Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 09:55 AM EDT

PDB ID	:	1PVO
Title	:	X-ray crystal structure of Rho transcription termination factor in complex with ssRNA substrate and ANPPNP
Authors	:	Skordalakes, E.; Berger, J.M.
Deposited on	:	2003-06-27
Resolution	:	3.00 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 ⓘ 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 ⓘ) were used in the production of this report:

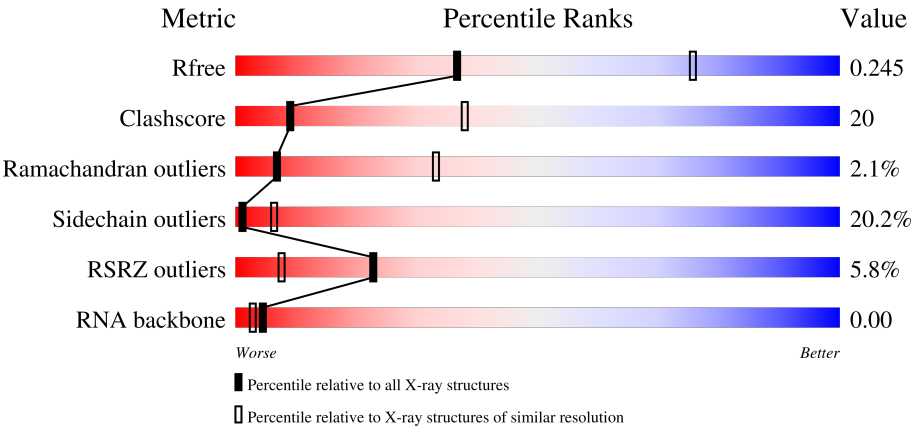
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	G	2	50% 50%
1	H	2	100% 50% 50%
1	J	2	100% 100%
1	K	2	100% 100%

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Mol	Chain	Length	Quality of chain
1	L	2	50% 50%
2	A	419	7% 55% 34% 9%
2	B	419	9% 43% 32% 11% 15%
2	C	419	3% 53% 35% 9%
2	D	419	3% 47% 39% 11%
2	E	419	4% 55% 35% 7%
2	F	419	6% 51% 34% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	A	601	X	-	-	-
3	ANP	B	602	X	-	-	-
3	ANP	C	603	X	-	-	-
3	ANP	D	604	X	-	-	-
3	ANP	E	605	X	-	-	-
3	ANP	F	606	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19246 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.

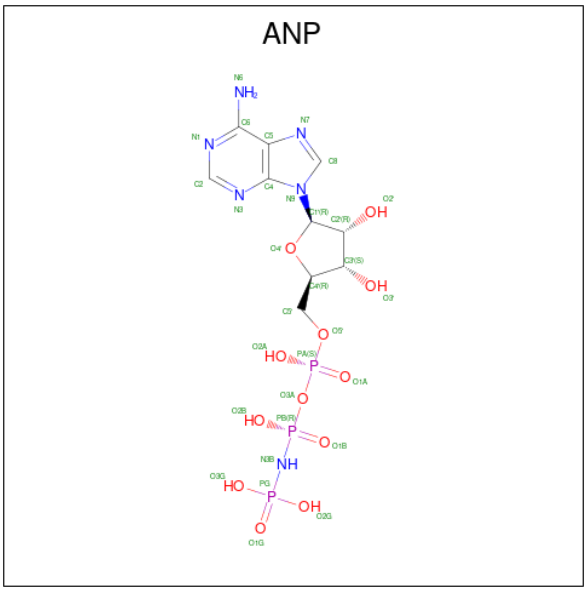
- Molecule 1 is a RNA chain called 5'-R(P*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			

- Molecule 2 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	B	358	Total	C	N	O	S	0	0	0
			2813	1776	494	529	14			
2	C	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3201	2020	561	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	5	Total	O	0	0
			5	5		
4	D	4	Total	O	0	0
			4	4		
4	E	2	Total	O	0	0
			2	2		
4	F	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

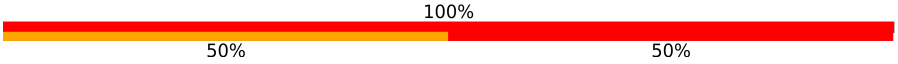
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-R(P*UP*C)-3'

Chain G:

• Molecule 1: 5'-R(P*UP*C)-3'

Chain H:

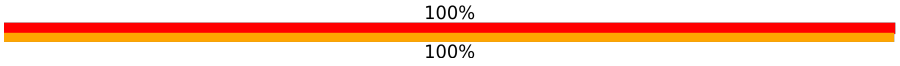


• Molecule 1: 5'-R(P*UP*C)-3'

Chain J:

• Molecule 1: 5'-R(P*UP*C)-3'

Chain K:

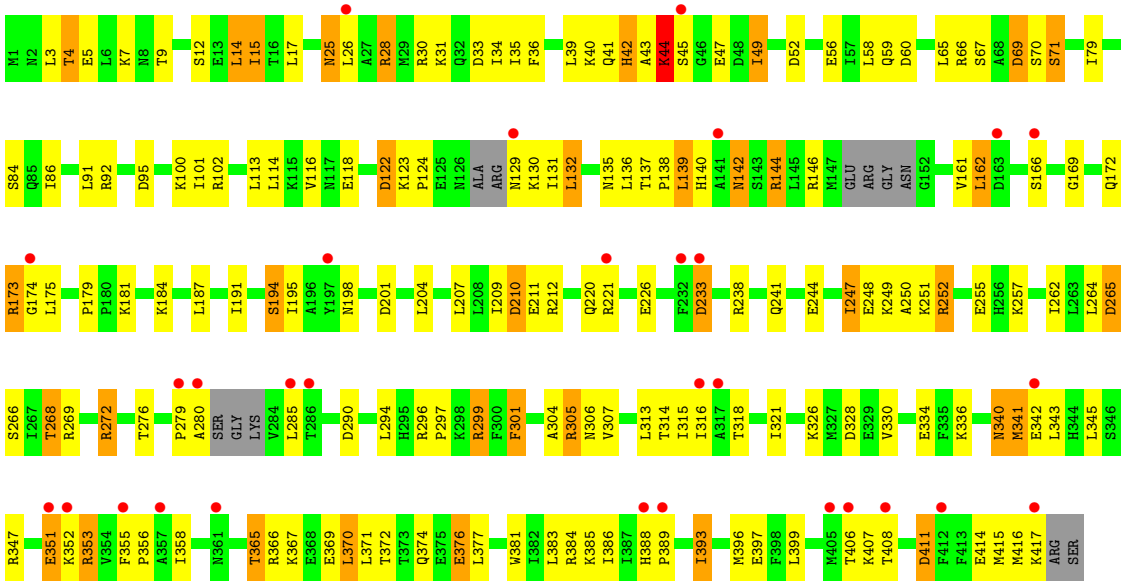


• Molecule 1: 5'-R(P*UP*C)-3'

Chain L:

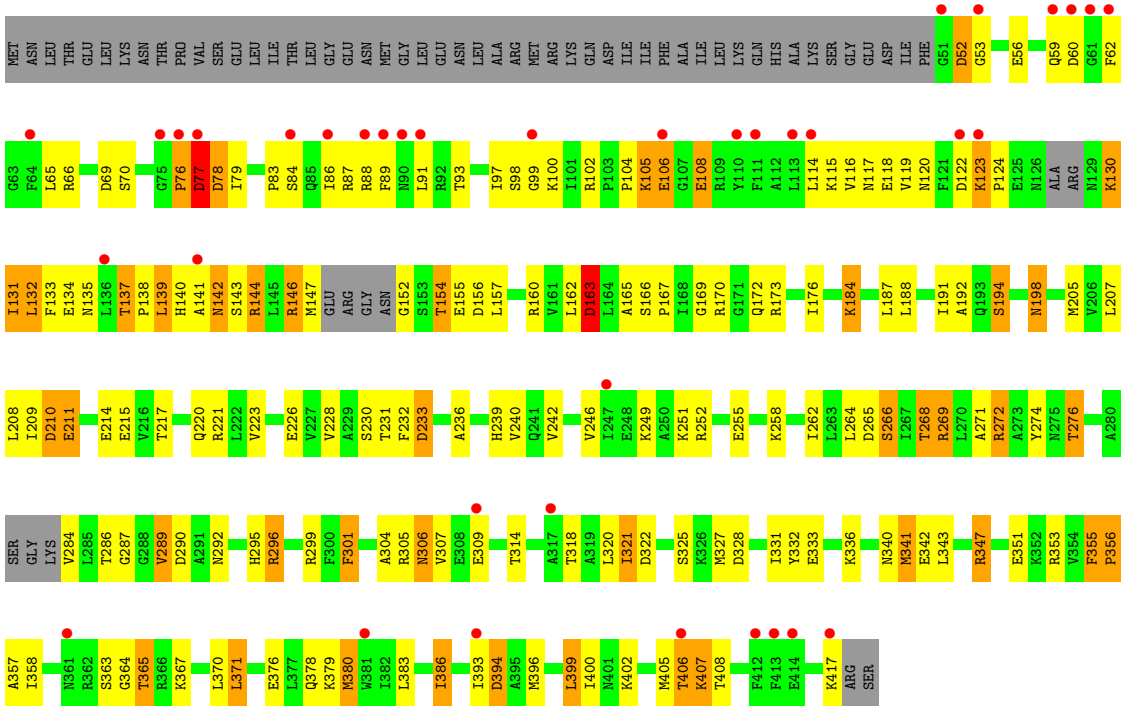
• Molecule 2: Transcription termination factor rho

Chain A:



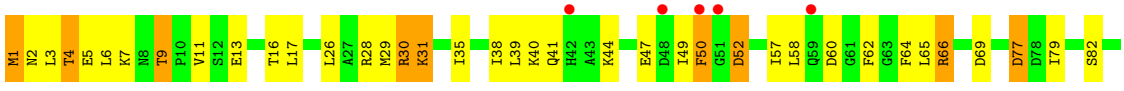
• Molecule 2: Transcription termination factor rho

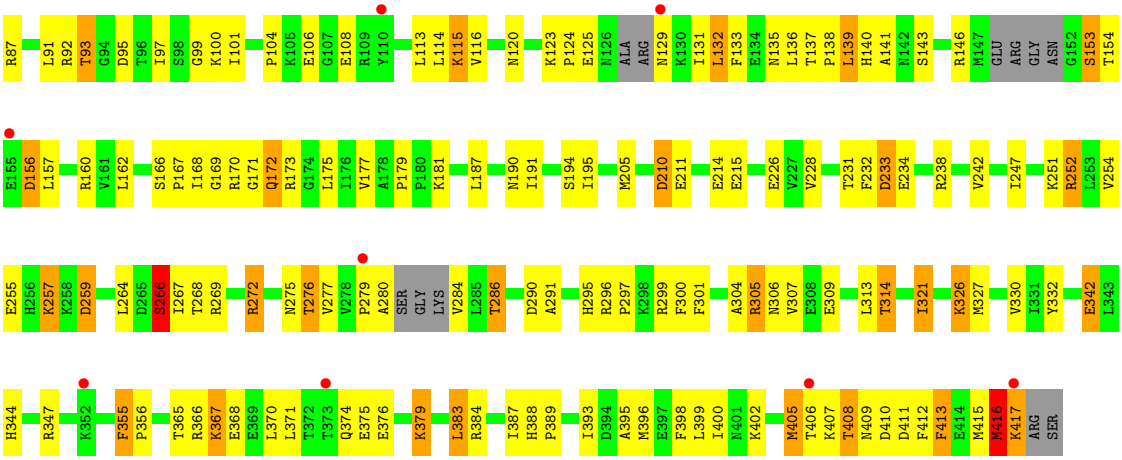
Chain B:



• Molecule 2: Transcription termination factor rho

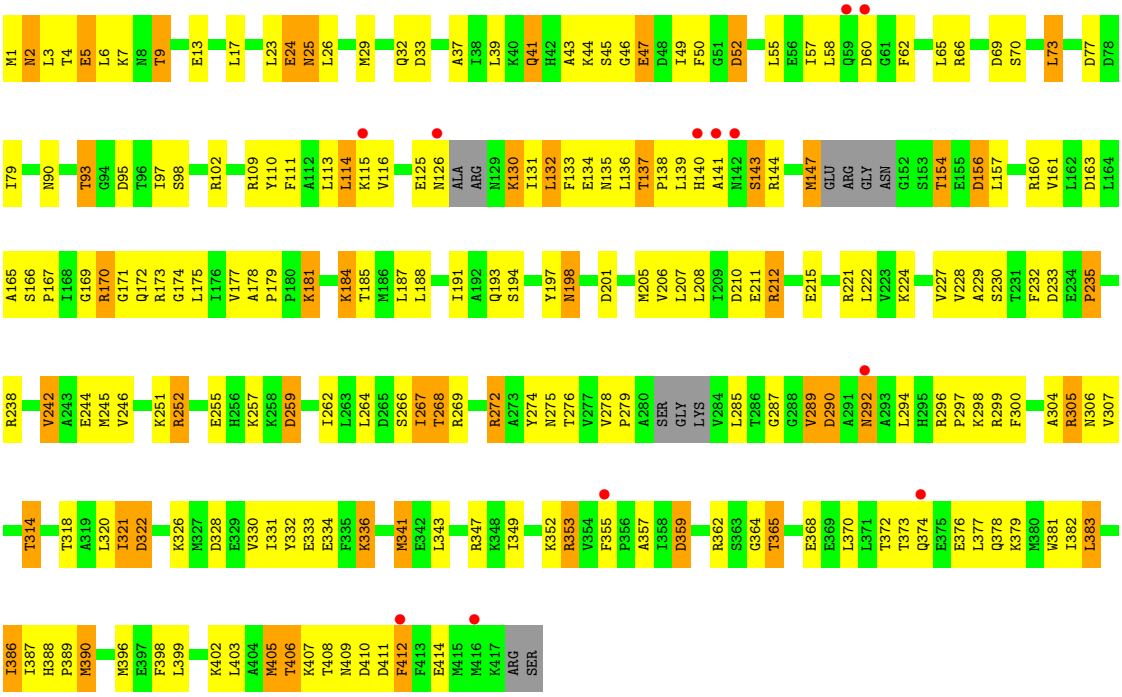
Chain C:





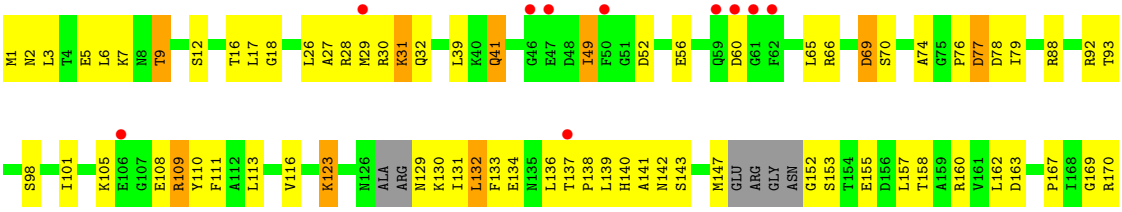
• Molecule 2: Transcription termination factor rho

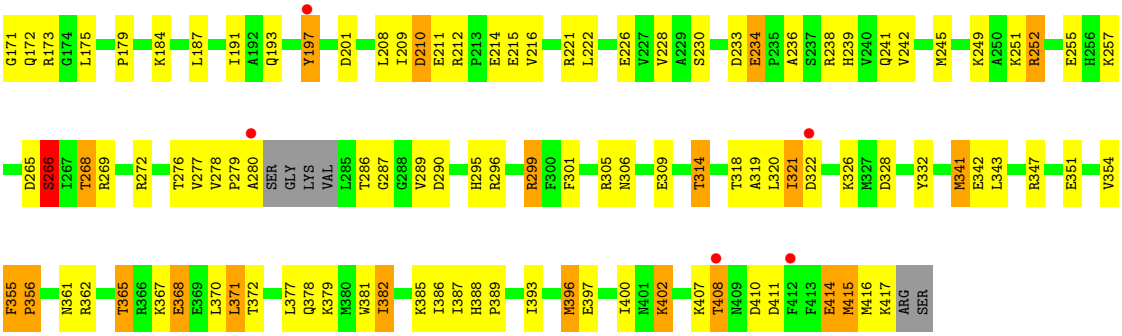
Chain D:



• Molecule 2: Transcription termination factor rho

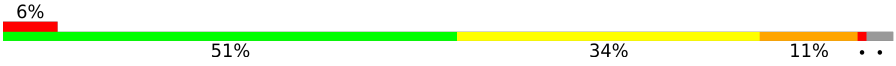
Chain E:

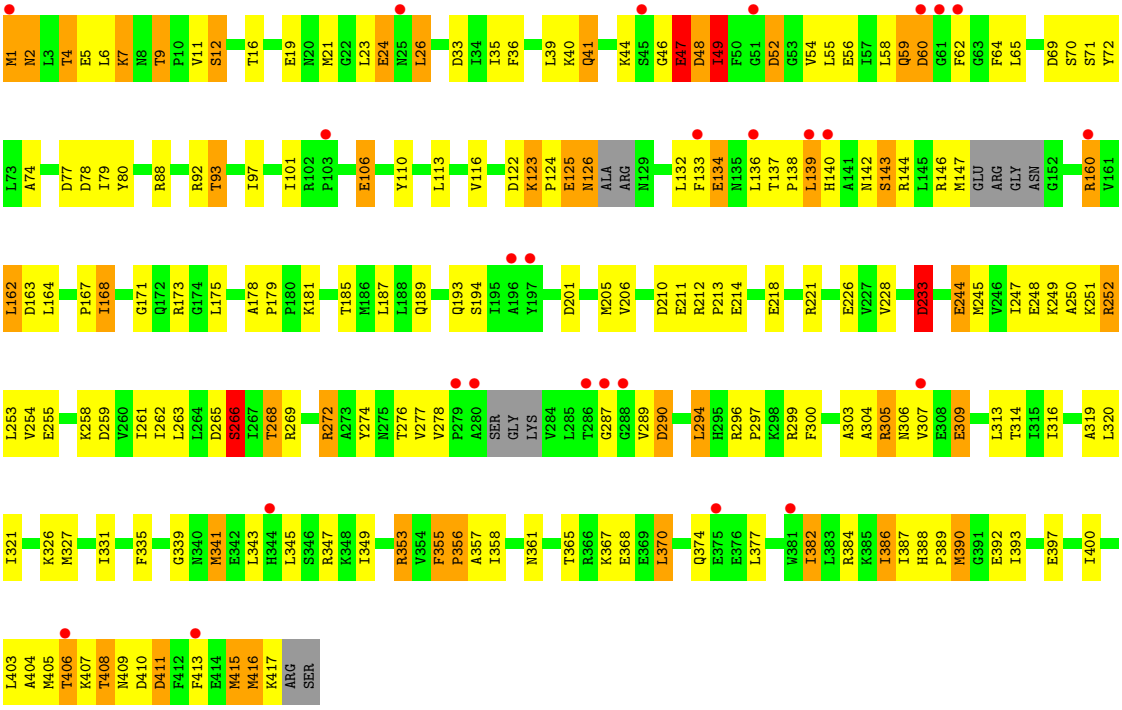




• Molecule 2: Transcription termination factor rho

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.25Å 204.65Å 147.79Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.00) 96.3 (29.88-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.271 , 0.304 0.239 , 0.245	Depositor DCC
R_{free} test set	3403 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 114.4	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	0.92	EDS
Total number of atoms	19246	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	G	0.69	0/43	1.40	1/64 (1.6%)
1	H	0.80	0/43	1.34	1/64 (1.6%)
1	J	0.82	0/43	1.05	0/64
1	K	0.98	0/43	1.54	1/64 (1.6%)
1	L	0.69	0/43	1.39	1/64 (1.6%)
2	A	0.42	0/3253	0.71	11/4379 (0.3%)
2	B	0.43	0/2854	0.71	9/3844 (0.2%)
2	C	0.56	0/3253	0.76	7/4379 (0.2%)
2	D	0.51	0/3253	0.75	10/4379 (0.2%)
2	E	0.49	0/3246	0.74	11/4369 (0.3%)
2	F	0.42	0/3253	0.70	14/4379 (0.3%)
All	All	0.48	0/19327	0.74	66/26049 (0.3%)

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
2	B	0	1
2	E	0	3
2	F	1	1
All	All	1	5

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	77	ASP	CB-CG-OD2	7.04	124.64	118.30
1	G	1	U	P-O3'-C3'	6.65	127.68	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	95	ASP	CB-CG-OD2	6.63	124.26	118.30
2	A	265	ASP	CB-CG-OD2	6.28	123.95	118.30
2	F	233	ASP	CB-CG-OD2	6.25	123.92	118.30
2	F	355	PHE	N-CA-C	6.21	127.77	111.00
2	D	156	ASP	CB-CG-OD2	6.13	123.81	118.30
2	E	163	ASP	CB-CG-OD2	6.08	123.77	118.30
2	E	77	ASP	CB-CG-OD2	6.07	123.76	118.30
2	D	290	ASP	CB-CG-OD2	5.97	123.67	118.30
2	A	95	ASP	CB-CG-OD2	5.97	123.67	118.30
1	K	1	U	P-O3'-C3'	5.94	126.83	119.70
2	E	69	ASP	CB-CG-OD2	5.93	123.64	118.30
2	B	265	ASP	CB-CG-OD2	5.92	123.63	118.30
1	L	1	U	P-O3'-C3'	5.85	126.72	119.70
2	A	201	ASP	CB-CG-OD2	5.83	123.55	118.30
2	D	328	ASP	CB-CG-OD2	5.75	123.47	118.30
2	F	163	ASP	CB-CG-OD2	5.73	123.46	118.30
2	F	69	ASP	CB-CG-OD2	5.71	123.44	118.30
2	A	328	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	233	ASP	CB-CG-OD2	5.66	123.40	118.30
2	E	210	ASP	CB-CG-OD2	5.66	123.39	118.30
2	D	52	ASP	CB-CG-OD2	5.62	123.36	118.30
2	C	259	ASP	CB-CG-OD2	5.61	123.35	118.30
2	C	210	ASP	CB-CG-OD2	5.61	123.35	118.30
2	F	77	ASP	CB-CG-OD2	5.59	123.34	118.30
2	F	33	ASP	CB-CG-OD2	5.57	123.31	118.30
2	B	77	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	78	ASP	CB-CG-OD2	5.53	123.28	118.30
2	E	52	ASP	CB-CG-OD2	5.53	123.27	118.30
2	A	122	ASP	CB-CG-OD2	5.52	123.27	118.30
2	F	411	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	163	ASP	CB-CG-OD2	5.47	123.23	118.30
2	E	201	ASP	CB-CG-OD2	5.45	123.21	118.30
2	E	78	ASP	CB-CG-OD2	5.44	123.19	118.30
2	F	265	ASP	CB-CG-OD2	5.35	123.11	118.30
2	F	48	ASP	CB-CG-OD2	5.34	123.11	118.30
2	A	411	ASP	CB-CG-OD2	5.34	123.10	118.30
2	B	69	ASP	CB-CG-OD2	5.32	123.09	118.30
2	F	52	ASP	CB-CG-OD2	5.32	123.09	118.30
2	C	411	ASP	CB-CG-OD2	5.31	123.08	118.30
2	A	33	ASP	CB-CG-OD2	5.31	123.08	118.30
2	D	201	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	265	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	U	P-O3'-C3'	5.29	126.04	119.70
2	C	233	ASP	CB-CG-OD2	5.28	123.05	118.30
2	E	328	ASP	CB-CG-OD2	5.26	123.04	118.30
2	E	233	ASP	CB-CG-OD2	5.26	123.03	118.30
2	C	410	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	156	ASP	CB-CG-OD2	5.25	123.03	118.30
2	A	69	ASP	CB-CG-OD2	5.25	123.02	118.30
2	F	259	ASP	CB-CG-OD2	5.21	122.99	118.30
2	F	60	ASP	CB-CG-OD2	5.20	122.98	118.30
2	A	60	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	60	ASP	CB-CG-OD2	5.18	122.97	118.30
2	D	411	ASP	CB-CG-OD2	5.17	122.95	118.30
2	C	156	ASP	CB-CG-OD2	5.14	122.93	118.30
2	D	259	ASP	CB-CG-OD2	5.13	122.91	118.30
2	F	290	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	210	ASP	CB-CG-OD2	5.09	122.88	118.30
2	A	233	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	33	ASP	CB-CG-OD2	5.09	122.88	118.30
2	E	290	ASP	CB-CG-OD2	5.03	122.82	118.30
2	F	210	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	394	ASP	CB-CG-OD2	5.00	122.80	118.30
2	C	52	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	355	PHE	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	355	PHE	Peptide
2	E	266	SER	Peptide
2	E	355	PHE	Peptide
2	E	371	LEU	Peptide
2	F	24	GLU	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	G	40	0	22	0	0
1	H	40	0	22	2	0
1	J	40	0	22	3	0
1	K	40	0	22	4	0
1	L	40	0	22	3	0
2	A	3208	0	3284	116	0
2	B	2813	0	2870	126	0
2	C	3208	0	3284	152	0
2	D	3208	0	3284	149	0
2	E	3201	0	3275	142	0
2	F	3208	0	3284	124	0
3	A	31	0	7	3	0
3	B	31	0	7	0	0
3	C	31	0	7	0	0
3	D	31	0	7	0	0
3	E	31	0	7	0	0
3	F	31	0	7	0	0
4	A	1	0	0	0	0
4	C	5	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	1	0
4	F	2	0	0	0	0
All	All	19246	0	19433	778	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 20.

All (778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:HG3	2:B:272:ARG:HH11	1.01	1.10
2:C:355:PHE:HB2	2:C:356:PRO:HD3	1.26	1.09
2:F:353:ARG:HG3	2:F:353:ARG:HH11	1.06	1.09
2:C:30:ARG:HG2	2:C:30:ARG:HH11	1.14	1.09
2:C:272:ARG:HG3	2:C:272:ARG:HH11	0.92	1.09
2:A:265:ASP:O	2:A:318:THR:HB	1.61	1.00
2:E:140:HIS:CB	2:E:306:ASN:HB2	1.93	0.98
2:F:167:PRO:HD2	2:F:365:THR:HG22	1.44	0.98
2:E:1:MET:HG3	2:E:2:ASN:H	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ARG:HG3	2:B:296:ARG:HH11	1.26	0.96
2:A:272:ARG:HG3	2:A:272:ARG:HH11	1.29	0.95
2:C:379:LYS:HG3	2:C:412:PHE:CD1	2.01	0.95
2:F:23:LEU:HD21	2:F:41:GLN:HG3	1.44	0.95
2:C:405:MET:O	2:C:406:THR:HG23	1.66	0.95
2:C:355:PHE:CB	2:C:356:PRO:HD3	1.96	0.94
2:D:131:ILE:HG22	2:D:133:PHE:HD2	1.33	0.94
2:E:167:PRO:O	2:E:365:THR:HG21	1.67	0.94
2:C:141:ALA:CB	2:C:370:LEU:HB2	1.99	0.93
2:B:169:GLY:H	2:B:172:GLN:HG3	1.37	0.89
2:C:272:ARG:HG3	2:C:272:ARG:NH1	1.72	0.89
2:B:140:HIS:HA	2:B:306:ASN:HD22	1.37	0.88
2:C:141:ALA:O	2:C:370:LEU:HB3	1.74	0.87
2:C:141:ALA:HB1	2:C:370:LEU:HB2	1.54	0.86
2:D:266:SER:OG	2:D:269:ARG:HG2	1.75	0.86
2:D:131:ILE:CG2	2:D:133:PHE:HD2	1.89	0.85
2:A:49:ILE:CG2	2:A:101:ILE:HG13	2.07	0.84
2:E:139:LEU:HD11	2:F:218:GLU:OE1	1.77	0.84
2:E:299:ARG:HG3	2:E:299:ARG:HH11	1.42	0.84
2:F:147:MET:HG2	2:F:194:SER:HB3	1.58	0.84
2:D:141:ALA:HB1	2:D:370:LEU:HB2	1.60	0.83
2:E:208:LEU:HB3	2:E:211:GLU:HG3	1.59	0.83
2:F:167:PRO:HD2	2:F:365:THR:CG2	2.06	0.83
2:D:275:ASN:HD21	2:D:290:ASP:H	1.27	0.83
2:E:140:HIS:CB	2:E:306:ASN:CB	2.55	0.83
2:E:266:SER:HB2	2:E:269:ARG:H	1.42	0.83
2:C:355:PHE:HB2	2:C:356:PRO:CD	2.08	0.82
2:D:131:ILE:HG22	2:D:133:PHE:CD2	2.14	0.82
2:E:140:HIS:HA	2:E:306:ASN:CB	2.09	0.82
2:B:141:ALA:CB	2:B:370:LEU:HB2	2.10	0.82
2:B:140:HIS:CB	2:B:306:ASN:HB3	2.10	0.81
2:B:236:ALA:HA	2:B:239:HIS:HD2	1.46	0.81
2:A:4:THR:HG21	2:A:52:ASP:OD2	1.81	0.80
2:B:137:THR:HG22	2:B:305:ARG:HB2	1.63	0.80
2:F:353:ARG:HG3	2:F:353:ARG:NH1	1.85	0.80
2:F:356:PRO:HD2	2:F:400:ILE:HD11	1.64	0.80
2:A:49:ILE:HG22	2:A:101:ILE:HG13	1.64	0.79
2:E:136:LEU:HD13	2:F:221:ARG:NH2	1.98	0.79
2:C:135:ASN:HB3	2:C:307:VAL:HG13	1.64	0.79
2:F:171:GLY:H	2:F:314:THR:HB	1.47	0.79
2:A:140:HIS:HA	2:A:306:ASN:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:379:LYS:HG3	2:C:412:PHE:CG	2.18	0.79
2:B:272:ARG:HG3	2:B:272:ARG:NH1	1.81	0.78
2:B:296:ARG:HG3	2:B:296:ARG:NH1	1.93	0.78
2:A:173:ARG:H	2:A:340:ASN:HD21	1.31	0.77
2:C:275:ASN:HD21	2:C:290:ASP:H	1.33	0.77
2:C:280:ALA:C	2:C:284:VAL:N	2.37	0.76
2:A:294:LEU:HD13	2:A:334:GLU:HG3	1.68	0.76
2:D:194:SER:O	2:D:198:ASN:HB2	1.86	0.76
2:E:169:GLY:H	2:E:172:GLN:HG3	1.51	0.76
2:F:92:ARG:HH22	2:F:133:PHE:HE2	1.34	0.75
2:A:172:GLN:HE22	2:A:371:LEU:HD11	1.51	0.75
2:E:226:GLU:OE2	2:E:249:LYS:HE2	1.87	0.75
2:B:272:ARG:HH11	2:B:272:ARG:CG	1.90	0.75
2:C:30:ARG:HH11	2:C:30:ARG:CG	1.99	0.75
2:B:266:SER:HA	2:B:318:THR:O	1.87	0.74
2:E:140:HIS:CA	2:E:306:ASN:CB	2.65	0.74
2:C:30:ARG:HG2	2:C:30:ARG:NH1	1.93	0.74
2:B:141:ALA:HB3	2:B:370:LEU:HB2	1.68	0.73
2:D:140:HIS:HA	2:D:306:ASN:CB	2.18	0.73
2:A:372:THR:HG23	2:A:376:GLU:HB3	1.70	0.73
2:B:341:MET:HG2	2:B:342:GLU:N	2.03	0.73
2:A:388:HIS:HB3	2:A:389:PRO:HD3	1.70	0.73
2:D:174:GLY:HA2	2:D:341:MET:HG3	1.71	0.72
2:C:170:ARG:HD3	2:C:259:ASP:OD2	1.89	0.72
2:F:307:VAL:HG13	2:F:309:GLU:HG2	1.71	0.72
2:D:272:ARG:HH11	2:D:272:ARG:CG	2.01	0.72
2:D:137:THR:CG2	2:D:305:ARG:HB2	2.19	0.72
2:B:139:LEU:HD13	2:B:367:LYS:HD2	1.71	0.72
2:C:162:LEU:HD21	2:C:168:ILE:CD1	2.20	0.72
2:F:147:MET:HG2	2:F:194:SER:CB	2.20	0.71
2:C:402:LYS:O	2:C:405:MET:HG3	1.91	0.71
2:A:251:LYS:O	2:A:255:GLU:HG3	1.90	0.71
2:D:3:LEU:HD22	2:D:79:ILE:HD11	1.73	0.71
2:C:141:ALA:HB3	2:C:370:LEU:HB2	1.73	0.71
2:F:23:LEU:CD2	2:F:41:GLN:HG3	2.20	0.71
2:D:268:THR:O	2:D:272:ARG:HG2	1.91	0.70
2:E:169:GLY:H	2:E:172:GLN:CG	2.04	0.70
2:C:379:LYS:CG	2:C:412:PHE:CD1	2.75	0.70
2:D:177:VAL:CG1	2:D:321:ILE:HD12	2.21	0.70
2:B:295:HIS:CD2	2:C:233:ASP:O	2.44	0.70
2:A:139:LEU:HD22	2:A:367:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:GLY:H	2:D:172:GLN:CG	2.05	0.69
2:F:266:SER:HB2	2:F:269:ARG:H	1.58	0.69
2:B:132:LEU:HD22	2:B:251:LYS:HD3	1.74	0.69
2:C:356:PRO:HD2	2:C:400:ILE:HD11	1.74	0.69
2:A:195:ILE:HG21	2:A:204:LEU:HD13	1.72	0.69
2:E:171:GLY:H	2:E:314:THR:HG22	1.57	0.69
2:A:355:PHE:HB2	2:A:356:PRO:HD3	1.73	0.69
2:B:266:SER:OG	2:B:269:ARG:HB2	1.93	0.69
2:E:137:THR:HG23	2:E:305:ARG:HB2	1.74	0.69
2:E:138:PRO:HD2	2:E:306:ASN:O	1.92	0.68
2:D:5:GLU:O	2:D:9:THR:HG22	1.94	0.68
2:C:140:HIS:HA	2:C:306:ASN:CB	2.24	0.67
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.24	0.67
2:E:299:ARG:HG3	2:E:299:ARG:NH1	2.04	0.67
2:F:140:HIS:HA	2:F:306:ASN:HB2	1.74	0.67
2:C:162:LEU:HD21	2:C:168:ILE:HD12	1.77	0.67
2:D:230:SER:HB3	2:D:242:VAL:HG21	1.77	0.67
2:A:181:LYS:HA	3:A:601:ANP:O1B	1.95	0.66
2:C:355:PHE:CB	2:C:356:PRO:CD	2.68	0.66
2:D:136:LEU:HD12	2:E:221:ARG:NH2	2.09	0.66
2:C:7:LYS:HE2	2:C:77:ASP:OD1	1.95	0.66
2:D:251:LYS:O	2:D:255:GLU:HG3	1.95	0.66
2:D:321:ILE:HD11	2:D:332:TYR:CD2	2.30	0.66
2:C:191:ILE:O	2:C:195:ILE:HG13	1.96	0.66
2:A:135:ASN:HB3	2:A:307:VAL:HG13	1.77	0.66
2:C:231:THR:OG1	2:C:233:ASP:HB2	1.94	0.66
2:C:177:VAL:HG13	2:C:321:ILE:HD12	1.77	0.66
2:F:341:MET:HA	2:F:365:THR:HA	1.78	0.66
2:D:131:ILE:CG2	2:D:133:PHE:CD2	2.74	0.65
2:D:272:ARG:HH11	2:D:272:ARG:CB	2.08	0.65
2:B:137:THR:CG2	2:B:305:ARG:HB2	2.27	0.65
2:C:266:SER:HB2	2:C:269:ARG:HB2	1.77	0.65
2:E:268:THR:CG2	2:E:320:LEU:H	2.10	0.65
2:C:277:VAL:O	2:C:277:VAL:HG12	1.96	0.65
2:E:131:ILE:HG22	2:E:134:GLU:HG2	1.78	0.65
2:D:102:ARG:HG2	2:D:114:LEU:HB2	1.77	0.65
2:A:341:MET:HG2	2:A:342:GLU:N	2.10	0.65
2:F:189:GLN:O	2:F:193:GLN:HG3	1.97	0.65
2:A:341:MET:HB2	2:A:365:THR:HB	1.79	0.64
2:E:140:HIS:CA	2:E:306:ASN:HB3	2.28	0.64
2:B:210:ASP:HB2	2:B:269:ARG:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:LEU:N	2:D:255:GLU:OE2	2.29	0.64
2:F:294:LEU:O	2:F:297:PRO:HD2	1.97	0.64
2:D:290:ASP:OD1	2:D:292:ASN:HB3	1.98	0.64
2:B:226:GLU:OE1	2:B:249:LYS:HE2	1.97	0.64
2:B:194:SER:O	2:B:198:ASN:HB2	1.97	0.63
2:E:171:GLY:H	2:E:314:THR:CG2	2.11	0.63
2:A:172:GLN:NE2	2:A:371:LEU:HD11	2.14	0.63
2:D:156:ASP:OD1	2:D:160:ARG:HG2	1.98	0.63
2:D:294:LEU:HD13	2:D:334:GLU:HG3	1.80	0.63
2:D:1:MET:HG3	2:D:2:ASN:H	1.62	0.63
2:E:136:LEU:HD13	2:F:221:ARG:HH21	1.64	0.63
2:A:140:HIS:HA	2:A:306:ASN:CB	2.28	0.63
2:A:299:ARG:HB3	2:A:299:ARG:HH11	1.63	0.63
2:C:5:GLU:O	2:C:9:THR:HG22	1.99	0.63
2:F:46:GLY:O	2:F:48:ASP:N	2.31	0.63
2:A:169:GLY:H	2:A:172:GLN:CG	2.12	0.63
2:A:173:ARG:NH2	2:B:214:GLU:OE2	2.31	0.63
2:B:141:ALA:O	2:B:142:ASN:C	2.37	0.62
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.79	0.62
2:A:173:ARG:HH22	2:B:214:GLU:CD	2.02	0.62
2:B:228:VAL:CG1	2:B:242:VAL:HG13	2.28	0.62
2:D:294:LEU:O	2:D:298:LYS:HG3	1.99	0.62
2:E:3:LEU:HD12	2:E:39:LEU:HD11	1.82	0.62
2:A:169:GLY:HA3	2:A:371:LEU:HD21	1.81	0.62
1:J:1:U:H5'	2:D:62:PHE:CZ	2.34	0.62
2:E:1:MET:HG3	2:E:2:ASN:N	2.07	0.62
2:A:41:GLN:C	2:A:43:ALA:H	2.03	0.62
2:D:141:ALA:HB1	2:D:370:LEU:CB	2.30	0.62
2:B:207:LEU:HD23	2:B:264:LEU:HD13	1.82	0.62
2:D:321:ILE:HD11	2:D:332:TYR:CE2	2.35	0.62
2:A:272:ARG:HH11	2:A:272:ARG:CG	2.08	0.62
2:F:134:GLU:O	2:F:134:GLU:HG2	1.99	0.62
2:A:268:THR:O	2:A:272:ARG:HG2	2.00	0.62
2:C:257:LYS:HE2	2:C:309:GLU:O	2.00	0.62
2:D:169:GLY:O	2:D:172:GLN:HG2	2.00	0.62
2:F:272:ARG:HH11	2:F:272:ARG:HB3	1.65	0.62
2:A:173:ARG:N	2:A:340:ASN:HD21	1.96	0.61
2:A:272:ARG:HG3	2:A:272:ARG:NH1	2.08	0.61
2:D:272:ARG:HH11	2:D:272:ARG:HG3	1.63	0.61
2:F:343:LEU:HD11	2:F:358:ILE:HG12	1.80	0.61
2:D:267:ILE:HG22	2:D:318:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:GLU:O	2:F:9:THR:HG22	1.99	0.61
2:D:359:ASP:OD2	2:D:362:ARG:HD2	2.01	0.61
2:D:39:LEU:HB3	2:D:111:PHE:CZ	2.36	0.61
2:E:141:ALA:O	2:E:371:LEU:HG	2.00	0.61
2:B:141:ALA:HB1	2:B:370:LEU:HB2	1.82	0.61
2:C:173:ARG:NH1	2:C:304:ALA:O	2.34	0.61
2:B:62:PHE:HB3	2:B:83:PRO:HG3	1.83	0.60
2:B:307:VAL:HG12	2:B:309:GLU:H	1.66	0.60
2:C:141:ALA:HA	2:C:371:LEU:HD21	1.82	0.60
2:F:16:THR:HA	2:F:19:GLU:HB2	1.82	0.60
2:C:296:ARG:HB2	2:C:297:PRO:HD3	1.83	0.60
2:E:132:LEU:HD22	2:E:251:LYS:HG2	1.84	0.60
2:A:355:PHE:HB3	3:A:601:ANP:HN61	1.67	0.60
2:B:140:HIS:HA	2:B:306:ASN:ND2	2.13	0.60
2:C:272:ARG:HH11	2:C:272:ARG:CG	1.86	0.60
2:D:173:ARG:NH1	2:D:304:ALA:O	2.35	0.60
2:D:113:LEU:HD21	2:D:116:VAL:HG22	1.83	0.59
2:E:252:ARG:NH1	2:E:255:GLU:OE2	2.35	0.59
2:D:141:ALA:CB	2:D:370:LEU:HB2	2.30	0.59
2:D:268:THR:HA	2:D:331:ILE:HG21	1.84	0.59
2:B:228:VAL:HG12	2:B:242:VAL:HG13	1.83	0.59
2:C:79:ILE:HD13	2:C:101:ILE:HG21	1.84	0.59
2:F:252:ARG:HA	2:F:255:GLU:OE1	2.02	0.59
2:B:268:THR:O	2:B:272:ARG:HG2	2.02	0.59
2:E:56:GLU:HG3	2:E:245:MET:HE1	1.85	0.59
2:D:321:ILE:O	2:D:322:ASP:HB2	2.02	0.59
2:E:268:THR:HG21	2:E:320:LEU:H	1.66	0.59
2:F:168:ILE:HG21	2:F:316:ILE:HD11	1.85	0.59
2:A:173:ARG:H	2:A:340:ASN:ND2	2.00	0.59
2:A:252:ARG:NH1	2:A:255:GLU:CD	2.56	0.59
2:F:272:ARG:HD2	2:F:327:MET:SD	2.43	0.59
2:B:98:SER:HB2	2:B:118:GLU:HB2	1.84	0.59
2:C:92:ARG:CZ	2:C:131:ILE:HD11	2.33	0.58
2:C:156:ASP:O	2:C:160:ARG:HG3	2.02	0.58
2:D:174:GLY:CA	2:D:341:MET:HG3	2.32	0.58
2:C:139:LEU:HD22	2:C:367:LYS:HD2	1.84	0.58
1:L:1:U:H4'	1:L:2:C:O5'	2.02	0.58
1:H:2:C:N3	2:C:66:ARG:NH2	2.50	0.58
2:A:142:ASN:N	2:A:142:ASN:HD22	2.02	0.58
2:C:167:PRO:HG2	2:C:368:GLU:HG2	1.85	0.58
2:C:383:LEU:HD11	2:C:399:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:LYS:HA	2:E:27:ALA:O	2.02	0.58
1:L:2:C:H5	2:F:110:TYR:HH	1.50	0.58
2:A:355:PHE:HB3	3:A:601:ANP:N6	2.19	0.58
2:C:160:ARG:NH2	2:C:406:THR:O	2.37	0.58
2:D:252:ARG:HD2	2:E:28:ARG:NH2	2.18	0.58
2:F:388:HIS:HB3	2:F:389:PRO:HD3	1.85	0.58
2:C:104:PRO:HA	2:C:108:GLU:OE1	2.04	0.58
2:F:58:LEU:HG	2:F:59:GLN:H	1.69	0.58
2:A:138:PRO:HD2	2:A:306:ASN:O	2.04	0.58
2:D:65:LEU:HB2	2:D:79:ILE:HB	1.84	0.58
2:D:135:ASN:HB3	2:D:307:VAL:HG13	1.86	0.58
2:D:131:ILE:HA	2:D:255:GLU:OE2	2.04	0.57
2:A:14:LEU:HD11	2:A:35:ILE:HG13	1.84	0.57
2:A:358:ILE:HB	2:A:396:MET:HE1	1.86	0.57
2:F:367:LYS:HD3	2:F:370:LEU:HD11	1.86	0.57
2:C:113:LEU:HD21	2:C:116:VAL:HG22	1.87	0.57
2:D:140:HIS:HA	2:D:306:ASN:HB3	1.86	0.57
2:E:160:ARG:HG2	2:E:408:THR:OG1	2.04	0.57
2:A:43:ALA:C	2:A:45:SER:H	2.07	0.57
2:A:116:VAL:HG12	2:A:124:PRO:HG3	1.86	0.57
2:B:173:ARG:HD3	2:B:304:ALA:HB3	1.87	0.57
2:E:321:ILE:HD11	2:E:332:TYR:CG	2.40	0.57
2:E:184:LYS:HG3	2:E:318:THR:HG21	1.87	0.57
2:E:382:ILE:O	2:E:386:ILE:HG23	2.05	0.57
2:A:132:LEU:HD13	2:A:251:LYS:HA	1.86	0.56
2:B:333:GLU:O	2:B:336:LYS:HB2	2.05	0.56
2:E:140:HIS:HA	2:E:306:ASN:ND2	2.20	0.56
2:B:376:GLU:O	2:B:380:MET:HG2	2.06	0.56
2:E:141:ALA:O	2:E:371:LEU:CD2	2.53	0.56
2:E:321:ILE:HD11	2:E:332:TYR:CB	2.36	0.56
2:F:185:THR:O	2:F:189:GLN:HG3	2.05	0.56
2:C:140:HIS:CB	2:C:306:ASN:HB2	2.35	0.56
2:D:211:GLU:HG3	2:D:215:GLU:HB3	1.86	0.56
2:D:272:ARG:HG3	2:D:272:ARG:NH1	2.20	0.56
2:E:347:ARG:O	2:E:351:GLU:HG2	2.05	0.56
2:F:123:LYS:HG3	2:F:126:ASN:HB2	1.87	0.56
2:C:169:GLY:H	2:C:172:GLN:HG2	1.70	0.56
2:C:106:GLU:C	2:C:108:GLU:H	2.07	0.56
2:E:266:SER:HB3	2:E:320:LEU:HG	1.87	0.56
2:D:333:GLU:O	2:D:336:LYS:HB2	2.06	0.56
1:J:1:U:O2	2:D:110:TYR:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:ASP:HB2	2:C:62:PHE:HE2	1.70	0.56
2:A:5:GLU:O	2:A:9:THR:HG23	2.06	0.56
2:A:132:LEU:HD22	2:A:251:LYS:HD3	1.88	0.56
2:A:252:ARG:HH12	2:A:255:GLU:CD	2.09	0.56
2:C:132:LEU:HD13	2:C:251:LYS:HA	1.88	0.56
2:D:147:MET:HB3	2:D:194:SER:OG	2.05	0.56
2:D:161:VAL:HG11	2:D:396:MET:HE2	1.87	0.56
2:E:141:ALA:CB	2:E:370:LEU:HB2	2.35	0.56
2:C:58:LEU:HD12	2:C:62:PHE:CZ	2.41	0.56
2:D:167:PRO:O	2:D:365:THR:HG21	2.05	0.56
2:A:146:ARG:NH2	2:A:376:GLU:OE1	2.37	0.56
2:F:211:GLU:HG3	2:F:212:ARG:N	2.21	0.56
2:C:30:ARG:CG	2:C:30:ARG:NH1	2.64	0.55
2:D:238:ARG:O	2:D:242:VAL:HG23	2.05	0.55
2:A:169:GLY:H	2:A:172:GLN:HG2	1.71	0.55
2:D:210:ASP:OD1	2:D:232:PHE:HA	2.05	0.55
2:F:142:ASN:O	2:F:143:SER:C	2.44	0.55
2:A:49:ILE:HG22	2:A:101:ILE:O	2.06	0.55
2:B:176:ILE:HB	2:B:318:THR:HG22	1.88	0.55
2:C:99:GLY:HA3	2:C:115:LYS:O	2.07	0.55
2:C:284:VAL:HG12	2:C:291:ALA:HB3	1.88	0.55
2:D:137:THR:HG22	2:D:305:ARG:HB2	1.88	0.55
2:E:268:THR:HG21	2:E:320:LEU:N	2.22	0.55
2:E:131:ILE:HG23	2:E:133:PHE:H	1.71	0.55
2:D:187:LEU:HD11	2:D:343:LEU:HD23	1.87	0.55
2:E:214:GLU:HG2	2:E:215:GLU:N	2.21	0.55
2:D:137:THR:HG23	2:D:305:ARG:HB2	1.87	0.55
2:E:299:ARG:HH11	2:E:299:ARG:CG	2.17	0.55
2:A:304:ALA:HB2	2:A:315:ILE:HG13	1.88	0.55
2:B:65:LEU:HD21	2:B:97:ILE:HB	1.89	0.55
2:C:136:LEU:HD13	2:D:221:ARG:NH2	2.22	0.55
2:A:42:HIS:HD2	2:A:47:GLU:HB3	1.73	0.54
2:A:250:ALA:HB1	2:A:313:LEU:HD13	1.89	0.54
2:D:207:LEU:HD23	2:D:264:LEU:HD13	1.89	0.54
2:C:141:ALA:HA	2:C:371:LEU:CD2	2.36	0.54
2:B:86:ILE:HA	2:B:91:LEU:HD12	1.88	0.54
2:D:290:ASP:OD1	2:D:292:ASN:CB	2.55	0.54
2:A:374:GLN:HA	2:A:377:LEU:HD12	1.87	0.54
2:D:147:MET:HE1	2:D:191:ILE:HG23	1.89	0.54
2:D:268:THR:CG2	2:D:320:LEU:H	2.21	0.54
2:F:353:ARG:HH11	2:F:353:ARG:CG	1.97	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:PRO:HA	2:B:108:GLU:OE1	2.07	0.54
2:C:277:VAL:O	2:C:277:VAL:CG1	2.55	0.54
2:F:272:ARG:O	2:F:276:THR:HG23	2.08	0.54
2:D:140:HIS:HA	2:D:306:ASN:HB2	1.89	0.54
2:C:143:SER:OG	2:C:170:ARG:HD2	2.08	0.54
2:F:274:TYR:CD2	2:F:297:PRO:HG3	2.43	0.54
2:B:192:ALA:HB1	2:B:223:VAL:HG22	1.90	0.54
1:K:2:C:H5	2:E:110:TYR:HH	1.54	0.53
2:A:43:ALA:C	2:A:45:SER:N	2.61	0.53
2:A:269:ARG:HA	2:A:272:ARG:HG2	1.89	0.53
2:E:140:HIS:HA	2:E:306:ASN:HD22	1.71	0.53
2:E:269:ARG:HA	2:E:272:ARG:HG2	1.90	0.53
2:E:356:PRO:HG2	2:E:400:ILE:HG12	1.91	0.53
2:F:244:GLU:HA	2:F:247:ILE:HG22	1.90	0.53
2:A:65:LEU:HB2	2:A:79:ILE:HB	1.89	0.53
2:B:207:LEU:HD11	2:B:242:VAL:HG12	1.91	0.53
2:E:141:ALA:HB1	2:E:370:LEU:HB2	1.90	0.53
2:F:160:ARG:O	2:F:164:LEU:HG	2.08	0.53
2:B:167:PRO:O	2:B:365:THR:HG21	2.08	0.53
2:F:253:LEU:O	2:F:258:LYS:HB2	2.07	0.53
2:A:36:PHE:O	2:A:40:LYS:HB2	2.07	0.53
2:C:326:LYS:O	2:C:330:VAL:HG23	2.08	0.53
2:C:91:LEU:HD13	2:C:97:ILE:CD1	2.38	0.53
2:C:135:ASN:HB3	2:C:307:VAL:CG1	2.37	0.53
2:D:268:THR:HG21	2:D:320:LEU:H	1.73	0.53
2:C:295:HIS:NE2	2:D:235:PRO:HD3	2.24	0.53
2:B:289:VAL:HG12	2:B:327:MET:HB2	1.89	0.53
2:C:91:LEU:HD13	2:C:97:ILE:HD11	1.90	0.53
2:D:73:LEU:HD12	2:D:238:ARG:NE	2.24	0.53
2:E:173:ARG:NH2	2:F:214:GLU:OE2	2.42	0.53
2:B:140:HIS:HA	2:B:306:ASN:HB3	1.91	0.53
2:C:166:SER:HA	2:C:365:THR:HG23	1.91	0.53
2:C:187:LEU:O	2:C:191:ILE:HG13	2.09	0.53
2:E:171:GLY:N	2:E:314:THR:HG22	2.23	0.53
2:A:174:GLY:HA3	2:A:316:ILE:HD12	1.90	0.52
2:B:141:ALA:HB3	2:B:370:LEU:CB	2.37	0.52
2:C:375:GLU:CD	2:C:375:GLU:H	2.12	0.52
2:D:60:ASP:HB2	2:D:62:PHE:CE2	2.44	0.52
2:A:210:ASP:OD2	2:A:269:ARG:HD2	2.08	0.52
2:F:54:VAL:HG21	2:F:249:LYS:HD2	1.92	0.52
2:F:411:ASP:O	2:F:415:MET:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:HIS:CA	2:B:306:ASN:HB3	2.38	0.52
2:C:60:ASP:HB2	2:C:62:PHE:CE2	2.45	0.52
2:F:403:LEU:C	2:F:405:MET:H	2.12	0.52
2:F:46:GLY:C	2:F:48:ASP:H	2.12	0.52
2:A:86:ILE:HA	2:A:91:LEU:HD12	1.91	0.52
2:A:238:ARG:NH1	2:A:241:GLN:OE1	2.43	0.52
2:C:4:THR:HG22	2:C:5:GLU:N	2.25	0.52
2:F:261:ILE:HG12	2:F:314:THR:CG2	2.39	0.52
2:E:3:LEU:O	2:E:6:LEU:HB2	2.10	0.52
2:A:135:ASN:HB3	2:A:307:VAL:CG1	2.40	0.52
2:B:141:ALA:HB1	2:B:371:LEU:HG	1.91	0.52
2:B:269:ARG:NH1	2:B:272:ARG:HH12	2.08	0.52
2:D:275:ASN:ND2	2:D:290:ASP:H	2.02	0.52
2:A:169:GLY:H	2:A:172:GLN:HE21	1.57	0.51
2:D:206:VAL:HB	2:D:227:VAL:HG22	1.92	0.51
2:E:140:HIS:CB	2:E:306:ASN:HB3	2.37	0.51
2:D:269:ARG:HA	2:D:272:ARG:HG2	1.92	0.51
2:A:144:ARG:HD3	2:A:146:ARG:CZ	2.41	0.51
2:A:175:LEU:HD13	2:A:301:PHE:CZ	2.45	0.51
2:C:62:PHE:HE1	2:C:64:PHE:HE2	1.58	0.51
2:A:369:GLU:HG2	2:A:370:LEU:N	2.26	0.51
2:B:272:ARG:NH1	2:B:272:ARG:CG	2.59	0.51
2:D:154:THR:O	2:D:157:LEU:HB2	2.11	0.51
2:B:132:LEU:HD13	2:B:251:LYS:HG2	1.93	0.51
2:A:166:SER:HB2	2:A:341:MET:HG3	1.92	0.51
2:D:353:ARG:HD2	2:D:355:PHE:CZ	2.46	0.51
2:E:49:ILE:CG2	2:E:101:ILE:HG13	2.39	0.51
2:F:187:LEU:HD22	2:F:345:LEU:HD21	1.92	0.51
1:J:2:C:H42	2:D:66:ARG:HH12	1.59	0.51
2:A:356:PRO:HB2	2:A:396:MET:CE	2.41	0.51
2:C:321:ILE:HD11	2:C:332:TYR:CD2	2.46	0.51
2:E:368:GLU:HB3	2:E:377:LEU:HD11	1.92	0.51
2:A:266:SER:OG	2:A:269:ARG:HB2	2.10	0.51
2:F:138:PRO:C	2:F:140:HIS:H	2.14	0.51
2:F:162:LEU:CD1	2:F:187:LEU:HD11	2.41	0.51
2:B:207:LEU:HD13	2:B:246:VAL:HG21	1.93	0.51
2:D:169:GLY:H	2:D:172:GLN:HG3	1.76	0.51
2:B:340:ASN:ND2	2:C:214:GLU:OE2	2.42	0.50
2:E:197:TYR:C	2:E:197:TYR:CD2	2.84	0.50
2:F:4:THR:HB	2:F:52:ASP:OD1	2.10	0.50
2:E:139:LEU:O	2:E:141:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:THR:HA	2:F:331:ILE:HG21	1.94	0.50
2:B:160:ARG:HE	2:B:408:THR:HB	1.77	0.50
2:C:139:LEU:O	2:C:141:ALA:N	2.44	0.50
2:E:173:ARG:HH21	2:F:212:ARG:HD2	1.76	0.50
2:E:143:SER:OG	2:E:170:ARG:HD2	2.11	0.50
2:F:247:ILE:HB	2:F:300:PHE:CE1	2.47	0.50
1:K:2:C:H42	2:E:66:ARG:HH12	1.60	0.50
2:B:144:ARG:HD3	2:B:371:LEU:O	2.11	0.50
2:B:402:LYS:O	2:B:405:MET:HB2	2.11	0.50
2:C:140:HIS:HA	2:C:306:ASN:HB3	1.93	0.50
2:D:170:ARG:HD3	2:D:259:ASP:OD2	2.10	0.50
2:F:36:PHE:CZ	2:F:40:LYS:HE3	2.46	0.50
2:F:175:LEU:HD11	2:F:319:ALA:HB2	1.94	0.50
2:A:41:GLN:C	2:A:43:ALA:N	2.65	0.50
2:A:140:HIS:CA	2:A:306:ASN:HB3	2.40	0.50
2:B:144:ARG:NH2	2:B:163:ASP:CG	2.65	0.50
2:B:268:THR:CG2	2:B:320:LEU:H	2.25	0.50
2:C:140:HIS:CA	2:C:306:ASN:HB3	2.42	0.50
2:E:169:GLY:HA3	2:E:371:LEU:HD21	1.93	0.50
2:C:95:ASP:OD1	2:C:120:ASN:ND2	2.34	0.50
2:D:132:LEU:HD22	2:D:251:LYS:HD3	1.93	0.50
2:D:197:TYR:HD2	2:D:198:ASN:HD22	1.59	0.50
2:D:294:LEU:CD1	2:D:334:GLU:HG3	2.41	0.50
2:E:1:MET:CG	2:E:2:ASN:H	2.05	0.50
2:E:402:LYS:HD3	2:E:415:MET:HG2	1.93	0.50
2:E:49:ILE:HG22	2:E:101:ILE:HG13	1.94	0.50
2:F:46:GLY:C	2:F:47:GLU:HG3	2.32	0.50
2:F:55:LEU:O	2:F:93:THR:HA	2.12	0.50
2:A:187:LEU:HG	2:A:191:ILE:HD11	1.94	0.49
2:F:23:LEU:HB3	2:F:26:LEU:HD21	1.93	0.49
2:B:272:ARG:HD2	2:B:327:MET:CE	2.42	0.49
2:B:295:HIS:HD2	2:C:233:ASP:O	1.92	0.49
2:F:123:LYS:O	2:F:125:GLU:N	2.44	0.49
2:A:272:ARG:CG	2:A:272:ARG:NH1	2.73	0.49
2:C:140:HIS:CA	2:C:306:ASN:CB	2.90	0.49
2:C:173:ARG:HD3	2:C:301:PHE:O	2.11	0.49
2:D:57:ILE:H	2:D:93:THR:HB	1.77	0.49
2:D:272:ARG:HH11	2:D:272:ARG:HB3	1.77	0.49
2:A:42:HIS:CD2	2:A:47:GLU:HB3	2.46	0.49
2:B:169:GLY:H	2:B:172:GLN:CG	2.18	0.49
2:C:140:HIS:CB	2:C:306:ASN:CB	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187:LEU:O	2:E:191:ILE:HD12	2.11	0.49
2:A:31:LYS:HA	2:A:34:ILE:HD12	1.94	0.49
2:A:296:ARG:HB2	2:A:297:PRO:HD3	1.93	0.49
2:B:356:PRO:C	2:B:358:ILE:H	2.16	0.49
2:C:268:THR:O	2:C:272:ARG:HG2	2.12	0.49
2:F:71:SER:HB3	2:F:228:VAL:HG13	1.94	0.49
2:A:388:HIS:HB3	2:A:389:PRO:CD	2.42	0.49
2:C:123:LYS:C	2:C:125:GLU:H	2.16	0.49
2:C:154:THR:HA	2:C:157:LEU:HD12	1.94	0.49
2:E:386:ILE:HG13	2:E:387:ILE:N	2.28	0.49
2:F:58:LEU:O	2:F:60:ASP:N	2.45	0.49
2:C:172:GLN:NE2	2:C:371:LEU:HD11	2.28	0.49
2:C:266:SER:CB	2:C:269:ARG:HG2	2.42	0.49
2:F:65:LEU:HB2	2:F:79:ILE:HB	1.95	0.49
2:C:139:LEU:CD2	2:C:367:LYS:HD2	2.43	0.49
2:E:129:ASN:N	4:E:606:HOH:O	2.45	0.49
2:B:210:ASP:OD1	2:B:232:PHE:HA	2.13	0.49
2:F:56:GLU:HA	2:F:93:THR:HB	1.94	0.49
2:C:383:LEU:HD11	2:C:399:LEU:CD1	2.42	0.48
2:A:169:GLY:N	2:A:172:GLN:HE21	2.11	0.48
2:C:342:GLU:HG3	2:C:344:HIS:CE1	2.48	0.48
2:F:113:LEU:HD21	2:F:116:VAL:HG22	1.95	0.48
2:B:269:ARG:HA	2:B:269:ARG:HD3	1.68	0.48
2:F:386:ILE:O	2:F:386:ILE:HG13	2.10	0.48
2:F:382:ILE:O	2:F:386:ILE:HG23	2.12	0.48
2:F:79:ILE:HD13	2:F:101:ILE:HG21	1.94	0.48
2:B:405:MET:O	2:B:406:THR:HB	2.13	0.48
2:E:187:LEU:HD21	2:E:343:LEU:HD23	1.96	0.48
2:B:173:ARG:HH22	2:C:214:GLU:CD	2.17	0.48
2:C:168:ILE:HA	2:C:172:GLN:HG2	1.95	0.48
2:D:274:TYR:CD2	2:D:297:PRO:HG3	2.49	0.48
2:E:187:LEU:HG	2:E:191:ILE:CD1	2.44	0.48
2:E:341:MET:HG2	2:E:342:GLU:N	2.29	0.48
2:F:49:ILE:O	2:F:101:ILE:HG12	2.14	0.48
2:F:132:LEU:HD22	2:F:251:LYS:HD3	1.96	0.48
2:A:179:PRO:HD2	2:A:345:LEU:O	2.13	0.48
2:B:325:SER:HB3	2:B:328:ASP:HB2	1.96	0.48
2:C:171:GLY:H	2:C:314:THR:HB	1.79	0.48
2:D:136:LEU:HD12	2:E:221:ARG:HH21	1.77	0.48
2:D:132:LEU:HD13	2:D:251:LYS:HA	1.96	0.48
2:D:208:LEU:HD12	2:D:229:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ASN:HB3	2:B:307:VAL:HG13	1.94	0.48
2:B:152:GLY:N	2:B:407:LYS:HZ1	2.11	0.48
2:C:131:ILE:HA	2:C:255:GLU:OE2	2.14	0.48
2:F:92:ARG:HH21	2:F:252:ARG:NH2	2.12	0.48
2:A:142:ASN:HD22	2:A:142:ASN:H	1.62	0.47
2:B:166:SER:HA	2:B:365:THR:HG22	1.95	0.47
2:C:123:LYS:O	2:C:125:GLU:N	2.47	0.47
2:D:165:ALA:O	2:D:364:GLY:HA2	2.14	0.47
2:A:194:SER:O	2:A:198:ASN:HB2	2.13	0.47
2:C:153:SER:OG	2:C:154:THR:N	2.46	0.47
2:D:266:SER:HB3	2:D:269:ARG:HB2	1.95	0.47
2:C:272:ARG:HD2	2:C:327:MET:CE	2.44	0.47
2:D:141:ALA:HB3	2:D:370:LEU:CD1	2.44	0.47
2:A:70:SER:O	2:A:71:SER:HB2	2.14	0.47
2:B:307:VAL:HG12	2:B:309:GLU:N	2.30	0.47
2:E:295:HIS:CD2	2:F:233:ASP:O	2.67	0.47
2:A:39:LEU:O	2:A:49:ILE:HD11	2.14	0.47
2:D:398:PHE:O	2:D:402:LYS:HG3	2.15	0.47
2:E:173:ARG:HH22	2:F:214:GLU:CD	2.18	0.47
2:E:266:SER:HA	2:E:318:THR:O	2.13	0.47
2:F:387:ILE:HA	2:F:390:MET:SD	2.54	0.47
2:A:187:LEU:O	2:A:191:ILE:HG13	2.14	0.47
2:B:272:ARG:O	2:B:276:THR:HG23	2.15	0.47
2:C:214:GLU:HG2	2:C:215:GLU:N	2.30	0.47
2:D:132:LEU:HD13	2:D:251:LYS:HG2	1.95	0.47
2:E:361:ASN:ND2	2:E:388:HIS:O	2.47	0.47
2:F:355:PHE:O	2:F:357:ALA:N	2.48	0.47
2:F:406:THR:HB	2:F:410:ASP:HB2	1.96	0.47
2:A:244:GLU:HA	2:A:247:ILE:HG22	1.97	0.47
2:B:165:ALA:O	2:B:364:GLY:HA2	2.15	0.47
2:C:177:VAL:CG1	2:C:321:ILE:HD12	2.43	0.47
2:C:379:LYS:HB2	2:C:412:PHE:CZ	2.50	0.47
2:D:24:GLU:O	2:D:25:ASN:C	2.52	0.47
2:D:377:LEU:HG	2:D:381:TRP:HD1	1.79	0.47
2:D:382:ILE:O	2:D:386:ILE:HG22	2.14	0.47
2:A:226:GLU:OE2	2:A:249:LYS:HE2	2.15	0.47
2:D:134:GLU:OE1	2:E:31:LYS:N	2.46	0.47
2:E:212:ARG:O	2:E:216:VAL:HG23	2.15	0.47
2:E:396:MET:O	2:E:400:ILE:HG13	2.14	0.47
2:F:58:LEU:HG	2:F:59:GLN:N	2.30	0.47
2:F:248:GLU:OE2	2:F:248:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:PHE:HE1	2:C:251:LYS:HZ2	1.61	0.47
2:C:141:ALA:HB3	2:C:370:LEU:HD12	1.97	0.47
2:C:167:PRO:O	2:C:365:THR:HG21	2.15	0.47
2:C:171:GLY:H	2:C:314:THR:CG2	2.27	0.47
2:C:286:THR:O	2:C:286:THR:OG1	2.29	0.47
2:B:231:THR:C	2:B:233:ASP:N	2.69	0.46
2:D:228:VAL:CG1	2:D:242:VAL:HG12	2.45	0.46
2:E:236:ALA:HA	2:E:239:HIS:HD2	1.79	0.46
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.97	0.46
2:D:383:LEU:O	2:D:387:ILE:HG13	2.15	0.46
2:E:7:LYS:HE2	2:E:77:ASP:OD1	2.15	0.46
2:A:44:LYS:HG3	2:A:47:GLU:HG3	1.96	0.46
2:C:136:LEU:HD13	2:D:221:ARG:HH21	1.81	0.46
2:D:2:ASN:HD22	2:D:50:PHE:HB2	1.79	0.46
2:D:353:ARG:HD2	2:D:355:PHE:HZ	1.79	0.46
2:A:252:ARG:HH11	2:A:252:ARG:HA	1.80	0.46
2:B:296:ARG:HH11	2:B:296:ARG:CG	2.10	0.46
2:C:272:ARG:O	2:C:276:THR:HG23	2.16	0.46
2:D:169:GLY:H	2:D:172:GLN:HG2	1.79	0.46
2:B:228:VAL:HG12	2:B:242:VAL:CG1	2.45	0.46
2:D:46:GLY:O	2:D:47:GLU:CB	2.64	0.46
2:F:58:LEU:C	2:F:60:ASP:H	2.19	0.46
2:A:352:LYS:HD2	2:A:393:ILE:HG21	1.97	0.46
2:B:52:ASP:HA	2:B:97:ILE:O	2.15	0.46
2:B:406:THR:OG1	2:B:407:LYS:N	2.46	0.46
2:C:57:ILE:H	2:C:93:THR:HB	1.79	0.46
2:B:131:ILE:HB	2:B:133:PHE:HD2	1.81	0.46
2:C:50:PHE:HE1	2:C:100:LYS:HE2	1.81	0.46
2:E:65:LEU:HB2	2:E:79:ILE:HB	1.97	0.46
2:E:141:ALA:O	2:E:371:LEU:CG	2.63	0.46
2:E:193:GLN:NE2	2:E:222:LEU:HD13	2.31	0.46
1:L:2:C:H5	2:F:110:TYR:OH	1.99	0.46
2:B:105:LYS:O	2:B:106:GLU:C	2.54	0.46
2:B:187:LEU:O	2:B:191:ILE:HD12	2.16	0.46
2:E:382:ILE:H	2:E:382:ILE:HG13	1.67	0.46
2:B:236:ALA:HA	2:B:239:HIS:CD2	2.37	0.46
2:D:132:LEU:HD21	2:D:305:ARG:HD2	1.96	0.46
2:E:354:VAL:HG12	2:E:354:VAL:O	2.15	0.46
2:C:160:ARG:HE	2:C:408:THR:HG23	1.81	0.46
2:E:210:ASP:HB2	2:E:269:ARG:HB3	1.96	0.46
2:D:373:THR:O	2:D:376:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:HIS:CD2	2:D:233:ASP:O	2.68	0.45
2:C:387:ILE:HG21	2:C:395:ALA:HB1	1.97	0.45
2:D:388:HIS:HB3	2:D:389:PRO:HD3	1.98	0.45
2:F:36:PHE:HZ	2:F:40:LYS:HE3	1.80	0.45
2:B:205:MET:O	2:B:262:ILE:HA	2.16	0.45
2:B:217:THR:HA	2:B:220:GLN:HB2	1.97	0.45
2:D:272:ARG:CG	2:D:272:ARG:NH1	2.68	0.45
2:E:321:ILE:HD11	2:E:332:TYR:CD2	2.51	0.45
2:E:321:ILE:HD13	2:E:321:ILE:HA	1.65	0.45
2:C:6:LEU:O	2:C:9:THR:HG23	2.16	0.45
2:C:366:ARG:NH1	2:D:212:ARG:NH1	2.64	0.45
2:E:410:ASP:O	2:E:414:GLU:HB2	2.16	0.45
2:C:137:THR:HG21	2:C:305:ARG:NH1	2.32	0.45
2:E:139:LEU:C	2:E:141:ALA:N	2.68	0.45
2:F:160:ARG:HD3	2:F:408:THR:OG1	2.17	0.45
2:A:15:ILE:HG23	2:A:26:LEU:HB2	1.99	0.45
2:A:262:ILE:HD12	2:A:313:LEU:HD11	1.99	0.45
2:D:147:MET:CE	2:D:191:ILE:HG23	2.46	0.45
2:F:304:ALA:O	2:F:305:ARG:HB3	2.17	0.45
2:A:169:GLY:O	2:A:172:GLN:HG2	2.17	0.45
2:C:272:ARG:HD2	2:C:327:MET:SD	2.57	0.45
2:C:387:ILE:CG2	2:C:395:ALA:HB1	2.47	0.45
2:F:247:ILE:O	2:F:250:ALA:HB3	2.16	0.45
2:A:248:GLU:O	2:A:252:ARG:HG2	2.16	0.45
2:B:269:ARG:HH11	2:B:272:ARG:HH12	1.64	0.45
2:A:207:LEU:HD23	2:A:264:LEU:HD13	1.99	0.45
2:B:290:ASP:C	2:B:290:ASP:OD1	2.54	0.45
2:D:26:LEU:HA	2:D:29:MET:HG3	1.98	0.45
2:D:65:LEU:HD21	2:D:97:ILE:HB	1.99	0.45
2:E:123:LYS:H	2:E:123:LYS:HG2	1.56	0.45
2:E:152:GLY:HA2	2:E:407:LYS:HE2	1.99	0.45
2:B:143:SER:HB3	2:B:170:ARG:HB2	1.99	0.44
2:E:113:LEU:HD21	2:E:116:VAL:HG22	1.99	0.44
2:E:137:THR:HG23	2:E:305:ARG:CB	2.42	0.44
2:A:49:ILE:HG23	2:A:101:ILE:HG13	1.97	0.44
2:A:56:GLU:HB3	2:A:66:ARG:HE	1.82	0.44
2:C:284:VAL:HG12	2:C:291:ALA:CB	2.46	0.44
2:F:206:VAL:HG22	2:F:263:LEU:HD12	1.98	0.44
2:C:171:GLY:HA2	2:C:313:LEU:O	2.17	0.44
2:C:266:SER:HB2	2:C:269:ARG:CB	2.46	0.44
2:E:137:THR:HG22	2:F:214:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:TYR:CG	2:F:245:MET:HG2	2.53	0.44
2:F:92:ARG:NH2	2:F:252:ARG:NH2	2.65	0.44
2:A:266:SER:HA	2:A:318:THR:O	2.17	0.44
2:E:105:LYS:N	2:E:108:GLU:OE1	2.45	0.44
2:E:184:LYS:CG	2:E:318:THR:HG21	2.48	0.44
2:B:211:GLU:HG2	2:B:215:GLU:HB3	1.99	0.44
2:C:141:ALA:O	2:C:370:LEU:CB	2.57	0.44
2:E:272:ARG:HG3	2:E:272:ARG:HH11	1.83	0.44
2:A:139:LEU:HA	2:B:214:GLU:HB2	1.99	0.44
2:A:304:ALA:HB2	2:A:315:ILE:CG1	2.48	0.44
2:B:240:VAL:HG13	2:B:274:TYR:CZ	2.52	0.44
2:D:184:LYS:HG2	2:D:185:THR:N	2.32	0.44
2:F:268:THR:CG2	2:F:320:LEU:H	2.30	0.44
2:B:173:ARG:CD	2:B:301:PHE:O	2.66	0.44
2:C:1:MET:CG	2:C:2:ASN:H	2.31	0.44
2:D:137:THR:CG2	2:D:305:ARG:CB	2.95	0.44
2:E:131:ILE:HG22	2:E:134:GLU:CG	2.47	0.44
2:E:228:VAL:HG12	2:E:242:VAL:CG1	2.47	0.44
2:A:14:LEU:CD1	2:A:35:ILE:HG13	2.47	0.44
2:D:144:ARG:HH12	2:D:372:THR:HG22	1.83	0.44
2:D:160:ARG:CZ	2:D:408:THR:HB	2.47	0.44
2:D:252:ARG:HD3	2:D:252:ARG:HA	1.86	0.44
2:D:264:LEU:HD22	2:D:300:PHE:CE2	2.53	0.44
2:E:268:THR:HG22	2:E:319:ALA:HA	2.00	0.44
2:F:403:LEU:O	2:F:405:MET:N	2.50	0.44
2:A:139:LEU:HD13	2:A:367:LYS:NZ	2.32	0.44
2:B:396:MET:O	2:B:400:ILE:HG12	2.18	0.44
2:E:141:ALA:O	2:E:371:LEU:HD23	2.18	0.44
2:F:296:ARG:HB2	2:F:297:PRO:HD3	1.99	0.44
2:B:123:LYS:HG2	2:B:124:PRO:HD2	2.00	0.43
2:B:134:GLU:OE1	2:C:31:LYS:N	2.51	0.43
2:D:174:GLY:HA2	2:D:341:MET:CG	2.46	0.43
2:E:228:VAL:CG1	2:E:242:VAL:HG13	2.47	0.43
2:B:130:LYS:HD3	2:B:130:LYS:H	1.83	0.43
2:D:289:VAL:HG11	2:D:330:VAL:HG11	2.00	0.43
2:E:238:ARG:NH1	2:E:241:GLN:OE1	2.46	0.43
2:E:295:HIS:HD2	2:F:233:ASP:O	2.01	0.43
2:F:138:PRO:O	2:F:140:HIS:N	2.50	0.43
2:B:89:PHE:CE2	2:B:116:VAL:HG21	2.52	0.43
2:B:321:ILE:HD11	2:B:332:TYR:CG	2.53	0.43
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:LEU:HD21	2:D:41:GLN:HG3	2.00	0.43
2:D:387:ILE:O	2:D:390:MET:HB2	2.17	0.43
2:D:398:PHE:CE1	2:D:402:LYS:HE2	2.53	0.43
2:F:266:SER:HB3	2:F:320:LEU:HG	1.99	0.43
2:D:141:ALA:CB	2:D:370:LEU:CB	2.94	0.43
2:E:139:LEU:O	2:E:140:HIS:C	2.56	0.43
2:E:381:TRP:CH2	2:F:353:ARG:HD3	2.53	0.43
2:B:52:ASP:HB2	2:B:53:GLY:H	1.64	0.43
2:B:76:PRO:O	2:B:78:ASP:N	2.52	0.43
2:D:238:ARG:O	2:D:242:VAL:CG2	2.67	0.43
2:E:132:LEU:HD22	2:E:251:LYS:HE2	2.01	0.43
2:F:62:PHE:HE1	2:F:64:PHE:HE2	1.67	0.43
2:F:160:ARG:HD3	2:F:408:THR:CB	2.48	0.43
2:F:294:LEU:C	2:F:297:PRO:HD2	2.38	0.43
1:H:1:U:H4'	1:H:2:C:O5'	2.19	0.43
2:A:326:LYS:O	2:A:330:VAL:HG23	2.18	0.43
2:B:386:ILE:O	2:B:386:ILE:HG13	2.18	0.43
2:C:252:ARG:HA	2:C:252:ARG:HD3	1.75	0.43
2:B:356:PRO:HB2	2:B:396:MET:HE1	2.00	0.43
2:C:79:ILE:HD13	2:C:101:ILE:CG2	2.48	0.43
2:D:46:GLY:O	2:D:47:GLU:HB2	2.19	0.43
2:D:131:ILE:HG21	2:D:133:PHE:HD2	1.78	0.43
2:D:289:VAL:CG1	2:D:330:VAL:HG11	2.49	0.43
2:D:410:ASP:O	2:D:414:GLU:HB2	2.19	0.43
2:F:272:ARG:HH11	2:F:272:ARG:CB	2.31	0.43
2:F:74:ALA:HA	2:F:78:ASP:OD2	2.19	0.43
2:F:250:ALA:O	2:F:254:VAL:HG23	2.19	0.43
2:B:99:GLY:HA2	2:B:117:ASN:HB2	2.01	0.43
2:C:205:MET:HE3	2:C:226:GLU:OE1	2.19	0.43
2:C:416:MET:HB3	2:C:417:LYS:H	1.70	0.43
2:A:351:GLU:C	2:A:353:ARG:H	2.22	0.42
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.00	0.42
2:C:228:VAL:CG1	2:C:242:VAL:HG13	2.48	0.42
2:E:130:LYS:HE3	2:F:12:SER:N	2.34	0.42
2:A:137:THR:HG21	2:A:305:ARG:NH1	2.34	0.42
2:E:5:GLU:O	2:E:9:THR:CG2	2.67	0.42
2:E:101:ILE:HD12	2:E:111:PHE:HD1	1.84	0.42
2:F:106:GLU:H	2:F:106:GLU:HG2	1.45	0.42
2:F:349:ILE:HD11	2:F:392:GLU:HB3	2.00	0.42
2:B:154:THR:HA	2:B:157:LEU:HG	2.01	0.42
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:HIS:HA	2:C:306:ASN:HB2	2.00	0.42
2:E:133:PHE:HE1	2:E:251:LYS:HZ3	1.65	0.42
2:B:138:PRO:C	2:B:140:HIS:H	2.23	0.42
2:D:205:MET:O	2:D:262:ILE:HA	2.19	0.42
2:F:416:MET:H	2:F:416:MET:HG2	1.57	0.42
1:K:2:C:H5	2:E:110:TYR:CZ	2.38	0.42
1:K:2:C:H5	2:E:110:TYR:OH	2.03	0.42
2:A:179:PRO:CD	2:A:345:LEU:O	2.67	0.42
2:A:294:LEU:CD1	2:A:334:GLU:HG3	2.43	0.42
2:C:264:LEU:HD22	2:C:300:PHE:CE2	2.55	0.42
2:D:178:ALA:HA	2:D:179:PRO:HD3	1.94	0.42
2:E:66:ARG:HG2	2:E:66:ARG:HH11	1.84	0.42
2:A:296:ARG:HG3	2:A:296:ARG:HH11	1.84	0.42
2:C:65:LEU:HD12	2:C:79:ILE:HD12	2.01	0.42
2:C:146:ARG:NH2	2:C:376:GLU:OE1	2.53	0.42
2:D:379:LYS:HG3	2:D:412:PHE:CD1	2.55	0.42
2:E:230:SER:HA	2:E:234:GLU:OE1	2.20	0.42
2:A:113:LEU:HD21	2:A:116:VAL:HG22	2.01	0.42
2:B:169:GLY:O	2:B:172:GLN:HG2	2.19	0.42
2:C:106:GLU:C	2:C:108:GLU:N	2.73	0.42
2:C:138:PRO:HD2	2:C:306:ASN:O	2.20	0.42
2:C:175:LEU:HD13	2:C:301:PHE:CZ	2.55	0.42
2:C:234:GLU:OE2	2:C:238:ARG:HG2	2.20	0.42
2:D:6:LEU:O	2:D:9:THR:HG23	2.20	0.42
2:D:174:GLY:CA	2:D:341:MET:CG	2.96	0.42
2:E:378:GLN:O	2:E:382:ILE:HG13	2.19	0.42
2:F:123:LYS:H	2:F:123:LYS:HG2	1.48	0.42
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.83	0.42
2:B:209:ILE:O	2:B:230:SER:O	2.38	0.42
2:E:388:HIS:HB3	2:E:389:PRO:HD3	2.01	0.42
2:F:19:GLU:C	2:F:21:MET:H	2.22	0.42
2:F:353:ARG:NH1	2:F:353:ARG:CG	2.65	0.42
2:B:130:LYS:O	2:B:255:GLU:HG2	2.20	0.42
2:C:210:ASP:OD1	2:C:232:PHE:HA	2.19	0.42
2:F:62:PHE:HB2	2:F:80:TYR:CE1	2.54	0.42
2:F:178:ALA:HA	2:F:179:PRO:HD3	1.85	0.42
2:B:231:THR:OG1	2:B:233:ASP:HB2	2.20	0.41
2:C:379:LYS:HB2	2:C:412:PHE:CE1	2.55	0.41
2:D:55:LEU:HB2	2:D:97:ILE:HD12	2.02	0.41
2:A:136:LEU:HD13	2:B:221:ARG:HH21	1.84	0.41
2:B:268:THR:HG21	2:B:320:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:PHE:HE1	2:C:64:PHE:CE2	2.37	0.41
2:D:188:LEU:HD23	2:D:188:LEU:HA	1.96	0.41
2:A:356:PRO:HB2	2:A:396:MET:HE3	2.02	0.41
2:D:408:THR:HG23	2:D:409:ASN:N	2.35	0.41
2:A:28:ARG:HD3	2:A:28:ARG:HA	1.87	0.41
2:A:100:LYS:O	2:A:114:LEU:N	2.50	0.41
2:A:162:LEU:HD11	2:A:343:LEU:HD22	2.01	0.41
2:D:134:GLU:OE2	2:E:29:MET:O	2.39	0.41
2:D:403:LEU:C	2:D:405:MET:H	2.24	0.41
2:E:1:MET:CG	2:E:2:ASN:N	2.77	0.41
2:E:18:GLY:HA3	2:E:26:LEU:CD1	2.50	0.41
2:E:32:GLN:HB3	2:E:76:PRO:HD2	2.01	0.41
2:E:92:ARG:NH2	2:E:131:ILE:HD11	2.35	0.41
2:C:146:ARG:HH21	2:C:376:GLU:CD	2.24	0.41
2:E:139:LEU:HD22	2:E:367:LYS:HG3	2.02	0.41
2:F:331:ILE:O	2:F:335:PHE:HD1	2.03	0.41
2:A:279:PRO:O	2:A:280:ALA:C	2.59	0.41
2:B:351:GLU:C	2:B:353:ARG:H	2.24	0.41
2:E:66:ARG:NH1	2:E:74:ALA:HA	2.35	0.41
2:E:141:ALA:HB3	2:E:370:LEU:HB2	2.02	0.41
2:A:161:VAL:HG11	2:A:396:MET:HE1	2.02	0.41
2:D:171:GLY:H	2:D:314:THR:HB	1.85	0.41
2:F:46:GLY:C	2:F:48:ASP:N	2.74	0.41
2:F:205:MET:O	2:F:262:ILE:HA	2.21	0.41
2:B:173:ARG:HD3	2:B:301:PHE:O	2.20	0.41
2:B:173:ARG:NH2	2:C:214:GLU:OE2	2.54	0.41
2:B:380:MET:HG2	2:B:380:MET:H	1.71	0.41
2:C:123:LYS:C	2:C:125:GLU:N	2.74	0.41
2:C:398:PHE:O	2:C:402:LYS:HG3	2.21	0.41
2:D:349:ILE:H	2:D:349:ILE:HG13	1.64	0.41
2:E:49:ILE:HG22	2:E:49:ILE:O	2.21	0.41
2:E:209:ILE:HG22	2:E:210:ASP:N	2.34	0.41
2:E:279:PRO:O	2:E:280:ALA:C	2.59	0.41
2:B:119:VAL:HG12	2:B:120:ASN:HD22	1.85	0.41
2:C:1:MET:HE2	2:C:1:MET:HB2	1.94	0.41
2:C:409:ASN:O	2:C:413:PHE:HB2	2.21	0.41
2:D:406:THR:HB	2:D:407:LYS:H	1.55	0.41
2:E:142:ASN:O	2:E:143:SER:HB3	2.21	0.41
2:E:167:PRO:HD2	2:E:365:THR:HG23	2.03	0.41
2:F:4:THR:HA	2:F:7:LYS:HG3	2.02	0.41
2:F:52:ASP:HA	2:F:97:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:LYS:HA	2:B:124:PRO:HD3	1.95	0.41
2:D:166:SER:HA	2:D:365:THR:HG22	2.03	0.41
2:E:41:GLN:HE21	2:E:41:GLN:HB3	1.69	0.41
2:C:171:GLY:H	2:C:314:THR:CB	2.35	0.40
2:D:37:ALA:O	2:D:41:GLN:HB2	2.21	0.40
2:F:274:TYR:HD2	2:F:297:PRO:HG3	1.85	0.40
2:A:44:LYS:HG3	2:A:47:GLU:CG	2.52	0.40
2:C:179:PRO:HA	2:C:321:ILE:O	2.22	0.40
2:C:272:ARG:O	2:C:276:THR:CG2	2.69	0.40
2:D:175:LEU:HD12	2:D:175:LEU:HA	1.95	0.40
2:D:278:VAL:HA	2:D:279:PRO:HD3	1.92	0.40
2:E:252:ARG:HD3	2:E:252:ARG:HA	1.83	0.40
2:F:1:MET:HB2	2:F:2:ASN:H	1.58	0.40
2:A:388:HIS:CB	2:A:389:PRO:HD3	2.43	0.40
2:B:322:ASP:HB3	2:B:347:ARG:NH1	2.37	0.40
2:E:109:ARG:HD2	2:E:110:TYR:CE2	2.56	0.40
2:E:187:LEU:HG	2:E:191:ILE:HD12	2.03	0.40
2:B:138:PRO:C	2:B:140:HIS:N	2.75	0.40
2:B:146:ARG:HH12	2:B:376:GLU:CD	2.24	0.40
2:B:343:LEU:HD12	2:B:363:SER:OG	2.22	0.40
2:E:137:THR:HG21	2:F:213:PRO:HB2	2.03	0.40
2:E:179:PRO:HA	2:E:321:ILE:O	2.20	0.40
2:F:309:GLU:HG2	2:F:309:GLU:H	1.50	0.40
2:F:361:ASN:OD1	2:F:388:HIS:HA	2.20	0.40
2:B:184:LYS:HB3	2:B:184:LYS:HE3	1.41	0.40
2:B:271:ALA:HB3	2:B:331:ILE:HD13	2.03	0.40
2:C:254:VAL:HG21	2:C:313:LEU:HB2	2.03	0.40
2:C:279:PRO:O	2:C:280:ALA:CB	2.68	0.40
2:D:386:ILE:O	2:D:386:ILE:HG13	2.17	0.40
2:F:303:ALA:O	2:F:313:LEU:HD23	2.22	0.40
2:F:339:GLY:C	2:F:341:MET:H	2.25	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
2	A	400/419 (96%)	367 (92%)	30 (8%)	3 (1%)	19 57
2	B	350/419 (84%)	313 (89%)	25 (7%)	12 (3%)	3 20
2	C	400/419 (96%)	361 (90%)	32 (8%)	7 (2%)	8 37
2	D	400/419 (96%)	363 (91%)	27 (7%)	10 (2%)	5 28
2	E	399/419 (95%)	370 (93%)	25 (6%)	4 (1%)	15 53
2	F	400/419 (96%)	351 (88%)	35 (9%)	14 (4%)	3 20
All	All	2349/2514 (93%)	2125 (90%)	174 (7%)	50 (2%)	7 33

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	356	PRO
2	C	50	PHE
2	C	355	PHE
2	D	47	GLU
2	D	181	LYS
2	E	266	SER
2	F	47	GLU
2	F	49	ILE
2	F	266	SER
2	F	407	LYS
2	A	25	ASN
2	A	42	HIS
2	B	142	ASN
2	B	266	SER
2	D	25	ASN
2	D	292	ASN
2	D	357	ALA
2	F	44	LYS
2	F	59	GLN
2	F	143	SER
2	B	59	GLN
2	B	77	ASP
2	B	106	GLU
2	B	139	LEU
2	B	406	THR
2	C	139	LEU
2	C	407	LYS

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Mol	Chain	Res	Type
2	D	43	ALA
2	F	139	LEU
2	F	404	ALA
2	B	76	PRO
2	B	287	GLY
2	C	266	SER
2	D	143	SER
2	D	359	ASP
2	E	31	LYS
2	F	124	PRO
2	F	181	LYS
2	A	44	LYS
2	B	355	PHE
2	B	357	ALA
2	D	287	GLY
2	D	368	GLU
2	E	356	PRO
2	F	305	ARG
2	C	416	MET
2	F	356	PRO
2	F	287	GLY
2	E	287	GLY
2	C	124	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
2	A	350/359 (98%)	271 (77%)	79 (23%)	1 4
2	B	306/359 (85%)	242 (79%)	64 (21%)	1 5
2	C	350/359 (98%)	284 (81%)	66 (19%)	1 8
2	D	350/359 (98%)	273 (78%)	77 (22%)	1 4
2	E	349/359 (97%)	289 (83%)	60 (17%)	2 10
2	F	350/359 (98%)	280 (80%)	70 (20%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2055/2154 (95%)	1639 (80%)	416 (20%)	1 6

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	LEU
2	A	4	THR
2	A	7	LYS
2	A	12	SER
2	A	14	LEU
2	A	15	ILE
2	A	17	LEU
2	A	25	ASN
2	A	28	ARG
2	A	30	ARG
2	A	44	LYS
2	A	49	ILE
2	A	58	LEU
2	A	59	GLN
2	A	67	SER
2	A	69	ASP
2	A	71	SER
2	A	84	SER
2	A	92	ARG
2	A	102	ARG
2	A	118	GLU
2	A	122	ASP
2	A	123	LYS
2	A	129	ASN
2	A	130	LYS
2	A	131	ILE
2	A	132	LEU
2	A	139	LEU
2	A	142	ASN
2	A	144	ARG
2	A	162	LEU
2	A	173	ARG
2	A	184	LYS
2	A	194	SER
2	A	209	ILE
2	A	211	GLU
2	A	212	ARG

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Mol	Chain	Res	Type
2	A	220	GLN
2	A	221	ARG
2	A	233	ASP
2	A	247	ILE
2	A	252	ARG
2	A	257	LYS
2	A	268	THR
2	A	272	ARG
2	A	276	THR
2	A	285	LEU
2	A	290	ASP
2	A	299	ARG
2	A	301	PHE
2	A	305	ARG
2	A	314	THR
2	A	321	ILE
2	A	336	LYS
2	A	340	ASN
2	A	341	MET
2	A	347	ARG
2	A	351	GLU
2	A	353	ARG
2	A	365	THR
2	A	366	ARG
2	A	370	LEU
2	A	376	GLU
2	A	381	TRP
2	A	383	LEU
2	A	384	ARG
2	A	385	LYS
2	A	386	ILE
2	A	393	ILE
2	A	397	GLU
2	A	399	LEU
2	A	406	THR
2	A	407	LYS
2	A	408	THR
2	A	411	ASP
2	A	414	GLU
2	A	415	MET
2	A	416	MET
2	A	417	LYS

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Mol	Chain	Res	Type
2	B	52	ASP
2	B	56	GLU
2	B	66	ARG
2	B	70	SER
2	B	77	ASP
2	B	84	SER
2	B	87	ARG
2	B	88	ARG
2	B	93	THR
2	B	100	LYS
2	B	102	ARG
2	B	105	LYS
2	B	108	GLU
2	B	114	LEU
2	B	115	LYS
2	B	122	ASP
2	B	123	LYS
2	B	130	LYS
2	B	131	ILE
2	B	132	LEU
2	B	137	THR
2	B	144	ARG
2	B	146	ARG
2	B	147	MET
2	B	154	THR
2	B	155	GLU
2	B	162	LEU
2	B	163	ASP
2	B	184	LYS
2	B	194	SER
2	B	198	ASN
2	B	208	LEU
2	B	210	ASP
2	B	211	GLU
2	B	252	ARG
2	B	258	LYS
2	B	268	THR
2	B	269	ARG
2	B	272	ARG
2	B	276	THR
2	B	284	VAL
2	B	286	THR

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Mol	Chain	Res	Type
2	B	289	VAL
2	B	292	ASN
2	B	296	ARG
2	B	299	ARG
2	B	301	PHE
2	B	306	ASN
2	B	314	THR
2	B	321	ILE
2	B	341	MET
2	B	347	ARG
2	B	365	THR
2	B	371	LEU
2	B	378	GLN
2	B	379	LYS
2	B	380	MET
2	B	383	LEU
2	B	386	ILE
2	B	393	ILE
2	B	394	ASP
2	B	399	LEU
2	B	407	LYS
2	B	417	LYS
2	C	1	MET
2	C	3	LEU
2	C	4	THR
2	C	9	THR
2	C	11	VAL
2	C	13	GLU
2	C	16	THR
2	C	17	LEU
2	C	26	LEU
2	C	28	ARG
2	C	29	MET
2	C	30	ARG
2	C	31	LYS
2	C	35	ILE
2	C	38	ILE
2	C	39	LEU
2	C	40	LYS
2	C	41	GLN
2	C	44	LYS
2	C	47	GLU

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Mol	Chain	Res	Type
2	C	49	ILE
2	C	52	ASP
2	C	66	ARG
2	C	69	ASP
2	C	77	ASP
2	C	82	SER
2	C	87	ARG
2	C	93	THR
2	C	114	LEU
2	C	115	LYS
2	C	129	ASN
2	C	132	LEU
2	C	153	SER
2	C	172	GLN
2	C	181	LYS
2	C	190	ASN
2	C	194	SER
2	C	211	GLU
2	C	247	ILE
2	C	252	ARG
2	C	257	LYS
2	C	266	SER
2	C	267	ILE
2	C	272	ARG
2	C	276	THR
2	C	286	THR
2	C	299	ARG
2	C	305	ARG
2	C	314	THR
2	C	321	ILE
2	C	326	LYS
2	C	342	GLU
2	C	347	ARG
2	C	367	LYS
2	C	374	GLN
2	C	379	LYS
2	C	383	LEU
2	C	384	ARG
2	C	393	ILE
2	C	396	MET
2	C	405	MET
2	C	408	THR

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Mol	Chain	Res	Type
2	C	413	PHE
2	C	415	MET
2	C	416	MET
2	C	417	LYS
2	D	2	ASN
2	D	4	THR
2	D	5	GLU
2	D	7	LYS
2	D	9	THR
2	D	13	GLU
2	D	17	LEU
2	D	24	GLU
2	D	32	GLN
2	D	41	GLN
2	D	44	LYS
2	D	45	SER
2	D	49	ILE
2	D	52	ASP
2	D	58	LEU
2	D	69	ASP
2	D	70	SER
2	D	73	LEU
2	D	90	ASN
2	D	93	THR
2	D	98	SER
2	D	109	ARG
2	D	114	LEU
2	D	115	LYS
2	D	125	GLU
2	D	126	ASN
2	D	130	LYS
2	D	132	LEU
2	D	137	THR
2	D	138	PRO
2	D	139	LEU
2	D	143	SER
2	D	147	MET
2	D	154	THR
2	D	163	ASP
2	D	170	ARG
2	D	181	LYS
2	D	184	LYS

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Mol	Chain	Res	Type
2	D	193	GLN
2	D	198	ASN
2	D	212	ARG
2	D	222	LEU
2	D	224	LYS
2	D	235	PRO
2	D	242	VAL
2	D	244	GLU
2	D	245	MET
2	D	252	ARG
2	D	257	LYS
2	D	267	ILE
2	D	268	THR
2	D	272	ARG
2	D	276	THR
2	D	285	LEU
2	D	289	VAL
2	D	296	ARG
2	D	299	ARG
2	D	305	ARG
2	D	314	THR
2	D	321	ILE
2	D	322	ASP
2	D	326	LYS
2	D	336	LYS
2	D	341	MET
2	D	347	ARG
2	D	352	LYS
2	D	353	ARG
2	D	365	THR
2	D	374	GLN
2	D	378	GLN
2	D	383	LEU
2	D	386	ILE
2	D	390	MET
2	D	399	LEU
2	D	405	MET
2	D	406	THR
2	D	412	PHE
2	E	9	THR
2	E	12	SER
2	E	16	THR

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Mol	Chain	Res	Type
2	E	17	LEU
2	E	30	ARG
2	E	41	GLN
2	E	49	ILE
2	E	60	ASP
2	E	69	ASP
2	E	70	SER
2	E	88	ARG
2	E	93	THR
2	E	98	SER
2	E	109	ARG
2	E	123	LYS
2	E	132	LEU
2	E	147	MET
2	E	153	SER
2	E	155	GLU
2	E	157	LEU
2	E	158	THR
2	E	162	LEU
2	E	175	LEU
2	E	197	TYR
2	E	234	GLU
2	E	252	ARG
2	E	257	LYS
2	E	268	THR
2	E	276	THR
2	E	277	VAL
2	E	278	VAL
2	E	286	THR
2	E	289	VAL
2	E	296	ARG
2	E	299	ARG
2	E	301	PHE
2	E	309	GLU
2	E	314	THR
2	E	321	ILE
2	E	322	ASP
2	E	326	LYS
2	E	341	MET
2	E	355	PHE
2	E	362	ARG
2	E	365	THR

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Mol	Chain	Res	Type
2	E	368	GLU
2	E	372	THR
2	E	379	LYS
2	E	382	ILE
2	E	385	LYS
2	E	393	ILE
2	E	396	MET
2	E	397	GLU
2	E	402	LYS
2	E	408	THR
2	E	411	ASP
2	E	414	GLU
2	E	415	MET
2	E	416	MET
2	E	417	LYS
2	F	1	MET
2	F	2	ASN
2	F	4	THR
2	F	6	LEU
2	F	7	LYS
2	F	9	THR
2	F	11	VAL
2	F	12	SER
2	F	24	GLU
2	F	26	LEU
2	F	35	ILE
2	F	39	LEU
2	F	41	GLN
2	F	47	GLU
2	F	49	ILE
2	F	70	SER
2	F	88	ARG
2	F	93	THR
2	F	106	GLU
2	F	122	ASP
2	F	123	LYS
2	F	125	GLU
2	F	126	ASN
2	F	134	GLU
2	F	136	LEU
2	F	137	THR
2	F	139	LEU

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Mol	Chain	Res	Type
2	F	144	ARG
2	F	146	ARG
2	F	160	ARG
2	F	162	LEU
2	F	168	ILE
2	F	173	ARG
2	F	201	ASP
2	F	226	GLU
2	F	233	ASP
2	F	244	GLU
2	F	252	ARG
2	F	266	SER
2	F	268	THR
2	F	272	ARG
2	F	277	VAL
2	F	278	VAL
2	F	289	VAL
2	F	290	ASP
2	F	294	LEU
2	F	299	ARG
2	F	309	GLU
2	F	321	ILE
2	F	326	LYS
2	F	341	MET
2	F	347	ARG
2	F	353	ARG
2	F	368	GLU
2	F	370	LEU
2	F	374	GLN
2	F	377	LEU
2	F	382	ILE
2	F	384	ARG
2	F	386	ILE
2	F	390	MET
2	F	393	ILE
2	F	397	GLU
2	F	406	THR
2	F	408	THR
2	F	409	ASN
2	F	413	PHE
2	F	415	MET
2	F	416	MET

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Mol	Chain	Res	Type
2	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	42	HIS
2	A	142	ASN
2	A	172	GLN
2	A	198	ASN
2	A	340	ASN
2	B	120	ASN
2	B	198	ASN
2	B	295	HIS
2	B	306	ASN
2	C	59	GLN
2	C	142	ASN
2	C	172	GLN
2	C	190	ASN
2	C	275	ASN
2	C	306	ASN
2	C	344	HIS
2	C	409	ASN
2	D	32	GLN
2	D	41	GLN
2	D	172	GLN
2	D	198	ASN
2	D	275	ASN
2	D	344	HIS
2	D	361	ASN
2	E	41	GLN
2	E	193	GLN
2	E	295	HIS
2	E	306	ASN
2	E	344	HIS
2	F	41	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/2 (100%)	1 (50%)	1 (50%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	H	2/2 (100%)	1 (50%)	1 (50%)
1	J	1/2 (50%)	0	0
1	K	2/2 (100%)	1 (50%)	1 (50%)
1	L	2/2 (100%)	1 (50%)	1 (50%)
All	All	9/10 (90%)	4 (44%)	4 (44%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	H	2	C
1	K	2	C
1	L	2	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	1	U
1	H	1	U
1	K	1	U
1	L	1	U

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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ANP	B	602	-	29,33,33	4.21	12 (41%)	31,52,52	2.76	16 (51%)
3	ANP	D	604	-	29,33,33	4.28	13 (44%)	31,52,52	2.69	15 (48%)
3	ANP	F	606	-	29,33,33	4.23	13 (44%)	31,52,52	2.69	15 (48%)
3	ANP	E	605	-	29,33,33	4.33	13 (44%)	31,52,52	2.70	15 (48%)
3	ANP	C	603	-	29,33,33	4.25	11 (37%)	31,52,52	2.68	14 (45%)
3	ANP	A	601	-	29,33,33	4.16	14 (48%)	31,52,52	2.87	16 (51%)

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
3	ANP	B	602	-	3/3/7/8	6/14/38/38	0/3/3/3
3	ANP	D	604	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	F	606	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	E	605	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	C	603	-	3/3/7/8	7/14/38/38	0/3/3/3
3	ANP	A	601	-	3/3/7/8	4/14/38/38	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	605	ANP	C2'-C1'	-14.09	1.32	1.53
3	D	604	ANP	C2'-C1'	-13.82	1.32	1.53
3	F	606	ANP	C2'-C1'	-13.57	1.33	1.53
3	C	603	ANP	C2'-C1'	-13.53	1.33	1.53
3	A	601	ANP	C2'-C1'	-13.26	1.33	1.53
3	B	602	ANP	C2'-C1'	-13.22	1.33	1.53
3	D	604	ANP	O2'-C2'	-8.90	1.22	1.43
3	B	602	ANP	O3'-C3'	-8.89	1.22	1.43
3	E	605	ANP	O2'-C2'	-8.88	1.22	1.43
3	B	602	ANP	O2'-C2'	-8.87	1.22	1.43
3	C	603	ANP	O3'-C3'	-8.82	1.22	1.43
3	C	603	ANP	O2'-C2'	-8.81	1.22	1.43
3	E	605	ANP	O3'-C3'	-8.79	1.22	1.43
3	F	606	ANP	O2'-C2'	-8.71	1.22	1.43
3	D	604	ANP	O3'-C3'	-8.66	1.22	1.43
3	F	606	ANP	O3'-C3'	-8.65	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ANP	O2'-C2'	-8.63	1.22	1.43
3	A	601	ANP	O3'-C3'	-8.57	1.22	1.43
3	E	605	ANP	C3'-C4'	-8.02	1.32	1.53
3	D	604	ANP	C3'-C4'	-7.98	1.32	1.53
3	C	603	ANP	C3'-C4'	-7.92	1.32	1.53
3	B	602	ANP	C3'-C4'	-7.85	1.32	1.53
3	A	601	ANP	C3'-C4'	-7.62	1.33	1.53
3	F	606	ANP	C3'-C4'	-7.61	1.33	1.53
3	E	605	ANP	C2'-C3'	-7.59	1.32	1.53
3	C	603	ANP	C2'-C3'	-7.58	1.32	1.53
3	F	606	ANP	C2'-C3'	-7.49	1.32	1.53
3	B	602	ANP	C2'-C3'	-7.46	1.32	1.53
3	D	604	ANP	C2'-C3'	-7.36	1.33	1.53
3	A	601	ANP	C2'-C3'	-7.19	1.33	1.53
3	A	601	ANP	PG-O1G	3.57	1.51	1.46
3	E	605	ANP	PG-O1G	3.47	1.51	1.46
3	D	604	ANP	PG-O1G	3.42	1.51	1.46
3	F	606	ANP	PG-O1G	3.40	1.51	1.46
3	C	603	ANP	PG-O1G	3.39	1.51	1.46
3	B	602	ANP	PG-O1G	3.37	1.51	1.46
3	F	606	ANP	O4'-C1'	3.31	1.45	1.41
3	F	606	ANP	PB-O1B	3.13	1.51	1.46
3	C	603	ANP	O4'-C1'	3.09	1.45	1.41
3	D	604	ANP	O4'-C1'	3.00	1.45	1.41
3	E	605	ANP	PB-O1B	2.99	1.50	1.46
3	A	601	ANP	PB-O1B	2.98	1.50	1.46
3	B	602	ANP	PB-O1B	2.96	1.50	1.46
3	C	603	ANP	PB-O1B	2.95	1.50	1.46
3	B	602	ANP	O4'-C1'	2.90	1.45	1.41
3	D	604	ANP	PB-O1B	2.89	1.50	1.46
3	E	605	ANP	O4'-C1'	2.84	1.45	1.41
3	F	606	ANP	C5-C4	2.51	1.47	1.40
3	B	602	ANP	C5-C4	2.45	1.47	1.40
3	A	601	ANP	C5-C4	2.45	1.47	1.40
3	E	605	ANP	C5-C4	2.45	1.47	1.40
3	A	601	ANP	O4'-C1'	2.39	1.44	1.41
3	D	604	ANP	C5-C4	2.37	1.47	1.40
3	C	603	ANP	C5-C4	2.35	1.47	1.40
3	B	602	ANP	PG-O3G	-2.33	1.50	1.56
3	D	604	ANP	PG-O3G	-2.28	1.50	1.56
3	E	605	ANP	PG-O3G	-2.28	1.50	1.56
3	A	601	ANP	PB-O3A	2.27	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	606	ANP	PG-O2G	-2.25	1.50	1.56
3	F	606	ANP	PG-O3G	-2.25	1.50	1.56
3	F	606	ANP	PB-O2B	-2.25	1.50	1.56
3	D	604	ANP	PG-O2G	-2.25	1.50	1.56
3	E	605	ANP	PG-O2G	-2.24	1.50	1.56
3	A	601	ANP	PG-O2G	-2.22	1.50	1.56
3	B	602	ANP	PG-O2G	-2.20	1.50	1.56
3	A	601	ANP	PG-O3G	-2.20	1.50	1.56
3	F	606	ANP	C2-N3	2.18	1.35	1.32
3	D	604	ANP	PB-O2B	-2.17	1.50	1.56
3	C	603	ANP	PB-O2B	-2.15	1.51	1.56
3	E	605	ANP	C2-N3	2.11	1.35	1.32
3	E	605	ANP	PB-O2B	-2.11	1.51	1.56
3	D	604	ANP	C2-N3	2.06	1.35	1.32
3	C	603	ANP	C2-N3	2.06	1.35	1.32
3	B	602	ANP	PB-O2B	-2.03	1.51	1.56
3	A	601	ANP	C2-N3	2.02	1.35	1.32
3	A	601	ANP	PB-O2B	-2.01	1.51	1.56

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	ANP	C3'-C2'-C1'	5.85	109.79	100.98
3	C	603	ANP	C3'-C2'-C1'	5.79	109.70	100.98
3	B	602	ANP	C3'-C2'-C1'	5.65	109.48	100.98
3	D	604	ANP	C3'-C2'-C1'	5.56	109.34	100.98
3	E	605	ANP	C3'-C2'-C1'	5.47	109.22	100.98
3	A	601	ANP	O1G-PG-N3B	-5.46	103.73	111.77
3	D	604	ANP	O1G-PG-N3B	-5.10	104.26	111.77
3	F	606	ANP	C3'-C2'-C1'	5.04	108.56	100.98
3	A	601	ANP	O3'-C3'-C4'	4.91	125.25	111.05
3	F	606	ANP	O1G-PG-N3B	-4.86	104.62	111.77
3	B	602	ANP	O2B-PB-O1B	4.82	120.02	109.92
3	F	606	ANP	O3'-C3'-C4'	4.79	124.90	111.05
3	E	605	ANP	O2B-PB-O1B	4.73	119.84	109.92
3	E	605	ANP	O1G-PG-N3B	-4.70	104.85	111.77
3	C	603	ANP	O3'-C3'-C4'	4.65	124.50	111.05
3	E	605	ANP	O3'-C3'-C4'	4.65	124.50	111.05
3	D	604	ANP	O3'-C3'-C4'	4.57	124.27	111.05
3	F	606	ANP	O4'-C4'-C5'	4.57	124.40	109.37
3	C	603	ANP	O4'-C4'-C5'	4.40	123.84	109.37
3	B	602	ANP	O1G-PG-N3B	-4.39	105.30	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ANP	O3'-C3'-C4'	4.31	123.52	111.05
3	D	604	ANP	O2B-PB-O1B	4.29	118.92	109.92
3	F	606	ANP	O2B-PB-O1B	4.26	118.86	109.92
3	A	601	ANP	O2B-PB-O1B	4.24	118.81	109.92
3	C	603	ANP	O1G-PG-N3B	-4.23	105.54	111.77
3	C	603	ANP	O2B-PB-O1B	4.18	118.69	109.92
3	B	602	ANP	O4'-C4'-C5'	4.14	122.99	109.37
3	A	601	ANP	O3'-C3'-C2'	4.10	125.07	111.82
3	C	603	ANP	PB-O3A-PA	-3.99	118.56	132.62
3	A	601	ANP	O4'-C4'-C5'	3.99	122.49	109.37
3	D	604	ANP	O3'-C3'-C2'	3.86	124.31	111.82
3	A	601	ANP	O1B-PB-N3B	-3.84	106.12	111.77
3	D	604	ANP	O2'-C2'-C3'	3.77	124.02	111.82
3	B	602	ANP	O1B-PB-N3B	-3.74	106.26	111.77
3	E	605	ANP	PB-O3A-PA	-3.71	119.54	132.62
3	A	601	ANP	O2'-C2'-C3'	3.70	123.79	111.82
3	C	603	ANP	O2'-C2'-C1'	3.70	124.52	110.85
3	A	601	ANP	N3-C2-N1	-3.69	122.91	128.68
3	F	606	ANP	O3'-C3'-C2'	3.68	123.72	111.82
3	B	602	ANP	O3'-C3'-C2'	3.64	123.60	111.82
3	C	603	ANP	O3'-C3'-C2'	3.62	123.53	111.82
3	E	605	ANP	O4'-C4'-C5'	3.61	121.24	109.37
3	E	605	ANP	O2'-C2'-C3'	3.60	123.48	111.82
3	F	606	ANP	PB-O3A-PA	-3.60	119.94	132.62
3	E	605	ANP	O3'-C3'-C2'	3.60	123.45	111.82
3	D	604	ANP	O4'-C4'-C5'	3.57	121.12	109.37
3	E	605	ANP	O2'-C2'-C1'	3.54	123.92	110.85
3	B	602	ANP	N3-C2-N1	-3.53	123.17	128.68
3	F	606	ANP	N3-C2-N1	-3.52	123.18	128.68
3	D	604	ANP	O2'-C2'-C1'	3.51	123.81	110.85
3	F	606	ANP	C2'-C3'-C4'	3.50	109.44	102.64
3	B	602	ANP	PB-O3A-PA	-3.49	120.33	132.62
3	A	601	ANP	O2'-C2'-C1'	3.47	123.65	110.85
3	D	604	ANP	PB-O3A-PA	-3.45	120.45	132.62
3	C	603	ANP	N3-C2-N1	-3.45	123.29	128.68
3	C	603	ANP	O2'-C2'-C3'	3.34	122.64	111.82
3	E	605	ANP	N3-C2-N1	-3.33	123.48	128.68
3	B	602	ANP	C2'-C3'-C4'	3.32	109.10	102.64
3	C	603	ANP	C2'-C3'-C4'	3.32	109.08	102.64
3	B	602	ANP	O2'-C2'-C1'	3.31	123.07	110.85
3	D	604	ANP	N3-C2-N1	-3.30	123.52	128.68
3	F	606	ANP	O2'-C2'-C1'	3.27	122.92	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	ANP	C2'-C3'-C4'	3.17	108.79	102.64
3	E	605	ANP	C2'-C3'-C4'	3.10	108.66	102.64
3	B	602	ANP	O2'-C2'-C3'	3.07	121.76	111.82
3	B	602	ANP	O2G-PG-O3G	3.02	115.67	107.64
3	D	604	ANP	C2'-C3'-C4'	3.00	108.47	102.64
3	B	602	ANP	O4'-C4'-C3'	2.98	111.02	105.11
3	A	601	ANP	PB-O3A-PA	-2.98	122.14	132.62
3	A	601	ANP	O2G-PG-O3G	2.97	115.54	107.64
3	A	601	ANP	C5'-C4'-C3'	2.95	126.22	115.18
3	F	606	ANP	O2G-PG-O3G	2.94	115.46	107.64
3	E	605	ANP	O2G-PG-O3G	2.86	115.26	107.64
3	E	605	ANP	O1B-PB-N3B	-2.83	107.60	111.77
3	D	604	ANP	O2G-PG-O3G	2.74	114.92	107.64
3	F	606	ANP	C5'-C4'-C3'	2.67	125.18	115.18
3	F	606	ANP	O2'-C2'-C3'	2.66	120.42	111.82
3	F	606	ANP	O4'-C4'-C3'	2.64	110.33	105.11
3	C	603	ANP	O4'-C4'-C3'	2.63	110.32	105.11
3	B	602	ANP	C5'-C4'-C3'	2.61	124.96	115.18
3	A	601	ANP	O4'-C4'-C3'	2.56	110.19	105.11
3	D	604	ANP	O4'-C4'-C3'	2.45	109.96	105.11
3	D	604	ANP	O1B-PB-N3B	-2.44	108.18	111.77
3	C	603	ANP	C5'-C4'-C3'	2.41	124.21	115.18
3	E	605	ANP	O4'-C4'-C3'	2.34	109.75	105.11
3	E	605	ANP	C5'-C4'-C3'	2.32	123.89	115.18
3	C	603	ANP	O2G-PG-O3G	2.23	113.57	107.64
3	F	606	ANP	O4'-C1'-C2'	2.20	110.14	106.93
3	B	602	ANP	O4'-C1'-C2'	2.20	110.14	106.93
3	D	604	ANP	C5'-C4'-C3'	2.10	123.07	115.18
3	A	601	ANP	C1'-N9-C4	-2.07	123.00	126.64

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	ANP	C3'
3	A	601	ANP	C2'
3	A	601	ANP	C4'
3	B	602	ANP	C3'
3	B	602	ANP	C1'
3	B	602	ANP	C4'
3	C	603	ANP	C3'
3	C	603	ANP	C2'
3	C	603	ANP	C4'

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Mol	Chain	Res	Type	Atom
3	D	604	ANP	C3'
3	D	604	ANP	C2'
3	E	605	ANP	C3'
3	E	605	ANP	C2'
3	F	606	ANP	C3'
3	F	606	ANP	C4'

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ANP	PB-N3B-PG-O1G
3	A	601	ANP	PG-N3B-PB-O1B
3	A	601	ANP	C3'-C4'-C5'-O5'
3	B	602	ANP	PG-N3B-PB-O1B
3	B	602	ANP	O4'-C4'-C5'-O5'
3	C	603	ANP	PG-N3B-PB-O1B
3	C	603	ANP	PG-N3B-PB-O3A
3	C	603	ANP	C5'-O5'-PA-O3A
3	D	604	ANP	PB-N3B-PG-O1G
3	D	604	ANP	PG-N3B-PB-O1B
3	D	604	ANP	PG-N3B-PB-O3A
3	D	604	ANP	PA-O3A-PB-O1B
3	D	604	ANP	PA-O3A-PB-O2B
3	E	605	ANP	PG-N3B-PB-O1B
3	E	605	ANP	PG-N3B-PB-O3A
3	E	605	ANP	C5'-O5'-PA-O2A
3	F	606	ANP	PB-N3B-PG-O1G
3	F	606	ANP	PG-N3B-PB-O3A
3	F	606	ANP	C5'-O5'-PA-O1A
3	F	606	ANP	C3'-C4'-C5'-O5'
3	A	601	ANP	O4'-C4'-C5'-O5'
3	C	603	ANP	O4'-C4'-C5'-O5'
3	D	604	ANP	C3'-C4'-C5'-O5'
3	F	606	ANP	O4'-C4'-C5'-O5'
3	E	605	ANP	C5'-O5'-PA-O3A
3	C	603	ANP	C5'-O5'-PA-O1A
3	C	603	ANP	C5'-O5'-PA-O2A
3	E	605	ANP	C5'-O5'-PA-O1A
3	B	602	ANP	C3'-C4'-C5'-O5'
3	B	602	ANP	C4'-C5'-O5'-PA
3	F	606	ANP	C4'-C5'-O5'-PA
3	C	603	ANP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	B	602	ANP	PB-O3A-PA-O1A
3	B	602	ANP	C5'-O5'-PA-O1A
3	E	605	ANP	C3'-C4'-C5'-O5'

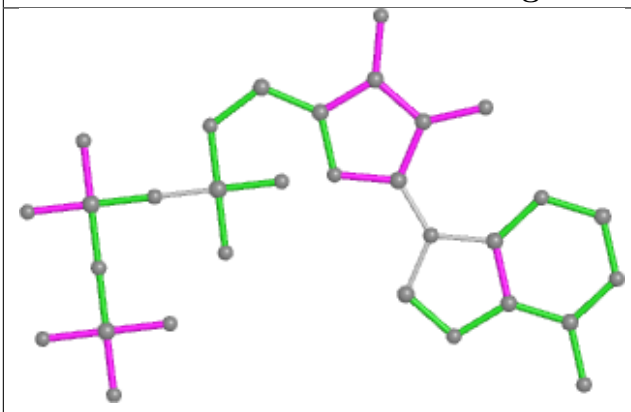
There are no ring outliers.

1 monomer is involved in 3 short contacts:

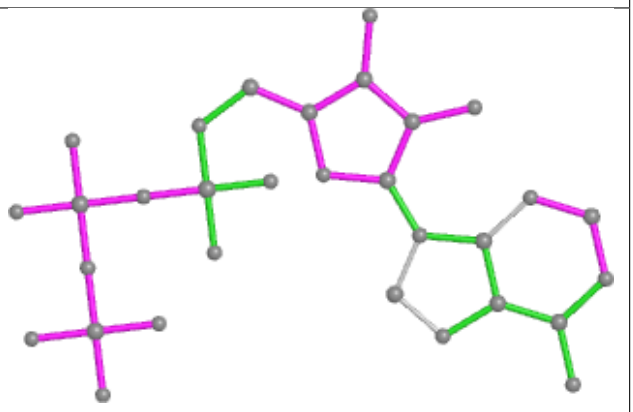
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ANP	3	0

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.

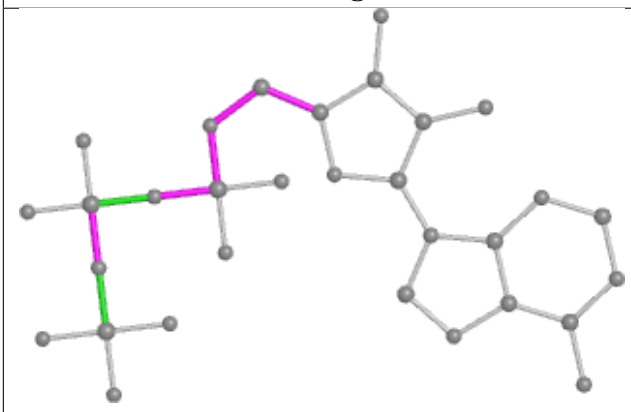
Ligand ANP B 602



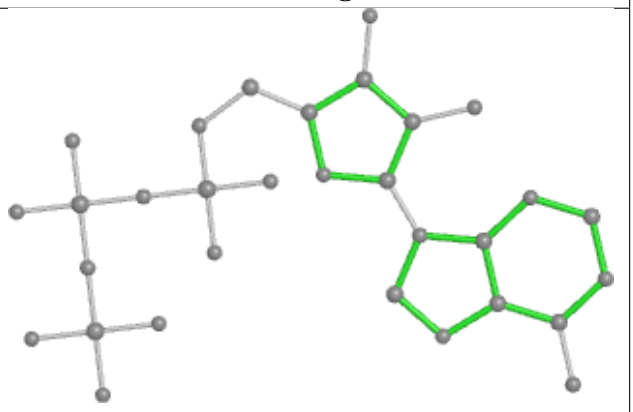
Bond lengths



Bond angles

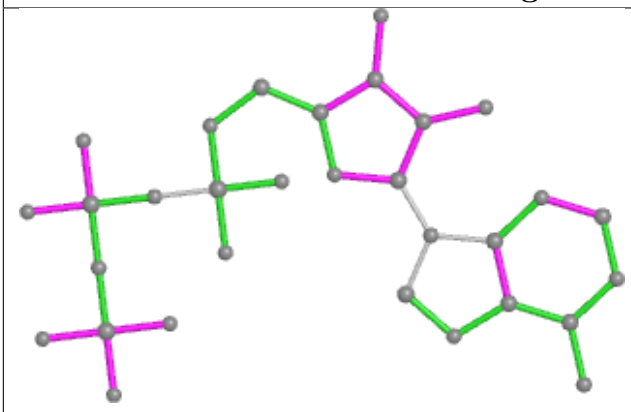


Torsions

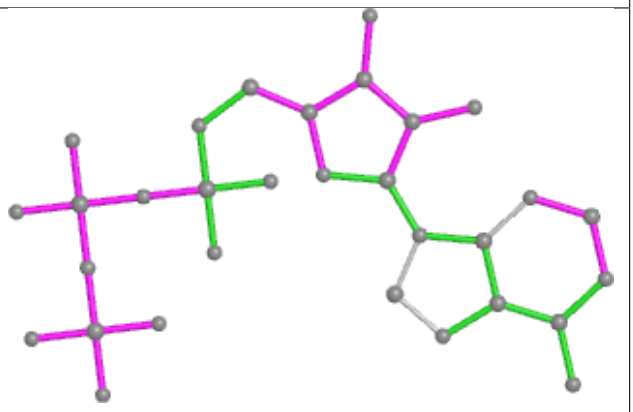


Rings

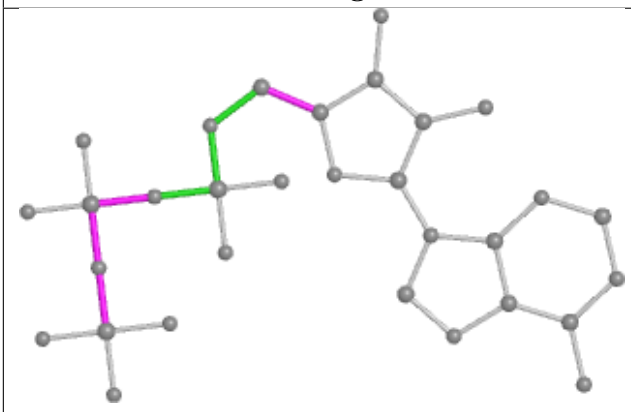
Ligand ANP D 604



Bond lengths



Bond angles



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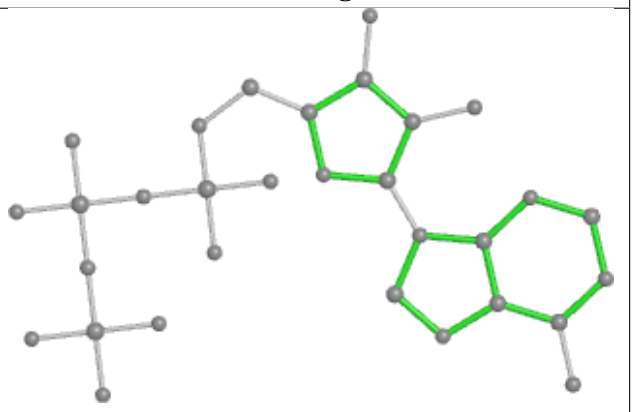
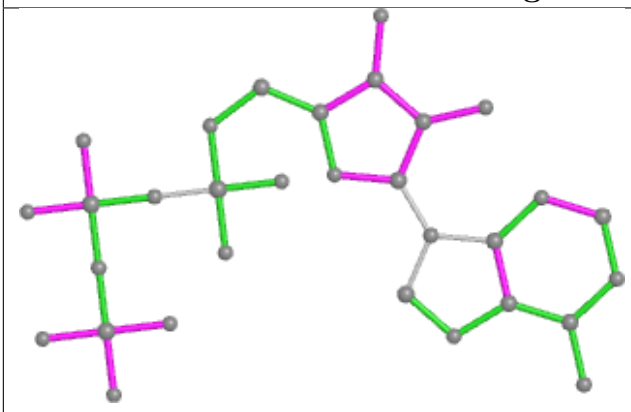
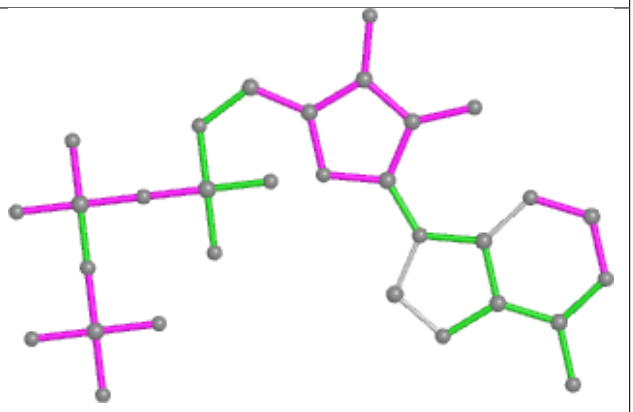


Rings

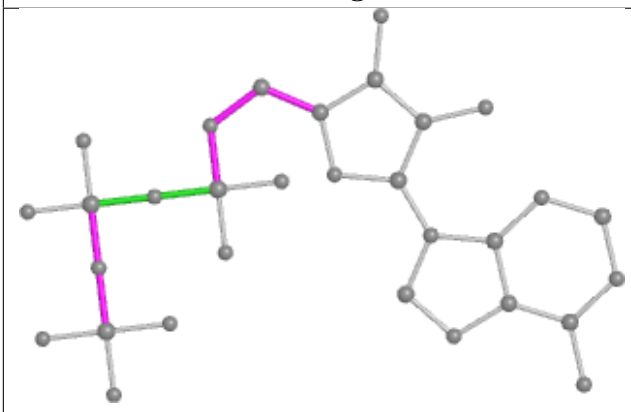
Ligand ANP F 606



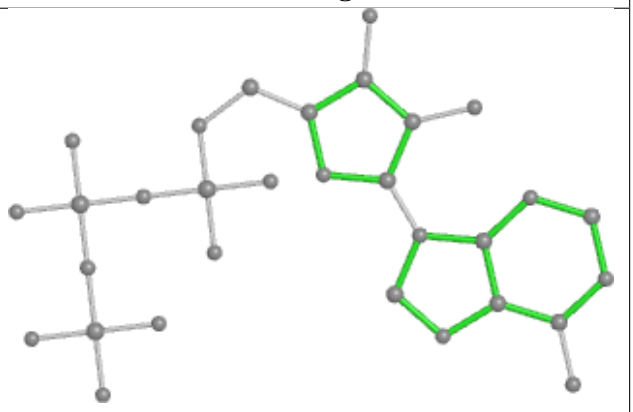
Bond lengths



Bond angles

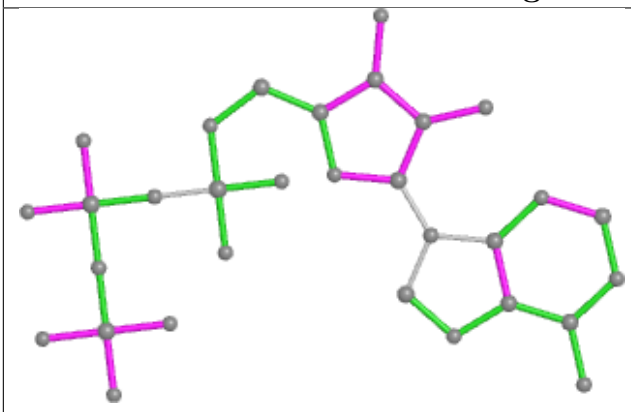


Torsions

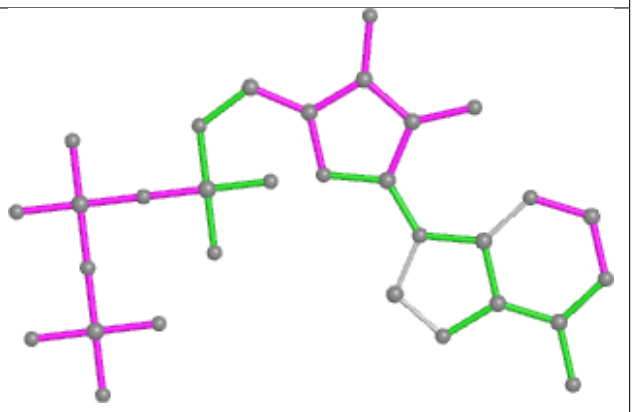


Rings

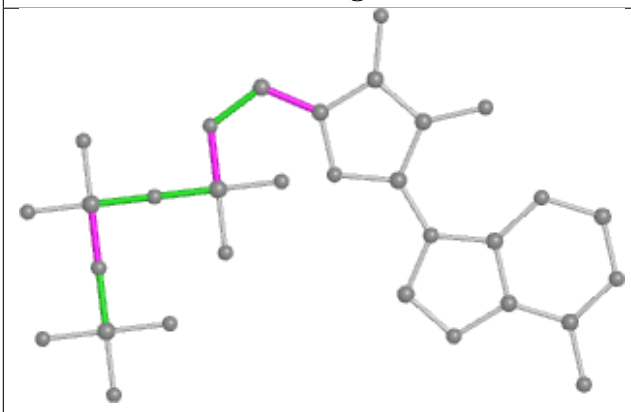
Ligand ANP E 605



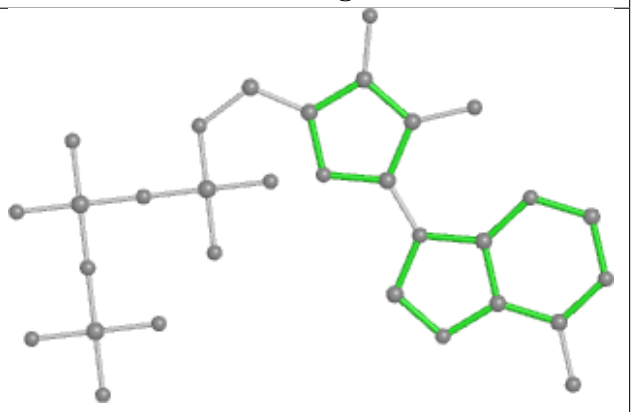
Bond lengths



Bond angles

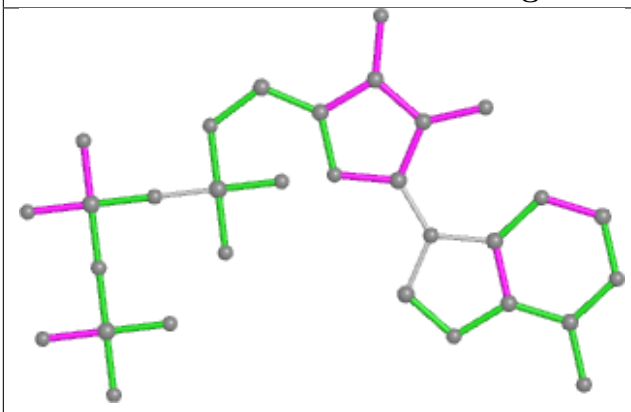


Torsions

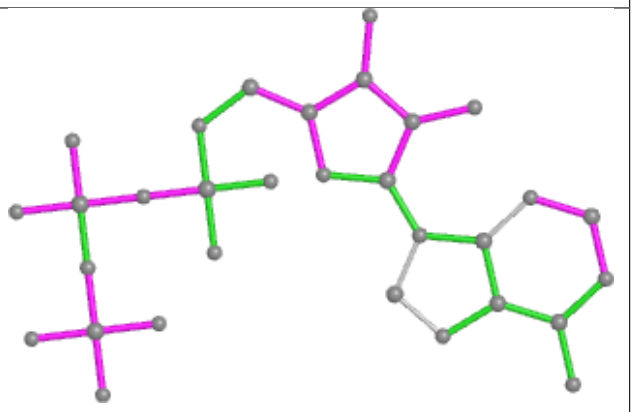


Rings

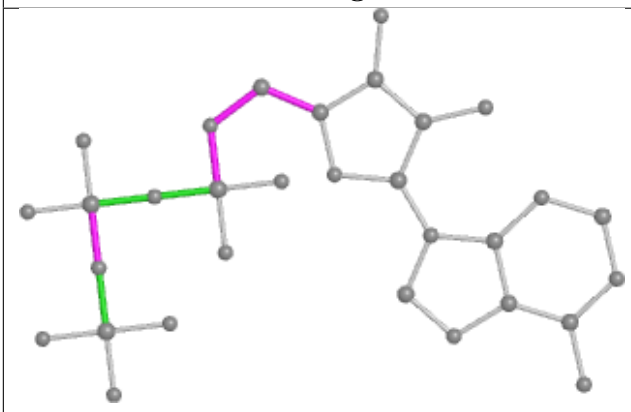
Ligand ANP C 603



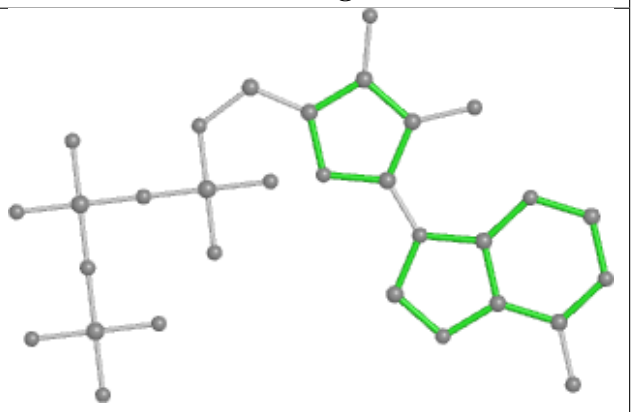
Bond lengths



Bond angles

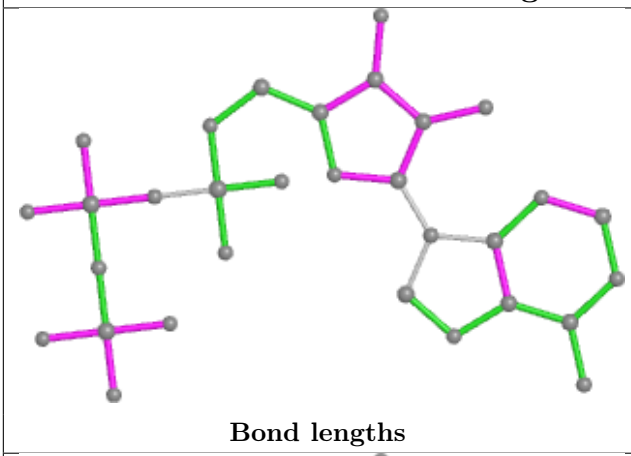


Torsions

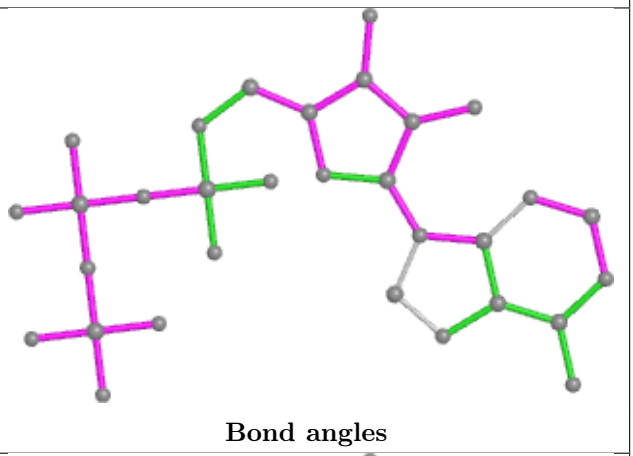


Rings

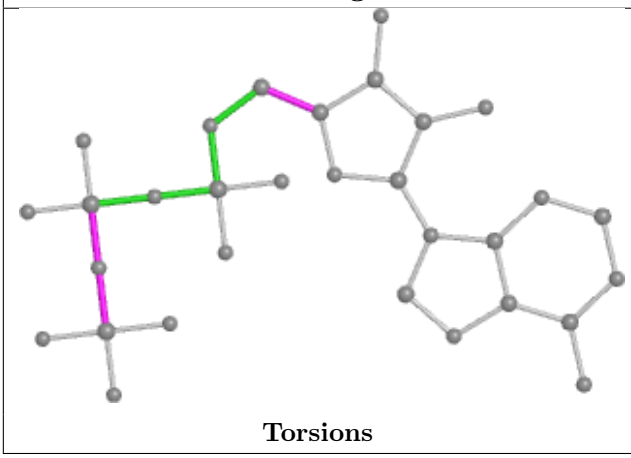
Ligand ANP A 601



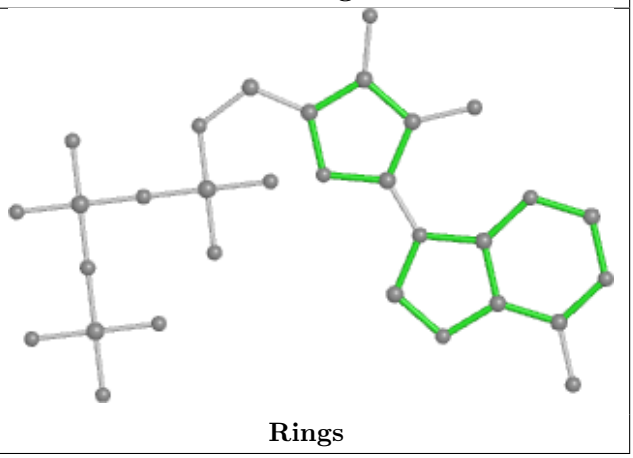
Bond lengths



Bond angles



Torsions



Rings

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	G	2/2 (100%)	1.31	0 100 100	150, 150, 150, 150	0
1	H	2/2 (100%)	2.53	2 (100%) 0 0	150, 150, 150, 150	0
1	J	2/2 (100%)	4.25	2 (100%) 0 0	150, 150, 150, 150	0
1	K	2/2 (100%)	3.93	2 (100%) 0 0	150, 150, 150, 150	0
1	L	2/2 (100%)	1.55	0 100 100	150, 150, 150, 150	0
2	A	408/419 (97%)	0.41	30 (7%) 14 4	42, 66, 114, 127	0
2	B	358/419 (85%)	0.53	37 (10%) 6 2	35, 65, 112, 127	0
2	C	408/419 (97%)	0.14	13 (3%) 47 20	20, 43, 96, 103	0
2	D	408/419 (97%)	0.14	12 (2%) 51 23	18, 46, 72, 124	0
2	E	407/419 (97%)	0.10	15 (3%) 41 17	21, 46, 85, 123	0
2	F	408/419 (97%)	0.32	26 (6%) 19 6	39, 65, 105, 119	0
All	All	2407/2524 (95%)	0.28	139 (5%) 23 7	18, 56, 104, 150	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	GLY	7.8
2	A	286	THR	6.1
2	A	412	PHE	6.1
2	B	88	ARG	6.0
1	K	2	C	5.7
2	B	75	GLY	5.6
2	A	129	ASN	5.5
2	C	417	LYS	5.2
2	A	141	ALA	5.2
2	B	106	GLU	5.2
2	D	355	PHE	5.2
2	A	417	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	J	2	C	4.9
2	B	414	GLU	4.7
2	B	86	ILE	4.6
2	E	46	GLY	4.4
2	F	25	ASN	4.4
2	B	84	SER	4.3
2	D	142	ASN	4.3
2	F	288	GLY	4.3
2	F	287	GLY	4.2
2	B	381	TRP	4.1
2	B	60	ASP	4.0
2	F	136	LEU	4.0
2	F	61	GLY	3.9
2	C	48	ASP	3.9
2	B	141	ALA	3.9
2	B	417	LYS	3.9
2	F	1	MET	3.7
2	A	355	PHE	3.7
2	B	114	LEU	3.7
1	J	1	U	3.6
2	C	406	THR	3.6
2	F	60	ASP	3.5
2	F	51	GLY	3.5
2	F	344	HIS	3.4
2	C	51	GLY	3.4
2	F	381	TRP	3.4
2	A	357	ALA	3.3
2	A	352	LYS	3.2
2	F	280	ALA	3.2
2	E	106	GLU	3.2
2	F	139	LEU	3.2
2	D	140	HIS	3.2
2	B	99	GLY	3.1
2	D	416	MET	3.1
2	D	412	PHE	3.1
2	D	59	GLN	3.1
2	A	279	PRO	3.0
2	B	113	LEU	3.0
2	B	90	ASN	3.0
2	F	413	PHE	3.0
2	F	196	ALA	3.0
2	E	60	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	322	ASP	3.0
2	A	406	THR	3.0
2	E	408	THR	2.9
2	F	406	THR	2.9
2	D	374	GLN	2.9
2	A	285	LEU	2.9
2	F	286	THR	2.9
2	A	408	THR	2.8
1	H	2	C	2.8
2	A	361	ASN	2.8
2	B	110	TYR	2.8
2	D	126	ASN	2.7
2	B	61	GLY	2.7
2	E	50	PHE	2.7
2	B	393	ILE	2.7
2	F	160	ARG	2.7
2	F	197	TYR	2.7
2	B	53	GLY	2.6
2	B	136	LEU	2.6
2	A	233	ASP	2.6
2	B	111	PHE	2.6
2	B	89	PHE	2.6
2	E	412	PHE	2.6
2	C	50	PHE	2.6
2	C	59	GLN	2.6
2	A	389	PRO	2.6
2	A	163	ASP	2.5
2	B	91	LEU	2.5
2	A	280	ALA	2.5
2	B	62	PHE	2.5
2	D	60	ASP	2.5
2	F	62	PHE	2.5
2	F	375	GLU	2.5
2	E	137	THR	2.5
2	A	405	MET	2.5
2	A	232	PHE	2.4
2	B	59	GLN	2.4
2	A	174	GLY	2.4
2	B	413	PHE	2.4
2	A	166	SER	2.4
2	A	197	TYR	2.4
2	B	412	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	47	GLU	2.3
2	B	123	LYS	2.3
2	A	342	GLU	2.3
2	C	155	GLU	2.3
2	F	103	PRO	2.3
2	D	115	LYS	2.3
2	B	406	THR	2.2
2	B	64	PHE	2.2
2	A	317	ALA	2.2
2	C	129	ASN	2.2
1	H	1	U	2.2
2	B	309	GLU	2.2
2	B	77	ASP	2.2
2	C	352	LYS	2.2
2	E	62	PHE	2.2
2	B	122	ASP	2.2
2	E	29	MET	2.2
2	A	351	GLU	2.2
2	E	61	GLY	2.2
1	K	1	U	2.2
2	B	317	ALA	2.2
2	E	197	TYR	2.2
2	F	279	PRO	2.2
2	F	140	HIS	2.2
2	C	279	PRO	2.1
2	E	280	ALA	2.1
2	F	45	SER	2.1
2	A	26	LEU	2.1
2	B	361	ASN	2.1
2	E	59	GLN	2.1
2	D	141	ALA	2.1
2	A	221	ARG	2.1
2	A	388	HIS	2.1
2	C	42	HIS	2.1
2	F	133	PHE	2.1
2	C	373	THR	2.1
2	D	292	ASN	2.1
2	B	247	ILE	2.1
2	A	316	ILE	2.1
2	C	110	TYR	2.0
2	B	76	PRO	2.0
2	F	307	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	45	SER	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)

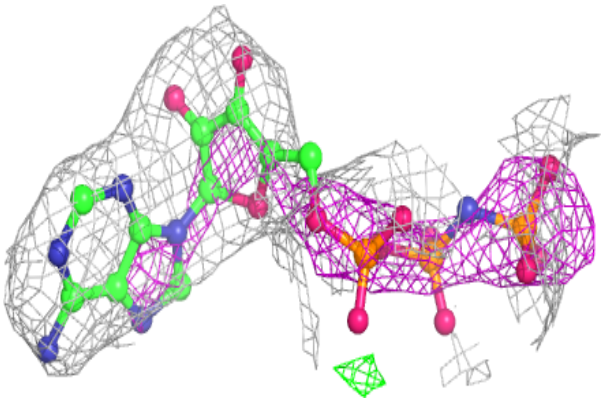
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

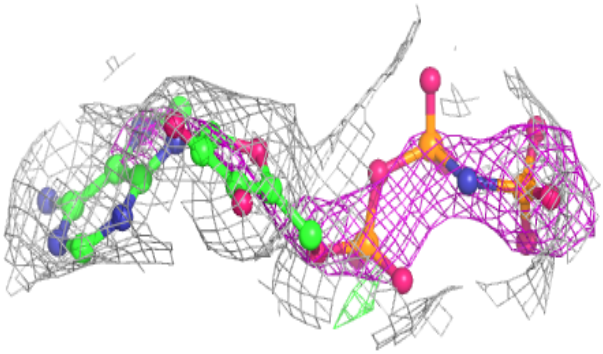
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANP	A	601	31/31	0.72	0.32	150,150,150,150	0
3	ANP	F	606	31/31	0.80	0.24	150,150,150,150	0
3	ANP	E	605	31/31	0.83	0.21	150,150,150,150	0
3	ANP	B	602	31/31	0.84	0.17	150,150,150,150	0
3	ANP	C	603	31/31	0.84	0.18	150,150,150,150	0
3	ANP	D	604	31/31	0.86	0.20	150,150,150,150	0

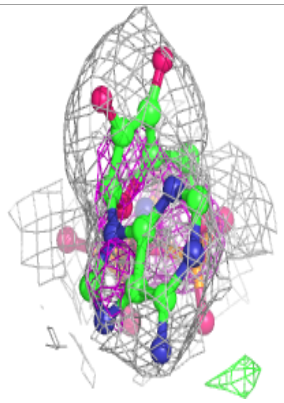
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 601:

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

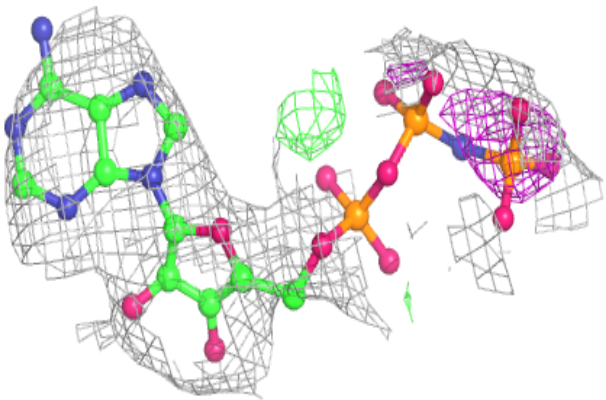


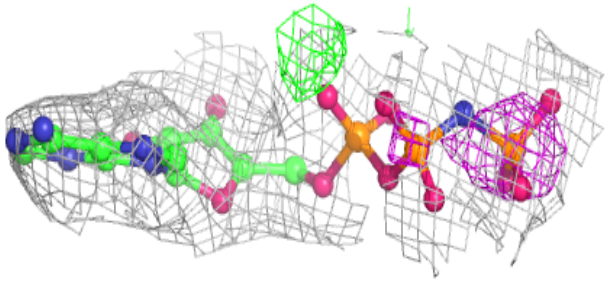


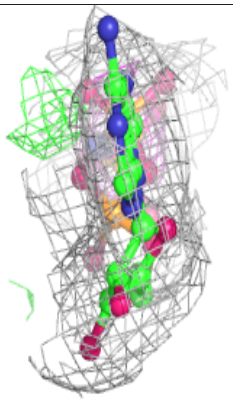


Electron density around ANP F 606:

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

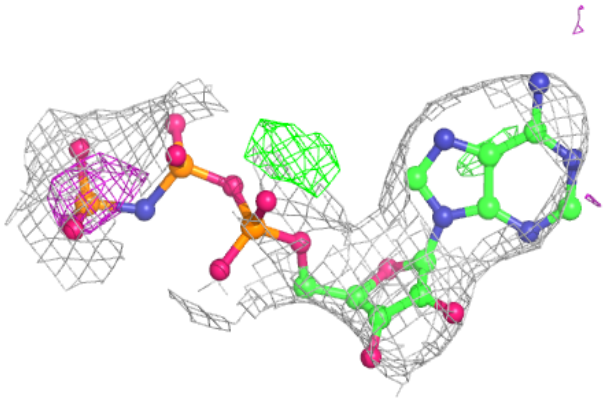


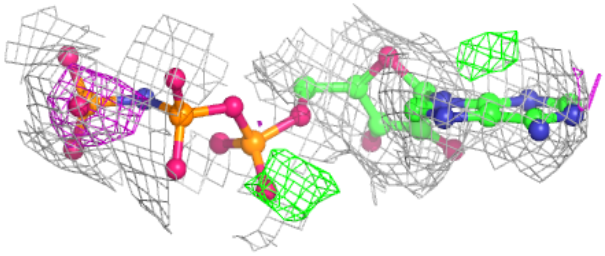


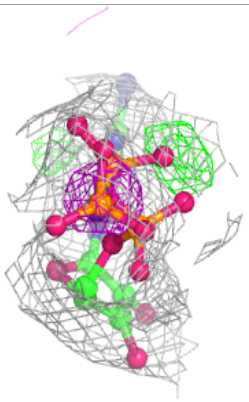


Electron density around ANP E 605:

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

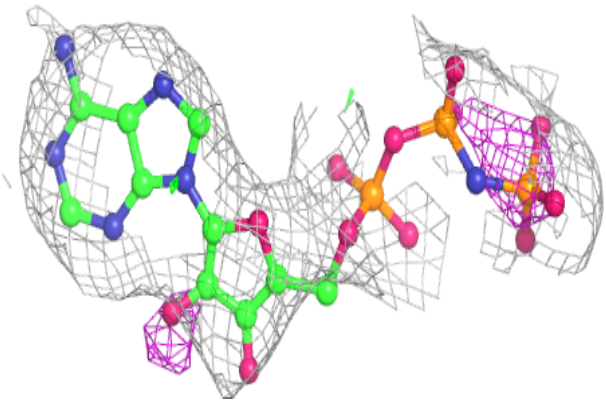


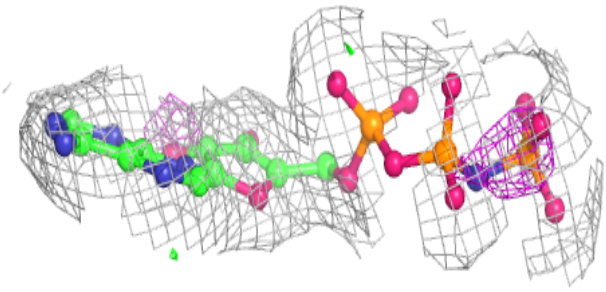


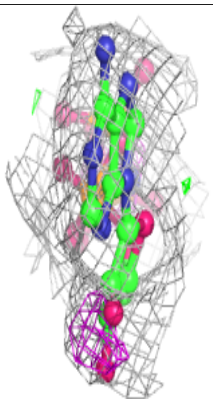


Electron density around ANP B 602:

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

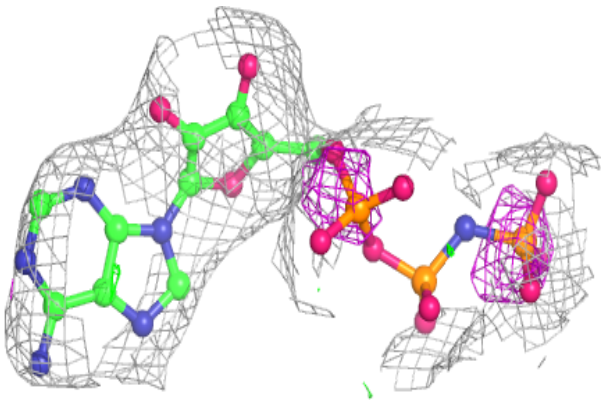


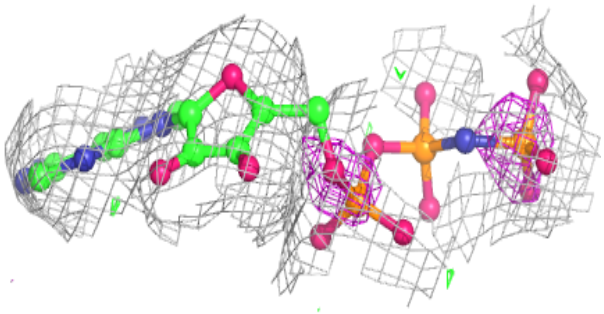


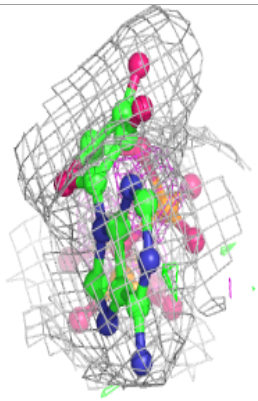


Electron density around ANP C 603:

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

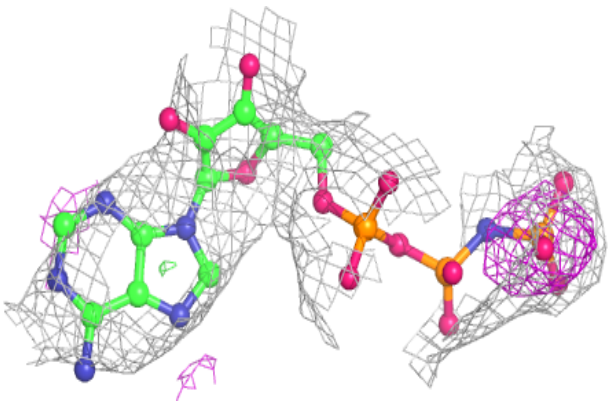


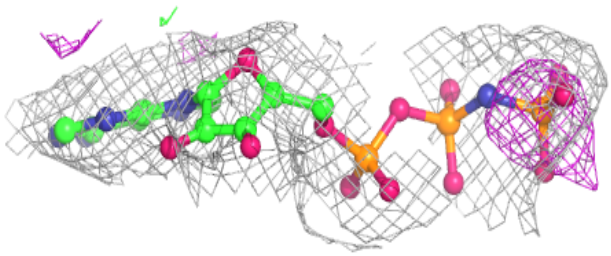


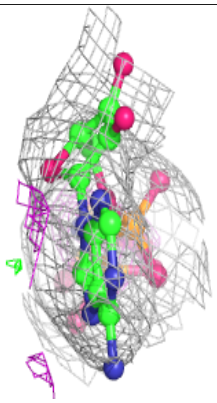


Electron density around ANP D 604:

$2mF_o$-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.