL:HG13	1.70	0.73
1:E:262:SER:HB2	1:E:265:SER:H	1.54	0.73
1:E:272:THR:O	1:E:276:VAL:HG23	1.88	0.73
2:C:400:ATP:H5'1	2:C:400:ATP:H8	1.54	0.73
1:A:60:ASN:C	1:A:60:ASN:HD22	1.90	0.72
1:E:2:LYS:HE3	1:E:87:ARG:O	1.89	0.72
1:B:276:VAL:HG12	1:B:280:LEU:HD12	1.69	0.72
1:D:53:GLY:O	1:D:56:TRP:CD1	2.41	0.72
1:D:28:LEU:HD23	1:D:330:ILE:HG21	1.69	0.72
1:E:54:GLU:HG3	1:E:55:ASN:HA	1.72	0.72
1:D:28:LEU:CD2	1:D:330:ILE:CG2	2.60	0.72
2:E:400:ATP:H5'1	2:E:400:ATP:C8	2.25	0.72
1:F:168:LYS:NZ	1:F:204:GLU:OE2	2.23	0.72
1:F:151:THR:HG23	1:F:154:GLU:OE2	1.89	0.71
1:C:237:PHE:N	1:C:237:PHE:CD2	2.55	0.71
1:D:142:ILE:CD1	1:D:276:VAL:HG22	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:HA2	1:A:106:GLN:HE21	1.54	0.71
1:B:53:GLY:O	1:B:56:TRP:CD1	2.43	0.70
1:D:151:THR:OG1	1:D:154:GLU:HG3	1.91	0.70
1:F:90:LEU:HD23	1:F:91:VAL:N	2.07	0.70
1:A:142:ILE:HD13	1:A:276:VAL:CG2	2.22	0.70
1:A:178:VAL:HG11	2:A:400:ATP:H5'2	1.72	0.70
1:D:1:MET:N	1:D:32:VAL:O	2.24	0.70
1:C:159:ASP:C	1:C:159:ASP:OD1	2.30	0.69
1:D:1:MET:CE	1:D:33:PHE:CD1	2.70	0.69
1:B:272:THR:O	1:B:276:VAL:HG23	1.92	0.69
1:A:142:ILE:HD13	1:A:276:VAL:HG22	1.73	0.69
1:F:54:GLU:O	1:F:54:GLU:HG3	1.93	0.69
1:D:10:VAL:O	1:D:10:VAL:CG1	2.30	0.69
1:B:2:LYS:HE2	1:B:87:ARG:O	1.92	0.68
1:B:227:GLU:HG3	1:B:258:PRO:HB3	1.74	0.68
1:F:217:MET:HE1	1:F:332:ARG:HD3	1.75	0.68
1:F:250:SER:OG	1:F:314:ARG:NH1	2.25	0.68
1:A:130:LYS:HE3	1:A:302:GLU:HG3	1.74	0.68
1:B:87:ARG:NH1	4:B:371:HOH:O	2.27	0.67
1:C:266:ARG:HG2	1:C:266:ARG:NH1	2.05	0.67
1:C:215:ALA:HB1	1:C:315:TYR:CE2	2.29	0.67
1:D:2:LYS:HE3	1:D:87:ARG:O	1.94	0.67
1:D:210:THR:CG2	1:D:230:GLN:HE21	2.07	0.67
1:E:320:THR:HG21	4:E:364:HOH:O	1.95	0.67
1:A:22:ARG:NH2	1:A:53:GLY:HA2	2.01	0.67
1:F:25:ALA:HA	1:F:28:LEU:HD11	1.77	0.67
1:F:160:GLN:O	1:F:161:LEU:HD23	1.95	0.66
1:C:276:VAL:HG12	1:C:280:LEU:HD12	1.78	0.66
1:C:54:GLU:OE2	1:C:55:ASN:N	2.29	0.66
1:E:276:VAL:HG12	1:E:280:LEU:HD12	1.77	0.66
1:D:66:LEU:HD11	1:D:114:ILE:HD12	1.77	0.65
1:C:90:LEU:CD1	1:C:334:VAL:HG13	2.27	0.65
1:C:217:MET:HE3	1:C:332:ARG:CD	2.26	0.65
1:D:56:TRP:CD1	1:D:56:TRP:N	2.64	0.65
1:B:295:ASP:OD1	1:B:295:ASP:N	2.30	0.65
1:D:90:LEU:CD1	1:D:334:VAL:HG13	2.27	0.65
1:F:186:ASP:N	1:F:186:ASP:OD1	2.29	0.65
1:C:159:ASP:OD1	1:C:160:GLN:N	2.30	0.65
1:D:12:GLU:N	1:D:12:GLU:OE1	2.30	0.64
1:E:151:THR:O	1:E:153:ASP:N	2.30	0.64
1:C:312:TYR:O	1:C:312:TYR:CD2	2.49	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:O	1:A:318:MET:HG2	1.97	0.64
1:F:290:LEU:CD2	1:F:298:VAL:HG11	2.26	0.64
2:F:400:ATP:H8	2:F:400:ATP:H5'1	1.61	0.64
1:B:99:LEU:H	1:B:102:ASP:CG	2.01	0.64
1:A:60:ASN:ND2	1:A:60:ASN:O	2.30	0.64
1:F:157:PRO:CB	1:F:160:GLN:CB	2.63	0.64
1:A:183:ARG:HD2	1:F:154:GLU:HG3	1.80	0.64
1:D:58:ASP:N	1:D:58:ASP:OD1	2.30	0.63
1:C:316:PRO:O	1:C:320:THR:HG23	1.99	0.63
1:B:64:ALA:HB1	1:B:76:LEU:O	1.98	0.63
1:C:272:THR:O	1:C:276:VAL:HG23	1.98	0.63
1:C:134:TYR:O	1:C:138:ARG:HG3	1.98	0.63
1:C:158:THR:OG1	1:C:159:ASP:N	2.30	0.63
1:D:339:ALA:O	1:D:340:GLY:C	2.37	0.63
1:E:60:ASN:C	1:E:60:ASN:ND2	2.51	0.63
1:B:142:ILE:CD1	1:B:276:VAL:HG22	2.28	0.62
1:A:22:ARG:NH2	1:A:54:GLU:H	1.97	0.62
1:B:262:SER:HB2	1:B:265:SER:H	1.63	0.62
1:B:142:ILE:HD13	1:B:276:VAL:HG22	1.81	0.62
1:D:340:GLY:HA3	1:E:30:THR:CB	2.30	0.62
1:B:99:LEU:HA	1:B:102:ASP:OD1	2.00	0.62
1:C:217:MET:HE2	1:C:224:ILE:HD11	1.81	0.62
1:D:315:TYR:HB3	1:D:316:PRO:HD3	1.81	0.62
1:E:103:GLY:HA2	1:E:106:GLN:HG2	1.81	0.62
1:A:103:GLY:CA	1:A:106:GLN:HE22	2.12	0.62
1:D:103:GLY:O	1:D:106:GLN:HG2	2.00	0.61
1:F:163:TYR:OH	1:F:184:GLU:HB2	1.99	0.61
1:B:117:VAL:HG12	1:B:118:GLY:N	2.15	0.61
1:B:178:VAL:HG11	2:B:400:ATP:H5'2	1.81	0.61
1:E:60:ASN:ND2	1:E:60:ASN:O	2.30	0.61
1:F:1:MET:HE1	1:F:334:VAL:HG11	1.81	0.61
1:F:188:GLN:O	1:F:192:GLU:HG2	2.01	0.61
1:E:151:THR:OG1	1:E:154:GLU:CG	2.49	0.61
1:F:191:VAL:O	1:F:195:ARG:HG3	2.00	0.61
1:C:23:GLU:OE1	1:C:326:ARG:NH1	2.34	0.61
1:D:62:ARG:HD2	1:D:79:GLU:OE1	2.00	0.61
1:D:290:LEU:HD13	1:D:298:VAL:HG11	1.82	0.61
1:E:22:ARG:HE	1:E:53:GLY:HA2	1.66	0.60
1:F:90:LEU:CD1	1:F:334:VAL:HG13	2.31	0.60
1:D:260:ASP:O	1:D:261:ILE:HG23	2.02	0.60
1:E:2:LYS:CE	1:E:87:ARG:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HD22	1:E:94:VAL:HG22	1.84	0.60
1:E:103:GLY:HA2	1:E:106:GLN:CG	2.31	0.60
1:F:90:LEU:CD2	1:F:91:VAL:N	2.65	0.60
1:F:290:LEU:HD23	1:F:298:VAL:CG1	2.32	0.60
1:B:168:LYS:HZ2	1:B:204:GLU:CD	2.05	0.60
1:D:276:VAL:HG12	1:D:280:LEU:HD12	1.82	0.60
1:E:151:THR:C	1:E:153:ASP:N	2.53	0.60
1:C:54:GLU:CD	1:C:55:ASN:H	2.05	0.60
1:D:98:LYS:O	1:D:99:LEU:HB2	2.01	0.60
1:B:3:ILE:HD12	1:B:90:LEU:HD13	1.83	0.59
1:F:230:GLN:O	1:F:230:GLN:HG2	2.00	0.59
1:C:237:PHE:H	1:C:237:PHE:HD2	1.49	0.59
1:B:210:THR:HG21	1:B:230:GLN:HE21	1.67	0.59
1:D:28:LEU:O	1:D:29:GLY:O	2.21	0.59
1:D:32:VAL:HG23	1:D:33:PHE:N	2.17	0.59
1:B:14:HIS:O	1:B:17:SER:HB3	2.03	0.59
1:C:142:ILE:HD13	1:C:276:VAL:HG22	1.84	0.59
1:D:210:THR:HG21	1:D:230:GLN:NE2	2.17	0.59
1:C:24:VAL:HG13	1:C:330:ILE:HD11	1.84	0.59
1:C:212:ILE:HG23	1:C:228:VAL:CG1	2.33	0.59
1:E:142:ILE:CD1	1:E:276:VAL:HG22	2.27	0.59
1:A:188:GLN:O	1:A:192:GLU:HG2	2.03	0.58
1:D:14:HIS:O	1:D:17:SER:HB3	2.02	0.58
1:B:217:MET:HE3	1:B:332:ARG:HB3	1.83	0.58
1:C:90:LEU:HD12	1:C:334:VAL:HG13	1.83	0.58
1:D:178:VAL:HG11	2:D:400:ATP:H5'2	1.85	0.58
1:A:172:SER:HB3	4:A:348:HOH:O	2.02	0.58
1:F:134:TYR:O	1:F:138:ARG:HG3	2.04	0.58
1:E:178:VAL:HG11	2:E:400:ATP:H5'2	1.86	0.57
1:E:183:ARG:CB	1:E:185:GLU:OE2	2.52	0.57
1:E:54:GLU:CG	1:E:55:ASN:HA	2.34	0.57
1:F:184:GLU:O	1:F:184:GLU:HG3	2.02	0.57
1:F:163:TYR:CD2	1:F:182:ALA:O	2.58	0.57
1:A:76:LEU:HD23	1:A:85:THR:HG22	1.86	0.57
1:A:83:TYR:CD1	1:A:83:TYR:C	2.77	0.57
1:F:53:GLY:O	1:F:56:TRP:CD1	2.56	0.57
1:D:119:CYS:HB3	1:D:123:SER:OG	2.05	0.57
1:F:90:LEU:HD12	1:F:334:VAL:HG13	1.87	0.57
1:A:55:ASN:N	1:A:55:ASN:OD1	2.37	0.57
1:F:163:TYR:HB3	1:F:164:PRO:HA	1.87	0.57
1:A:92:LEU:HD22	1:A:94:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG12	1:C:181:VAL:HG22	1.85	0.56
2:C:400:ATP:H5'1	2:C:400:ATP:C8	2.38	0.56
1:D:187:LEU:CD2	1:D:188:GLN:N	2.57	0.56
1:F:163:TYR:OH	1:F:184:GLU:HA	2.04	0.56
1:F:277:TYR:HE1	1:F:286:SER:HB2	1.70	0.56
1:B:60:ASN:HD22	1:B:60:ASN:C	2.09	0.56
1:D:187:LEU:HD23	1:D:187:LEU:C	2.26	0.56
1:B:315:TYR:HB3	1:B:316:PRO:HD3	1.88	0.56
1:C:237:PHE:N	1:C:237:PHE:HD2	2.03	0.56
1:C:302:GLU:OE1	1:C:304:ASN:OD1	2.23	0.56
1:B:27:HIS:ND1	1:B:326:ARG:HD3	2.20	0.56
1:B:250:SER:OG	1:B:314:ARG:NH1	2.30	0.56
1:C:144:THR:HB	1:C:145:PRO:HD2	1.87	0.56
1:B:66:LEU:HD21	1:B:109:LEU:HD23	1.87	0.56
1:B:117:VAL:CG1	1:B:118:GLY:N	2.69	0.56
1:A:77:VAL:O	1:A:83:TYR:HA	2.07	0.55
1:B:60:ASN:C	1:B:60:ASN:ND2	2.60	0.55
1:C:178:VAL:HG11	2:C:400:ATP:H5'2	1.88	0.55
1:A:183:ARG:NE	1:A:186:ASP:OD1	2.39	0.55
1:B:158:THR:O	1:B:159:ASP:C	2.43	0.55
2:B:400:ATP:H8	2:B:400:ATP:C5'	2.15	0.55
1:D:22:ARG:HG2	1:D:22:ARG:O	2.04	0.55
1:A:3:ILE:HG23	1:A:3:ILE:O	2.07	0.55
1:B:195:ARG:HA	1:B:198:ASP:O	2.06	0.55
1:F:290:LEU:HD23	1:F:298:VAL:HG11	1.86	0.55
1:F:151:THR:CG2	1:F:154:GLU:OE2	2.55	0.55
1:A:330:ILE:O	1:A:334:VAL:HG23	2.07	0.55
1:D:32:VAL:HG23	1:D:33:PHE:H	1.70	0.55
1:F:286:SER:OG	1:F:305:THR:HA	2.07	0.55
1:B:158:THR:OG1	1:B:159:ASP:N	2.40	0.55
1:B:172:SER:HB3	4:B:361:HOH:O	2.06	0.55
1:C:157:PRO:O	1:C:159:ASP:N	2.40	0.55
1:F:92:LEU:HD12	1:F:93:PRO:CD	2.37	0.55
1:B:92:LEU:HD22	1:B:94:VAL:CG2	2.38	0.54
1:F:92:LEU:HD12	1:F:93:PRO:HD2	1.88	0.54
1:F:163:TYR:OH	1:F:184:GLU:CA	2.56	0.54
1:E:255:VAL:HG12	1:E:256:THR:N	2.21	0.54
1:A:302:GLU:OE1	1:A:304:ASN:OD1	2.26	0.54
1:F:98:LYS:O	1:F:99:LEU:HB2	2.08	0.54
1:D:87:ARG:O	1:D:87:ARG:CG	2.56	0.54
1:F:160:GLN:C	1:F:161:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:THR:HB	1:C:205:GLU:OE2	2.08	0.53
1:D:109:LEU:HD13	1:D:116:TYR:CG	2.44	0.53
1:B:24:VAL:HG12	1:B:28:LEU:HD21	1.89	0.53
1:F:157:PRO:C	1:F:160:GLN:H	2.12	0.53
1:B:289:ASP:O	1:B:290:LEU:HD23	2.09	0.53
1:C:2:LYS:CE	1:C:87:ARG:O	2.57	0.53
1:E:255:VAL:CG1	1:E:256:THR:N	2.71	0.53
2:F:400:ATP:H5'1	2:F:400:ATP:C8	2.44	0.53
1:D:37:TYR:CD2	1:D:51:GLY:HA2	2.44	0.53
1:E:235:HIS:ND1	1:E:236:GLY:N	2.57	0.53
1:C:134:TYR:HA	1:C:144:THR:HG21	1.90	0.53
1:F:215:ALA:HB1	1:F:315:TYR:CE2	2.43	0.53
1:C:161:LEU:HD23	1:C:161:LEU:N	2.24	0.52
1:D:91:VAL:HG11	1:D:109:LEU:HD21	1.91	0.52
1:E:151:THR:C	1:E:153:ASP:H	2.11	0.52
1:A:290:LEU:HD13	1:A:298:VAL:HG11	1.91	0.52
1:C:181:VAL:HG21	1:C:187:LEU:HD13	1.91	0.52
1:A:48:LEU:O	1:A:61:CYS:HA	2.10	0.52
1:F:277:TYR:CE1	1:F:286:SER:HB2	2.45	0.52
1:C:117:VAL:HG13	4:C:352:HOH:O	2.10	0.52
1:E:90:LEU:HD11	1:E:334:VAL:HG13	1.91	0.52
1:F:230:GLN:O	1:F:230:GLN:CG	2.56	0.52
1:C:65:VAL:HG13	4:D:348:HOH:O	2.10	0.52
1:B:55:ASN:OD1	1:B:55:ASN:N	2.43	0.52
1:D:289:ASP:O	1:D:301:ASN:HB3	2.09	0.51
1:B:217:MET:HE1	1:B:332:ARG:HD3	1.93	0.51
1:B:232:THR:CG2	1:B:233:LEU:H	2.22	0.51
1:F:217:MET:HE1	1:F:332:ARG:CD	2.40	0.51
1:A:165:VAL:HG12	1:A:181:VAL:CG2	2.40	0.51
1:C:22:ARG:HE	1:C:53:GLY:HA2	1.75	0.51
1:C:257:VAL:HG21	1:C:317:ARG:HG2	1.91	0.51
1:F:83:TYR:CD1	1:F:83:TYR:C	2.84	0.51
1:A:163:TYR:HA	1:A:164:PRO:C	2.31	0.51
1:B:54:GLU:CG	1:B:55:ASN:HA	2.41	0.51
1:C:24:VAL:HG13	1:C:330:ILE:CD1	2.40	0.51
1:F:94:VAL:HA	1:F:306:PHE:CE2	2.45	0.51
1:F:142:ILE:HD13	1:F:276:VAL:CG2	2.36	0.51
1:A:134:TYR:O	1:A:138:ARG:HG3	2.11	0.51
1:F:290:LEU:HD22	1:F:298:VAL:HG11	1.92	0.51
1:B:1:MET:HE3	1:B:90:LEU:HB2	1.93	0.51
1:B:133:THR:HG23	1:B:280:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HB3	1:C:33:PHE:CD2	2.46	0.50
1:C:217:MET:CE	1:C:332:ARG:HD3	2.37	0.50
1:C:277:TYR:CE1	1:C:286:SER:HB2	2.47	0.50
1:B:99:LEU:N	1:B:102:ASP:OD1	2.42	0.50
1:F:178:VAL:HG11	2:F:400:ATP:H5'2	1.94	0.50
1:F:315:TYR:HB3	1:F:316:PRO:HD3	1.93	0.50
1:C:266:ARG:O	1:C:270:GLN:HG3	2.12	0.50
1:C:277:TYR:HE1	1:C:286:SER:HB2	1.76	0.50
1:C:54:GLU:O	1:C:55:ASN:HB2	2.11	0.50
1:D:184:GLU:O	1:D:187:LEU:HD22	2.12	0.50
1:C:163:TYR:HB3	1:C:164:PRO:HA	1.94	0.50
1:C:266:ARG:NH1	1:C:266:ARG:CG	2.70	0.50
1:B:277:TYR:CE1	1:B:286:SER:HB2	2.46	0.50
1:F:62:ARG:NH1	4:F:364:HOH:O	2.44	0.50
1:A:193:ALA:O	1:A:196:GLU:HB2	2.11	0.50
1:D:285:LEU:HD23	1:D:285:LEU:H	1.77	0.50
1:A:338:LEU:O	1:A:339:ALA:O	2.30	0.50
1:B:163:TYR:OH	1:B:184:GLU:HA	2.12	0.50
1:D:231:ILE:HD13	1:D:255:VAL:HG12	1.93	0.50
1:E:172:SER:HB3	4:E:362:HOH:O	2.11	0.50
1:B:66:LEU:HD23	1:B:108:LEU:HD23	1.94	0.49
1:F:290:LEU:CD2	1:F:298:VAL:CG1	2.90	0.49
1:B:144:THR:O	1:B:145:PRO:O	2.30	0.49
1:D:46:TRP:C	1:D:47:GLN:HG3	2.32	0.49
1:E:277:TYR:CE1	1:E:286:SER:HB2	2.47	0.49
1:A:183:ARG:CZ	1:A:185:GLU:OE1	2.60	0.49
1:E:37:TYR:CD1	1:E:52:PRO:HD3	2.48	0.49
1:D:184:GLU:O	1:D:184:GLU:HG3	2.11	0.49
1:B:66:LEU:HB3	1:B:108:LEU:HD21	1.95	0.49
1:E:151:THR:OG1	1:E:154:GLU:HG3	2.12	0.49
1:A:109:LEU:HD13	1:A:116:TYR:CG	2.48	0.49
1:F:163:TYR:OH	1:F:184:GLU:CB	2.60	0.49
1:E:231:ILE:O	1:E:234:SER:OG	2.25	0.49
1:F:156:ILE:O	1:F:158:THR:N	2.46	0.49
1:A:144:THR:HB	1:A:145:PRO:HD2	1.95	0.49
1:A:315:TYR:HB3	1:A:316:PRO:HD3	1.94	0.49
1:C:266:ARG:O	1:C:266:ARG:HG3	2.06	0.49
1:E:152:ALA:HB2	4:E:363:HOH:O	2.13	0.49
1:A:47:GLN:HB3	1:A:61:CYS:HB3	1.95	0.48
1:B:108:LEU:O	1:B:112:SER:OG	2.30	0.48
1:B:144:THR:C	1:B:145:PRO:O	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:THR:O	1:D:152:ALA:C	2.52	0.48
1:E:151:THR:O	1:E:152:ALA:C	2.51	0.48
1:F:109:LEU:HD13	1:F:116:TYR:CG	2.48	0.48
1:F:152:ALA:N	1:F:195:ARG:HH12	2.09	0.48
1:F:159:ASP:OD2	1:F:159:ASP:C	2.52	0.48
1:F:155:LYS:O	1:F:157:PRO:HD3	2.13	0.48
1:B:277:TYR:HE1	1:B:286:SER:HB2	1.77	0.48
1:C:230:GLN:NE2	1:C:235:HIS:HB2	2.28	0.48
1:E:28:LEU:HD12	1:E:28:LEU:O	2.13	0.48
1:E:18:VAL:HG13	1:E:53:GLY:H	1.77	0.48
1:A:210:THR:HG21	1:A:230:GLN:NE2	2.29	0.48
1:C:98:LYS:O	1:C:99:LEU:HB2	2.14	0.48
1:E:1:MET:HE2	1:E:33:PHE:CE1	2.48	0.48
1:E:320:THR:CG2	4:E:364:HOH:O	2.57	0.48
1:C:147:PHE:HB2	1:C:202:LEU:HD11	1.95	0.48
1:F:218:GLY:HA2	1:F:336:LEU:HD21	1.94	0.48
1:A:10:VAL:HG12	1:A:10:VAL:O	2.13	0.48
1:E:315:TYR:HB3	1:E:316:PRO:HD3	1.96	0.48
1:C:2:LYS:HE3	1:C:87:ARG:O	2.14	0.47
1:D:191:VAL:HG13	1:D:201:VAL:HG11	1.95	0.47
1:D:308:GLY:O	1:D:313:SER:HB3	2.14	0.47
1:C:217:MET:HE2	1:C:224:ILE:CD1	2.44	0.47
1:B:10:VAL:HG12	1:B:10:VAL:O	2.13	0.47
1:C:103:GLY:HA2	1:C:106:GLN:HG3	1.97	0.47
1:C:168:LYS:HB3	1:C:178:VAL:HG22	1.97	0.47
1:F:168:LYS:CE	1:F:204:GLU:OE2	2.61	0.47
1:F:5:ILE:O	1:F:5:ILE:HG22	2.13	0.47
1:A:22:ARG:HE	1:A:53:GLY:HA3	1.80	0.47
1:D:129:ASP:HB3	1:D:132:LEU:HD12	1.96	0.47
1:A:102:ASP:HB3	1:A:128:MET:HG2	1.95	0.47
1:A:103:GLY:C	1:A:106:GLN:NE2	2.68	0.47
1:D:106:GLN:HA	1:D:109:LEU:HB2	1.97	0.47
1:F:316:PRO:CB	1:F:326:ARG:NH1	2.77	0.47
1:D:285:LEU:HB3	1:D:333:LEU:HD21	1.97	0.47
1:E:54:GLU:HG2	1:E:55:ASN:ND2	2.30	0.47
1:E:237:PHE:N	1:E:237:PHE:CD2	2.81	0.47
1:B:106:GLN:HE21	1:B:106:GLN:HB3	1.50	0.47
1:D:3:ILE:HG23	1:D:35:PRO:HA	1.97	0.47
1:A:163:TYR:HB3	1:A:164:PRO:HA	1.97	0.46
1:C:3:ILE:HG23	1:C:3:ILE:O	2.15	0.46
1:D:311:SER:HA	1:D:326:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:THR:HG23	1:C:280:LEU:HD11	1.97	0.46
1:D:223:LEU:HD11	1:D:277:TYR:CD2	2.50	0.46
1:D:260:ASP:O	1:D:261:ILE:CG2	2.61	0.46
1:B:27:HIS:CE1	1:B:326:ARG:CD	2.91	0.46
1:F:66:LEU:HD21	1:F:109:LEU:HD23	1.97	0.46
1:C:217:MET:CE	1:C:224:ILE:HD11	2.44	0.46
1:F:163:TYR:N	1:F:163:TYR:CD1	2.84	0.46
1:A:54:GLU:OE1	1:A:54:GLU:CA	2.30	0.46
1:D:37:TYR:CD1	1:D:52:PRO:HD3	2.51	0.46
1:D:285:LEU:HD23	1:D:285:LEU:N	2.30	0.46
1:A:83:TYR:CD1	1:A:83:TYR:O	2.69	0.46
1:A:183:ARG:NH2	1:A:185:GLU:HB2	2.10	0.46
1:C:90:LEU:HD23	1:C:91:VAL:H	1.81	0.46
1:F:101:GLU:HA	4:F:354:HOH:O	2.13	0.46
1:F:192:GLU:HG2	1:F:192:GLU:H	1.59	0.46
1:B:102:ASP:HB2	1:B:104:ALA:H	1.81	0.46
1:D:290:LEU:HD13	1:D:298:VAL:HG12	1.97	0.46
1:E:108:LEU:HD13	1:F:108:LEU:CD1	2.13	0.46
1:B:312:TYR:C	1:B:312:TYR:CD2	2.89	0.46
1:C:153:ASP:OD2	1:C:154:GLU:HG3	2.16	0.46
1:C:163:TYR:N	1:C:163:TYR:CD1	2.83	0.46
1:C:188:GLN:O	1:C:192:GLU:HG2	2.16	0.46
1:C:305:THR:HG23	4:C:361:HOH:O	2.15	0.46
1:A:108:LEU:HD13	1:B:108:LEU:HD13	1.98	0.45
1:A:142:ILE:HD13	1:A:276:VAL:HG23	1.97	0.45
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.80	0.45
1:C:22:ARG:O	1:C:26:THR:HG23	2.17	0.45
1:A:334:VAL:O	1:A:338:LEU:HD12	2.16	0.45
1:B:129:ASP:HB3	1:B:132:LEU:HD12	1.97	0.45
1:A:257:VAL:HA	1:A:258:PRO:HA	1.81	0.45
1:C:230:GLN:HE21	1:C:235:HIS:HB2	1.79	0.45
1:A:66:LEU:HD21	1:A:109:LEU:HD23	1.98	0.45
1:A:167:VAL:HG22	1:A:203:ILE:HG12	1.99	0.45
1:B:76:LEU:HD23	1:B:85:THR:HG22	1.99	0.45
1:C:90:LEU:CD2	1:C:91:VAL:N	2.79	0.45
1:D:4:GLY:HA3	1:D:88:LEU:HD13	1.99	0.45
1:D:64:ALA:HB1	1:D:76:LEU:O	2.17	0.45
1:F:151:THR:C	1:F:195:ARG:HH22	2.20	0.45
1:C:40:ILE:HD11	1:C:46:TRP:CZ2	2.52	0.45
1:C:157:PRO:C	1:C:159:ASP:H	2.20	0.45
1:D:66:LEU:HD21	1:D:109:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:CD1	1:D:298:VAL:HG11	2.46	0.45
1:D:330:ILE:O	1:D:334:VAL:HG23	2.17	0.45
1:E:290:LEU:HD23	1:E:300:LEU:HA	1.98	0.45
1:F:190:ALA:O	1:F:193:ALA:HB3	2.17	0.45
1:A:147:PHE:HA	1:A:203:ILE:O	2.17	0.45
1:C:185:GLU:H	1:C:185:GLU:HG3	1.42	0.45
1:D:90:LEU:HD23	1:D:91:VAL:H	1.82	0.45
1:C:83:TYR:CD1	1:C:83:TYR:C	2.90	0.44
1:C:90:LEU:HD23	1:C:91:VAL:N	2.32	0.44
1:A:210:THR:CG2	1:A:230:GLN:HE21	2.29	0.44
1:C:102:ASP:HB3	1:C:128:MET:HG2	1.99	0.44
1:D:120:ASP:O	1:D:124:SER:OG	2.31	0.44
1:C:83:TYR:CE2	1:D:78:LEU:HB3	2.52	0.44
1:D:1:MET:HE3	1:D:1:MET:HB3	1.67	0.44
1:F:92:LEU:HD12	1:F:92:LEU:C	2.37	0.44
1:F:163:TYR:CD2	1:F:182:ALA:C	2.91	0.44
1:A:210:THR:HG21	1:A:230:GLN:HE21	1.81	0.44
1:B:168:LYS:NZ	1:B:204:GLU:CD	2.71	0.44
1:C:6:ILE:HA	1:C:38:LEU:O	2.17	0.44
1:C:215:ALA:HB1	1:C:315:TYR:CD2	2.51	0.44
1:D:338:LEU:C	1:D:340:GLY:H	2.21	0.44
1:A:171:ARG:HH21	1:A:200:LYS:HB3	1.82	0.44
1:A:54:GLU:HB3	1:A:55:ASN:H	1.29	0.44
1:A:165:VAL:HG12	1:A:181:VAL:HG22	1.99	0.44
1:C:157:PRO:C	1:C:159:ASP:N	2.65	0.44
1:E:184:GLU:HB3	4:E:359:HOH:O	2.18	0.44
1:B:64:ALA:HB2	1:B:77:VAL:HA	1.99	0.44
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.81	0.44
1:D:212:ILE:HG22	1:D:290:LEU:HB2	1.99	0.44
1:D:330:ILE:O	1:D:331:ASP:C	2.56	0.44
1:C:144:THR:HB	1:C:145:PRO:CD	2.47	0.43
1:B:128:MET:O	1:B:128:MET:HG3	2.16	0.43
1:E:132:LEU:HD11	1:F:122:GLN:HE21	1.83	0.43
1:E:132:LEU:HD11	1:F:122:GLN:NE2	2.33	0.43
1:E:250:SER:OG	1:E:314:ARG:NH1	2.51	0.43
1:B:99:LEU:CA	1:B:102:ASP:OD1	2.66	0.43
1:B:230:GLN:HB2	1:B:259:ALA:CB	2.48	0.43
1:F:154:GLU:HG2	1:F:155:LYS:N	2.34	0.43
1:F:158:THR:OG1	1:F:159:ASP:N	2.50	0.43
1:D:159:ASP:OD2	1:D:160:GLN:N	2.51	0.43
1:D:187:LEU:O	1:D:188:GLN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:THR:C	1:F:160:GLN:N	2.71	0.43
1:F:163:TYR:HD2	1:F:182:ALA:C	2.22	0.43
1:F:17:SER:HA	1:F:96:HIS:CD2	2.53	0.43
1:F:92:LEU:HD12	1:F:93:PRO:N	2.32	0.43
1:B:22:ARG:HE	1:B:53:GLY:HA2	1.83	0.43
1:E:211:GLU:HG3	1:E:234:SER:HB3	2.00	0.43
1:B:66:LEU:HD23	1:B:108:LEU:CD2	2.49	0.43
1:D:49:CYS:HB3	1:D:61:CYS:HB3	2.00	0.43
1:F:25:ALA:O	1:F:28:LEU:HD12	2.18	0.43
1:B:92:LEU:HD22	1:B:94:VAL:HG23	2.00	0.43
1:B:316:PRO:O	1:B:317:ARG:C	2.57	0.43
1:E:103:GLY:CA	1:E:106:GLN:HG2	2.46	0.43
1:F:173:GLY:C	1:F:175:SER:N	2.70	0.43
1:A:24:VAL:O	1:A:28:LEU:HD23	2.18	0.43
1:D:90:LEU:HD12	1:D:334:VAL:HG13	2.01	0.43
1:F:181:VAL:HG21	1:F:187:LEU:HD13	2.01	0.43
1:A:183:ARG:HB3	1:A:185:GLU:OE2	2.19	0.42
1:B:315:TYR:N	1:B:316:PRO:CD	2.81	0.42
1:E:90:LEU:CD1	1:E:334:VAL:HG13	2.48	0.42
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.89	0.42
2:B:400:ATP:C8	2:B:400:ATP:C5'	2.93	0.42
1:D:109:LEU:HD13	1:D:116:TYR:CB	2.48	0.42
1:F:101:GLU:OE2	1:F:306:PHE:N	2.44	0.42
1:E:54:GLU:HA	1:E:55:ASN:HA	1.76	0.42
1:E:183:ARG:CB	4:E:381:HOH:O	2.67	0.42
1:F:162:THR:HB	1:F:205:GLU:OE2	2.20	0.42
1:F:167:VAL:O	1:F:178:VAL:HA	2.20	0.42
1:E:332:ARG:O	1:E:336:LEU:HG	2.20	0.42
1:A:215:ALA:HB1	1:A:315:TYR:CE2	2.54	0.42
1:B:120:ASP:HB3	1:B:123:SER:H	1.85	0.42
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.93	0.42
1:C:187:LEU:O	1:C:191:VAL:HG23	2.19	0.42
1:D:62:ARG:HH11	1:D:62:ARG:CG	2.32	0.42
1:F:70:ARG:HG2	1:F:112:SER:O	2.19	0.42
1:C:73:HIS:O	1:C:73:HIS:ND1	2.53	0.42
1:D:248:SER:HA	1:D:249:GLY:HA2	1.83	0.42
1:D:146:ASN:HB2	1:D:205:GLU:HB2	2.02	0.42
1:A:162:THR:O	1:A:165:VAL:CG2	2.63	0.41
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.35	0.41
1:B:159:ASP:OD2	1:B:160:GLN:CB	2.63	0.41
1:C:133:THR:CG2	1:C:280:LEU:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LEU:HG	1:D:298:VAL:HG21	2.02	0.41
1:D:316:PRO:O	1:D:320:THR:HG23	2.20	0.41
1:E:147:PHE:HA	1:E:203:ILE:O	2.20	0.41
1:F:129:ASP:OD1	1:F:131:SER:OG	2.32	0.41
1:B:1:MET:HE3	1:B:90:LEU:HD12	2.02	0.41
1:E:330:ILE:O	1:E:334:VAL:HG23	2.21	0.41
1:F:37:TYR:O	1:F:48:LEU:HD12	2.19	0.41
1:F:170:ALA:CB	1:F:200:LYS:HD3	2.50	0.41
1:C:16:ILE:HG22	1:C:96:HIS:CD2	2.56	0.41
1:E:187:LEU:O	1:E:188:GLN:C	2.57	0.41
1:F:302:GLU:OE1	1:F:304:ASN:OD1	2.39	0.41
1:E:123:SER:HB3	1:E:280:LEU:O	2.20	0.41
1:B:94:VAL:HA	1:B:306:PHE:CE2	2.56	0.41
1:B:106:GLN:H	1:B:106:GLN:HG2	1.08	0.41
1:B:168:LYS:HG2	1:B:202:LEU:HB3	2.02	0.41
1:C:157:PRO:O	1:C:158:THR:C	2.59	0.41
1:C:212:ILE:CG2	1:C:228:VAL:CG1	2.98	0.41
1:A:25:ALA:HA	1:A:28:LEU:HD21	2.03	0.41
1:D:217:MET:HE3	1:D:332:ARG:HB3	2.02	0.41
1:F:117:VAL:HG11	1:F:333:LEU:HB3	2.03	0.41
1:A:13:GLU:HG2	1:A:16:ILE:HD12	2.02	0.41
1:B:290:LEU:CD2	1:B:300:LEU:HA	2.51	0.41
1:E:290:LEU:CD2	1:E:300:LEU:HA	2.50	0.41
1:A:325:SER:O	1:A:328:ASP:N	2.53	0.41
1:B:143:ALA:C	1:B:144:THR:CG2	2.88	0.41
1:B:286:SER:OG	1:B:305:THR:HA	2.21	0.41
1:E:142:ILE:HD13	1:E:276:VAL:CG2	2.32	0.41
1:F:195:ARG:C	1:F:197:TYR:H	2.23	0.41
1:B:32:VAL:HG23	1:B:33:PHE:H	1.86	0.41
1:C:90:LEU:HD11	1:C:334:VAL:HG13	2.00	0.41
1:E:27:HIS:CE1	1:E:326:ARG:HD2	2.55	0.41
1:E:49:CYS:HB3	1:E:61:CYS:SG	2.61	0.41
1:E:220:GLY:HA3	1:E:221:PRO:HD3	1.89	0.41
1:F:163:TYR:HD1	1:F:163:TYR:H	1.66	0.41
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.92	0.41
1:B:37:TYR:CD2	1:B:51:GLY:HA2	2.56	0.41
1:B:54:GLU:HA	1:B:55:ASN:HA	1.62	0.41
1:B:158:THR:C	1:B:160:GLN:N	2.71	0.41
1:D:32:VAL:CG2	1:D:33:PHE:CD2	3.04	0.41
1:B:144:THR:O	1:B:145:PRO:C	2.58	0.40
1:A:90:LEU:HD12	1:A:334:VAL:HG13	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLY:HA3	1:B:88:LEU:HD13	2.03	0.40
1:B:49:CYS:HB3	1:B:61:CYS:SG	2.61	0.40
1:C:28:LEU:H	1:C:28:LEU:HG	1.73	0.40
1:C:159:ASP:CG	1:C:160:GLN:N	2.74	0.40
1:D:10:VAL:HG22	1:D:42:LYS:O	2.21	0.40
1:E:3:ILE:HD12	1:E:90:LEU:HD13	2.03	0.40
1:F:41:THR:C	1:F:43:SER:H	2.24	0.40
1:F:165:VAL:CG1	1:F:166:PHE:N	2.84	0.40
1:F:195:ARG:C	1:F:197:TYR:N	2.75	0.40
1:C:220:GLY:HA3	1:C:221:PRO:HD3	1.88	0.40
1:D:187:LEU:C	1:D:189:GLY:N	2.69	0.40
1:E:28:LEU:H	1:E:28:LEU:HG	1.71	0.40
1:F:138:ARG:NH1	1:F:147:PHE:CE1	2.90	0.40
1:B:168:LYS:NZ	1:B:204:GLU:OE2	2.42	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	323/346 (93%)	308 (95%)	13 (4%)	2 (1%)	25	57
1	B	325/346 (94%)	306 (94%)	19 (6%)	0	100	100
1	C	327/346 (94%)	307 (94%)	17 (5%)	3 (1%)	17	49
1	D	323/346 (93%)	302 (94%)	19 (6%)	2 (1%)	25	57
1	E	327/346 (94%)	306 (94%)	20 (6%)	1 (0%)	41	71
1	F	323/346 (93%)	303 (94%)	17 (5%)	3 (1%)	17	49
All	All	1948/2076 (94%)	1832 (94%)	105 (5%)	11 (1%)	25	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	PRO
1	C	158	THR
1	D	29	GLY
1	F	152	ALA
1	E	221	PRO
1	F	221	PRO
1	C	221	PRO
1	A	94	VAL
1	D	157	PRO
1	A	221	PRO
1	F	93	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	254/283 (90%)	229 (90%)	25 (10%)	8 28
1	B	256/283 (90%)	231 (90%)	25 (10%)	8 28
1	C	257/283 (91%)	230 (90%)	27 (10%)	7 25
1	D	255/283 (90%)	229 (90%)	26 (10%)	7 26
1	E	257/283 (91%)	242 (94%)	15 (6%)	20 50
1	F	252/283 (89%)	227 (90%)	25 (10%)	8 27
All	All	1531/1698 (90%)	1388 (91%)	143 (9%)	9 31

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	11	SER
1	A	28	LEU
1	A	32	VAL
1	A	54	GLU
1	A	55	ASN
1	A	60	ASN
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	79	GLU
1	A	85	THR
1	A	90	LEU
1	A	106	GLN
1	A	110	GLU
1	A	139	SER
1	A	179	SER
1	A	183	ARG
1	A	184	GLU
1	A	196	GLU
1	A	233	LEU
1	A	262	SER
1	A	263	THR
1	A	286	SER
1	A	309	MET
1	A	332	ARG
1	A	336	LEU
1	B	28	LEU
1	B	32	VAL
1	B	43	SER
1	B	55	ASN
1	B	60	ASN
1	B	90	LEU
1	B	105	ILE
1	B	106	GLN
1	B	120	ASP
1	B	128	MET
1	B	144	THR
1	B	145	PRO
1	B	159	ASP
1	B	172	SER
1	B	210	THR
1	B	233	LEU
1	B	250	SER
1	B	252	ASN
1	B	262	SER
1	B	264	THR
1	B	267	SER
1	B	286	SER
1	B	295	ASP
1	B	320	THR
1	B	336	LEU

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Mol	Chain	Res	Type
1	C	12	GLU
1	C	28	LEU
1	C	32	VAL
1	C	47	GLN
1	C	54	GLU
1	C	60	ASN
1	C	62	ARG
1	C	83	TYR
1	C	85	THR
1	C	90	LEU
1	C	92	LEU
1	C	106	GLN
1	C	133	THR
1	C	135	LEU
1	C	153	ASP
1	C	159	ASP
1	C	165	VAL
1	C	179	SER
1	C	185	GLU
1	C	224	ILE
1	C	237	PHE
1	C	248	SER
1	C	250	SER
1	C	263	THR
1	C	266	ARG
1	C	286	SER
1	C	336	LEU
1	D	0	HIS
1	D	1	MET
1	D	11	SER
1	D	12	GLU
1	D	32	VAL
1	D	56	TRP
1	D	58	ASP
1	D	60	ASN
1	D	61	CYS
1	D	62	ARG
1	D	87	ARG
1	D	90	LEU
1	D	92	LEU
1	D	106	GLN
1	D	124	SER

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Mol	Chain	Res	Type
1	D	133	THR
1	D	151	THR
1	D	160	GLN
1	D	186	ASP
1	D	187	LEU
1	D	212	ILE
1	D	229	ASP
1	D	248	SER
1	D	250	SER
1	D	256	THR
1	D	336	LEU
1	E	-1	SER
1	E	1	MET
1	E	28	LEU
1	E	55	ASN
1	E	60	ASN
1	E	62	ARG
1	E	90	LEU
1	E	106	GLN
1	E	133	THR
1	E	151	THR
1	E	154	GLU
1	E	165	VAL
1	E	179	SER
1	E	188	GLN
1	E	305	THR
1	F	28	LEU
1	F	32	VAL
1	F	60	ASN
1	F	62	ARG
1	F	84	GLU
1	F	90	LEU
1	F	92	LEU
1	F	151	THR
1	F	158	THR
1	F	159	ASP
1	F	160	GLN
1	F	161	LEU
1	F	165	VAL
1	F	172	SER
1	F	184	GLU
1	F	186	ASP

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Mol	Chain	Res	Type
1	F	192	GLU
1	F	199	SER
1	F	202	LEU
1	F	212	ILE
1	F	232	THR
1	F	262	SER
1	F	286	SER
1	F	305	THR
1	F	336	LEU

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	60	ASN
1	A	106	GLN
1	A	270	GLN
1	B	27	HIS
1	B	60	ASN
1	B	106	GLN
1	B	270	GLN
1	C	0	HIS
1	C	55	ASN
1	C	60	ASN
1	C	106	GLN
1	D	230	GLN
1	E	0	HIS
1	E	27	HIS
1	E	55	ASN
1	F	60	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)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	A	400	3	26,33,33	1.05	2 (7%)	31,52,52	1.63	5 (16%)
2	ATP	C	400	3	26,33,33	0.97	1 (3%)	31,52,52	1.53	4 (12%)
2	ATP	B	400	3	26,33,33	1.04	1 (3%)	31,52,52	1.55	4 (12%)
2	ATP	E	400	3	26,33,33	1.11	1 (3%)	31,52,52	1.38	3 (9%)
2	ATP	F	400	3	26,33,33	1.02	1 (3%)	31,52,52	1.56	4 (12%)
2	ATP	D	400	3	26,33,33	1.07	1 (3%)	31,52,52	1.46	3 (9%)

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
2	ATP	A	400	3	-	8/18/38/38	0/3/3/3
2	ATP	C	400	3	-	6/18/38/38	0/3/3/3
2	ATP	B	400	3	-	7/18/38/38	0/3/3/3
2	ATP	E	400	3	-	7/18/38/38	0/3/3/3
2	ATP	F	400	3	-	6/18/38/38	0/3/3/3
2	ATP	D	400	3	-	9/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	ATP	O4'-C1'	3.47	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	ATP	O4'-C1'	2.91	1.45	1.41
2	A	400	ATP	O4'-C1'	2.53	1.44	1.41
2	F	400	ATP	O4'-C1'	2.36	1.44	1.41
2	B	400	ATP	PG-O2G	2.30	1.63	1.54
2	A	400	ATP	PG-O2G	2.25	1.63	1.54
2	C	400	ATP	O4'-C1'	2.08	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	ATP	N3-C2-N1	-4.65	121.41	128.68
2	B	400	ATP	N3-C2-N1	-4.61	121.47	128.68
2	F	400	ATP	N3-C2-N1	-4.60	121.49	128.68
2	A	400	ATP	N3-C2-N1	-4.47	121.69	128.68
2	E	400	ATP	N3-C2-N1	-4.27	122.00	128.68
2	D	400	ATP	N3-C2-N1	-4.16	122.18	128.68
2	F	400	ATP	PB-O3B-PG	-3.79	119.83	132.83
2	D	400	ATP	PB-O3B-PG	-3.65	120.30	132.83
2	C	400	ATP	PB-O3B-PG	-3.65	120.31	132.83
2	A	400	ATP	PB-O3B-PG	-3.56	120.61	132.83
2	B	400	ATP	PB-O3B-PG	-3.54	120.69	132.83
2	E	400	ATP	PB-O3B-PG	-3.51	120.77	132.83
2	A	400	ATP	C3'-C2'-C1'	3.41	106.11	100.98
2	B	400	ATP	C4-C5-N7	-2.88	106.39	109.40
2	C	400	ATP	PA-O3A-PB	-2.69	123.61	132.83
2	E	400	ATP	C5'-C4'-C3'	-2.68	105.12	115.18
2	D	400	ATP	PA-O3A-PB	-2.53	124.16	132.83
2	B	400	ATP	PA-O3A-PB	-2.43	124.48	132.83
2	F	400	ATP	C5'-C4'-C3'	-2.43	106.08	115.18
2	A	400	ATP	PA-O3A-PB	-2.38	124.65	132.83
2	F	400	ATP	PA-O3A-PB	-2.29	124.96	132.83
2	A	400	ATP	C4-C5-N7	-2.29	107.02	109.40
2	C	400	ATP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	C5'-O5'-PA-O1A
2	A	400	ATP	C5'-O5'-PA-O2A
2	B	400	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	400	ATP	C5'-O5'-PA-O2A
2	C	400	ATP	C5'-O5'-PA-O1A
2	C	400	ATP	C5'-O5'-PA-O2A
2	D	400	ATP	PB-O3B-PG-O2G
2	D	400	ATP	C5'-O5'-PA-O1A
2	D	400	ATP	C5'-O5'-PA-O2A
2	E	400	ATP	C5'-O5'-PA-O1A
2	E	400	ATP	C5'-O5'-PA-O2A
2	F	400	ATP	C5'-O5'-PA-O2A
2	A	400	ATP	PA-O3A-PB-O1B
2	D	400	ATP	PB-O3A-PA-O5'
2	A	400	ATP	PB-O3B-PG-O3G
2	E	400	ATP	C5'-O5'-PA-O3A
2	F	400	ATP	C5'-O5'-PA-O3A
2	E	400	ATP	PG-O3B-PB-O2B
2	F	400	ATP	PG-O3B-PB-O2B
2	F	400	ATP	C5'-O5'-PA-O1A
2	B	400	ATP	PG-O3B-PB-O2B
2	C	400	ATP	PG-O3B-PB-O2B
2	E	400	ATP	PA-O3A-PB-O1B
2	D	400	ATP	PA-O3A-PB-O3B
2	B	400	ATP	PA-O3A-PB-O1B
2	C	400	ATP	PA-O3A-PB-O1B
2	E	400	ATP	PG-O3B-PB-O1B
2	C	400	ATP	O4'-C4'-C5'-O5'
2	E	400	ATP	O4'-C4'-C5'-O5'
2	A	400	ATP	C5'-O5'-PA-O3A
2	B	400	ATP	C5'-O5'-PA-O3A
2	C	400	ATP	C5'-O5'-PA-O3A
2	D	400	ATP	C5'-O5'-PA-O3A
2	A	400	ATP	O4'-C4'-C5'-O5'
2	B	400	ATP	O4'-C4'-C5'-O5'
2	A	400	ATP	PG-O3B-PB-O2B
2	B	400	ATP	PG-O3B-PB-O1B
2	D	400	ATP	PG-O3B-PB-O2B
2	D	400	ATP	PA-O3A-PB-O1B
2	F	400	ATP	PG-O3B-PB-O1B
2	D	400	ATP	O4'-C4'-C5'-O5'
2	F	400	ATP	O4'-C4'-C5'-O5'

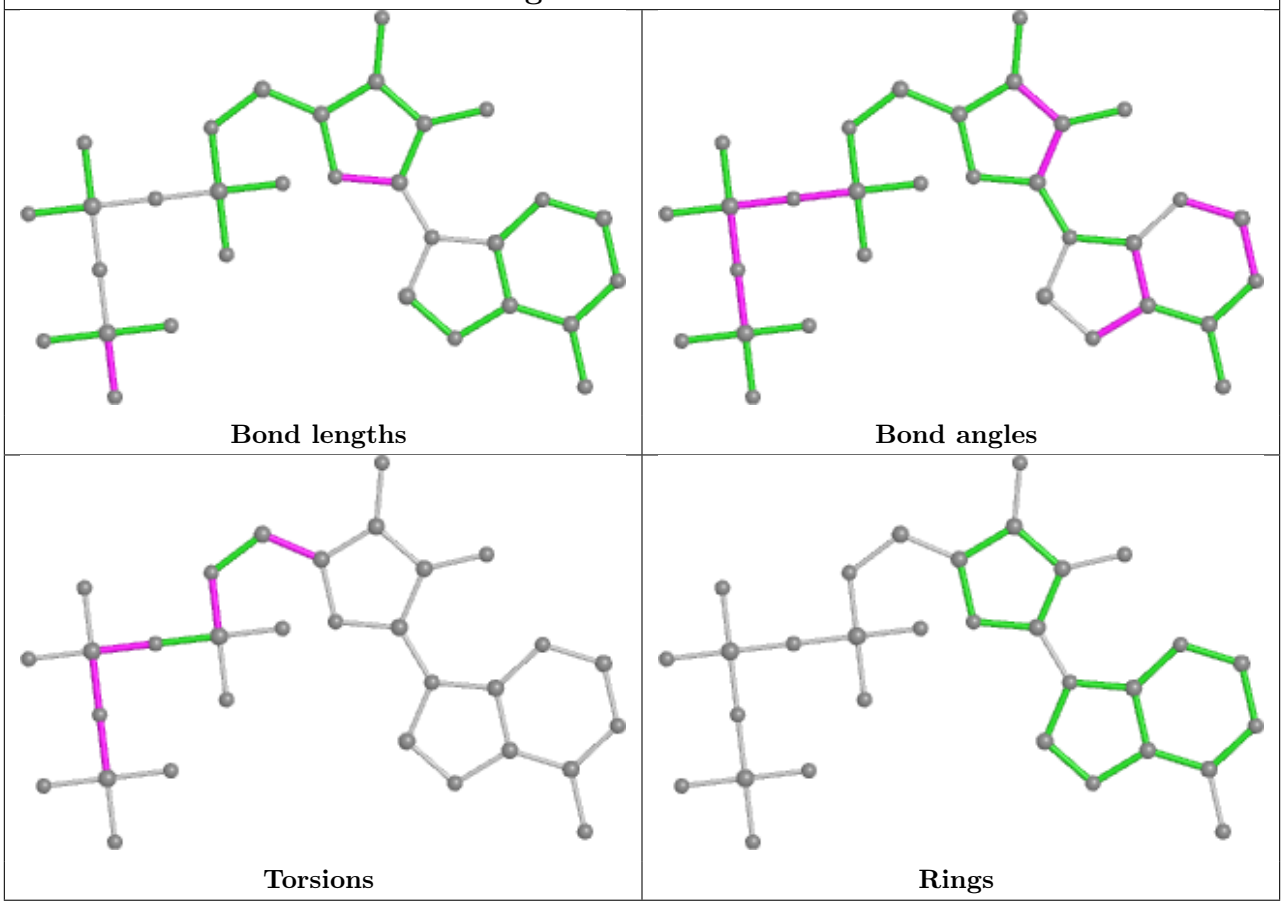
There are no ring outliers.

6 monomers are involved in 20 short contacts:

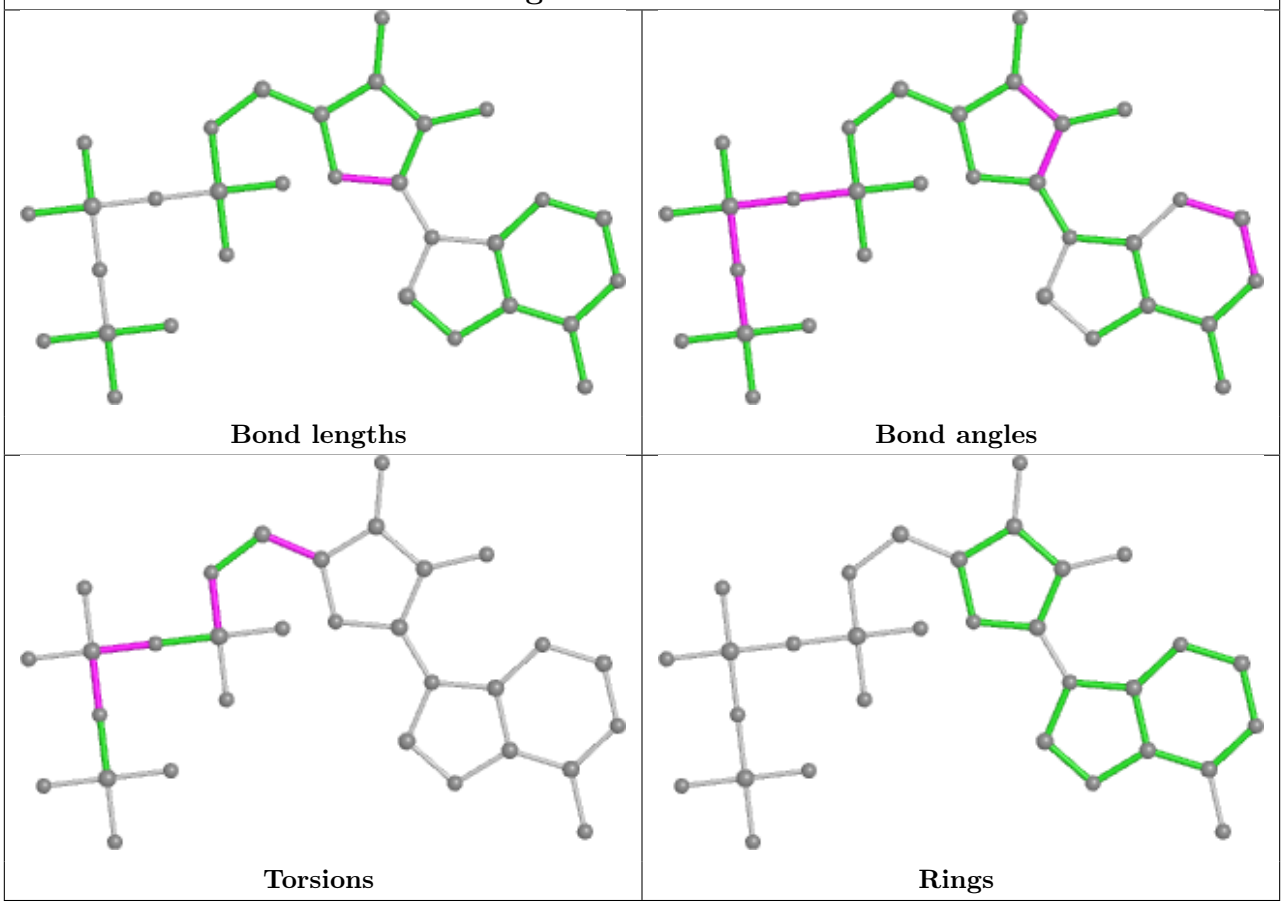
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	ATP	3	0
2	C	400	ATP	3	0
2	B	400	ATP	5	0
2	E	400	ATP	3	0
2	F	400	ATP	3	0
2	D	400	ATP	3	0

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

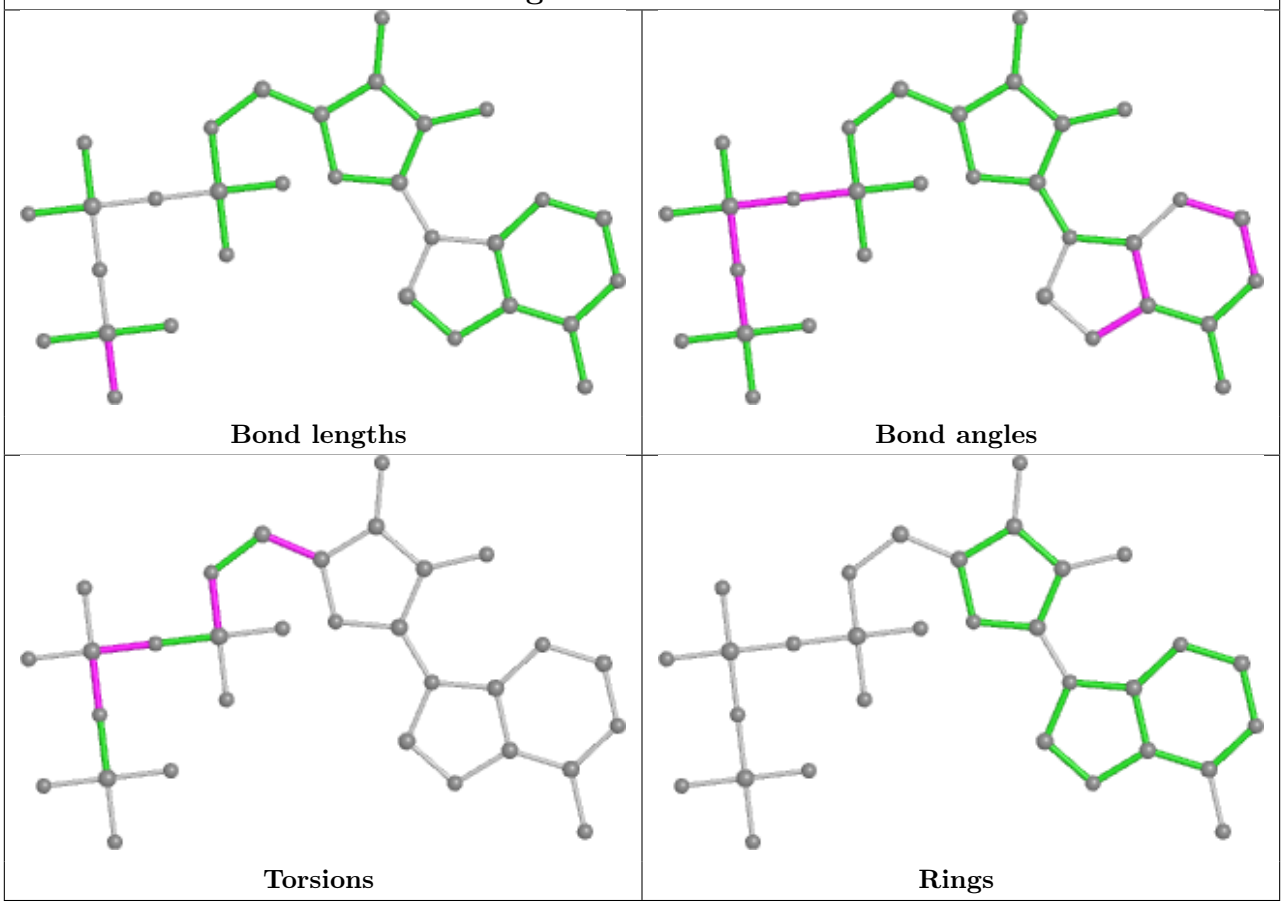
Ligand ATP A 400



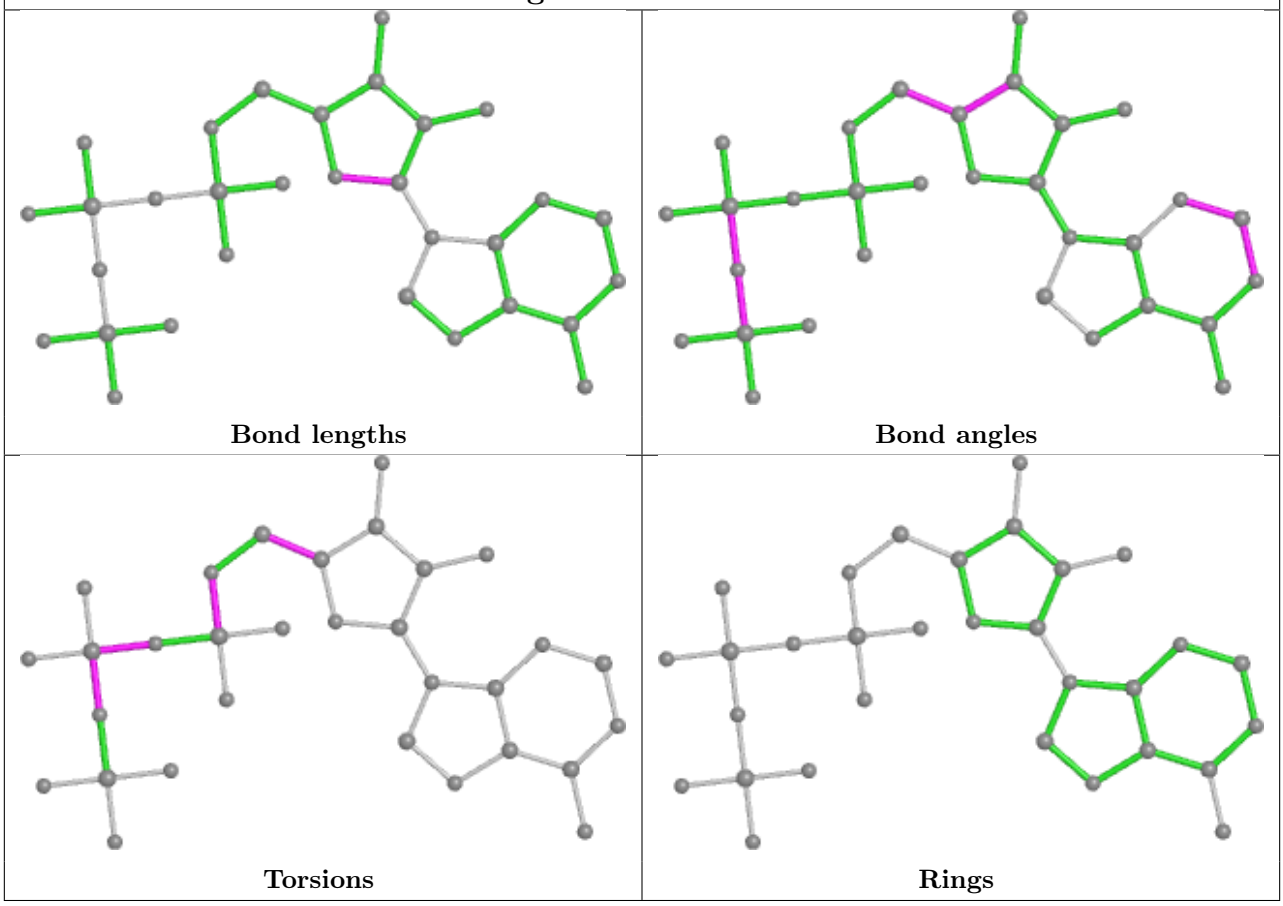
Ligand ATP C 400



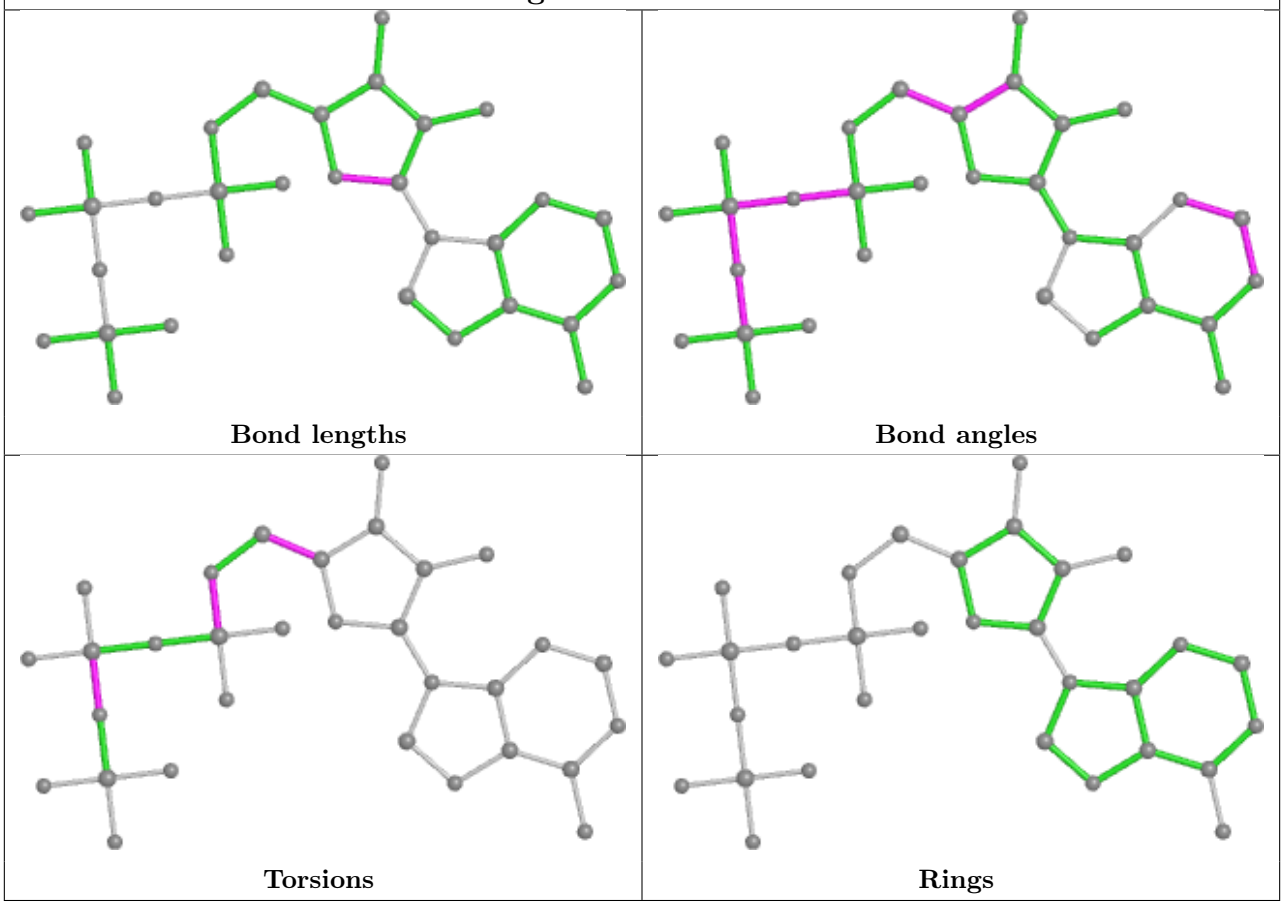
Ligand ATP B 400



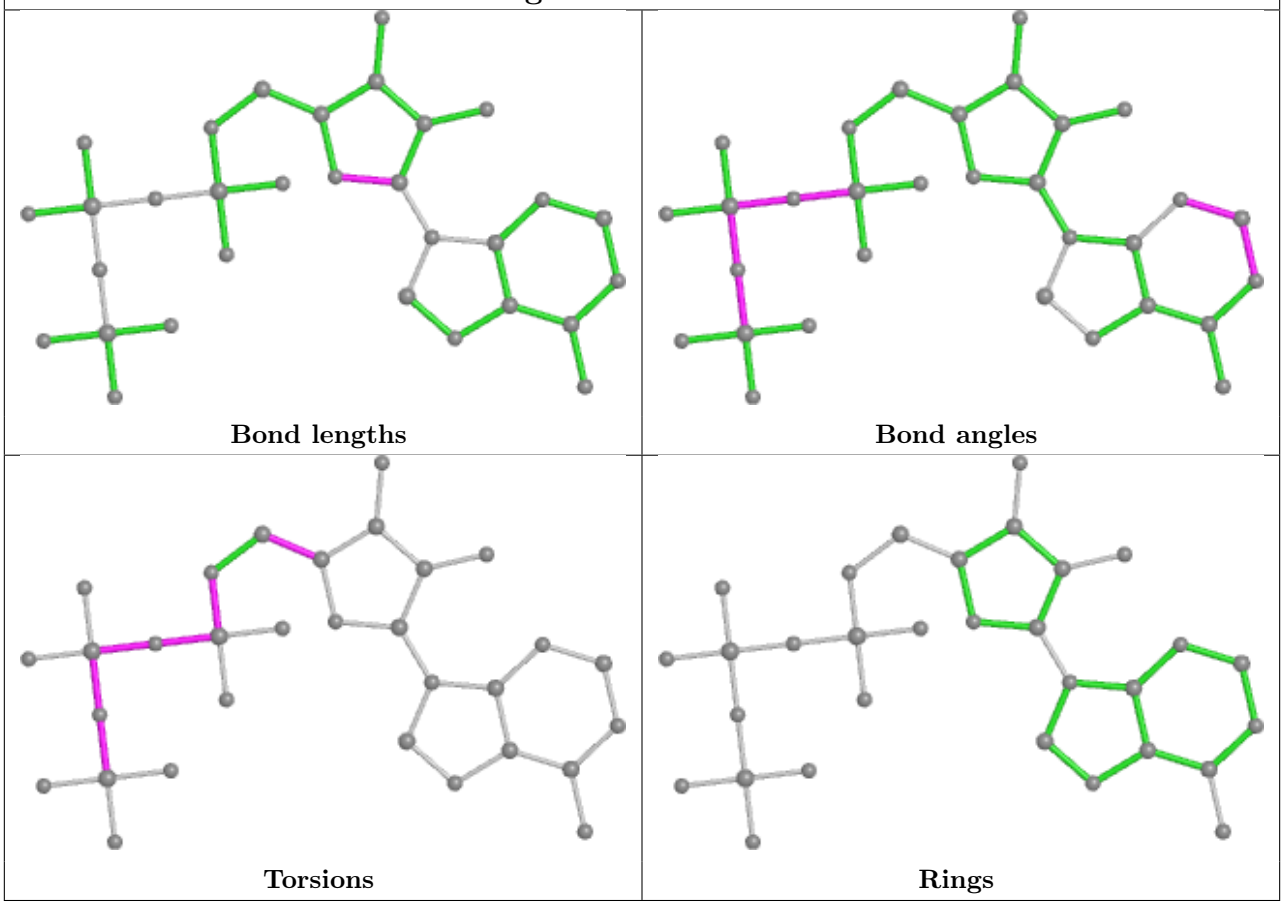
Ligand ATP E 400



Ligand ATP F 400



Ligand ATP D 400



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	327/346 (94%)	-0.56	0	100	100	17, 36, 76, 104	0
1	B	329/346 (95%)	-0.54	0	100	100	17, 35, 69, 87	0
1	C	331/346 (95%)	-0.53	0	100	100	19, 34, 70, 87	0
1	D	327/346 (94%)	-0.44	2 (0%)	89	77	20, 40, 87, 105	0
1	E	331/346 (95%)	-0.52	0	100	100	20, 40, 76, 99	0
1	F	327/346 (94%)	-0.32	4 (1%)	79	60	17, 44, 97, 141	0
All	All	1972/2076 (94%)	-0.48	6 (0%)	94	87	17, 38, 79, 141	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	GLN	3.9
1	D	186	ASP	2.5
1	F	164	PRO	2.5
1	F	152	ALA	2.4
1	F	157	PRO	2.1
1	D	162	THR	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)

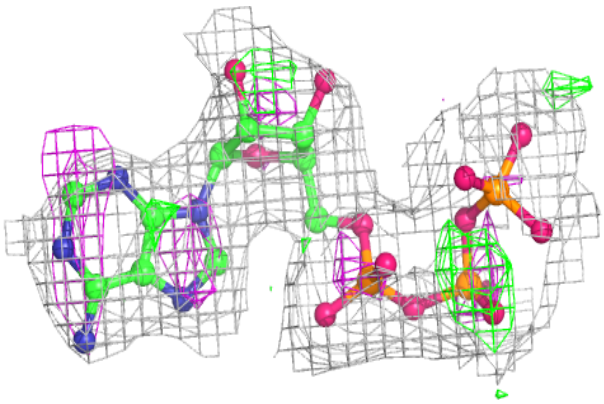
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

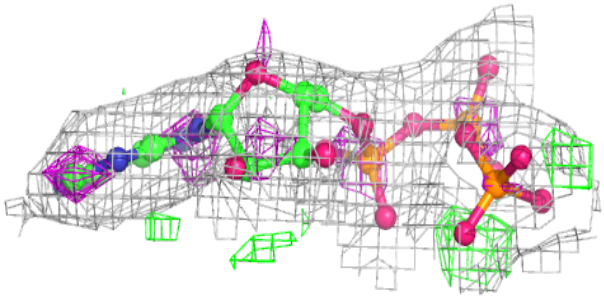
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	A	400	31/31	0.93	0.17	2,7,12,19	0
2	ATP	E	400	31/31	0.93	0.18	8,16,23,25	0
2	ATP	F	400	31/31	0.93	0.15	2,9,18,19	0
2	ATP	C	400	31/31	0.94	0.16	11,18,23,32	0
2	ATP	D	400	31/31	0.94	0.14	5,13,16,20	0
3	MG	A	500	1/1	0.94	0.20	9,9,9,9	0
2	ATP	B	400	31/31	0.95	0.14	4,10,14,16	0
3	MG	B	500	1/1	0.95	0.19	2,2,2,2	0
3	MG	D	501	1/1	0.95	0.10	2,2,2,2	0
3	MG	C	500	1/1	0.96	0.27	6,6,6,6	0
3	MG	D	500	1/1	0.96	0.18	7,7,7,7	0
3	MG	A	501	1/1	0.96	0.14	2,2,2,2	0
3	MG	F	500	1/1	0.96	0.21	8,8,8,8	0
3	MG	E	501	1/1	0.98	0.15	2,2,2,2	0
3	MG	E	500	1/1	0.99	0.16	6,6,6,6	0
3	MG	B	501	1/1	0.99	0.17	2,2,2,2	0
3	MG	C	501	1/1	0.99	0.19	2,2,2,2	0
3	MG	F	501	1/1	0.99	0.14	2,2,2,2	0

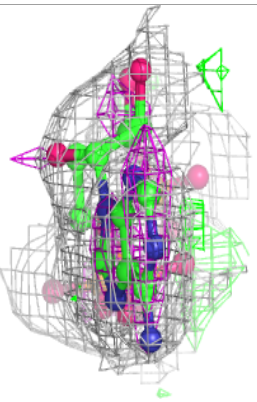
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 400:

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

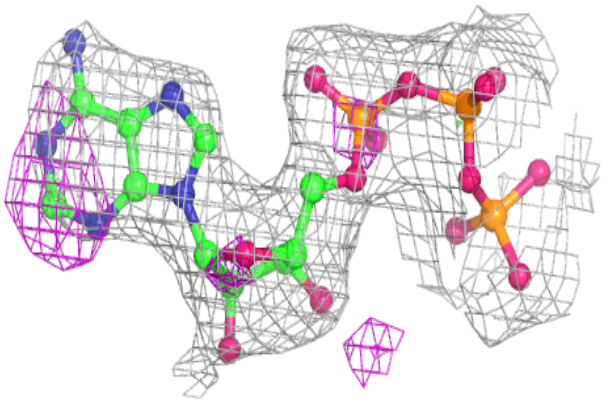


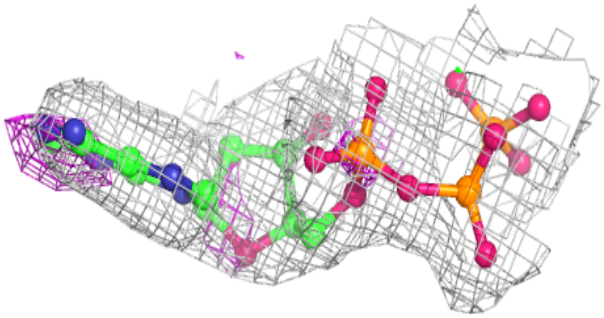


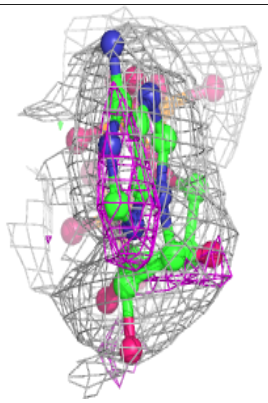


Electron density around ATP E 400:

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

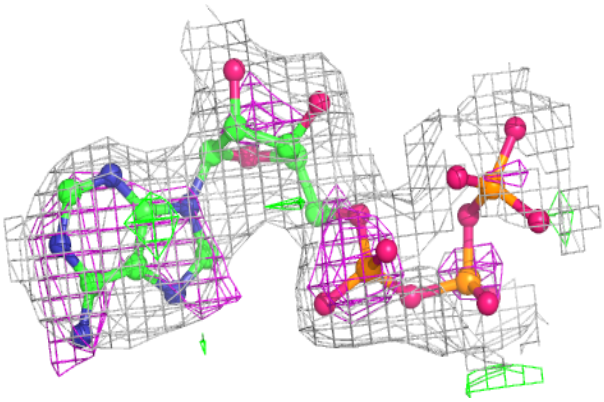


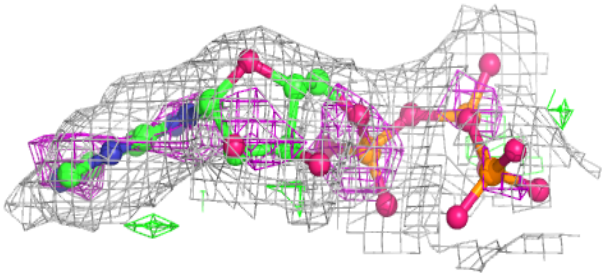


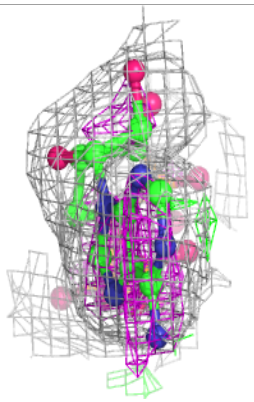


Electron density around ATP F 400:

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

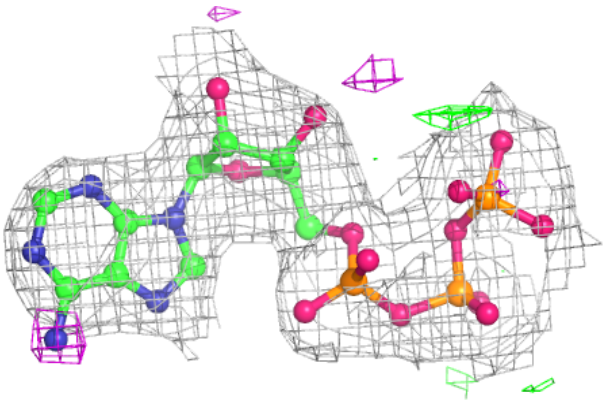


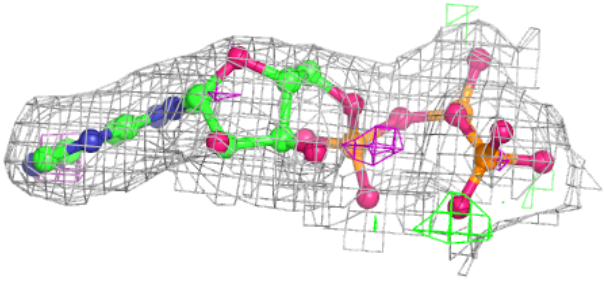


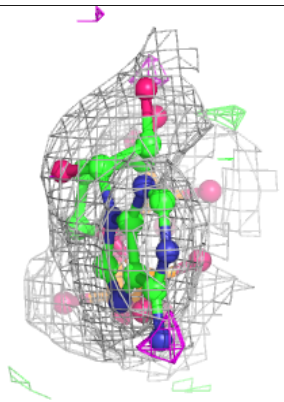


Electron density around ATP C 400:

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

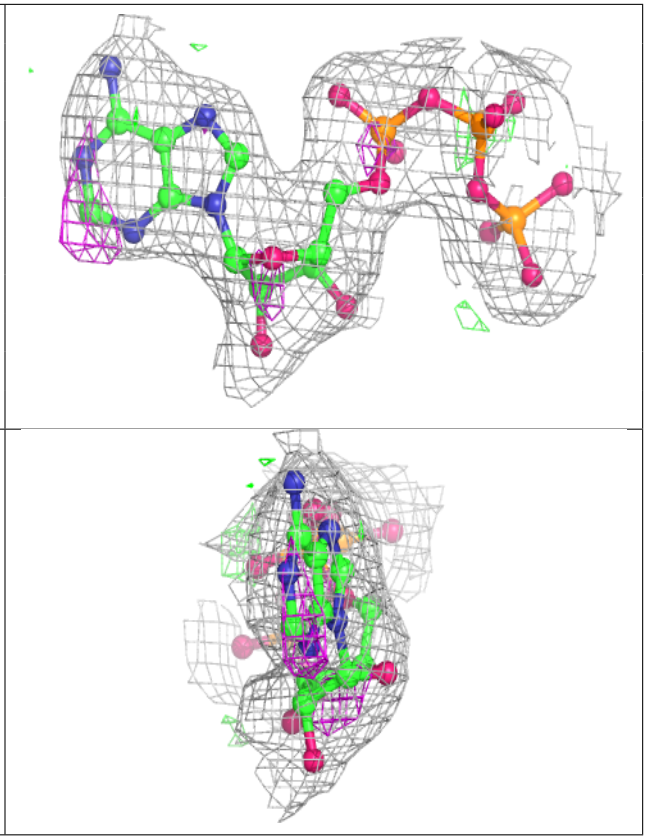


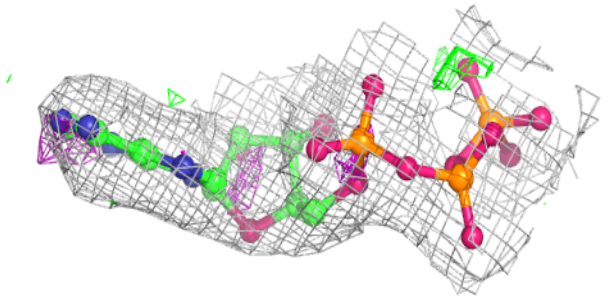




Electron density around ATP D 400:

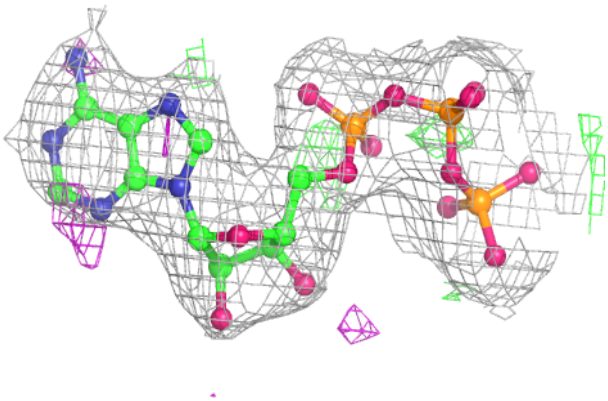
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

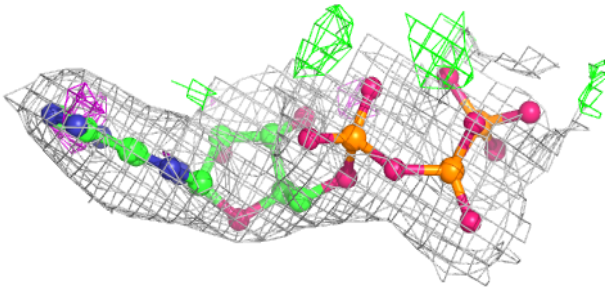


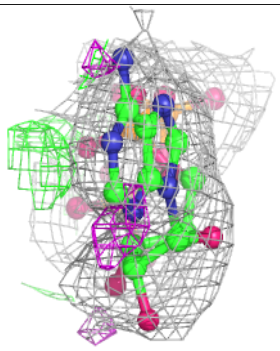


Electron density around ATP B 400:

$2mF_o$-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.