



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:06 PM UTC

PDB ID : 1PVO / pdb_00001pvo
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

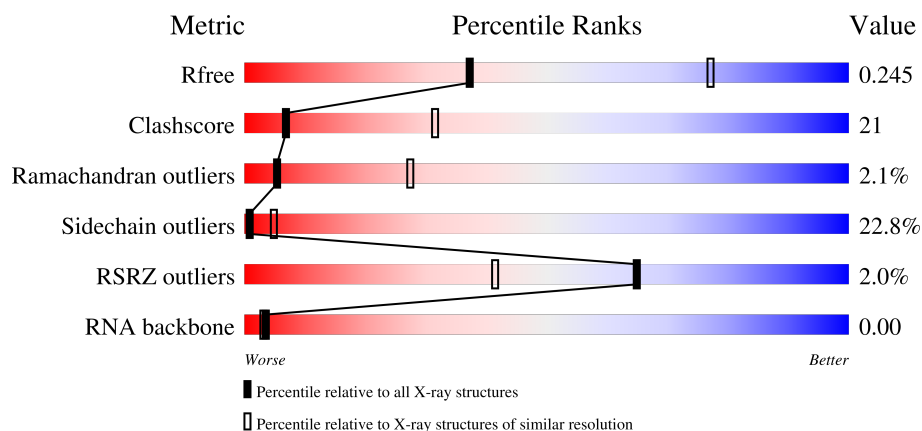
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	2	100%
1	H	2	100%
1	J	2	100%
1	K	2	50% 50%

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Mol	Chain	Length	Quality of chain
1	L	2	100%
2	A	419	% 53% 36% 9% .
2	B	419	3% 43% 31% 11% 15%
2	C	419	2% 50% 38% 8% . .
2	D	419	% 47% 39% 11% .
2	E	419	% 54% 35% 8% .
2	F	419	2% 50% 36% 10% . .

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	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

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.

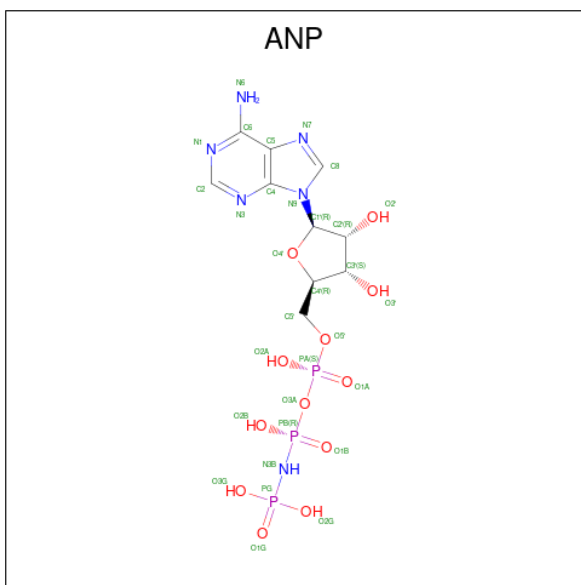
- Molecule 1 is a RNA chain called 5'-R(P*UP*C)-3'.

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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is water.

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

3 Residue-property plots

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

- Molecule 1: 5'-R(P*UP*C)-3'

Chain G:  100%

 U1 C2

- Molecule 1: 5'-R(P*UP*C)-3'

Chain H:  100%

 U1 C2

- Molecule 1: 5'-R(P*UP*C)-3'

Chain J:  100%
100%

 U1 C2

- Molecule 1: 5'-R(P*UP*C)-3'

Chain K:  100%
50% 50%

 U1 C2

- Molecule 1: 5'-R(P*UP*C)-3'

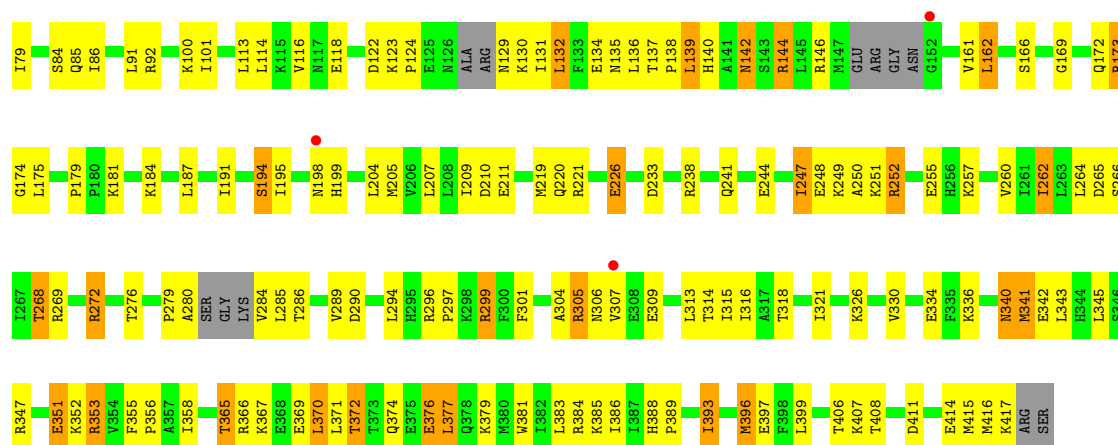
Chain L:  100%

 U1 C2

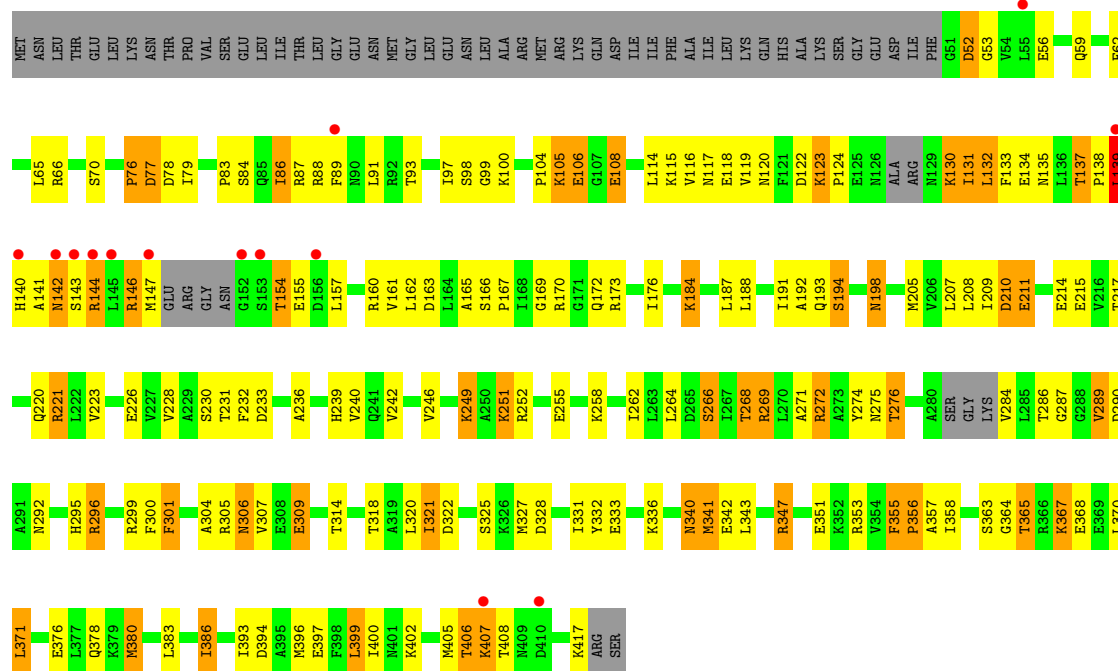
- Molecule 2: Transcription termination factor rho

Chain A:  %
53% 36% 9% .

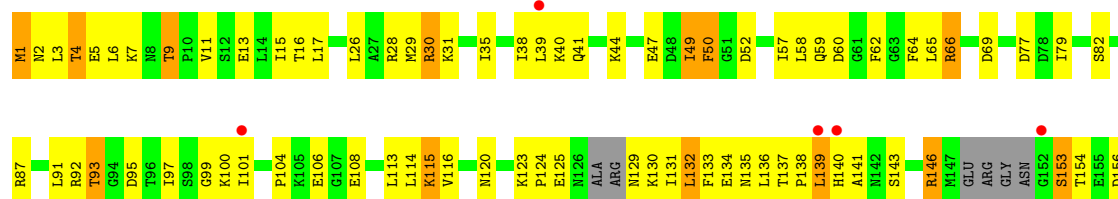
 K1 K2 K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60 K61 K62 K63 K64 K65 K66 K67 K68 K69 K70 K71

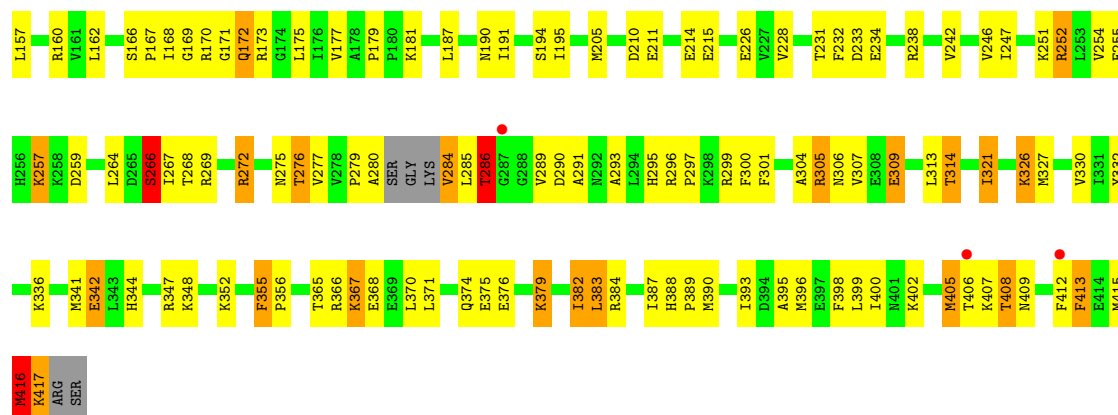


• Molecule 2: Transcription termination factor rho

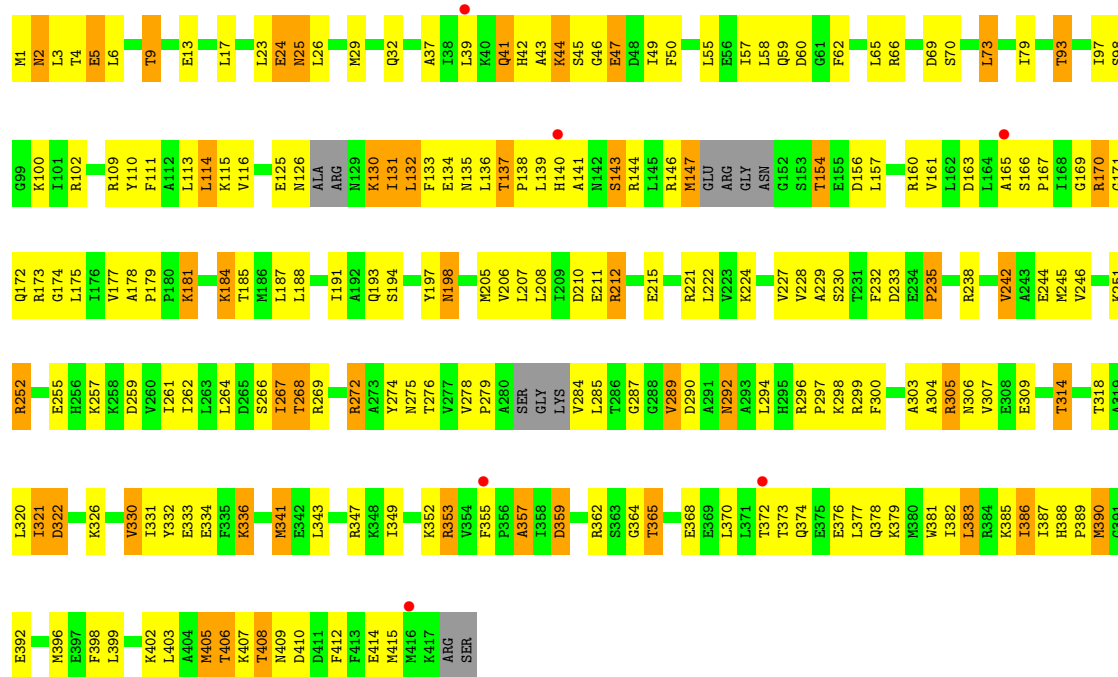


• Molecule 2: Transcription termination factor rho

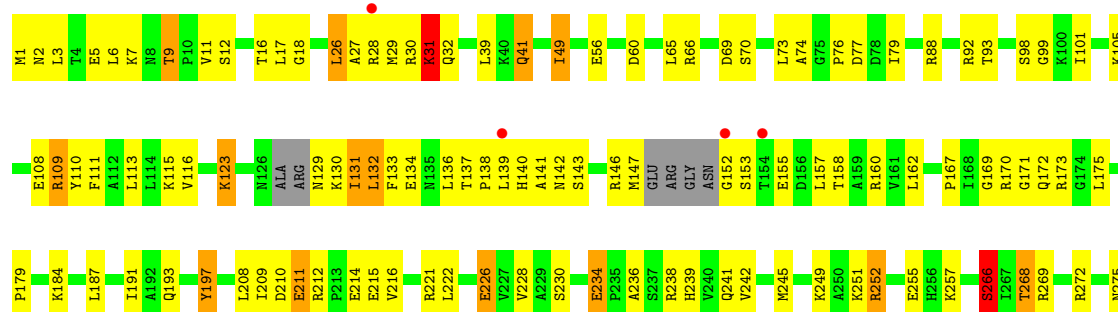




• Molecule 2: Transcription termination factor rho

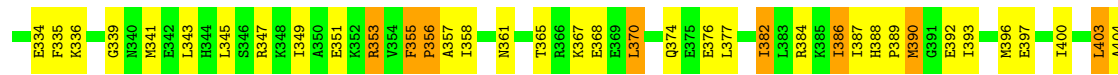
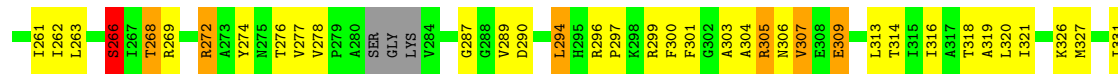
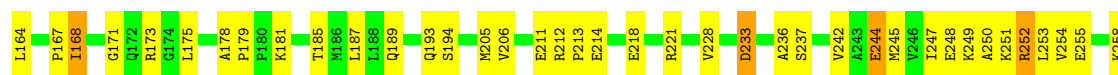
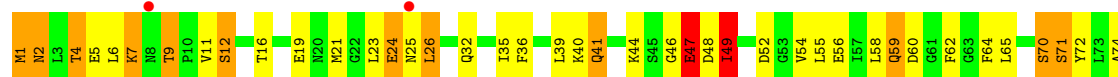


• Molecule 2: Transcription termination factor rho





• Molecule 2: Transcription termination factor rho



4 Data and refinement statistics

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 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.00) 96.1 (20.00-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 102.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/43	1.17	0/64
1	H	0.72	0/43	1.11	0/64
1	J	0.74	0/43	0.90	0/64
1	K	0.87	0/43	1.37	0/64
1	L	0.61	0/43	1.24	0/64
2	A	0.53	0/3253	0.87	0/4379
2	B	0.56	0/2854	0.89	0/3844
2	C	0.71	0/3253	0.98	2/4379 (0.0%)
2	D	0.63	0/3253	0.92	2/4379 (0.0%)
2	E	0.62	0/3246	0.92	3/4369 (0.1%)
2	F	0.52	0/3253	0.86	4/4379 (0.1%)
All	All	0.60	0/19327	0.91	11/26049 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	3
2	F	1	1
All	All	1	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	355	PHE	N-CA-C	8.12	127.77	109.81
2	D	408	THR	N-CA-C	5.95	117.44	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	25	ASN	N-CA-C	5.88	118.52	110.24
2	D	415	MET	N-CA-C	-5.64	108.19	114.62
2	E	99	GLY	N-CA-C	5.42	118.39	110.63
2	F	153	SER	N-CA-C	5.37	118.69	110.36
2	E	26	LEU	N-CA-C	5.27	117.10	111.36
2	C	293	ALA	N-CA-C	5.26	117.01	111.28
2	F	406	THR	N-CA-C	5.09	114.75	108.19
2	C	286	THR	N-CA-C	5.08	116.18	107.28
2	E	211	GLU	N-CA-C	5.00	117.85	110.59

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

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	123	0
2	B	2813	0	2870	133	0
2	C	3208	0	3284	162	0
2	D	3208	0	3284	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3201	0	3275	147	0
2	F	3208	0	3284	133	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	823	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 21.

All (823) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:147:MET:HE1	2:D:191:ILE:HG23	1.60	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:272:ARG:HD2	2:B:327:MET:HE2	1.59	0.81
2:B:140:HIS:CB	2:B:306:ASN:HB3	2.10	0.81
2:C:280:ALA:C	2:C:284:VAL:N	2.37	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:173:ARG:HH22	2:B:214:GLU:CD	2.02	0.67
2:B:141:ALA:O	2:B:142:ASN:C	2.37	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:A:41:GLN:C	2:A:43:ALA:H	2.03	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
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:A:252:ARG:NH1	2:A:255:GLU:CD	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:VAL:HG21	2:B:396:MET:HE1	1.79	0.63
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.79	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: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:43:ALA:C	2:A:45:SER:H	2.07	0.61
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
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:A:252:ARG:HH12	2:A:255:GLU:CD	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:ARG:NH1	2:C:304:ALA:O	2.34	0.61
2:C:106:GLU:C	2:C:108:GLU:H	2.07	0.60
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:F:142:ASN:O	2:F:143:SER:C	2.44	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: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:43:ALA:C	2:A:45:SER:N	2.61	0.59
2:A:173:ARG:H	2:A:340:ASN:ND2	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:275:ASN:HD22	2:B:327:MET:HE1	1.68	0.57
2:D:390:MET:HE1	2:D:398:PHE:CD2	2.39	0.57
2:E:160:ARG:HG2	2:E:408:THR:OG1	2.04	0.57
2:C:375:GLU:CD	2:C:375:GLU:H	2.12	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:F:46:GLY:C	2:F:48:ASP:H	2.12	0.57
2:F:403:LEU:C	2:F:405:MET:H	2.12	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:B:356:PRO:HB2	2:B:396:MET:HE2	1.86	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: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
2:E:356:PRO:HB2	2:E:396:MET:HE2	1.87	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: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: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: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:56:GLU:HG3	2:E:245:MET:HE1	1.88	0.55
2:E:197:TYR:C	2:E:197:TYR:CD2	2.84	0.55
2:F:138:PRO:C	2:F:140:HIS:H	2.14	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:161:VAL:HG21	2:D:396:MET:HE1	1.88	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:B:144:ARG:NH2	2:B:163:ASP:CG	2.65	0.54
2:A:41:GLN:C	2:A:43:ALA:N	2.65	0.54
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:F:46:GLY:C	2:F:47:GLU:HG3	2.32	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:B:275:ASN:ND2	2:B:327:MET:HE1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:ASP:OD1	2:D:292:ASN:CB	2.55	0.54
2:E:275:ASN:ND2	2:E:327:MET:HE1	2.22	0.54
2:A:374:GLN:HA	2:A:377:LEU:HD12	1.87	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
2:B:104:PRO:HA	2:B:108:GLU:OE1	2.07	0.54
2:B:356:PRO:C	2:B:358:ILE:H	2.16	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
1:K:2:C:H5	2:E:110:TYR:HH	1.54	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:C:205:MET:HE3	2:C:226:GLU:OE1	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
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:123:LYS:C	2:C:125:GLU:H	2.16	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:B:173:ARG:HH22	2:C:214:GLU:CD	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:272:ARG:HD2	2:C:327:MET:HE2	1.91	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: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
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:356:PRO:HB2	2:F:396:MET:HE2	1.92	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:E:173:ARG:HH22	2:F:214:GLU:CD	2.18	0.52
2:A:135:ASN:HB3	2:A:307:VAL:CG1	2.40	0.52
2:A:358:ILE:HB	2:A:396:MET:HE2	1.92	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:A:161:VAL:HG11	2:A:396:MET:HE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:GLU:O	2:D:25:ASN:C	2.52	0.51
2:E:368:GLU:HB3	2:E:377:LEU:HD11	1.92	0.51
2:F:58:LEU:C	2:F:60:ASP:H	2.19	0.51
2:A:266:SER:OG	2:A:269:ARG:HB2	2.10	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:105:LYS:O	2:B:106:GLU:C	2.54	0.50
2:B:340:ASN:ND2	2:C:214:GLU:OE2	2.42	0.50
2:F:4:THR:HB	2:F:52:ASP:OD1	2.10	0.50
2:A:356:PRO:HB2	2:A:396:MET:HE3	1.93	0.50
2:E:139:LEU:O	2:E:141:ALA:N	2.44	0.50
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:C:402:LYS:HA	2:C:405:MET:HE2	1.94	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:140:HIS:CA	2:A:306:ASN:HB3	2.40	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: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:295:HIS:HD2	2:C:233:ASP:O	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:290:ASP:C	2:B:290:ASP:OD1	2.54	0.49
2:C:140:HIS:CB	2:C:306:ASN:CB	2.90	0.49
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: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: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:C:390:MET:HE1	2:C:398:PHE:HB2	1.94	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: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:139:LEU:O	2:E:140:HIS:C	2.56	0.48
2:E:139:LEU:C	2:E:141:ALA:N	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:351:GLU:C	2:A:353:ARG:H	2.22	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
2:F:294:LEU:C	2:F:297:PRO:HD2	2.38	0.48
2:B:135:ASN:HB3	2:B:307:VAL:HG13	1.94	0.48
2:B:231:THR:C	2:B:233:ASP:N	2.69	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: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:138:PRO:C	2:B:140:HIS:H	2.23	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:F:147:MET:HE1	2:F:162:LEU:HD22	1.96	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: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:21:MET:HE1	2:A:38:ILE:HG23	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:106:GLU:C	2:C:108:GLU:N	2.73	0.47
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: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:B:341:MET:HE2	2:B:343:LEU:HB2	1.97	0.46
2:C:205:MET:HE2	2:C:246:VAL:HG13	1.96	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:F:19:GLU:C	2:F:21:MET:H	2.22	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: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:C:57:ILE:H	2:C:93:THR:HB	1.79	0.46
2:D:403:LEU:C	2:D:405:MET:H	2.24	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:C:146:ARG:HH21	2:C:376:GLU:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:173:ARG:NH2	2:B:214:GLU:CD	2.70	0.46
2:B:187:LEU:O	2:B:191:ILE:HD12	2.16	0.46
2:B:351:GLU:C	2:B:353:ARG:H	2.24	0.46
2:C:272:ARG:HD2	2:C:327:MET:CE	2.44	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:279:PRO:O	2:E:280:ALA:C	2.59	0.46
2:E:354:VAL:HG12	2:E:354:VAL:O	2.15	0.46
2:C:123:LYS:C	2:C:125:GLU:N	2.74	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
2:C:214:GLU:HG2	2:C:215:GLU:N	2.30	0.45
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: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:C:168:ILE:HD11	2:C:341:MET:HE3	1.99	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:B:146:ARG:HH12	2:B:376:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:339:GLY:C	2:F:341:MET:H	2.25	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:C:1:MET:HE2	2:C:1:MET:HB2	1.90	0.45
2:A:207:LEU:HD23	2:A:264:LEU:HD13	1.99	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:D:355:PHE:C	2:D:357:ALA:N	2.76	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:E:245:MET:CA	2:E:245:MET:HE2	2.47	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:B:138:PRO:C	2:B:140:HIS:N	2.75	0.44
2:C:138:PRO:C	2:C:140:HIS:H	2.26	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:D:131:ILE:O	2:D:132:LEU:C	2.60	0.44
2:E:137:THR:HG22	2:F:214:GLU:HB3	1.98	0.44
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:A:279:PRO:O	2:A:280:ALA:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:PHE:HZ	2:D:251:LYS:HZ3	1.58	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:335:PHE:O	2:F:336:LYS:C	2.61	0.44
2:F:403:LEU:O	2:F:405:MET:N	2.50	0.44
2:A:58:LEU:O	2:A:59:GLN:C	2.61	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:B:406:THR:OG1	2:B:407:LYS:N	2.46	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:161:VAL:CG2	2:D:396:MET:HE1	2.48	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
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: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:A:205:MET:HE3	2:A:260:VAL:CG1	2.47	0.43
2:E:132:LEU:HD22	2:E:251:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:294:LEU:C	2:E:297:PRO:HD2	2.44	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
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: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:D:146:ARG:C	2:D:147:MET:HG2	2.43	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:416:MET:HB3	2:C:417:LYS:H	1.70	0.43
2:A:139:LEU:HD13	2:A:367:LYS:HZ2	1.83	0.42
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.00	0.42
2:D:355:PHE:C	2:D:357:ALA:H	2.26	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:F:46:GLY:C	2:F:48:ASP:N	2.74	0.42
2:F:301:PHE:C	2:F:303:ALA:H	2.27	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
2:C:140:HIS:HA	2:C:306:ASN:HB2	2.00	0.42
2:E:140:HIS:HA	2:E:306:ASN:CG	2.44	0.42
2:B:205:MET:HE2	2:B:246:VAL:HG13	2.01	0.42
2:D:42:HIS:C	2:D:44:LYS:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:139:LEU:C	2:C:141:ALA:N	2.77	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:F:123:LYS:C	2:F:125:GLU:H	2.27	0.41
2:A:6:LEU:C	2:A:8:ASN:H	2.28	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
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:E:401:ASN:O	2:E:405:MET:HE3	2.19	0.41
2:C:285:LEU:C	2:C:286:THR:HG22	2.46	0.41
2:D:408:THR:HG23	2:D:409:ASN:N	2.35	0.41
2:F:266:SER:H	2:F:318:THR:HG1	1.65	0.41
2:A:28:ARG:HD3	2:A:28:ARG:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:49:ILE:O	2:C:50:PHE:C	2.63	0.41
2:C:286:THR:O	2:C:286:THR:OG1	2.29	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:F:403:LEU:C	2:F:405:MET:N	2.76	0.41
2:D:171:GLY:H	2:D:314:THR:HB	1.85	0.41
2:F:70:SER:O	2:F:71:SER:C	2.63	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: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:73:LEU:O	2:E:74:ALA:C	2.62	0.41
2:E:209:ILE:HG22	2:E:210:ASP:N	2.34	0.41
2:A:219:MET:HE2	2:A:219:MET:HB2	1.91	0.41
2:B:119:VAL:HG12	2:B:120:ASN:HD22	1.85	0.41
2:C:409:ASN:O	2:C:413:PHE:HB2	2.21	0.41
2:D:303:ALA:O	2:D:304:ALA:C	2.63	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
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:C:382:ILE:O	2:C:383:LEU:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:ILE:HG22	2:E:49:ILE:O	2.21	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:272:ARG:CD	2:B:327:MET:HE2	2.39	0.40
2:B:300:PHE:CD2	2:B:300:PHE:C	3.00	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:236:ALA:O	2:F:237:SER:C	2.64	0.40
2:F:303:ALA:O	2:F:313:LEU:HD23	2.22	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%)	16 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	350/419 (84%)	313 (89%)	25 (7%)	12 (3%)	3	17
2	C	400/419 (96%)	361 (90%)	32 (8%)	7 (2%)	6	31
2	D	400/419 (96%)	363 (91%)	27 (7%)	10 (2%)	4	23
2	E	399/419 (95%)	370 (93%)	25 (6%)	4 (1%)	12	45
2	F	400/419 (96%)	351 (88%)	35 (9%)	14 (4%)	3	16
All	All	2349/2514 (93%)	2125 (90%)	174 (7%)	50 (2%)	5	27

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
2	D	43	ALA
2	F	139	LEU
2	F	404	ALA

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Mol	Chain	Res	Type
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 ⓘ

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%)	259 (74%)	91 (26%)	0	3
2	B	306/359 (85%)	234 (76%)	72 (24%)	1	4
2	C	350/359 (98%)	274 (78%)	76 (22%)	1	6
2	D	350/359 (98%)	268 (77%)	82 (23%)	1	4
2	E	349/359 (97%)	279 (80%)	70 (20%)	1	7
2	F	350/359 (98%)	273 (78%)	77 (22%)	1	5
All	All	2055/2154 (95%)	1587 (77%)	468 (23%)	1	5

All (468) 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	11	VAL
2	A	12	SER
2	A	14	LEU
2	A	15	ILE
2	A	17	LEU
2	A	21	MET
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	85	GLN
2	A	92	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	134	GLU
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	199	HIS
2	A	209	ILE
2	A	211	GLU
2	A	220	GLN
2	A	221	ARG
2	A	226	GLU

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Mol	Chain	Res	Type
2	A	233	ASP
2	A	247	ILE
2	A	252	ARG
2	A	257	LYS
2	A	262	ILE
2	A	268	THR
2	A	272	ARG
2	A	276	THR
2	A	284	VAL
2	A	285	LEU
2	A	286	THR
2	A	289	VAL
2	A	290	ASP
2	A	299	ARG
2	A	305	ARG
2	A	309	GLU
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	372	THR
2	A	376	GLU
2	A	377	LEU
2	A	379	LYS
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	396	MET
2	A	397	GLU
2	A	399	LEU
2	A	406	THR
2	A	407	LYS

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Mol	Chain	Res	Type
2	A	408	THR
2	A	411	ASP
2	A	414	GLU
2	A	415	MET
2	A	416	MET
2	A	417	LYS
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	86	ILE
2	B	87	ARG
2	B	88	ARG
2	B	93	THR
2	B	100	LYS
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	139	LEU
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	184	LYS
2	B	193	GLN
2	B	194	SER
2	B	198	ASN
2	B	208	LEU
2	B	210	ASP
2	B	211	GLU
2	B	221	ARG

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Mol	Chain	Res	Type
2	B	249	LYS
2	B	251	LYS
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
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	309	GLU
2	B	314	THR
2	B	321	ILE
2	B	340	ASN
2	B	341	MET
2	B	347	ARG
2	B	365	THR
2	B	367	LYS
2	B	368	GLU
2	B	371	LEU
2	B	378	GLN
2	B	380	MET
2	B	383	LEU
2	B	386	ILE
2	B	393	ILE
2	B	394	ASP
2	B	397	GLU
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

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Mol	Chain	Res	Type
2	C	15	ILE
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	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
2	C	49	ILE
2	C	52	ASP
2	C	59	GLN
2	C	66	ARG
2	C	69	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	130	LYS
2	C	132	LEU
2	C	134	GLU
2	C	146	ARG
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

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Mol	Chain	Res	Type
2	C	284	VAL
2	C	286	THR
2	C	289	VAL
2	C	299	ARG
2	C	305	ARG
2	C	309	GLU
2	C	314	THR
2	C	321	ILE
2	C	326	LYS
2	C	336	LYS
2	C	342	GLU
2	C	347	ARG
2	C	348	LYS
2	C	352	LYS
2	C	367	LYS
2	C	374	GLN
2	C	379	LYS
2	C	382	ILE
2	C	383	LEU
2	C	384	ARG
2	C	393	ILE
2	C	396	MET
2	C	405	MET
2	C	408	THR
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	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	58	LEU
2	D	59	GLN

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Mol	Chain	Res	Type
2	D	69	ASP
2	D	70	SER
2	D	73	LEU
2	D	93	THR
2	D	98	SER
2	D	100	LYS
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	131	ILE
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
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	261	ILE
2	D	267	ILE
2	D	268	THR
2	D	272	ARG
2	D	276	THR
2	D	284	VAL
2	D	285	LEU

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Mol	Chain	Res	Type
2	D	289	VAL
2	D	296	ARG
2	D	299	ARG
2	D	305	ARG
2	D	309	GLU
2	D	314	THR
2	D	321	ILE
2	D	322	ASP
2	D	326	LYS
2	D	330	VAL
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	385	LYS
2	D	386	ILE
2	D	390	MET
2	D	392	GLU
2	D	399	LEU
2	D	405	MET
2	D	406	THR
2	E	9	THR
2	E	11	VAL
2	E	12	SER
2	E	16	THR
2	E	17	LEU
2	E	30	ARG
2	E	31	LYS
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

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Mol	Chain	Res	Type
2	E	115	LYS
2	E	123	LYS
2	E	131	ILE
2	E	132	LEU
2	E	146	ARG
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	226	GLU
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	318	THR
2	E	321	ILE
2	E	322	ASP
2	E	326	LYS
2	E	327	MET
2	E	341	MET
2	E	355	PHE
2	E	362	ARG
2	E	365	THR
2	E	368	GLU
2	E	369	GLU
2	E	372	THR
2	E	379	LYS
2	E	382	ILE

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Mol	Chain	Res	Type
2	E	385	LYS
2	E	386	ILE
2	E	393	ILE
2	E	396	MET
2	E	397	GLU
2	E	400	ILE
2	E	402	LYS
2	E	408	THR
2	E	411	ASP
2	E	414	GLU
2	E	415	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	32	GLN
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	71	SER
2	F	86	ILE
2	F	88	ARG
2	F	93	THR
2	F	106	GLU
2	F	114	LEU
2	F	115	LYS
2	F	122	ASP
2	F	123	LYS
2	F	125	GLU
2	F	126	ASN
2	F	134	GLU
2	F	136	LEU

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Mol	Chain	Res	Type
2	F	137	THR
2	F	139	LEU
2	F	144	ARG
2	F	160	ARG
2	F	162	LEU
2	F	168	ILE
2	F	173	ARG
2	F	233	ASP
2	F	242	VAL
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	307	VAL
2	F	309	GLU
2	F	321	ILE
2	F	326	LYS
2	F	334	GLU
2	F	347	ARG
2	F	351	GLU
2	F	353	ARG
2	F	368	GLU
2	F	370	LEU
2	F	374	GLN
2	F	376	GLU
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	403	LEU
2	F	406	THR
2	F	408	THR

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Mol	Chain	Res	Type
2	F	409	ASN
2	F	413	PHE
2	F	415	MET
2	F	416	MET
2	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	32	GLN
2	A	42	HIS
2	A	135	ASN
2	A	142	ASN
2	A	172	GLN
2	A	198	ASN
2	A	275	ASN
2	A	295	HIS
2	A	340	ASN
2	A	388	HIS
2	A	409	ASN
2	B	85	GLN
2	B	120	ASN
2	B	126	ASN
2	B	198	ASN
2	B	292	ASN
2	B	295	HIS
2	B	306	ASN
2	C	25	ASN
2	C	59	GLN
2	C	142	ASN
2	C	172	GLN
2	C	275	ASN
2	C	292	ASN
2	C	306	ASN
2	C	344	HIS
2	D	32	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

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Mol	Chain	Res	Type
2	E	135	ASN
2	E	190	ASN
2	E	193	GLN
2	E	295	HIS
2	E	306	ASN
2	E	344	HIS
2	F	41	GLN
2	F	90	ASN
2	F	142	ASN
2	F	189	GLN
2	F	344	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/2 (100%)	1 (50%)	1 (50%)
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 oligosaccharides 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	F	606	-	33,33,33	3.51	17 (51%)	45,52,52	3.31	25 (55%)
3	ANP	E	605	-	33,33,33	3.58	17 (51%)	45,52,52	3.32	26 (57%)
3	ANP	D	604	-	33,33,33	3.54	17 (51%)	45,52,52	3.33	26 (57%)
3	ANP	B	602	-	33,33,33	3.52	16 (48%)	45,52,52	3.37	26 (57%)
3	ANP	A	601	-	33,33,33	3.50	17 (51%)	45,52,52	3.33	28 (62%)
3	ANP	C	603	-	33,33,33	3.52	15 (45%)	45,52,52	3.27	25 (55%)

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	F	606	-	2/2/7/8	6/18/38/38	0/3/3/3
3	ANP	E	605	-	2/2/7/8	5/18/38/38	0/3/3/3
3	ANP	D	604	-	2/2/7/8	6/18/38/38	0/3/3/3
3	ANP	B	602	-	3/3/7/8	8/18/38/38	0/3/3/3
3	ANP	A	601	-	3/3/7/8	6/18/38/38	0/3/3/3
3	ANP	C	603	-	3/3/7/8	7/18/38/38	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604	ANP	O2'-C2'	-8.46	1.22	1.43
3	B	602	ANP	O3'-C3'	-8.44	1.22	1.43
3	E	605	ANP	O2'-C2'	-8.44	1.22	1.43
3	B	602	ANP	O2'-C2'	-8.43	1.22	1.43
3	C	603	ANP	O3'-C3'	-8.38	1.22	1.43
3	C	603	ANP	O2'-C2'	-8.37	1.22	1.43
3	E	605	ANP	O3'-C3'	-8.35	1.22	1.43
3	F	606	ANP	O2'-C2'	-8.28	1.22	1.43
3	D	604	ANP	O3'-C3'	-8.23	1.22	1.43
3	F	606	ANP	O3'-C3'	-8.22	1.22	1.43
3	A	601	ANP	O2'-C2'	-8.20	1.22	1.43
3	A	601	ANP	O3'-C3'	-8.14	1.22	1.43
3	E	605	ANP	C3'-C4'	-8.08	1.32	1.53
3	D	604	ANP	C3'-C4'	-8.04	1.32	1.53
3	C	603	ANP	C3'-C4'	-7.98	1.32	1.53
3	B	602	ANP	C3'-C4'	-7.91	1.32	1.53
3	E	605	ANP	C2'-C3'	-7.68	1.32	1.53
3	A	601	ANP	C3'-C4'	-7.68	1.33	1.53
3	C	603	ANP	C2'-C3'	-7.67	1.32	1.53
3	F	606	ANP	C3'-C4'	-7.66	1.33	1.53
3	F	606	ANP	C2'-C3'	-7.58	1.32	1.53
3	B	602	ANP	C2'-C3'	-7.54	1.32	1.53
3	D	604	ANP	C2'-C3'	-7.44	1.33	1.53
3	A	601	ANP	C2'-C3'	-7.27	1.33	1.53
3	E	605	ANP	C2'-C1'	-6.71	1.32	1.53
3	D	604	ANP	C2'-C1'	-6.58	1.32	1.53
3	F	606	ANP	C2'-C1'	-6.46	1.33	1.53
3	C	603	ANP	C2'-C1'	-6.44	1.33	1.53
3	A	601	ANP	C2'-C1'	-6.31	1.33	1.53
3	B	602	ANP	C2'-C1'	-6.29	1.33	1.53
3	F	606	ANP	C5-C4	4.75	1.47	1.39
3	B	602	ANP	C5-C4	4.67	1.47	1.39
3	A	601	ANP	C5-C4	4.67	1.47	1.39
3	E	605	ANP	C5-C4	4.67	1.47	1.39
3	D	604	ANP	C5-C4	4.55	1.47	1.39
3	C	603	ANP	C5-C4	4.52	1.47	1.39
3	A	601	ANP	PG-O1G	3.72	1.51	1.46
3	E	605	ANP	C1'-N9	-3.66	1.36	1.46
3	A	601	ANP	C1'-N9	-3.64	1.36	1.46
3	E	605	ANP	PG-O1G	3.61	1.51	1.46
3	D	604	ANP	PG-O1G	3.57	1.51	1.46
3	F	606	ANP	PG-O1G	3.54	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	ANP	PG-O1G	3.53	1.51	1.46
3	D	604	ANP	C1'-N9	-3.52	1.36	1.46
3	B	602	ANP	PG-O1G	3.51	1.51	1.46
3	F	606	ANP	C1'-N9	-3.48	1.36	1.46
3	C	603	ANP	C1'-N9	-3.29	1.37	1.46
3	F	606	ANP	PB-O1B	3.26	1.51	1.46
3	B	602	ANP	C1'-N9	-3.16	1.37	1.46
3	E	605	ANP	PB-O1B	3.11	1.50	1.46
3	A	601	ANP	PB-O1B	3.10	1.50	1.46
3	B	602	ANP	PB-O1B	3.08	1.50	1.46
3	C	603	ANP	PB-O1B	3.07	1.50	1.46
3	D	604	ANP	PB-O1B	3.01	1.50	1.46
3	A	601	ANP	C8-N7	2.73	1.36	1.31
3	A	601	ANP	C5-C6	2.72	1.48	1.41
3	B	602	ANP	C5-C6	2.67	1.48	1.41
3	E	605	ANP	C8-N7	2.63	1.36	1.31
3	B	602	ANP	C8-N7	2.62	1.36	1.31
3	F	606	ANP	C8-N7	2.62	1.36	1.31
3	F	606	ANP	C5-C6	2.61	1.48	1.41
3	D	604	ANP	C4-N9	-2.54	1.32	1.37
3	E	605	ANP	C4-N9	-2.53	1.32	1.37
3	D	604	ANP	C5-C6	2.52	1.48	1.41
3	E	605	ANP	C5-C6	2.52	1.48	1.41
3	C	603	ANP	C8-N7	2.52	1.36	1.31
3	D	604	ANP	C8-N7	2.51	1.36	1.31
3	A	601	ANP	PA-O3A	2.51	1.62	1.59
3	C	603	ANP	C5-C6	2.48	1.47	1.41
3	C	603	ANP	C5-N7	-2.45	1.34	1.39
3	C	603	ANP	C4-N9	-2.41	1.32	1.37
3	B	602	ANP	PG-O3G	-2.38	1.50	1.56
3	D	604	ANP	C5-N7	-2.35	1.34	1.39
3	A	601	ANP	C4-N9	-2.35	1.32	1.37
3	B	602	ANP	C4-N9	-2.35	1.32	1.37
3	D	604	ANP	PG-O3G	-2.33	1.50	1.56
3	E	605	ANP	PG-O3G	-2.33	1.50	1.56
3	F	606	ANP	PG-O2G	-2.30	1.50	1.56
3	F	606	ANP	PG-O3G	-2.30	1.50	1.56
3	F	606	ANP	PB-O2B	-2.30	1.50	1.56
3	A	601	ANP	PB-O3A	2.30	1.61	1.59
3	D	604	ANP	PG-O2G	-2.30	1.50	1.56
3	E	605	ANP	PG-O2G	-2.29	1.50	1.56
3	D	604	ANP	C8-N9	-2.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ANP	PG-O2G	-2.27	1.50	1.56
3	E	605	ANP	C5-N7	-2.27	1.34	1.39
3	B	602	ANP	PG-O2G	-2.25	1.50	1.56
3	A	601	ANP	PG-O3G	-2.25	1.50	1.56
3	D	604	ANP	PB-O2B	-2.21	1.50	1.56
3	F	606	ANP	C4-N9	-2.21	1.33	1.37
3	F	606	ANP	C5-N7	-2.21	1.35	1.39
3	C	603	ANP	PB-O2B	-2.19	1.51	1.56
3	E	605	ANP	C8-N9	-2.17	1.33	1.37
3	B	602	ANP	C5-N7	-2.17	1.35	1.39
3	C	603	ANP	C8-N9	-2.16	1.33	1.37
3	E	605	ANP	PB-O2B	-2.15	1.51	1.56
3	B	602	ANP	PB-O2B	-2.08	1.51	1.56
3	F	606	ANP	C8-N9	-2.06	1.34	1.37
3	A	601	ANP	PB-O2B	-2.06	1.51	1.56

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ANP	C4-N9-C8	8.38	114.54	105.74
3	E	605	ANP	C4-N9-C8	8.14	114.29	105.74
3	D	604	ANP	C4-N9-C8	8.03	114.17	105.74
3	F	606	ANP	C4-N9-C8	7.90	114.04	105.74
3	B	602	ANP	C4-N9-C8	7.71	113.83	105.74
3	C	603	ANP	C4-N9-C8	7.70	113.82	105.74
3	B	602	ANP	O4'-C1'-N9	7.36	122.23	108.09
3	D	604	ANP	O4'-C1'-N9	7.31	122.12	108.09
3	C	603	ANP	O4'-C1'-N9	7.12	121.77	108.09
3	F	606	ANP	O4'-C1'-N9	7.09	121.70	108.09
3	E	605	ANP	O4'-C1'-N9	6.99	121.51	108.09
3	F	606	ANP	N3-C4-N9	6.24	137.79	127.17
3	E	605	ANP	N3-C4-N9	6.22	137.75	127.17
3	C	603	ANP	N3-C4-N9	6.11	137.55	127.17
3	D	604	ANP	N3-C4-N9	6.06	137.48	127.17
3	B	602	ANP	N3-C4-N9	6.05	137.46	127.17
3	A	601	ANP	N3-C4-N9	6.04	137.44	127.17
3	B	602	ANP	C2'-C1'-N9	5.55	127.10	113.30
3	A	601	ANP	O1G-PG-N3B	-5.46	103.73	111.77
3	A	601	ANP	N9-C8-N7	-5.23	106.51	113.94
3	E	605	ANP	C4'-O4'-C1'	-5.22	97.93	109.47
3	D	604	ANP	C4'-O4'-C1'	-5.15	98.09	109.47
3	D	604	ANP	O1G-PG-N3B	-5.10	104.26	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	ANP	C5-C4-N3	-5.09	119.71	126.72
3	E	605	ANP	C5-C4-N3	-5.07	119.73	126.72
3	F	606	ANP	C5-C4-N3	-5.06	119.75	126.72
3	B	602	ANP	C5-C4-N3	-5.04	119.77	126.72
3	D	604	ANP	N9-C8-N7	-5.01	106.83	113.94
3	D	604	ANP	C5-C4-N3	-5.00	119.84	126.72
3	E	605	ANP	N9-C8-N7	-4.97	106.89	113.94
3	A	601	ANP	O3'-C3'-C4'	4.93	125.25	111.08
3	A	601	ANP	O4'-C1'-N9	4.87	117.44	108.09
3	F	606	ANP	O1G-PG-N3B	-4.86	104.62	111.77
3	F	606	ANP	C4'-O4'-C1'	-4.84	98.78	109.47
3	C	603	ANP	N9-C8-N7	-4.83	107.08	113.94
3	C	603	ANP	C4'-O4'-C1'	-4.83	98.81	109.47
3	F	606	ANP	N9-C8-N7	-4.83	107.09	113.94
3	A	601	ANP	C5-C4-N3	-4.82	120.09	126.72
3	F	606	ANP	O3'-C3'-C4'	4.81	124.90	111.08
3	B	602	ANP	N9-C8-N7	-4.80	107.13	113.94
3	B	602	ANP	O2B-PB-O1B	4.73	120.02	109.87
3	F	606	ANP	O4'-C4'-C5'	4.70	124.40	109.33
3	E	605	ANP	O1G-PG-N3B	-4.70	104.85	111.77
3	C	603	ANP	O3'-C3'-C4'	4.67	124.50	111.08
3	E	605	ANP	O3'-C3'-C4'	4.67	124.50	111.08
3	E	605	ANP	O2B-PB-O1B	4.65	119.84	109.87
3	B	602	ANP	C4'-O4'-C1'	-4.60	99.32	109.47
3	D	604	ANP	O3'-C3'-C4'	4.59	124.27	111.08
3	C	603	ANP	O4'-C4'-C5'	4.53	123.84	109.33
3	A	601	ANP	C3'-C2'-C1'	4.40	109.79	101.46
3	F	606	ANP	C2'-C1'-N9	4.40	124.23	113.30
3	B	602	ANP	O1G-PG-N3B	-4.39	105.30	111.77
3	C	603	ANP	C3'-C2'-C1'	4.35	109.70	101.46
3	B	602	ANP	O3'-C3'-C4'	4.33	123.52	111.08
3	C	603	ANP	C2'-C1'-N9	4.32	124.04	113.30
3	B	602	ANP	O4'-C4'-C5'	4.26	122.99	109.33
3	D	604	ANP	C2'-C1'-N9	4.25	123.88	113.30
3	A	601	ANP	C4'-O4'-C1'	-4.25	100.08	109.47
3	B	602	ANP	C3'-C2'-C1'	4.24	109.48	101.46
3	C	603	ANP	O1G-PG-N3B	-4.23	105.54	111.77
3	D	604	ANP	O2B-PB-O1B	4.22	118.92	109.87
3	F	606	ANP	O2B-PB-O1B	4.19	118.86	109.87
3	C	603	ANP	O2'-C2'-C1'	4.19	124.52	110.10
3	A	601	ANP	O2B-PB-O1B	4.17	118.81	109.87
3	D	604	ANP	C3'-C2'-C1'	4.17	109.34	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ANP	O3'-C3'-C2'	4.14	125.07	111.82
3	C	603	ANP	O2B-PB-O1B	4.11	118.69	109.87
3	A	601	ANP	O4'-C4'-C5'	4.11	122.49	109.33
3	E	605	ANP	C3'-C2'-C1'	4.10	109.22	101.46
3	E	605	ANP	O2'-C2'-C1'	4.01	123.92	110.10
3	D	604	ANP	O2'-C2'-C1'	3.98	123.81	110.10
3	A	601	ANP	O2'-C2'-C1'	3.94	123.65	110.10
3	D	604	ANP	O3'-C3'-C2'	3.90	124.31	111.82
3	A	601	ANP	O1B-PB-N3B	-3.84	106.12	111.77
3	D	604	ANP	O2'-C2'-C3'	3.81	124.02	111.82
3	B	602	ANP	O2'-C2'-C1'	3.77	123.07	110.10
3	F	606	ANP	C3'-C2'-C1'	3.75	108.56	101.46
3	A	601	ANP	N3-C2-N1	-3.75	122.91	128.58
3	B	602	ANP	O1B-PB-N3B	-3.74	106.26	111.77
3	A	601	ANP	O2'-C2'-C3'	3.74	123.79	111.82
3	A	601	ANP	C2'-C1'-N9	3.73	122.58	113.30
3	F	606	ANP	O2'-C2'-C1'	3.72	122.92	110.10
3	E	605	ANP	O4'-C4'-C5'	3.72	121.24	109.33
3	F	606	ANP	O3'-C3'-C2'	3.71	123.72	111.82
3	D	604	ANP	O4'-C4'-C5'	3.68	121.12	109.33
3	B	602	ANP	O3'-C3'-C2'	3.67	123.60	111.82
3	E	605	ANP	C2'-C1'-N9	3.66	122.41	113.30
3	C	603	ANP	O3'-C3'-C2'	3.65	123.53	111.82
3	E	605	ANP	O2'-C2'-C3'	3.64	123.48	111.82
3	E	605	ANP	O3'-C3'-C2'	3.63	123.45	111.82
3	A	601	ANP	C2-N3-C4	3.61	120.65	111.83
3	B	602	ANP	N3-C2-N1	-3.58	123.17	128.58
3	B	602	ANP	C2-N3-C4	3.57	120.56	111.83
3	F	606	ANP	N3-C2-N1	-3.57	123.18	128.58
3	F	606	ANP	C2-N3-C4	3.54	120.48	111.83
3	F	606	ANP	C2'-C3'-C4'	3.54	109.44	102.61
3	C	603	ANP	C2-N3-C4	3.50	120.39	111.83
3	C	603	ANP	N3-C2-N1	-3.50	123.29	128.58
3	E	605	ANP	C2-N3-C4	3.45	120.26	111.83
3	D	604	ANP	C2-N3-C4	3.42	120.19	111.83
3	D	604	ANP	C5-N7-C8	3.38	108.76	103.45
3	C	603	ANP	O2'-C2'-C3'	3.38	122.64	111.82
3	E	605	ANP	N3-C2-N1	-3.37	123.48	128.58
3	A	601	ANP	C5-N7-C8	3.37	108.75	103.45
3	B	602	ANP	C2'-C3'-C4'	3.36	109.10	102.61
3	C	603	ANP	C2'-C3'-C4'	3.35	109.08	102.61
3	D	604	ANP	N3-C2-N1	-3.35	123.52	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	ANP	C5-N7-C8	3.28	108.61	103.45
3	F	606	ANP	C5-N7-C8	3.24	108.54	103.45
3	E	605	ANP	C5-N7-C8	3.23	108.52	103.45
3	B	602	ANP	C5-N7-C8	3.22	108.52	103.45
3	A	601	ANP	C2'-C3'-C4'	3.20	108.79	102.61
3	E	605	ANP	C2'-C3'-C4'	3.13	108.66	102.61
3	B	602	ANP	O2'-C2'-C3'	3.10	121.76	111.82
3	A	601	ANP	C5-C4-N9	-3.10	102.44	105.81
3	F	606	ANP	C5-C4-N9	-3.07	102.46	105.81
3	A	601	ANP	C5'-C4'-C3'	3.06	126.22	115.21
3	D	604	ANP	C2'-C3'-C4'	3.03	108.47	102.61
3	E	605	ANP	C5-C4-N9	-3.02	102.52	105.81
3	B	602	ANP	O2G-PG-O3G	3.01	115.67	107.59
3	A	601	ANP	O2G-PG-O3G	2.96	115.54	107.59
3	B	602	ANP	O4'-C4'-C3'	2.95	111.02	105.15
3	F	606	ANP	O2G-PG-O3G	2.93	115.46	107.59
3	D	604	ANP	C5-C4-N9	-2.87	102.69	105.81
3	E	605	ANP	O2G-PG-O3G	2.86	115.26	107.59
3	E	605	ANP	O1B-PB-N3B	-2.83	107.60	111.77
3	C	603	ANP	C5-C4-N9	-2.82	102.74	105.81
3	E	605	ANP	C1'-N9-C8	-2.79	120.90	127.09
3	B	602	ANP	C5-C4-N9	-2.79	102.77	105.81
3	F	606	ANP	C5'-C4'-C3'	2.77	125.18	115.21
3	D	604	ANP	O2G-PG-O3G	2.73	114.92	107.59
3	B	602	ANP	C1'-N9-C8	-2.72	121.06	127.09
3	B	602	ANP	C5'-C4'-C3'	2.71	124.96	115.21
3	C	603	ANP	C1'-N9-C8	-2.69	121.12	127.09
3	F	606	ANP	O2'-C2'-C3'	2.68	120.42	111.82
3	F	606	ANP	C1'-N9-C8	-2.67	121.18	127.09
3	D	604	ANP	C4-C5-N7	-2.66	107.55	110.58
3	F	606	ANP	O4'-C4'-C3'	2.61	110.33	105.15
3	C	603	ANP	O4'-C4'-C3'	2.60	110.32	105.15
3	D	604	ANP	C1'-N9-C8	-2.58	121.37	127.09
3	A	601	ANP	O4'-C4'-C3'	2.54	110.19	105.15
3	A	601	ANP	C4-C5-N7	-2.52	107.70	110.58
3	C	603	ANP	C5'-C4'-C3'	2.50	124.21	115.21
3	C	603	ANP	C4-C5-N7	-2.48	107.75	110.58
3	B	602	ANP	C4-C5-N7	-2.47	107.75	110.58
3	E	605	ANP	C4-C5-N7	-2.45	107.78	110.58
3	D	604	ANP	O1B-PB-N3B	-2.44	108.18	111.77
3	D	604	ANP	O4'-C4'-C3'	2.42	109.96	105.15
3	E	605	ANP	C5'-C4'-C3'	2.41	123.89	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	606	ANP	C4-C5-N7	-2.37	107.87	110.58
3	E	605	ANP	O4'-C4'-C3'	2.32	109.75	105.15
3	C	603	ANP	O2G-PG-O3G	2.23	113.57	107.59
3	A	601	ANP	C1'-N9-C8	-2.20	122.22	127.09
3	D	604	ANP	C5'-C4'-C3'	2.18	123.07	115.21
3	A	601	ANP	C6-C5-N7	2.14	136.21	132.09
3	A	601	ANP	C2-N1-C6	2.01	122.03	118.73

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	ANP	C4'
3	A	601	ANP	C2'
3	A	601	ANP	C3'
3	B	602	ANP	C4'
3	B	602	ANP	C1'
3	B	602	ANP	C3'
3	C	603	ANP	C4'
3	C	603	ANP	C2'
3	C	603	ANP	C3'
3	D	604	ANP	C2'
3	D	604	ANP	C3'
3	E	605	ANP	C2'
3	E	605	ANP	C3'
3	F	606	ANP	C4'
3	F	606	ANP	C3'

All (38) 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	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	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-O2B
3	E	605	ANP	PG-N3B-PB-O1B
3	E	605	ANP	PG-N3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
3	E	605	ANP	C5'-O5'-PA-O2A
3	E	605	ANP	C5'-O5'-PA-O3A
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	A	601	ANP	O4'-C4'-C5'-O5'
3	A	601	ANP	C3'-C4'-C5'-O5'
3	C	603	ANP	O4'-C4'-C5'-O5'
3	F	606	ANP	O4'-C4'-C5'-O5'
3	F	606	ANP	C3'-C4'-C5'-O5'
3	D	604	ANP	C3'-C4'-C5'-O5'
3	B	602	ANP	C2'-C1'-N9-C4
3	A	601	ANP	C2'-C1'-N9-C4
3	B	602	ANP	C2'-C1'-N9-C8
3	A	601	ANP	C2'-C1'-N9-C8
3	B	602	ANP	C3'-C4'-C5'-O5'
3	B	602	ANP	C5'-O5'-PA-O1A
3	C	603	ANP	C5'-O5'-PA-O1A
3	C	603	ANP	C5'-O5'-PA-O2A
3	C	603	ANP	C5'-O5'-PA-O3A
3	E	605	ANP	C5'-O5'-PA-O1A
3	B	602	ANP	C4'-C5'-O5'-PA
3	F	606	ANP	C4'-C5'-O5'-PA
3	C	603	ANP	C4'-C5'-O5'-PA
3	B	602	ANP	PB-O3A-PA-O1A
3	D	604	ANP	PA-O3A-PB-O1B

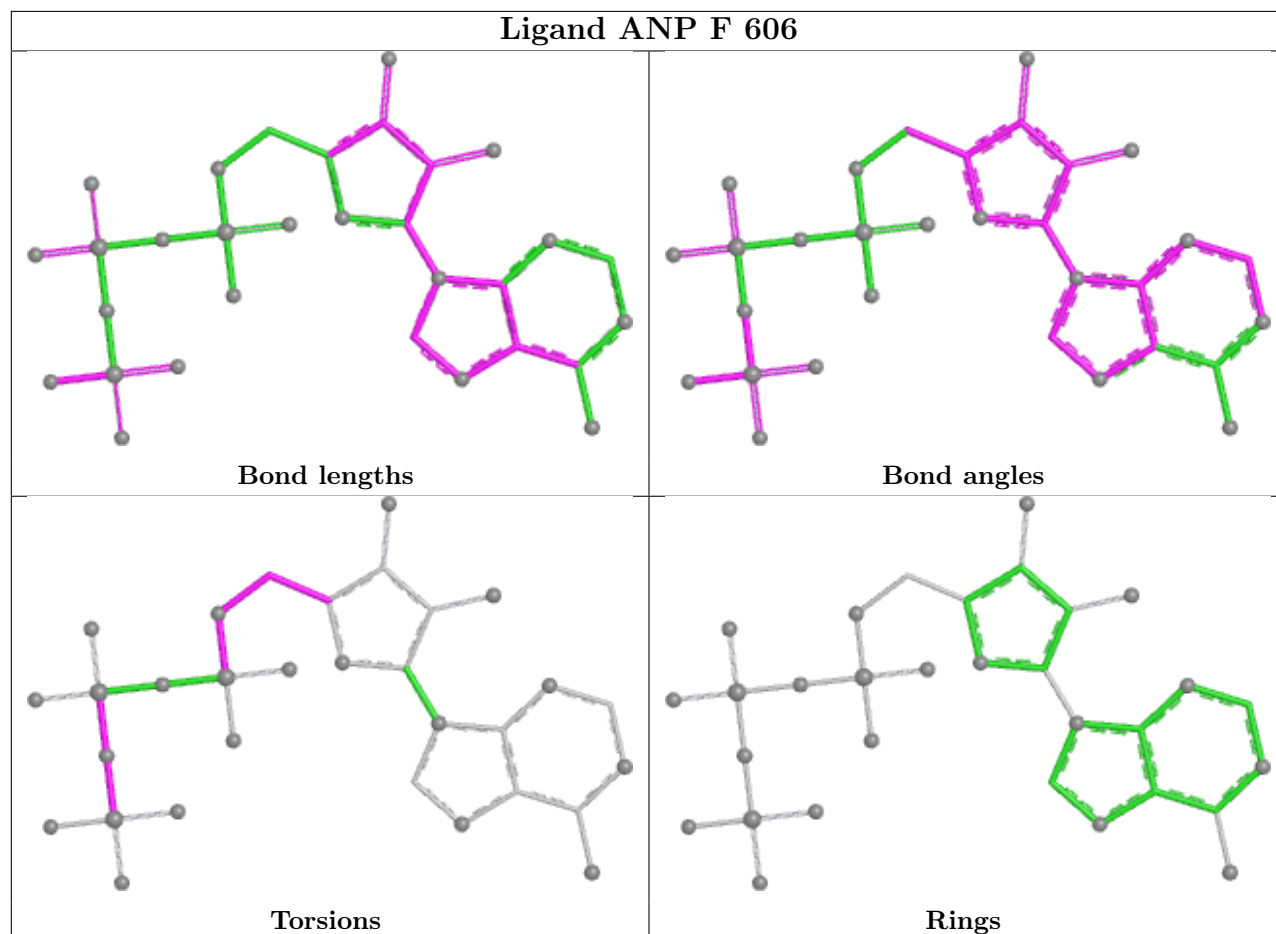
There are no ring outliers.

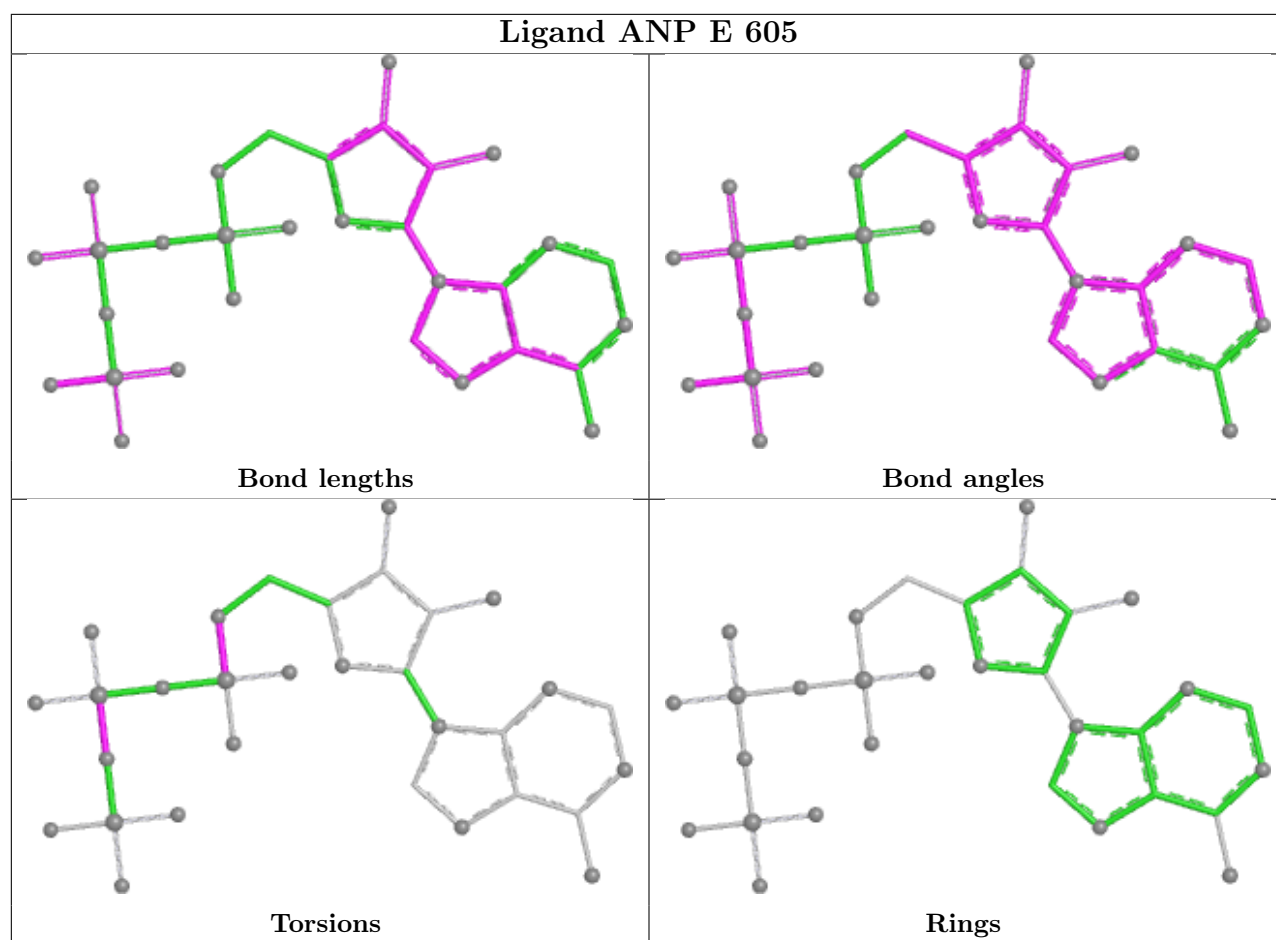
1 monomer is involved in 3 short contacts:

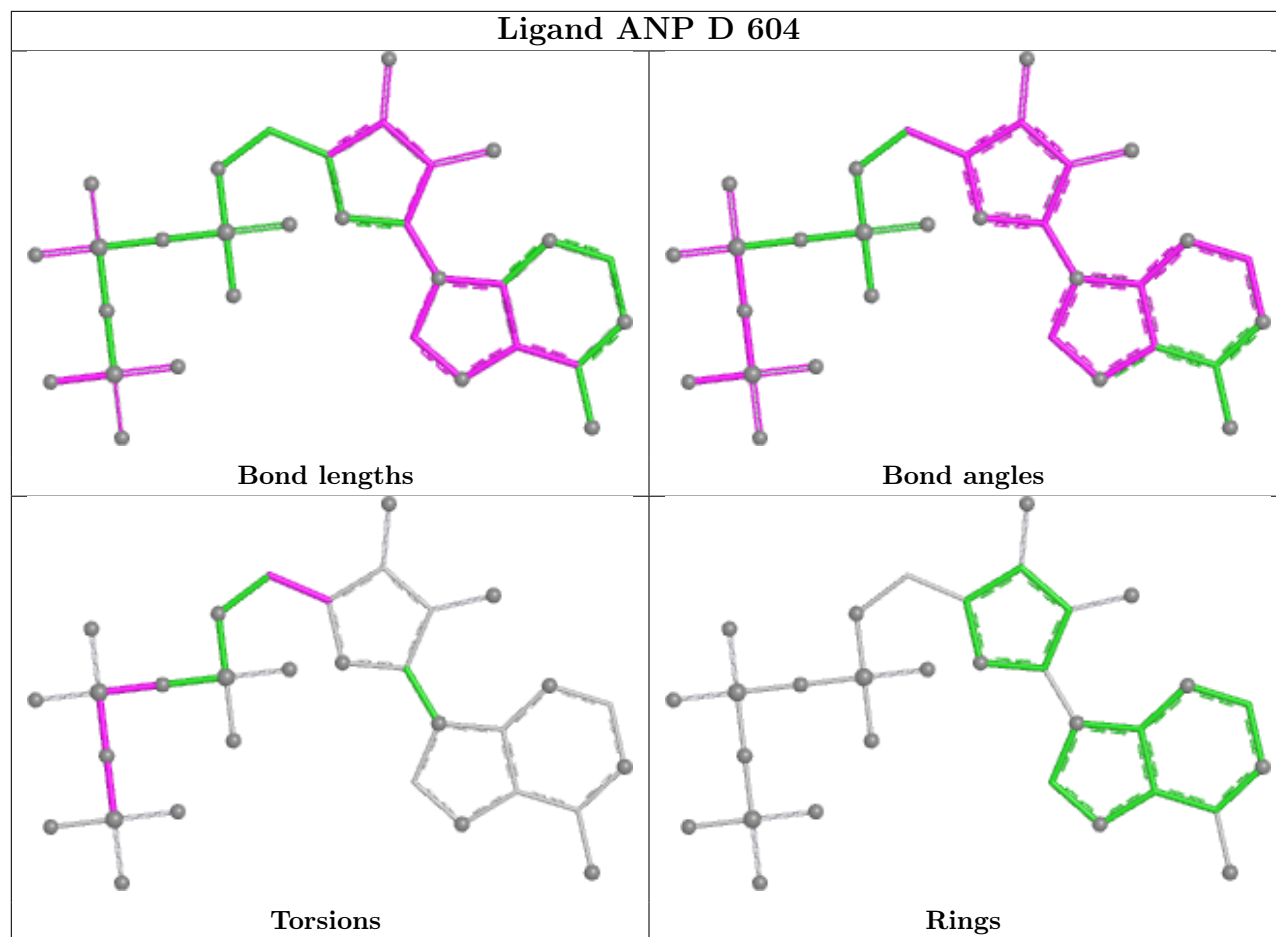
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ANP	3	0

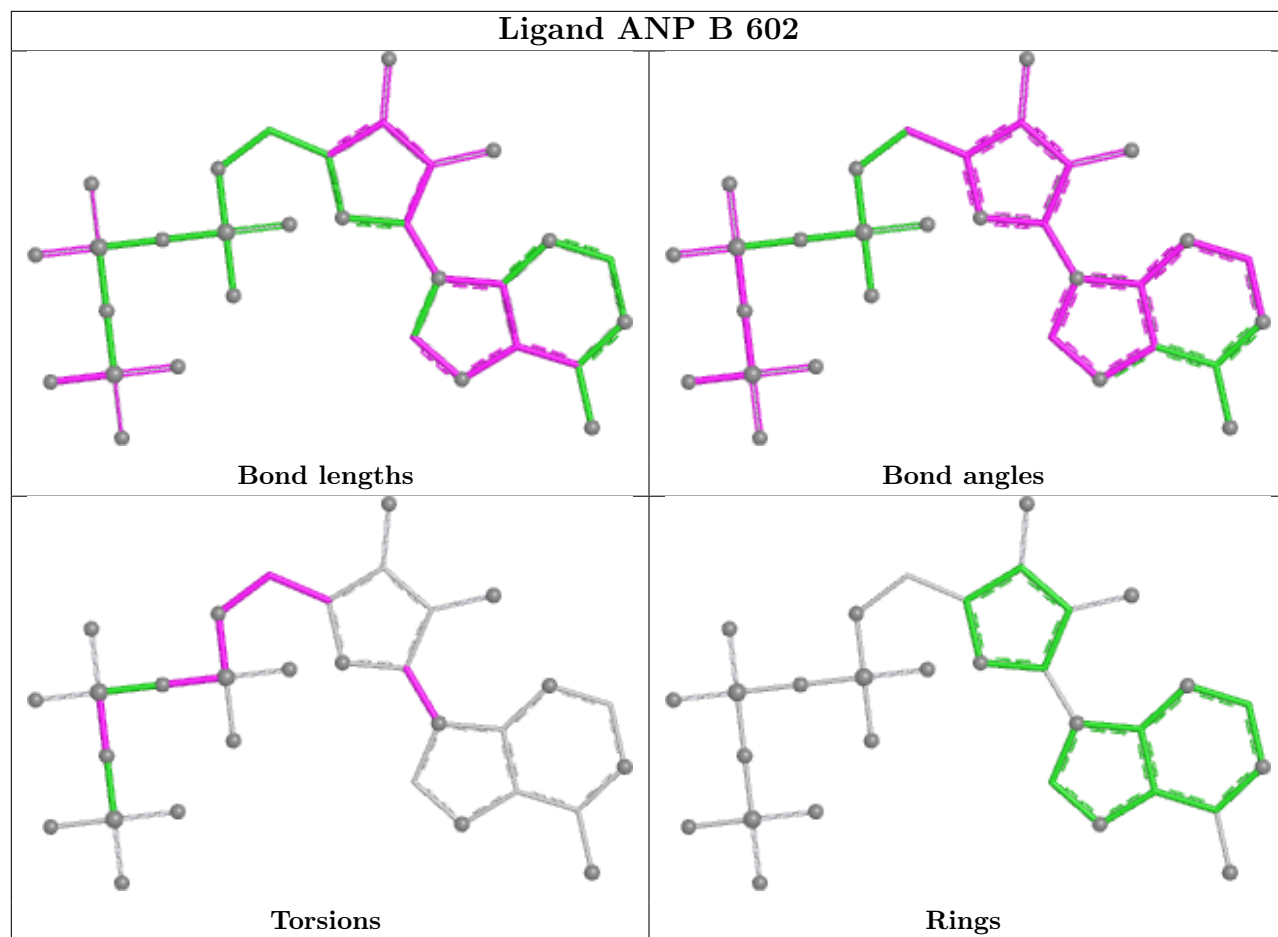
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

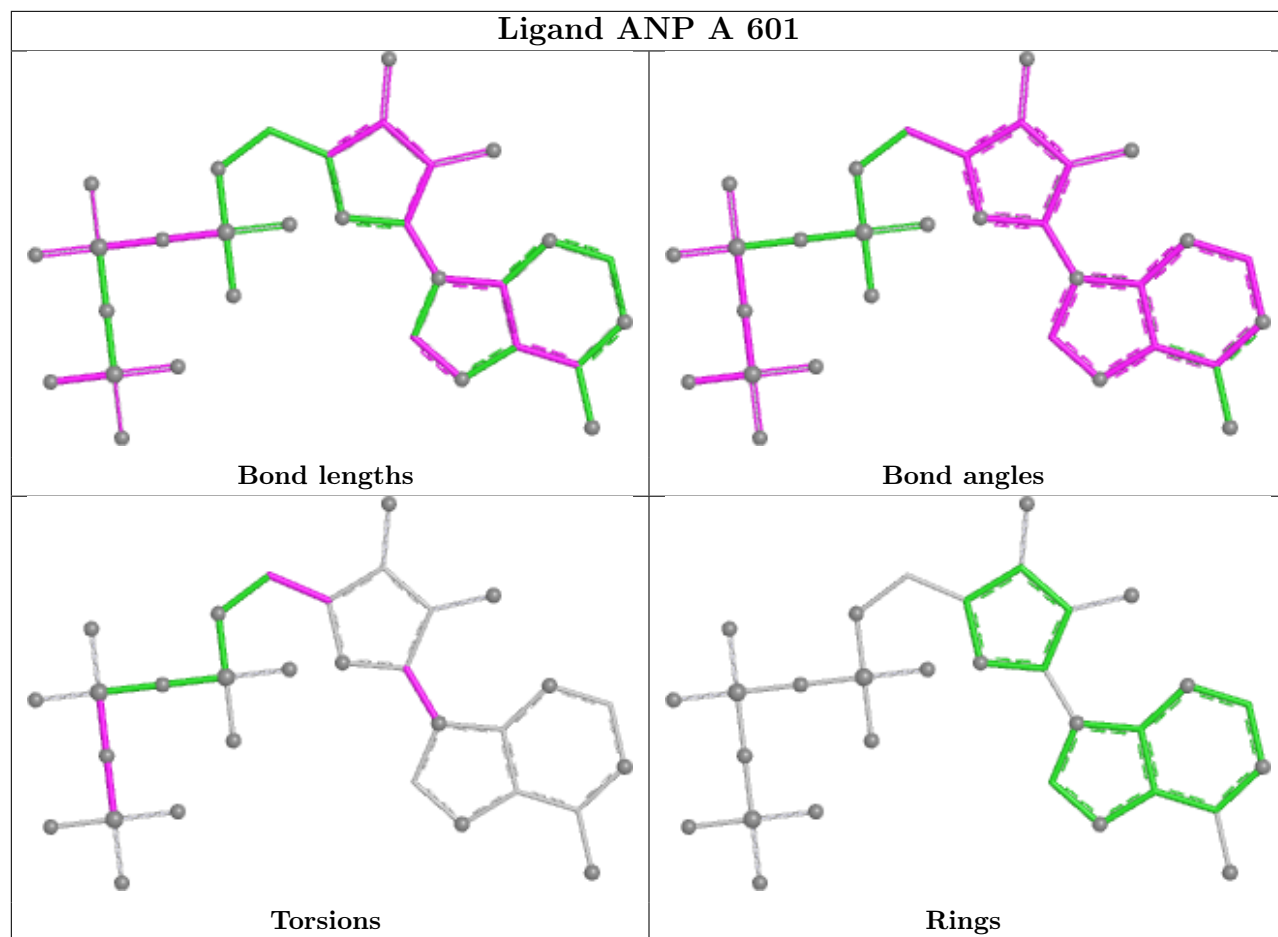
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

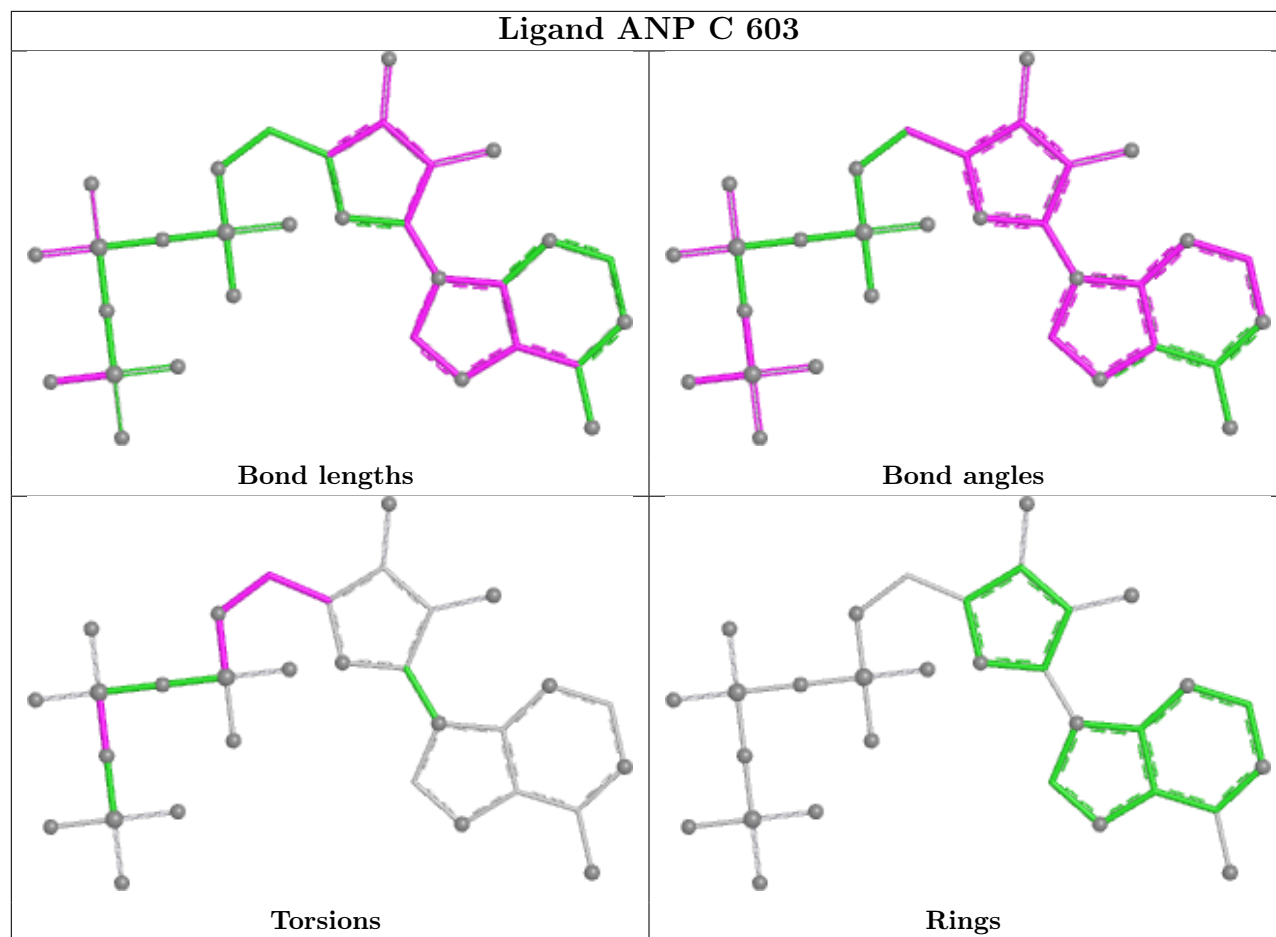












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	G	2/2 (100%)	0.92	0 100 100	150, 150, 150, 150	0
1	H	2/2 (100%)	1.77	0 100 100	150, 150, 150, 150	0
1	J	2/2 (100%)	2.58	2 (100%) 0 0	150, 150, 150, 150	0
1	K	2/2 (100%)	2.90	2 (100%) 0 0	150, 150, 150, 150	0
1	L	2/2 (100%)	1.29	0 100 100	150, 150, 150, 150	0
2	A	408/419 (97%)	-0.15	3 (0%) 84 66	42, 66, 114, 127	0
2	B	358/419 (85%)	0.04	14 (3%) 43 24	35, 65, 112, 127	0
2	C	408/419 (97%)	-0.29	8 (1%) 65 41	20, 43, 96, 103	0
2	D	408/419 (97%)	-0.33	6 (1%) 72 49	18, 46, 72, 124	0
2	E	407/419 (97%)	-0.30	5 (1%) 76 55	21, 46, 85, 123	0
2	F	408/419 (97%)	-0.23	7 (1%) 69 45	39, 65, 105, 119	0
All	All	2407/2524 (95%)	-0.21	47 (1%) 65 41	18, 56, 104, 150	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	152	GLY	5.5
2	B	139	LEU	5.3
2	B	145	LEU	5.0
2	D	355	PHE	4.8
2	B	140	HIS	4.1
2	B	55	LEU	3.7
2	B	143	SER	3.6
2	B	144	ARG	3.5
1	K	2	C	3.5
2	A	152	GLY	3.4
2	E	152	GLY	3.1
1	J	2	C	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	152	GLY	3.0
2	C	139	LEU	2.9
2	F	147	MET	2.9
2	B	153	SER	2.7
2	C	140	HIS	2.7
2	D	140	HIS	2.6
2	F	25	ASN	2.6
2	C	101	ILE	2.5
2	E	28	ARG	2.4
2	D	372	THR	2.4
2	F	8	ASN	2.4
1	K	1	U	2.4
2	C	152	GLY	2.3
2	E	154	THR	2.3
2	A	307	VAL	2.3
2	B	407	LYS	2.3
2	B	142	ASN	2.3
2	C	39	LEU	2.3
2	B	410	ASP	2.3
2	C	412	PHE	2.3
2	B	147	MET	2.2
2	E	139	LEU	2.2
2	F	132	LEU	2.2
2	C	287	GLY	2.2
2	A	198	ASN	2.2
2	F	409	ASN	2.1
1	J	1	U	2.1
2	D	165	ALA	2.1
2	B	89	PHE	2.1
2	B	156	ASP	2.1
2	D	416	MET	2.1
2	F	140	HIS	2.0
2	C	406	THR	2.0
2	E	407	LYS	2.0
2	D	39	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

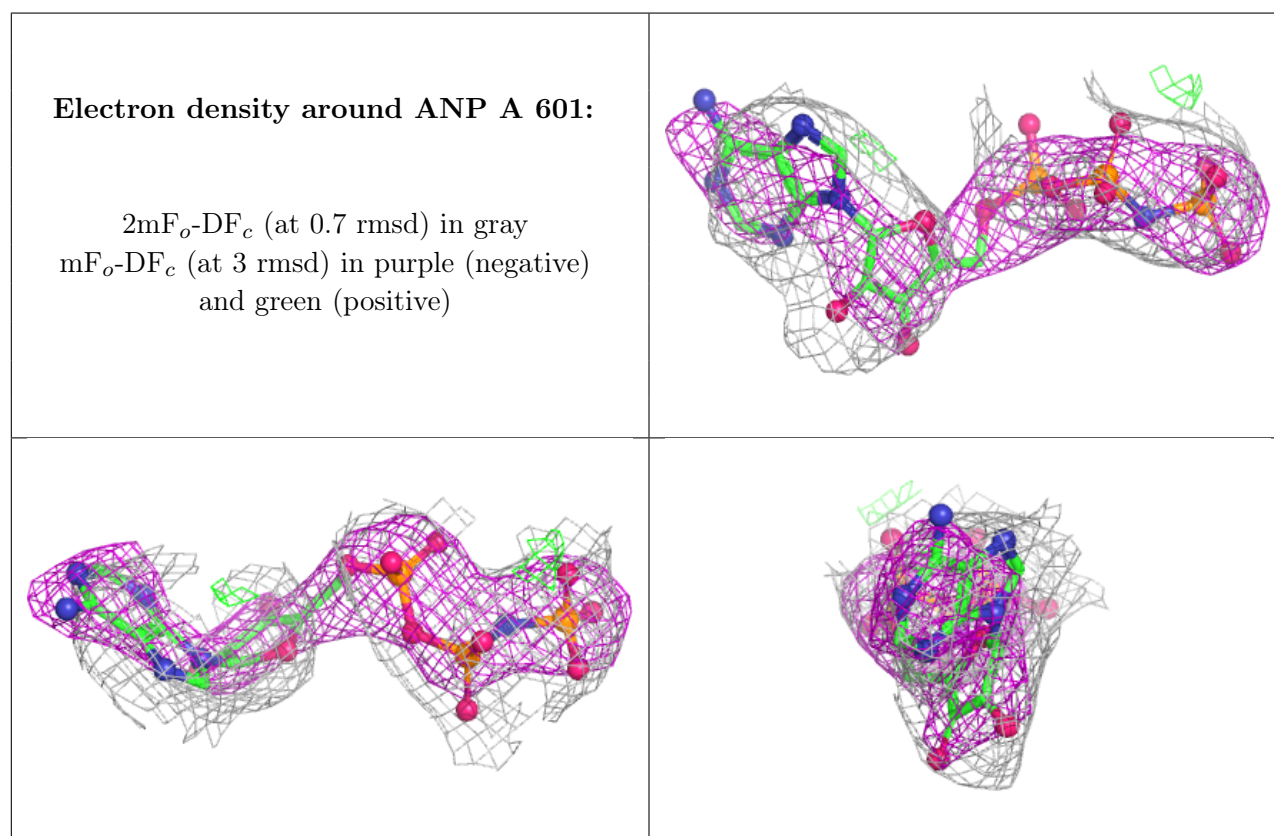
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

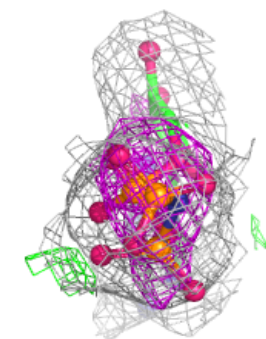
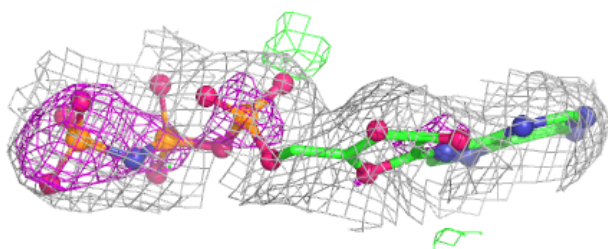
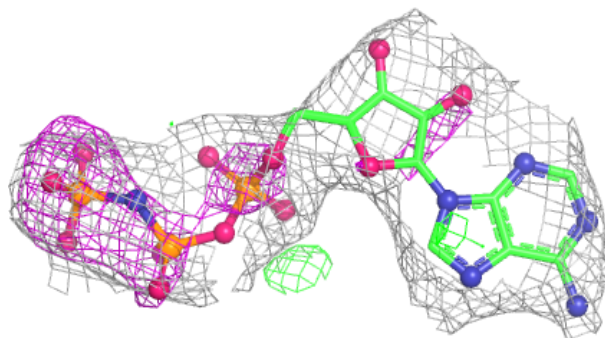
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	A	601	31/31	0.43	0.17	150,150,150,150	0
3	ANP	B	602	31/31	0.74	0.13	150,150,150,150	0
3	ANP	F	606	31/31	0.75	0.15	150,150,150,150	0
3	ANP	E	605	31/31	0.76	0.14	150,150,150,150	0
3	ANP	D	604	31/31	0.76	0.13	150,150,150,150	0
3	ANP	C	603	31/31	0.78	0.13	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.

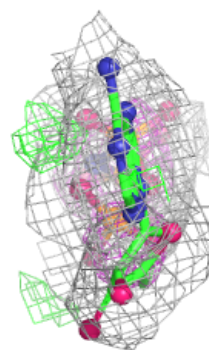
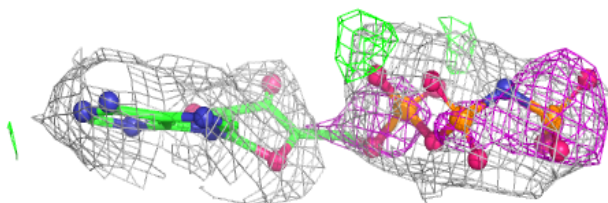
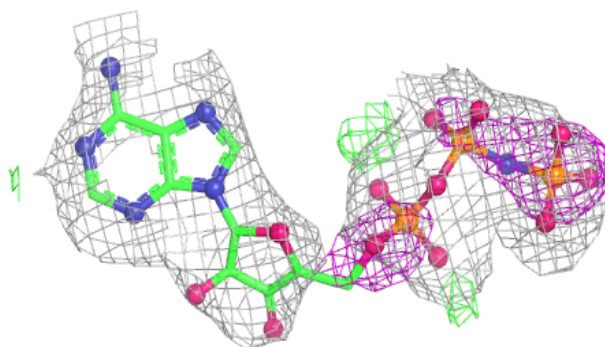


Electron density around ANP B 602:

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

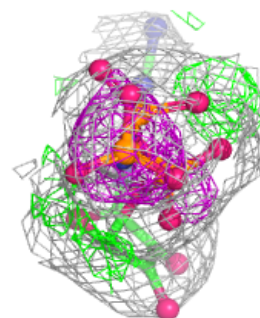
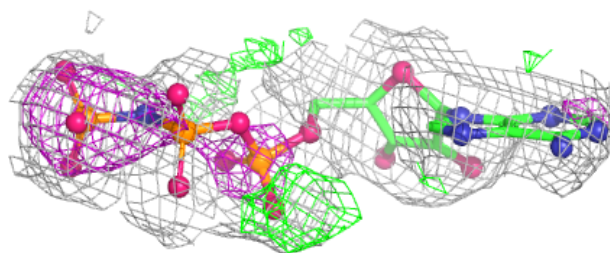
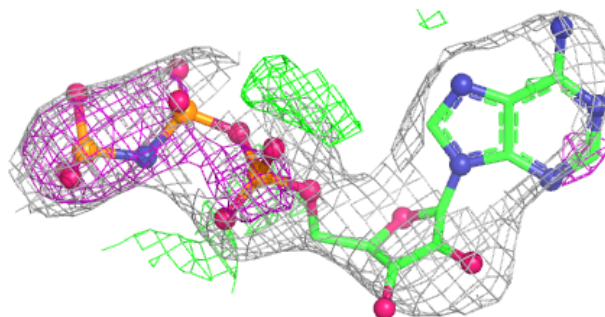
**Electron density around ANP F 606:**

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

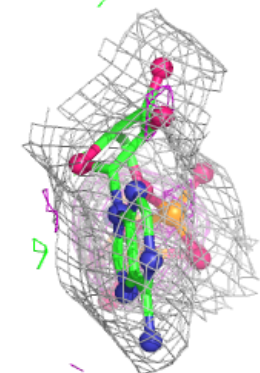
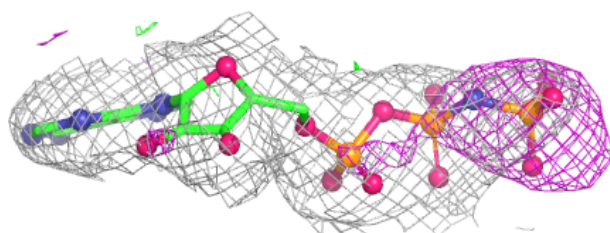
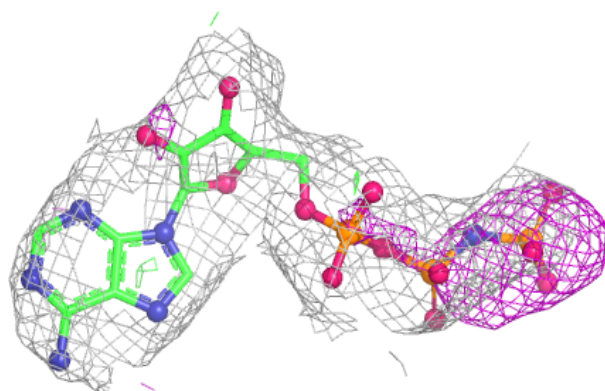


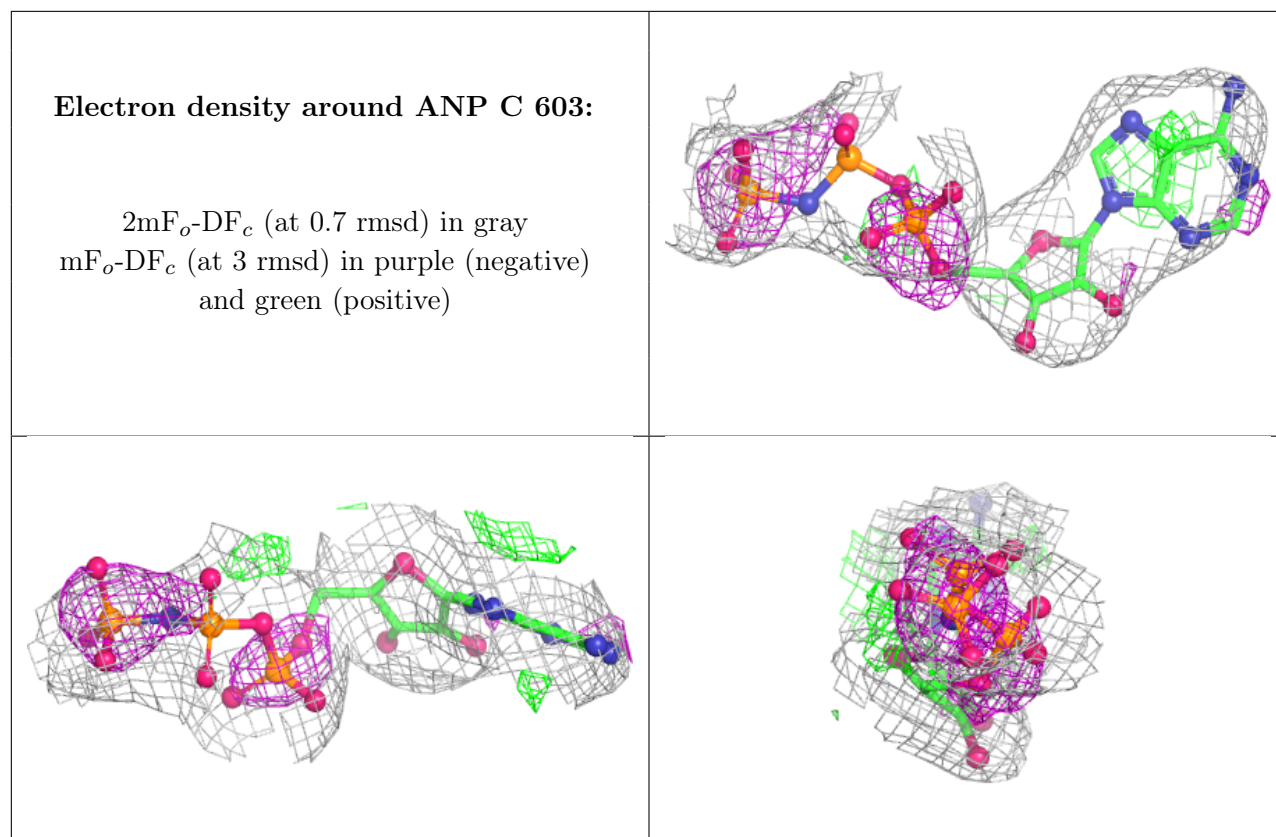
Electron density around ANP E 605:

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

**Electron density around ANP 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.