Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 03:56 PM EDT

PDB ID	:	4YIY
Title	:	Structure of MRB1590 bound to AMP-PNP
Authors	:	Shaw, P.L.R.; Schumacher, M.A.
Deposited on	:	2015-03-02
Resolution	:	3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

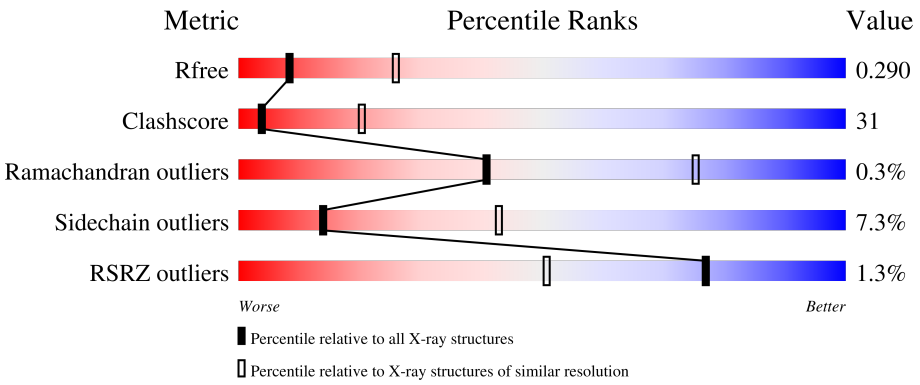
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

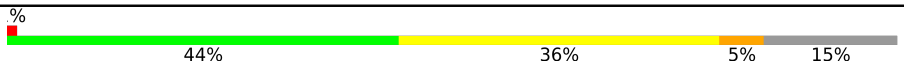
The reported resolution of this entry is 3.02 Å.

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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8916 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called kRNA Editing A6 Specific Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	577	4416	2763	782	845	26	0	0	0
1	A	577	4418	2763	783	846	26	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57ZF2
B	-10	HIS	-	expression tag	UNP Q57ZF2
B	-9	HIS	-	expression tag	UNP Q57ZF2
B	-8	HIS	-	expression tag	UNP Q57ZF2
B	-7	HIS	-	expression tag	UNP Q57ZF2
B	-6	HIS	-	expression tag	UNP Q57ZF2
B	-5	HIS	-	expression tag	UNP Q57ZF2
B	-4	SER	-	expression tag	UNP Q57ZF2
B	-3	SER	-	expression tag	UNP Q57ZF2
B	-2	GLY	-	expression tag	UNP Q57ZF2
B	-1	VAL	-	expression tag	UNP Q57ZF2
B	0	ASP	-	expression tag	UNP Q57ZF2
B	1	LEU	-	expression tag	UNP Q57ZF2
B	2	GLY	-	expression tag	UNP Q57ZF2
B	3	THR	-	expression tag	UNP Q57ZF2
B	4	GLU	-	expression tag	UNP Q57ZF2
B	5	ASN	-	expression tag	UNP Q57ZF2
B	6	LEU	-	expression tag	UNP Q57ZF2
B	7	TYR	-	expression tag	UNP Q57ZF2
B	8	PHE	-	expression tag	UNP Q57ZF2
B	9	GLN	-	expression tag	UNP Q57ZF2
B	10	SER	-	expression tag	UNP Q57ZF2
B	242	GLU	VAL	conflict	UNP Q57ZF2
A	-11	MET	-	initiating methionine	UNP Q57ZF2
A	-10	HIS	-	expression tag	UNP Q57ZF2

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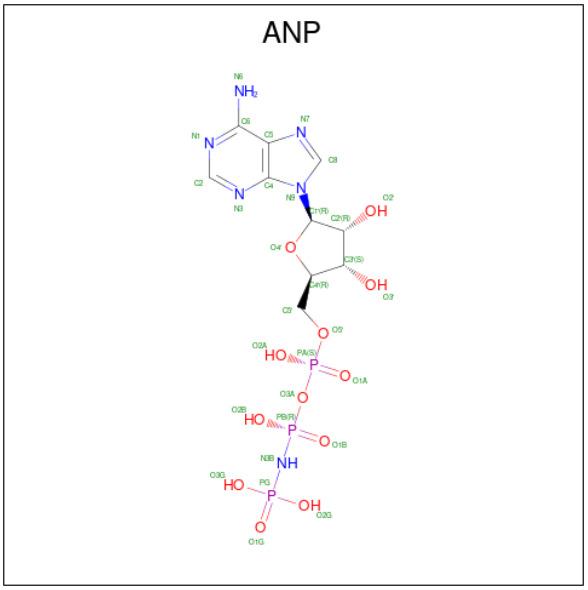
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q57ZF2
A	-8	HIS	-	expression tag	UNP Q57ZF2
A	-7	HIS	-	expression tag	UNP Q57ZF2
A	-6	HIS	-	expression tag	UNP Q57ZF2
A	-5	HIS	-	expression tag	UNP Q57ZF2
A	-4	SER	-	expression tag	UNP Q57ZF2
A	-3	SER	-	expression tag	UNP Q57ZF2
A	-2	GLY	-	expression tag	UNP Q57ZF2
A	-1	VAL	-	expression tag	UNP Q57ZF2
A	0	ASP	-	expression tag	UNP Q57ZF2
A	1	LEU	-	expression tag	UNP Q57ZF2
A	2	GLY	-	expression tag	UNP Q57ZF2
A	3	THR	-	expression tag	UNP Q57ZF2
A	4	GLU	-	expression tag	UNP Q57ZF2
A	5	ASN	-	expression tag	UNP Q57ZF2
A	6	LEU	-	expression tag	UNP Q57ZF2
A	7	TYR	-	expression tag	UNP Q57ZF2
A	8	PHE	-	expression tag	UNP Q57ZF2
A	9	GLN	-	expression tag	UNP Q57ZF2
A	10	SER	-	expression tag	UNP Q57ZF2
A	242	GLU	VAL	conflict	UNP Q57ZF2

- Molecule 2 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
			Total	C	N	O	P		
2	B	1	31	10	6	12	3	0	0
2	A	1	31	10	6	12	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	2	2	2	0	0
3	A	2	2	2	0	0

- Molecule 4 is water.

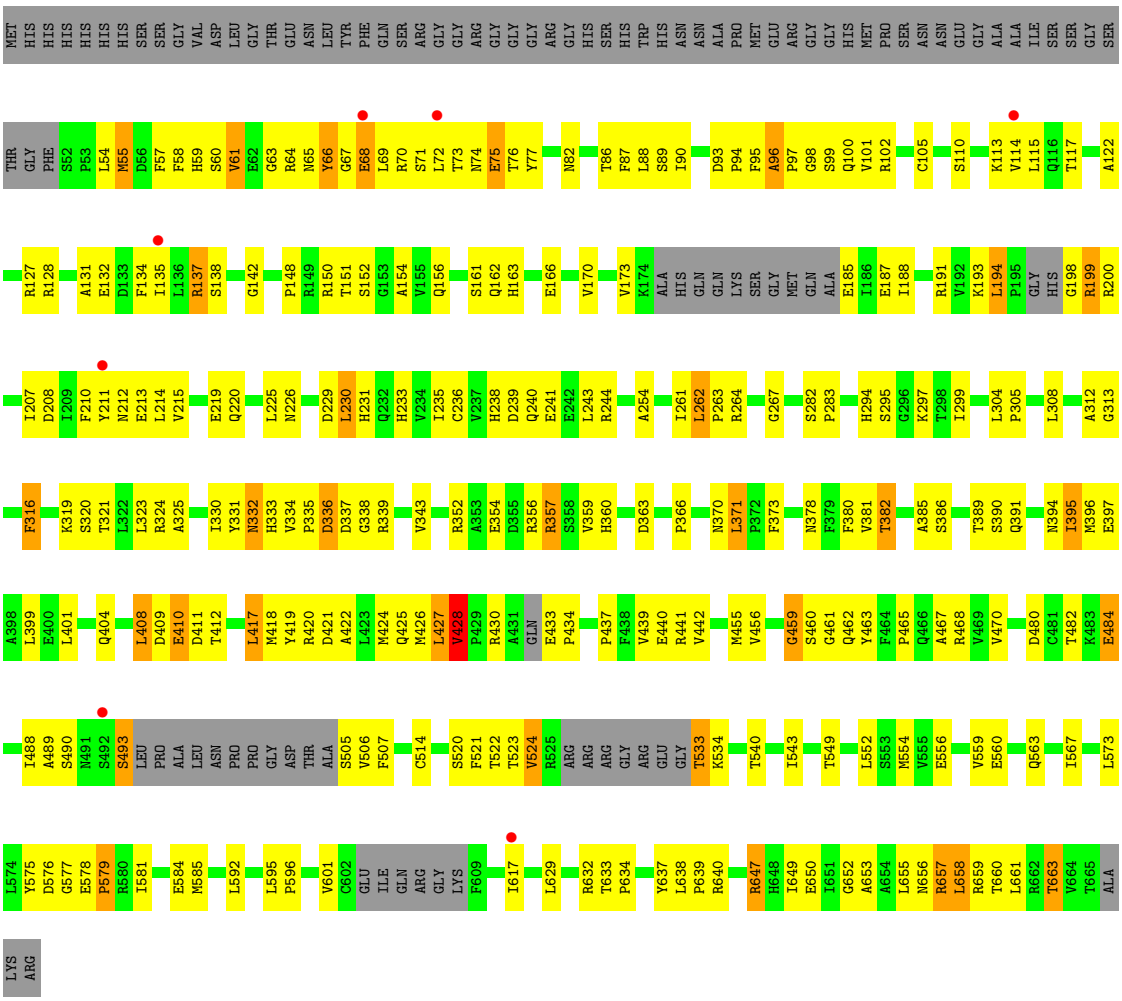
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	12	12	12	0	0
4	A	4	4	4	0	0

3 Residue-property plots (i)

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

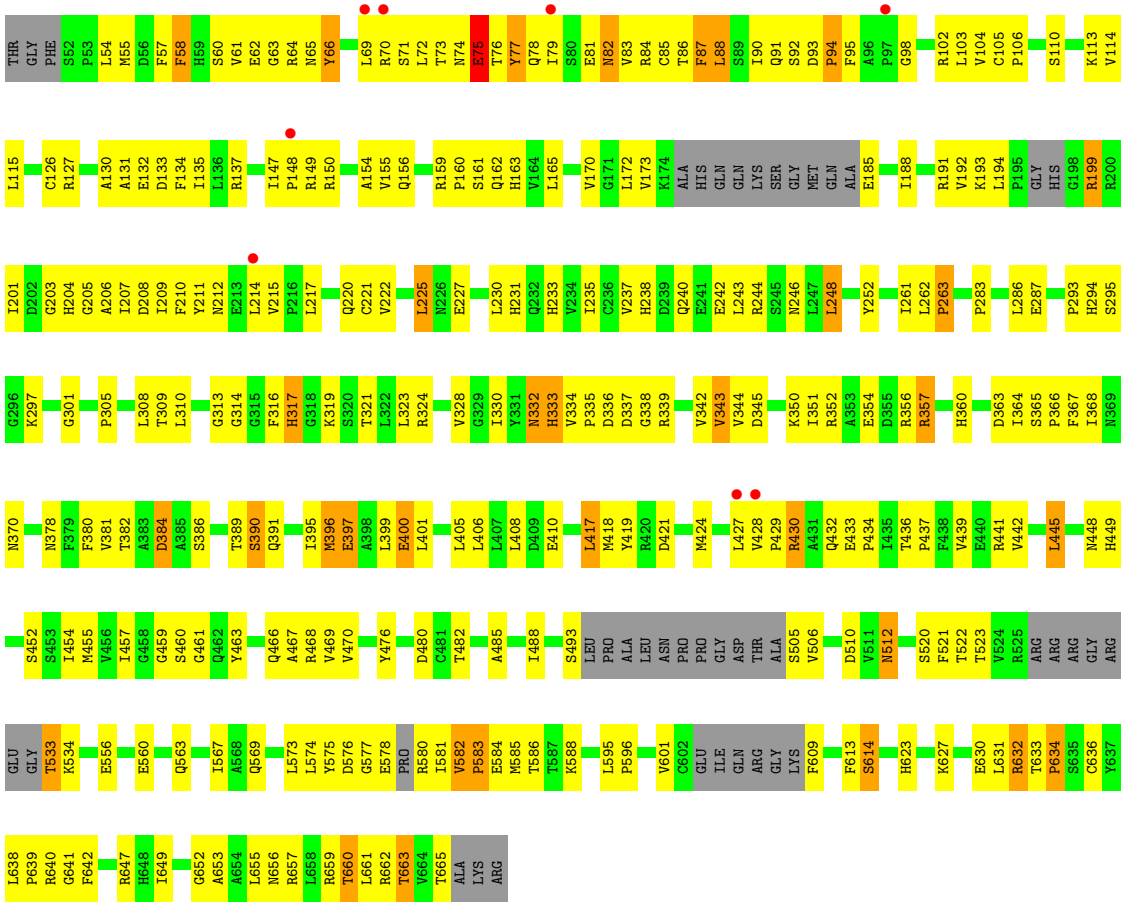
• Molecule 1: kRNA Editing A6 Specific Protein

Chain B:



• Molecule 1: kRNA Editing A6 Specific Protein

Chain A:


THR GLY PHE S52 P53 L54 M55 D56 F57 F58 H59 S60 V61 E62 G63 R64 N65 Y66 L69 R70 S71 L72 T73 N74 E75 T76 Y77 Q78 I79 S80 E81 N82 V83 R84 C85 T86 F87 L88 S89 I90 Q91 S92 D93 P94 F95 A96 P97 G98 R102 L103 V104 C105 P106 S110 K113 V114
L115 C126 R127 A130 A131 E132 D133 F134 I135 L136 R137 I147 P148 R149 R150 A154 V155 Q156 R159 P160 S161 Q162 H163 V164 L165 V170 G171 L172 V173 K174 ALA HIS GLN GLN LYS SER GLY MET GLN ALA E185 I188 R191 V192 K193 L194 P195 GLY HIS G198 R199 R200
I201 D202 G203 H204 G205 A206 I207 D208 I209 F210 Y211 N212 E213 L214 V215 P216 L217 Q220 C221 V222 L225 N226 E227 L230 H231 Q232 H233 V234 I235 G236 V237 H238 D239 Q240 E241 E242 L243 R244 S245 N246 L247 L248 Y252 I261 L262 P263 P283 L286 E287 P293 H294 S295
G296 K297 G301 P305 L308 T309 L310 G313 G314 G315 F316 H317 G318 K319 S320 T321 L322 L323 R324 V328 G329 I330 Y331 N332 H333 V334 P335 D336 D337 G338 R339 V342 V343 V344 D345 K350 I351 R352 A353 E354 D355 R356 R357 H360 D363 I364 S365 P366 F367 I368 N369
N370 N378 F379 F380 V381 T382 A383 D384 A385 S386 T389 S390 Q391 I395 M396 E397 A398 L399 E400 L401 L405 L406 L407 L408 D409 E410 L417 M418 Y419 R420 D421 M424 L427 V428 P429 R430 A431 Q432 E433 P434 T435 T436 P437 F438 V439 E440 R441 V442 L445 N448 H449
S452 S453 I454 M455 V456 I457 G458 G459 S460 G461 Q462 Y463 Q466 A467 R468 V469 V470 Y476 D480 C481 T482 A485 I488 S493 LEU PRO ALA LEU ASN PRO PRO GLY ASP THR ALA S505 V506 D510 V511 N512 S520 F521 T522 T523 V524 R525 ARG ARG ARG GLY ARG
GLU GLY T533 K534 E556 E560 Q563 I567 A568 Q569 L573 L574 Y575 D576 G577 E578 PRO R580 I581 V582 P583 E584 M585 T586 T587 K588 L595 P596 V601 C602 GLU ILE GLN ARG GLY LYS F609 F613 S614 H623 K627 E630 L631 R632 T633 P634 S635 C636 Y637
L638 P639 R640 G641 F642 R647 H648 I649 G652 A653 A654 L655 N656 R657 L658 R659 T660 L661 R662 T663 V664 T665 ALA LYS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.18Å 71.52Å 103.54Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	44.82 – 3.02 44.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.82-3.02) 97.6 (44.82-3.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.297 0.251 , 0.290	Depositor DCC
R_{free} test set	2004 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 14.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,k,-h-l 0.036 for -h-l,k,h 0.047 for h,-k,-h-l 0.378 for l,-k,h 0.044 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.78	1/4495 (0.0%)	0.82	13/6091 (0.2%)
1	B	0.77	0/4494	0.81	11/6091 (0.2%)
All	All	0.77	1/8989 (0.0%)	0.82	24/12182 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	PRO	N-CD	-13.53	1.28	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	631	LEU	N-CA-C	-10.11	83.70	111.00
1	B	657	ARG	CB-CA-C	-8.28	93.84	110.40
1	A	533	THR	N-CA-CB	-6.89	97.22	110.30
1	A	631	LEU	CB-CA-C	6.47	122.50	110.20
1	A	75	GLU	N-CA-C	-6.30	93.99	111.00
1	B	592	LEU	N-CA-C	6.12	127.52	111.00
1	B	408	LEU	N-CA-C	5.89	126.92	111.00
1	B	262	LEU	C-N-CD	5.79	140.56	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ARG	CB-CA-C	-5.56	99.29	110.40
1	A	262	LEU	C-N-CD	5.55	140.05	128.40
1	B	428	VAL	C-N-CD	5.51	139.97	128.40
1	A	88	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	647	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	390	SER	CB-CA-C	-5.43	99.78	110.10
1	A	317	HIS	N-CA-C	5.41	125.61	111.00
1	A	88	LEU	N-CA-C	5.39	125.56	111.00
1	B	198	GLY	N-CA-C	-5.38	99.64	113.10
1	A	582	VAL	C-N-CD	5.38	139.71	128.40
1	A	94	PRO	N-CA-C	5.35	126.02	112.10
1	B	658	LEU	N-CA-C	-5.17	97.04	111.00
1	B	404	GLN	N-CA-C	5.12	124.82	111.00
1	A	583	PRO	CA-N-CD	-5.09	104.37	111.50
1	B	459	GLY	N-CA-C	5.06	125.74	113.10
1	A	263	PRO	CA-N-CD	-5.01	104.48	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASP	Peptide
1	B	336	ASP	Peptide
1	B	96	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4418	0	4382	258	50
1	B	4416	0	4381	305	50
2	A	31	0	13	4	0
2	B	31	0	13	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	3	0
4	B	12	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8916	0	8789	544	50

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 31.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG23	1:B:115:LEU:CD1	1.70	1.21
1:B:576:ASP:OD2	1:B:634:PRO:HD2	1.03	1.19
1:A:57:PHE:O	1:A:60:SER:HB2	1.38	1.17
1:B:366:PRO:HG2	1:B:396:MET:HE3	1.27	1.16
1:A:244:ARG:NH2	1:A:332:ASN:OD1	1.78	1.16
1:B:430:ARG:HA	1:B:433:GLU:HB3	1.25	1.14
1:A:204:HIS:O	1:A:207:ILE:HG22	1.44	1.13
1:B:576:ASP:OD2	1:B:634:PRO:CD	1.97	1.13
1:B:244:ARG:HG2	1:B:343:VAL:HB	1.30	1.11
1:B:244:ARG:HH22	1:B:332:ASN:ND2	1.48	1.11
1:B:244:ARG:NH2	1:B:332:ASN:HD21	1.48	1.08
1:B:114:VAL:HG23	1:B:115:LEU:HD13	1.11	1.05
1:B:366:PRO:HG2	1:B:396:MET:CE	1.86	1.05
1:A:93:ASP:HB3	1:A:94:PRO:CD	1.87	1.05
1:B:54:LEU:HD11	1:B:58:PHE:CE2	1.93	1.03
1:B:137:ARG:NH1	1:B:334:VAL:HB	1.74	1.02
1:A:93:ASP:CB	1:A:94:PRO:HD2	1.86	1.00
1:B:66:TYR:OH	1:B:194:LEU:O	1.78	0.98
1:A:88:LEU:HD13	1:A:640:ARG:HD3	1.44	0.97
1:A:613:PHE:CZ	1:A:655:LEU:HD23	1.99	0.97
1:A:344:VAL:HG13	1:A:405:LEU:CD2	1.95	0.96
1:A:93:ASP:HB3	1:A:94:PRO:HD2	0.98	0.96
1:B:163:HIS:CE1	1:B:333:HIS:HE1	1.83	0.94
1:B:459:GLY:HA2	1:A:424:MET:HG2	1.46	0.94
1:B:576:ASP:CG	1:B:634:PRO:HD2	1.87	0.94
1:B:244:ARG:NH2	1:B:332:ASN:ND2	2.12	0.93
1:B:114:VAL:CG2	1:B:115:LEU:HD13	1.98	0.92
1:B:66:TYR:CE2	1:B:94:PRO:HG3	2.04	0.92
1:B:244:ARG:HH12	1:B:332:ASN:HD22	1.16	0.90
1:A:368:ILE:HD13	1:A:389:THR:HG22	1.52	0.90
1:A:460:SER:HB3	4:A:803:HOH:O	1.70	0.90
1:A:55:MET:HG3	1:A:207:ILE:HD11	1.52	0.90
1:B:653:ALA:HB1	1:B:657:ARG:HH12	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:HH22	1:B:332:ASN:HD21	1.04	0.89
1:B:370:ASN:O	1:B:371:LEU:HD23	1.72	0.88
1:B:66:TYR:HE2	1:B:94:PRO:HG3	1.38	0.88
1:B:137:ARG:HH12	1:B:334:VAL:HB	1.37	0.88
1:B:334:VAL:HG23	1:B:335:PRO:HD2	1.56	0.87
1:B:430:ARG:CA	1:B:433:GLU:HB3	2.04	0.87
1:B:163:HIS:CE1	1:B:333:HIS:CE1	2.62	0.86
1:B:58:PHE:O	1:B:61:VAL:HG23	1.75	0.86
1:B:638:LEU:HD23	1:B:639:PRO:HD2	1.57	0.85
1:A:344:VAL:CG1	1:A:405:LEU:HD23	2.06	0.85
1:B:88:LEU:HD13	1:B:640:ARG:HD3	1.56	0.85
1:B:524:VAL:HG21	1:B:575:TYR:HE1	1.42	0.84
1:B:163:HIS:HE1	1:B:333:HIS:HE1	1.23	0.83
1:A:127:ARG:HH21	1:A:294:HIS:HD2	1.24	0.83
1:B:386:SER:O	1:B:390:SER:OG	1.96	0.83
1:B:370:ASN:OD1	1:B:371:LEU:N	2.13	0.82
1:B:638:LEU:HD23	1:B:639:PRO:CD	2.09	0.82
1:B:460:SER:HB3	4:B:803:HOH:O	1.78	0.82
1:B:460:SER:O	4:B:801:HOH:O	1.95	0.82
1:B:128:ARG:HH11	1:B:128:ARG:HG2	1.45	0.81
1:A:344:VAL:CG1	1:A:405:LEU:CD2	2.59	0.81
2:B:701:ANP:O2A	1:A:386:SER:HB2	1.80	0.81
1:B:357:ARG:NH2	1:B:657:ARG:HG2	1.95	0.81
1:B:230:LEU:O	1:B:230:LEU:HD12	1.79	0.81
1:B:244:ARG:HG2	1:B:343:VAL:CB	2.10	0.81
1:B:210:PHE:O	1:B:215:VAL:HG23	1.81	0.80
1:B:356:ARG:HA	1:B:385:ALA:H	1.47	0.80
2:B:701:ANP:O1G	1:A:386:SER:OG	1.98	0.80
1:A:98:GLY:HA3	1:A:191:ARG:HG2	1.63	0.80
1:A:352:ARG:NH1	1:A:556:GLU:OE2	2.15	0.80
1:B:244:ARG:HH12	1:B:332:ASN:ND2	1.79	0.79
1:A:313:GLY:O	1:A:319:LYS:NZ	2.16	0.78
1:B:313:GLY:HA3	1:B:319:LYS:HE2	1.64	0.78
1:A:580:ARG:O	1:A:583:PRO:HD2	1.84	0.78
1:B:211:TYR:CD2	1:B:212:ASN:OD1	2.37	0.78
1:B:243:LEU:HD12	1:B:243:LEU:O	1.84	0.78
1:B:647:ARG:NH2	1:B:650:GLU:OE2	2.18	0.77
1:B:152:SER:OG	1:B:213:GLU:OE1	2.02	0.77
1:B:490:SER:O	1:B:493:SER:O	2.02	0.77
1:A:441:ARG:O	1:A:445:LEU:HD12	1.85	0.77
1:B:93:ASP:CG	1:B:94:PRO:HD2	2.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ANP:O3'	1:A:384:ASP:O	2.02	0.76
1:A:206:ALA:HA	1:A:209:ILE:HD12	1.67	0.76
1:B:334:VAL:CG2	1:B:335:PRO:HD2	2.16	0.75
1:B:321:THR:OG1	2:B:701:ANP:H5'2	1.87	0.75
1:B:573:LEU:HA	1:B:633:THR:HG21	1.68	0.75
1:B:524:VAL:HG21	1:B:575:TYR:CE1	2.22	0.75
1:B:430:ARG:HA	1:B:433:GLU:CB	2.12	0.74
1:B:386:SER:HB2	1:B:389:THR:HB	1.69	0.74
1:B:61:VAL:HA	1:B:64:ARG:HD2	1.70	0.74
1:B:244:ARG:NH1	1:B:332:ASN:ND2	2.34	0.74
1:A:208:ASP:OD1	1:A:212:ASN:ND2	2.20	0.73
1:B:354:GLU:O	1:B:390:SER:CB	2.37	0.73
1:A:248:LEU:HD12	1:A:252:TYR:O	1.88	0.73
1:B:117:THR:HG21	1:B:122:ALA:HB3	1.70	0.73
1:B:61:VAL:O	1:B:64:ARG:HB2	1.89	0.72
1:B:533:THR:OG1	1:B:534:LYS:N	2.20	0.72
1:B:73:THR:O	1:B:75:GLU:N	2.23	0.72
1:A:520:SER:O	1:A:660:THR:HG23	1.89	0.72
1:B:96:ALA:HB1	1:B:97:PRO:HD3	1.72	0.72
1:A:243:LEU:HD12	1:A:243:LEU:O	1.88	0.72
1:B:114:VAL:C	1:B:115:LEU:HD12	2.11	0.71
1:B:354:GLU:O	1:B:390:SER:HB2	1.90	0.71
1:A:613:PHE:CE2	1:A:655:LEU:HD23	2.25	0.71
1:A:137:ARG:HH12	1:A:334:VAL:HB	1.55	0.71
1:A:427:LEU:HG	1:A:428:VAL:HG13	1.70	0.71
1:A:72:LEU:N	1:A:72:LEU:HD12	2.06	0.71
1:A:57:PHE:O	1:A:60:SER:CB	2.30	0.71
1:A:173:VAL:O	1:A:185:GLU:N	2.24	0.70
1:B:66:TYR:HE2	1:B:94:PRO:CG	2.04	0.70
1:B:73:THR:HG22	1:B:74:ASN:OD1	1.91	0.70
1:B:244:ARG:CZ	1:B:332:ASN:ND2	2.54	0.70
1:A:368:ILE:HD13	1:A:389:THR:CG2	2.21	0.70
1:B:420:ARG:HH22	1:B:430:ARG:NH1	1.89	0.70
1:A:79:ILE:HD11	1:A:83:VAL:HG11	1.74	0.70
1:A:397:GLU:HG3	1:A:656:ASN:ND2	2.06	0.70
1:B:244:ARG:NH1	1:B:332:ASN:HD22	1.88	0.69
1:A:582:VAL:O	1:A:586:THR:OG1	2.08	0.69
1:A:194:LEU:HD12	1:A:194:LEU:N	2.08	0.69
1:B:397:GLU:HG3	1:B:656:ASN:ND2	2.08	0.69
1:A:127:ARG:HH21	1:A:294:HIS:CD2	2.10	0.69
1:A:581:ILE:HG23	1:A:585:MET:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG22	1:A:188:ILE:HG12	1.76	0.68
1:A:313:GLY:O	1:A:319:LYS:CE	2.41	0.68
1:A:576:ASP:OD2	1:A:634:PRO:HD2	1.94	0.67
1:B:54:LEU:CD1	1:B:58:PHE:CE2	2.76	0.67
1:B:236:CYS:O	1:B:240:GLN:HB2	1.94	0.67
1:B:267:GLY:HA2	1:A:384:ASP:OD2	1.95	0.67
1:B:244:ARG:CG	1:B:343:VAL:CG1	2.73	0.67
1:A:520:SER:O	1:A:660:THR:CG2	2.42	0.67
1:A:408:LEU:HB2	1:A:455:MET:HB2	1.77	0.66
1:A:410:GLU:OE1	1:A:457:ILE:HA	1.95	0.66
1:B:244:ARG:CZ	1:B:332:ASN:HD21	2.09	0.66
1:B:244:ARG:HG3	1:B:343:VAL:CG1	2.25	0.66
1:B:424:MET:HG3	1:A:459:GLY:HA2	1.78	0.66
1:A:368:ILE:CD1	1:A:389:THR:HG22	2.24	0.66
1:A:370:ASN:H	1:A:434:PRO:HB3	1.61	0.66
1:B:114:VAL:HG23	1:B:115:LEU:HD12	1.73	0.65
1:B:357:ARG:CZ	1:B:657:ARG:HG2	2.26	0.65
1:A:386:SER:HB3	1:A:389:THR:OG1	1.97	0.65
1:B:380:PHE:CZ	1:B:389:THR:CG2	2.79	0.65
1:B:93:ASP:CG	1:B:94:PRO:CD	2.64	0.65
1:B:522:THR:HG23	1:B:523:THR:N	2.12	0.65
1:B:522:THR:HG23	1:B:523:THR:HG23	1.79	0.65
1:B:523:THR:O	1:B:524:VAL:HG13	1.97	0.65
1:B:127:ARG:HH21	1:B:294:HIS:CD2	2.15	0.65
1:B:154:ALA:HB1	1:B:193:LYS:HB2	1.79	0.65
1:B:230:LEU:HD12	1:B:230:LEU:C	2.14	0.65
1:B:386:SER:HB3	2:A:701:ANP:O1G	1.98	0.64
1:A:54:LEU:HD13	1:A:77:TYR:CE2	2.31	0.64
1:A:132:GLU:OE2	1:A:172:LEU:N	2.30	0.64
1:B:357:ARG:NH2	1:B:657:ARG:CG	2.61	0.64
1:B:409:ASP:O	1:B:411:ASP:N	2.31	0.64
1:A:449:HIS:HD1	1:A:609:PHE:HE1	1.45	0.64
1:B:127:ARG:CG	1:B:238:HIS:HD2	2.09	0.64
1:B:514:CYS:O	1:B:663:THR:OG1	2.15	0.64
1:A:661:LEU:O	1:A:662:ARG:NH1	2.29	0.64
1:B:360:HIS:CE1	1:B:663:THR:H	2.16	0.63
1:B:420:ARG:HH12	1:B:430:ARG:HD3	1.63	0.63
1:A:321:THR:OG1	2:A:701:ANP:O2A	2.11	0.63
1:B:366:PRO:CG	1:B:396:MET:HE3	2.16	0.63
1:A:364:ILE:HD12	1:A:368:ILE:HD12	1.79	0.63
1:B:54:LEU:HD11	1:B:58:PHE:HE2	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:TYR:HD2	4:B:801:HOH:O	1.81	0.63
1:A:205:GLY:O	1:A:209:ILE:HG13	1.98	0.63
1:B:638:LEU:CD2	1:B:639:PRO:HD2	2.28	0.62
1:A:87:PHE:HD1	1:A:90:ILE:HD11	1.63	0.62
1:B:88:LEU:CD1	1:B:640:ARG:HD3	2.30	0.62
1:B:134:PHE:HB2	1:B:233:HIS:CD2	2.34	0.62
1:B:366:PRO:CG	1:B:396:MET:CE	2.72	0.62
1:B:419:TYR:OH	1:A:419:TYR:HE1	1.83	0.62
1:B:267:GLY:N	1:A:384:ASP:OD2	2.33	0.62
1:A:55:MET:HB2	1:A:211:TYR:CE2	2.34	0.62
1:A:134:PHE:HB2	1:A:233:HIS:CD2	2.35	0.62
1:B:137:ARG:NH1	1:B:334:VAL:CB	2.60	0.61
2:B:701:ANP:O2A	1:A:386:SER:CB	2.46	0.61
1:B:128:ARG:HG2	1:B:128:ARG:NH1	2.14	0.61
1:B:470:VAL:H	1:B:482:THR:HB	1.65	0.61
1:A:396:MET:CE	1:A:399:LEU:HD12	2.30	0.61
1:B:319:LYS:HB2	2:B:701:ANP:O1B	2.01	0.61
1:B:86:THR:HB	1:B:102:ARG:HB3	1.82	0.61
1:B:194:LEU:N	1:B:194:LEU:HD22	2.16	0.61
1:A:149:ARG:C	1:A:150:ARG:HG2	2.19	0.61
1:A:70:ARG:O	1:A:73:THR:HG22	2.01	0.60
1:A:408:LEU:HB2	1:A:455:MET:CB	2.31	0.60
1:B:211:TYR:HD2	1:B:212:ASN:OD1	1.81	0.60
1:B:132:GLU:OE1	4:B:802:HOH:O	2.17	0.60
1:A:133:ASP:O	1:A:137:ARG:HG2	2.02	0.60
1:B:420:ARG:HH22	1:B:430:ARG:HH11	1.47	0.60
1:A:69:LEU:O	1:A:72:LEU:HD13	2.01	0.60
1:A:76:THR:HG23	1:A:85:CYS:O	2.02	0.60
1:B:357:ARG:HH21	1:B:657:ARG:HA	1.67	0.60
1:A:88:LEU:CD1	1:A:640:ARG:HD3	2.28	0.60
1:B:170:VAL:HG22	1:B:188:ILE:HG12	1.82	0.60
1:A:149:ARG:O	1:A:150:ARG:HD3	2.02	0.59
1:A:391:GLN:HE22	1:A:418:MET:HE3	1.67	0.59
1:A:65:ASN:O	1:A:201:ILE:HD11	2.02	0.59
1:B:127:ARG:HE	1:B:238:HIS:CD2	2.21	0.59
1:B:66:TYR:CD2	1:B:94:PRO:HG3	2.38	0.59
1:B:76:THR:CG2	1:B:86:THR:OG1	2.50	0.59
1:A:73:THR:O	1:A:74:ASN:HB2	2.01	0.59
1:B:421:ASP:OD2	1:A:461:GLY:N	2.36	0.59
1:B:522:THR:HG23	1:B:523:THR:H	1.67	0.59
1:B:330:ILE:HG13	1:B:331:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:THR:HG22	1:B:540:THR:O	2.02	0.59
1:A:71:SER:O	1:A:75:GLU:OE1	2.21	0.59
1:A:396:MET:HE3	1:A:399:LEU:HD12	1.84	0.58
1:B:163:HIS:ND1	1:B:333:HIS:CE1	2.70	0.58
1:B:363:ASP:OD1	1:B:378:ASN:HA	2.02	0.58
1:B:658:LEU:HD12	1:B:659:ARG:H	1.66	0.58
1:B:199:ARG:O	1:B:199:ARG:HG2	2.01	0.58
1:A:308:LEU:HD23	1:A:467:ALA:HA	1.85	0.58
1:A:368:ILE:HD11	1:A:389:THR:HA	1.86	0.58
1:B:128:ARG:HH11	1:B:128:ARG:CG	2.16	0.58
1:A:72:LEU:HD12	1:A:72:LEU:H	1.65	0.58
1:A:581:ILE:HG23	1:A:585:MET:CG	2.33	0.58
1:B:127:ARG:HH21	1:B:294:HIS:HD2	1.49	0.58
1:B:173:VAL:O	1:B:185:GLU:N	2.37	0.57
1:B:231:HIS:O	1:B:235:ILE:HG13	2.03	0.57
1:B:267:GLY:CA	1:A:384:ASP:OD2	2.52	0.57
1:A:569:GLN:HE22	1:A:630:GLU:HA	1.68	0.57
1:B:395:ILE:O	1:B:399:LEU:HG	2.04	0.57
1:B:421:ASP:OD2	1:A:460:SER:HA	2.05	0.57
1:A:365:SER:N	1:A:366:PRO:CD	2.67	0.57
1:B:262:LEU:HD22	1:B:325:ALA:CB	2.35	0.57
1:B:267:GLY:CA	1:A:356:ARG:HB3	2.35	0.57
1:A:439:VAL:HG23	1:A:466:GLN:HG3	1.87	0.57
1:B:357:ARG:HH21	1:B:657:ARG:HG2	1.70	0.56
1:A:72:LEU:O	1:A:75:GLU:HB2	2.05	0.56
1:A:560:GLU:HB2	1:A:563:GLN:HG3	1.86	0.56
1:B:115:LEU:HD12	1:B:115:LEU:N	2.21	0.56
1:A:237:VAL:O	1:A:240:GLN:HB2	2.06	0.56
1:B:489:ALA:O	1:B:493:SER:HB2	2.06	0.56
1:B:576:ASP:CB	1:B:634:PRO:HD2	2.36	0.56
1:A:293:PRO:HG2	1:A:294:HIS:ND1	2.21	0.56
1:A:313:GLY:O	1:A:319:LYS:HE3	2.05	0.56
1:B:267:GLY:HA2	1:A:356:ARG:HB3	1.87	0.56
1:B:577:GLY:O	1:B:581:ILE:HB	2.06	0.55
1:A:92:SER:O	1:A:93:ASP:OD1	2.24	0.55
1:A:350:LYS:NZ	1:A:556:GLU:OE1	2.39	0.55
1:B:244:ARG:HG3	1:B:343:VAL:HG11	1.89	0.55
1:A:578:GLU:C	1:A:580:ARG:N	2.60	0.55
1:B:54:LEU:HD13	1:B:77:TYR:CE2	2.41	0.55
1:B:370:ASN:OD1	1:B:371:LEU:O	2.23	0.55
1:A:114:VAL:O	1:A:127:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:OD1	1:A:378:ASN:HA	2.06	0.55
1:A:295:SER:HB2	1:A:297:LYS:HD3	1.89	0.55
1:B:419:TYR:HH	1:A:419:TYR:HE1	1.55	0.55
1:B:366:PRO:HD2	1:B:396:MET:HE2	1.87	0.55
1:A:91:GLN:HG3	1:A:98:GLY:O	2.07	0.54
1:A:659:ARG:HG2	1:A:659:ARG:O	2.07	0.54
1:A:72:LEU:H	1:A:72:LEU:CD1	2.20	0.54
1:B:61:VAL:O	1:B:64:ARG:N	2.39	0.54
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.07	0.54
1:A:316:PHE:CZ	2:A:701:ANP:H4'	2.43	0.54
1:A:439:VAL:O	1:A:442:VAL:HG12	2.07	0.54
1:B:73:THR:C	1:B:75:GLU:H	2.11	0.54
1:A:86:THR:HB	1:A:102:ARG:HB3	1.89	0.53
1:A:334:VAL:HG23	1:A:335:PRO:HD2	1.89	0.53
1:A:401:LEU:HD13	1:A:649:ILE:HA	1.89	0.53
1:B:420:ARG:HH12	1:B:430:ARG:CD	2.21	0.53
1:B:243:LEU:HD22	1:B:299:ILE:HD11	1.89	0.53
1:B:319:LYS:HD2	1:B:456:VAL:HG13	1.90	0.53
1:B:408:LEU:HD23	1:B:418:MET:HE3	1.90	0.53
1:A:147:ILE:HB	1:A:148:PRO:HD3	1.90	0.53
1:B:87:PHE:HA	1:B:101:VAL:HG12	1.91	0.53
1:B:330:ILE:HD11	1:B:331:TYR:CE2	2.44	0.53
1:B:82:ASN:HB2	1:B:219:GLU:OE1	2.09	0.53
1:A:630:GLU:OE2	1:A:641:GLY:N	2.41	0.53
1:B:137:ARG:HH11	1:B:334:VAL:HB	1.70	0.53
1:A:72:LEU:O	1:A:75:GLU:CB	2.57	0.53
1:A:210:PHE:O	1:A:215:VAL:HG23	2.09	0.53
1:A:154:ALA:HB1	1:A:193:LYS:HB2	1.91	0.53
1:A:512:ASN:HB3	1:A:665:THR:OG1	2.09	0.53
1:A:639:PRO:HB2	1:A:642:PHE:CD1	2.43	0.53
1:A:54:LEU:HD13	1:A:77:TYR:HE2	1.73	0.52
1:A:334:VAL:CG2	1:A:335:PRO:HD2	2.39	0.52
1:A:653:ALA:HB1	1:A:657:ARG:HH12	1.74	0.52
1:B:360:HIS:HA	1:B:381:VAL:HG22	1.91	0.52
1:A:79:ILE:HD12	1:A:215:VAL:HG22	1.91	0.52
1:A:155:VAL:HG11	1:A:214:LEU:HD21	1.90	0.52
1:A:194:LEU:N	1:A:194:LEU:CD1	2.73	0.52
1:B:57:PHE:CE2	1:B:61:VAL:HG21	2.43	0.52
1:B:337:ASP:OD2	1:B:339:ARG:NE	2.33	0.52
1:A:244:ARG:NH1	4:A:801:HOH:O	2.42	0.52
1:B:137:ARG:HH12	1:B:334:VAL:CB	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PHE:CD1	1:B:214:LEU:HD12	2.45	0.52
1:A:161:SER:OG	1:A:162:GLN:N	2.42	0.52
1:B:58:PHE:HA	1:B:61:VAL:CG2	2.40	0.51
1:B:408:LEU:HB2	1:B:455:MET:HB3	1.92	0.51
1:A:283:PRO:HG2	1:A:286:LEU:HD12	1.92	0.51
1:A:613:PHE:CE2	1:A:655:LEU:CD2	2.93	0.51
1:B:67:GLY:O	1:B:69:LEU:N	2.43	0.51
1:B:439:VAL:O	1:B:442:VAL:HG12	2.11	0.51
1:A:476:TYR:HB3	2:A:701:ANP:N6	2.26	0.51
1:B:420:ARG:NH1	1:B:430:ARG:HD3	2.24	0.51
1:A:533:THR:OG1	1:A:534:LYS:N	2.41	0.51
1:A:72:LEU:N	1:A:72:LEU:CD1	2.73	0.51
1:A:113:LYS:HE2	1:A:227:GLU:OE2	2.11	0.51
1:B:76:THR:HG23	1:B:86:THR:HA	1.93	0.51
1:A:231:HIS:O	1:A:235:ILE:HG13	2.11	0.50
1:B:61:VAL:HG12	1:B:68:GLU:OE1	2.10	0.50
1:A:623:HIS:CD2	1:A:627:LYS:HE2	2.47	0.50
1:B:484:GLU:O	1:B:488:ILE:HG12	2.11	0.50
1:B:127:ARG:HG3	1:B:238:HIS:HD2	1.74	0.50
1:B:424:MET:HG3	1:A:459:GLY:CA	2.41	0.50
1:A:206:ALA:O	1:A:209:ILE:N	2.44	0.50
1:B:54:LEU:O	1:B:57:PHE:HB3	2.11	0.50
1:B:66:TYR:HE1	1:B:69:LEU:HD22	1.76	0.50
1:B:313:GLY:CA	1:B:319:LYS:HE2	2.40	0.50
1:B:397:GLU:HG3	1:B:656:ASN:HD22	1.77	0.50
1:A:78:GLN:HG3	1:A:84:ARG:HG3	1.93	0.50
1:A:137:ARG:HE	1:A:160:PRO:HB2	1.76	0.50
1:B:115:LEU:CD1	1:B:115:LEU:N	2.75	0.49
1:B:82:ASN:HB2	1:B:219:GLU:OE2	2.12	0.49
1:B:408:LEU:HB2	1:B:455:MET:CB	2.42	0.49
1:A:130:ALA:HB2	1:A:237:VAL:HG11	1.93	0.49
1:A:449:HIS:ND1	1:A:609:PHE:HE1	2.07	0.49
1:B:57:PHE:C	1:B:57:PHE:CD2	2.85	0.49
1:B:334:VAL:CG2	1:B:335:PRO:CD	2.89	0.49
1:A:54:LEU:HB2	1:A:77:TYR:CD2	2.47	0.49
1:A:391:GLN:HE22	1:A:418:MET:CE	2.24	0.49
1:B:655:LEU:O	1:B:661:LEU:HD13	2.13	0.49
1:A:61:VAL:O	1:A:61:VAL:HG12	2.13	0.49
1:A:357:ARG:HH21	1:A:657:ARG:HG2	1.77	0.49
1:A:470:VAL:H	1:A:482:THR:HB	1.77	0.49
1:A:354:GLU:O	1:A:390:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:OE2	1:A:613:PHE:HB3	2.13	0.49
1:A:66:TYR:CE1	1:A:94:PRO:HD3	2.48	0.49
1:A:313:GLY:N	1:A:319:LYS:HD3	2.28	0.49
1:B:134:PHE:C	1:B:134:PHE:CD2	2.86	0.49
1:A:344:VAL:HG13	1:A:405:LEU:HD21	1.88	0.49
1:B:58:PHE:HA	1:B:61:VAL:HG23	1.94	0.48
1:B:520:SER:HA	1:B:660:THR:O	2.13	0.48
1:B:194:LEU:N	1:B:194:LEU:CD2	2.76	0.48
1:A:310:LEU:HD11	1:A:463:TYR:HB3	1.96	0.48
1:B:225:LEU:HD21	1:B:230:LEU:CD2	2.43	0.48
1:B:652:GLY:O	1:B:656:ASN:HB2	2.13	0.48
1:B:76:THR:HG23	1:B:86:THR:CA	2.43	0.48
1:B:225:LEU:CD2	1:B:230:LEU:HD23	2.44	0.48
1:A:221:CYS:O	1:A:225:LEU:HD13	2.14	0.48
1:A:131:ALA:O	1:A:135:ILE:HG13	2.14	0.47
1:B:128:ARG:O	1:B:132:GLU:HG3	2.14	0.47
1:A:368:ILE:CD1	1:A:389:THR:HA	2.44	0.47
1:A:485:ALA:O	1:A:488:ILE:N	2.47	0.47
1:B:66:TYR:CE2	1:B:94:PRO:CG	2.85	0.47
1:B:76:THR:HG23	1:B:86:THR:OG1	2.13	0.47
1:B:352:ARG:NH1	1:B:556:GLU:OE2	2.47	0.47
1:B:543:ILE:O	1:B:549:THR:HA	2.14	0.47
1:A:114:VAL:HA	1:A:231:HIS:HD2	1.79	0.47
1:A:261:ILE:N	1:A:338:GLY:O	2.48	0.47
1:B:241:GLU:HG2	1:B:601:VAL:HG21	1.97	0.47
1:B:409:ASP:C	1:B:411:ASP:N	2.66	0.47
1:B:357:ARG:HH21	1:B:657:ARG:CA	2.27	0.47
1:B:573:LEU:CA	1:B:633:THR:HG21	2.38	0.47
1:B:578:GLU:N	1:B:579:PRO:HD2	2.30	0.47
1:A:79:ILE:HD11	1:A:83:VAL:CG1	2.44	0.47
1:A:82:ASN:OD1	1:A:82:ASN:N	2.48	0.47
1:B:439:VAL:HG13	1:B:440:GLU:HG2	1.95	0.47
1:A:54:LEU:HD11	1:A:58:PHE:CE2	2.49	0.47
1:A:287:GLU:HA	1:A:301:GLY:O	2.14	0.47
1:A:317:HIS:O	1:A:476:TYR:HD1	1.96	0.47
1:A:337:ASP:OD1	1:A:339:ARG:NH2	2.48	0.47
1:A:360:HIS:HB3	1:A:661:LEU:HD23	1.96	0.47
1:B:240:GLN:OE1	1:B:332:ASN:HB3	2.13	0.47
1:B:305:PRO:HG2	1:B:468:ARG:HG2	1.97	0.47
1:A:577:GLY:HA3	1:A:581:ILE:HD12	1.97	0.47
1:B:137:ARG:NH2	1:B:161:SER:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:O	1:A:194:LEU:CD1	2.63	0.47
1:B:226:ASN:OD1	1:B:229:ASP:OD2	2.32	0.46
1:B:391:GLN:HB3	1:B:417:LEU:HD12	1.97	0.46
1:A:79:ILE:HD12	1:A:215:VAL:CG2	2.46	0.46
1:A:337:ASP:OD2	1:A:339:ARG:NE	2.32	0.46
1:B:441:ARG:HB3	1:B:507:PHE:HZ	1.81	0.46
1:B:225:LEU:HD23	1:B:226:ASN:N	2.30	0.46
1:B:308:LEU:HD23	1:B:467:ALA:HA	1.98	0.46
1:B:373:PHE:N	1:B:373:PHE:CD1	2.79	0.46
1:A:581:ILE:HA	1:A:584:GLU:HB3	1.96	0.46
1:B:163:HIS:HD1	1:B:333:HIS:CE1	2.34	0.46
1:B:244:ARG:CG	1:B:343:VAL:HB	2.22	0.46
1:A:344:VAL:HG13	1:A:405:LEU:HD22	1.92	0.46
1:A:357:ARG:NH2	1:A:657:ARG:HG2	2.30	0.46
1:A:505:SER:OG	1:A:506:VAL:N	2.49	0.46
1:B:480:ASP:OD1	1:B:482:THR:HG22	2.15	0.46
1:A:93:ASP:CB	1:A:94:PRO:CD	2.61	0.46
1:A:127:ARG:HG3	1:A:238:HIS:HD2	1.80	0.46
1:A:127:ARG:NH2	1:A:294:HIS:HD2	2.02	0.46
1:B:352:ARG:HD3	1:B:554:MET:HB3	1.98	0.46
1:A:149:ARG:O	1:A:150:ARG:HG2	2.15	0.46
1:B:312:ALA:HB1	1:A:424:MET:HE1	1.96	0.46
1:A:448:ASN:HD22	1:A:505:SER:HB2	1.80	0.46
1:A:521:PHE:CE2	1:A:575:TYR:HA	2.50	0.46
1:A:58:PHE:O	1:A:62:GLU:N	2.49	0.46
1:A:69:LEU:HA	1:A:72:LEU:HD13	1.96	0.46
1:A:632:ARG:O	1:A:633:THR:C	2.53	0.46
1:B:76:THR:HG21	1:B:86:THR:OG1	2.15	0.46
1:B:380:PHE:CZ	1:B:389:THR:HG21	2.48	0.46
1:B:156:GLN:HB3	1:B:191:ARG:HB3	1.97	0.46
1:B:391:GLN:O	1:B:394:ASN:HB2	2.16	0.46
1:A:573:LEU:HD11	1:A:581:ILE:HD13	1.98	0.46
1:B:386:SER:HB2	1:B:389:THR:CB	2.43	0.45
1:A:339:ARG:O	1:A:342:VAL:HG13	2.16	0.45
1:B:96:ALA:O	1:B:98:GLY:N	2.50	0.45
1:B:262:LEU:HD22	1:B:325:ALA:HB2	1.97	0.45
1:A:114:VAL:HG23	1:A:115:LEU:HD13	1.99	0.45
1:B:95:PHE:O	1:B:95:PHE:CD1	2.70	0.45
1:B:113:LYS:HE3	1:B:231:HIS:ND1	2.31	0.45
1:B:127:ARG:NH2	1:B:294:HIS:HD2	2.14	0.45
1:A:344:VAL:HG12	1:A:345:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:PHE:CZ	1:B:72:LEU:HD11	2.52	0.45
1:B:127:ARG:HG3	1:B:238:HIS:CD2	2.51	0.45
1:B:131:ALA:O	1:B:135:ILE:HG13	2.16	0.45
1:A:396:MET:HE1	1:A:399:LEU:HD12	1.99	0.45
1:B:59:HIS:O	1:B:60:SER:C	2.51	0.45
1:B:382:THR:HG21	1:A:316:PHE:HZ	1.82	0.45
1:B:96:ALA:HB1	1:B:97:PRO:CD	2.44	0.45
1:B:263:PRO:O	1:B:263:PRO:HG2	2.16	0.45
1:B:461:GLY:N	1:A:421:ASP:OD2	2.46	0.45
1:A:165:LEU:HD21	1:A:563:GLN:NE2	2.32	0.45
1:A:360:HIS:CD2	1:A:663:THR:N	2.85	0.45
1:A:417:LEU:O	1:A:437:PRO:HA	2.17	0.45
1:B:57:PHE:O	1:B:60:SER:HB2	2.17	0.45
1:B:142:GLY:O	1:B:148:PRO:HD3	2.17	0.45
1:A:429:PRO:HB2	1:A:432:GLN:HG2	1.99	0.45
1:A:192:VAL:O	1:A:194:LEU:HD12	2.17	0.45
1:B:254:ALA:HB3	1:B:304:LEU:HD12	1.98	0.44
1:A:360:HIS:HA	1:A:381:VAL:HG22	1.99	0.44
1:A:244:ARG:NH1	1:A:343:VAL:HG12	2.31	0.44
1:B:336:ASP:O	1:B:338:GLY:N	2.50	0.44
1:A:351:ILE:HG13	1:A:406:LEU:HD22	1.98	0.44
1:B:424:MET:HE3	1:A:459:GLY:H	1.81	0.44
1:A:309:THR:HB	1:A:454:ILE:HG23	2.00	0.44
1:B:505:SER:OG	1:B:506:VAL:N	2.49	0.44
1:B:55:MET:HB2	1:B:207:ILE:HG12	2.00	0.44
1:B:336:ASP:O	1:B:337:ASP:C	2.57	0.44
1:B:426:MET:O	1:B:427:LEU:C	2.56	0.44
1:A:54:LEU:O	1:A:57:PHE:HB3	2.18	0.44
1:A:523:THR:HG21	1:A:660:THR:OG1	2.18	0.44
1:B:210:PHE:HD1	1:B:214:LEU:HD12	1.82	0.44
1:A:660:THR:HG23	1:A:660:THR:O	2.18	0.44
1:B:199:ARG:NH1	1:A:199:ARG:HD3	2.32	0.44
1:B:261:ILE:O	1:B:264:ARG:NH2	2.51	0.44
1:A:449:HIS:ND1	1:A:609:PHE:CE1	2.84	0.44
1:B:521:PHE:O	1:B:524:VAL:HG22	2.18	0.43
1:B:82:ASN:HB2	1:B:219:GLU:CD	2.38	0.43
1:B:244:ARG:CG	1:B:343:VAL:HG12	2.46	0.43
1:B:420:ARG:O	1:B:420:ARG:HG3	2.18	0.43
1:A:156:GLN:HB3	1:A:191:ARG:HB3	1.99	0.43
1:A:231:HIS:CE1	1:A:235:ILE:HD11	2.53	0.43
1:B:128:ARG:NH1	1:B:128:ARG:CG	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:O	1:B:390:SER:HB3	2.15	0.43
1:B:422:ALA:HB1	1:B:426:MET:HE2	2.00	0.43
1:B:581:ILE:HD11	1:B:585:MET:HE2	2.01	0.43
1:A:159:ARG:HA	1:A:160:PRO:HD2	1.72	0.43
1:A:163:HIS:CE1	1:A:333:HIS:HD1	2.35	0.43
1:A:367:PHE:CE2	1:A:395:ILE:HG21	2.53	0.43
1:A:395:ILE:O	1:A:399:LEU:HG	2.18	0.43
1:B:333:HIS:HB3	1:B:337:ASP:CB	2.48	0.43
1:B:401:LEU:HD13	1:B:649:ILE:HA	2.00	0.43
1:B:617:ILE:HD13	1:B:617:ILE:HA	1.89	0.43
1:B:653:ALA:HB1	1:B:657:ARG:NH1	2.17	0.43
1:A:61:VAL:HG12	1:A:201:ILE:HD12	2.00	0.43
1:A:206:ALA:O	1:A:209:ILE:HB	2.18	0.43
1:A:233:HIS:O	1:A:237:VAL:HG23	2.19	0.43
1:A:430:ARG:HH22	1:A:436:THR:HG23	1.84	0.43
1:B:225:LEU:HD21	1:B:230:LEU:HD23	1.99	0.43
1:A:242:GLU:O	1:A:246:ASN:CG	2.57	0.43
1:A:380:PHE:O	1:A:381:VAL:HG23	2.19	0.43
1:A:480:ASP:OD1	1:A:482:THR:HG22	2.18	0.43
1:B:523:THR:O	1:B:523:THR:OG1	2.33	0.43
1:B:560:GLU:HB2	1:B:563:GLN:HG3	2.00	0.43
1:A:54:LEU:HD13	1:A:77:TYR:CD2	2.54	0.43
1:A:94:PRO:HG2	1:A:95:PHE:HD2	1.84	0.43
1:A:222:VAL:O	1:A:225:LEU:HD22	2.18	0.43
1:B:73:THR:HG22	1:B:74:ASN:CG	2.39	0.43
1:B:409:ASP:C	1:B:411:ASP:H	2.22	0.43
1:A:324:ARG:O	1:A:328:VAL:HG22	2.19	0.43
1:A:659:ARG:O	1:A:659:ARG:CG	2.66	0.43
1:A:308:LEU:O	1:A:468:ARG:HB3	2.19	0.42
1:A:330:ILE:HD12	1:A:647:ARG:HD3	2.00	0.42
1:B:67:GLY:C	1:B:69:LEU:H	2.23	0.42
1:A:400:GLU:O	1:A:614:SER:HB2	2.19	0.42
1:A:428:VAL:O	1:A:428:VAL:HG23	2.18	0.42
1:B:166:GLU:HG2	1:B:629:LEU:HD11	2.00	0.42
1:A:636:CYS:SG	1:A:638:LEU:HB2	2.59	0.42
1:B:244:ARG:HG3	1:B:343:VAL:HG12	1.99	0.42
1:B:337:ASP:CG	1:B:339:ARG:HH21	2.23	0.42
1:B:437:PRO:HB2	1:B:439:VAL:HG12	2.02	0.42
1:A:82:ASN:O	1:A:106:PRO:HD2	2.19	0.42
1:A:305:PRO:HG2	1:A:468:ARG:HG2	2.00	0.42
1:A:401:LEU:HD11	1:A:652:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASP:OD1	1:B:339:ARG:NH2	2.52	0.42
1:A:360:HIS:HD2	1:A:663:THR:HB	1.85	0.42
1:B:397:GLU:CG	1:B:656:ASN:ND2	2.81	0.42
1:B:434:PRO:HD2	1:A:314:GLY:O	2.20	0.42
1:B:356:ARG:O	1:B:659:ARG:NH2	2.47	0.42
1:B:370:ASN:HB3	1:B:434:PRO:HB3	2.02	0.42
1:B:595:LEU:HD23	1:B:596:PRO:HD2	2.01	0.42
1:A:203:GLY:O	1:A:207:ILE:HB	2.20	0.42
1:A:360:HIS:CD2	1:A:663:THR:H	2.37	0.42
1:A:366:PRO:O	1:A:441:ARG:NE	2.52	0.42
1:B:409:ASP:O	1:B:410:GLU:C	2.58	0.42
1:A:405:LEU:HA	1:A:452:SER:O	2.20	0.42
1:B:295:SER:OG	1:B:297:LYS:HB2	2.20	0.42
1:B:543:ILE:HG13	1:B:552:LEU:HD11	2.02	0.42
1:B:57:PHE:CE2	1:B:72:LEU:HD11	2.55	0.41
1:B:425:GLN:O	1:B:428:VAL:O	2.36	0.41
1:B:370:ASN:C	1:B:371:LEU:HD23	2.38	0.41
1:A:126:CYS:HB2	1:A:601:VAL:HG23	2.01	0.41
1:B:89:SER:OG	1:B:90:ILE:N	2.54	0.41
1:B:97:PRO:HD2	1:B:98:GLY:H	1.85	0.41
1:B:235:ILE:O	1:B:239:ASP:HB2	2.20	0.41
1:A:433:GLU:HA	1:A:434:PRO:HD3	1.89	0.41
1:B:282:SER:HA	1:B:283:PRO:HD2	1.89	0.41
1:B:323:LEU:HD22	1:B:456:VAL:HG23	2.02	0.41
1:B:419:TYR:HB2	1:B:462:GLN:OE1	2.19	0.41
1:B:150:ARG:HG2	1:B:212:ASN:HB3	2.03	0.41
1:B:354:GLU:HG2	1:B:357:ARG:HB3	2.03	0.41
1:B:357:ARG:NH2	1:B:657:ARG:HA	2.35	0.41
1:A:82:ASN:O	1:A:105:CYS:HB2	2.20	0.41
1:A:573:LEU:N	1:A:633:THR:HG21	2.35	0.41
1:B:170:VAL:HA	1:B:187:GLU:O	2.20	0.41
1:A:73:THR:C	1:A:75:GLU:H	2.24	0.41
1:A:313:GLY:H	1:A:319:LYS:HD3	1.85	0.41
1:A:417:LEU:HB3	1:A:418:MET:HE2	2.03	0.41
1:B:100:GLN:H	1:B:100:GLN:HG3	1.67	0.41
1:B:320:SER:O	1:B:324:ARG:HG3	2.20	0.41
1:B:424:MET:CE	1:A:459:GLY:H	2.34	0.41
1:B:638:LEU:HD23	1:B:639:PRO:HD3	1.95	0.41
1:A:220:GLN:NE2	4:A:802:HOH:O	2.51	0.41
1:A:263:PRO:HG2	1:A:263:PRO:O	2.21	0.41
1:A:354:GLU:O	1:A:390:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:HB3	1:A:424:MET:HB2	2.03	0.41
1:A:595:LEU:HD23	1:A:596:PRO:HD2	2.03	0.41
1:A:638:LEU:HA	1:A:639:PRO:HD3	1.92	0.41
1:A:148:PRO:HG3	1:A:217:LEU:HG	2.02	0.41
1:B:54:LEU:HD13	1:B:77:TYR:CD2	2.56	0.40
1:B:408:LEU:HD12	1:B:408:LEU:N	2.36	0.40
1:B:647:ARG:HE	1:B:647:ARG:HB2	1.72	0.40
1:B:658:LEU:HD12	1:B:659:ARG:N	2.36	0.40
1:A:62:GLU:OE1	1:A:63:GLY:N	2.54	0.40
1:A:581:ILE:O	1:A:581:ILE:CG2	2.68	0.40
1:B:462:GLN:O	1:B:465:PRO:HD2	2.21	0.40
1:A:102:ARG:HG2	1:A:104:VAL:HG23	2.03	0.40
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.96	0.40
1:B:316:PHE:N	2:B:701:ANP:O2B	2.54	0.40
1:B:396:MET:HE1	1:B:507:PHE:HE1	1.85	0.40
1:B:357:ARG:NE	1:B:657:ARG:HG2	2.36	0.40
1:B:359:VAL:O	1:B:381:VAL:HA	2.22	0.40
1:A:344:VAL:O	1:A:345:ASP:C	2.56	0.40
1:A:522:THR:HG23	1:A:523:THR:N	2.35	0.40

All (50) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:C	1:A:580:ARG:NH1[2_455]	0.27	1.93
1:B:69:LEU:C	1:A:632:ARG:NH2[2_455]	0.39	1.81
1:B:70:ARG:CA	1:A:632:ARG:NE[2_455]	0.55	1.65
1:B:584:GLU:CD	1:A:64:ARG:NE[2_455]	0.57	1.63
1:B:584:GLU:CG	1:A:64:ARG:NH2[2_455]	0.63	1.57
1:B:64:ARG:N	1:A:580:ARG:CZ[2_455]	0.89	1.31
1:B:584:GLU:CD	1:A:64:ARG:CZ[2_455]	0.93	1.27
1:B:70:ARG:C	1:A:632:ARG:CD[2_455]	0.97	1.23
1:B:63:GLY:O	1:A:580:ARG:NH1[2_455]	1.07	1.13
1:B:70:ARG:O	1:A:632:ARG:CD[2_455]	1.09	1.11
1:B:70:ARG:N	1:A:632:ARG:NH2[2_455]	1.12	1.08
1:B:584:GLU:OE1	1:A:64:ARG:NE[2_455]	1.12	1.08
1:B:584:GLU:OE2	1:A:64:ARG:NE[2_455]	1.14	1.06
1:B:70:ARG:N	1:A:632:ARG:CZ[2_455]	1.17	1.03
1:B:584:GLU:OE1	1:A:64:ARG:NH1[2_455]	1.55	0.65
1:B:69:LEU:O	1:A:632:ARG:NH2[2_455]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:CB	1:A:632:ARG:NE[2_455]	1.64	0.56
1:B:63:GLY:O	1:A:580:ARG:CZ[2_455]	1.65	0.55
1:B:70:ARG:NH1	1:A:634:PRO:CB[2_455]	1.68	0.52
1:B:71:SER:N	1:A:632:ARG:CZ[2_455]	1.68	0.52
1:B:70:ARG:C	1:A:632:ARG:CZ[2_455]	1.70	0.50
1:B:64:ARG:C	1:A:580:ARG:NE[2_455]	1.72	0.48
1:B:69:LEU:O	1:A:632:ARG:CZ[2_455]	1.77	0.43
1:B:70:ARG:C	1:A:632:ARG:NH1[2_455]	1.79	0.41
1:B:70:ARG:C	1:A:632:ARG:CG[2_455]	1.79	0.41
1:B:70:ARG:O	1:A:632:ARG:CG[2_455]	1.79	0.41
1:B:64:ARG:CB	1:A:580:ARG:NH2[2_455]	1.80	0.40
1:B:64:ARG:C	1:A:580:ARG:CZ[2_455]	1.81	0.39
1:B:72:LEU:N	1:A:632:ARG:NH1[2_455]	1.83	0.37
1:B:584:GLU:CD	1:A:64:ARG:NH2[2_455]	1.83	0.37
1:B:64:ARG:C	1:A:580:ARG:NH2[2_455]	1.86	0.34
1:B:61:VAL:O	1:A:580:ARG:NH2[2_455]	1.91	0.29
1:B:584:GLU:CD	1:A:64:ARG:CD[2_455]	1.94	0.26
1:B:70:ARG:CB	1:A:632:ARG:CD[2_455]	1.95	0.25
1:B:69:LEU:O	1:A:632:ARG:NH1[2_455]	2.00	0.20
1:B:64:ARG:N	1:A:580:ARG:NE[2_455]	2.02	0.18
1:B:71:SER:N	1:A:632:ARG:NE[2_455]	2.02	0.18
1:B:69:LEU:N	1:A:632:ARG:NH2[2_455]	2.03	0.17
1:B:584:GLU:CD	1:A:64:ARG:NH1[2_455]	2.03	0.17
1:B:584:GLU:CG	1:A:64:ARG:NE[2_455]	2.04	0.16
1:B:584:GLU:CG	1:A:64:ARG:NH1[2_455]	2.04	0.16
1:B:63:GLY:O	1:A:580:ARG:NE[2_455]	2.07	0.13
1:B:71:SER:N	1:A:632:ARG:CG[2_455]	2.07	0.13
1:B:71:SER:CA	1:A:632:ARG:NH1[2_455]	2.09	0.11
1:B:64:ARG:O	1:A:580:ARG:CZ[2_455]	2.10	0.10
1:B:584:GLU:OE2	1:A:64:ARG:CZ[2_455]	2.11	0.09
1:B:64:ARG:O	1:A:580:ARG:NH2[2_455]	2.12	0.08
1:B:75:GLU:OE2	1:A:640:ARG:NH1[2_455]	2.14	0.06
1:B:71:SER:N	1:A:632:ARG:CD[2_455]	2.15	0.05
1:B:584:GLU:OE2	1:A:64:ARG:CD[2_455]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	563/680 (83%)	535 (95%)	28 (5%)	0	100	100
1	B	563/680 (83%)	534 (95%)	26 (5%)	3 (0%)	29	66
All	All	1126/1360 (83%)	1069 (95%)	54 (5%)	3 (0%)	41	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLU
1	B	410	GLU
1	B	579	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/567 (87%)	455 (93%)	36 (7%)	14	43
1	B	491/567 (87%)	455 (93%)	36 (7%)	14	43
All	All	982/1134 (87%)	910 (93%)	72 (7%)	14	43

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	MET
1	B	61	VAL
1	B	65	ASN
1	B	66	TYR
1	B	75	GLU
1	B	99	SER
1	B	105	CYS
1	B	110	SER
1	B	137	ARG

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Mol	Chain	Res	Type
1	B	138	SER
1	B	151	THR
1	B	162	GLN
1	B	194	LEU
1	B	200	ARG
1	B	208	ASP
1	B	220	GLN
1	B	230	LEU
1	B	316	PHE
1	B	332	ASN
1	B	357	ARG
1	B	371	LEU
1	B	382	THR
1	B	395	ILE
1	B	412	THR
1	B	417	LEU
1	B	427	LEU
1	B	428	VAL
1	B	484	GLU
1	B	493	SER
1	B	524	VAL
1	B	533	THR
1	B	559	VAL
1	B	567	ILE
1	B	632	ARG
1	B	637	TYR
1	B	663	THR
1	A	58	PHE
1	A	66	TYR
1	A	75	GLU
1	A	77	TYR
1	A	81	GLU
1	A	82	ASN
1	A	87	PHE
1	A	103	LEU
1	A	110	SER
1	A	199	ARG
1	A	225	LEU
1	A	230	LEU
1	A	248	LEU
1	A	332	ASN
1	A	333	HIS

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Mol	Chain	Res	Type
1	A	343	VAL
1	A	357	ARG
1	A	382	THR
1	A	384	ASP
1	A	396	MET
1	A	397	GLU
1	A	400	GLU
1	A	417	LEU
1	A	430	ARG
1	A	445	LEU
1	A	469	VAL
1	A	493	SER
1	A	510	ASP
1	A	512	ASN
1	A	567	ILE
1	A	574	LEU
1	A	588	LYS
1	A	614	SER
1	A	632	ARG
1	A	660	THR
1	A	663	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	ASN
1	B	82	ASN
1	B	163	HIS
1	B	220	GLN
1	B	226	ASN
1	B	238	HIS
1	B	281	GLN
1	B	332	ASN
1	B	333	HIS
1	B	369	ASN
1	B	656	ASN
1	A	91	GLN
1	A	231	HIS
1	A	240	GLN
1	A	281	GLN
1	A	391	GLN
1	A	448	ASN

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Mol	Chain	Res	Type
1	A	656	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ANP	B	701	3	29,33,33	1.86	5 (17%)	31,52,52	1.89	8 (25%)
2	ANP	A	701	3	29,33,33	1.98	9 (31%)	31,52,52	2.99	11 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	B	701	3	-	6/14/38/38	0/3/3/3
2	ANP	A	701	3	-	7/14/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	PG-N3B	4.66	1.75	1.63
2	B	701	ANP	PB-N3B	4.61	1.75	1.63
2	A	701	ANP	PB-O2B	-4.54	1.44	1.56
2	A	701	ANP	PG-O3G	-4.33	1.45	1.56
2	B	701	ANP	PB-O1B	3.36	1.51	1.46
2	B	701	ANP	PG-O1G	3.29	1.51	1.46
2	A	701	ANP	O4'-C4'	-3.13	1.38	1.45
2	A	701	ANP	PG-O2G	-2.90	1.48	1.56
2	A	701	ANP	PG-N3B	2.79	1.70	1.63
2	B	701	ANP	C5-C4	2.47	1.47	1.40
2	A	701	ANP	C5-N7	-2.32	1.31	1.39
2	A	701	ANP	C2'-C1'	-2.18	1.50	1.53
2	A	701	ANP	PA-O2A	-2.12	1.45	1.55
2	A	701	ANP	C2'-C3'	-2.02	1.47	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	ANP	O1G-PG-N3B	-11.17	95.32	111.77
2	A	701	ANP	O2B-PB-O1B	6.96	124.52	109.92
2	B	701	ANP	O1G-PG-N3B	-4.83	104.65	111.77
2	A	701	ANP	O1B-PB-N3B	-4.49	105.15	111.77
2	B	701	ANP	O2B-PB-O1B	4.05	118.41	109.92
2	B	701	ANP	C3'-C2'-C1'	3.51	106.26	100.98
2	B	701	ANP	PB-O3A-PA	-3.44	120.50	132.62
2	A	701	ANP	PB-O3A-PA	-3.32	120.91	132.62
2	B	701	ANP	N3-C2-N1	-3.18	123.71	128.68
2	A	701	ANP	O3A-PB-N3B	3.03	115.00	106.59
2	A	701	ANP	O4'-C1'-C2'	-2.94	102.63	106.93
2	A	701	ANP	N3-C2-N1	-2.88	124.18	128.68
2	A	701	ANP	N6-C6-N1	2.68	124.13	118.57
2	B	701	ANP	C4-C5-N7	-2.66	106.63	109.40
2	B	701	ANP	O1B-PB-N3B	-2.52	108.06	111.77
2	B	701	ANP	O2G-PG-O3G	2.33	113.84	107.64
2	A	701	ANP	O2G-PG-O3G	2.24	113.60	107.64
2	A	701	ANP	O3'-C3'-C2'	-2.23	104.62	111.82
2	A	701	ANP	O3'-C3'-C4'	-2.14	104.86	111.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B
2	B	701	ANP	PA-O3A-PB-O1B
2	A	701	ANP	PB-N3B-PG-O1G
2	A	701	ANP	PG-N3B-PB-O1B
2	A	701	ANP	PA-O3A-PB-O1B
2	A	701	ANP	C5'-O5'-PA-O1A
2	B	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	C5'-O5'-PA-O3A
2	B	701	ANP	C5'-O5'-PA-O2A
2	A	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C4'-C5'-O5'-PA
2	A	701	ANP	O4'-C4'-C5'-O5'

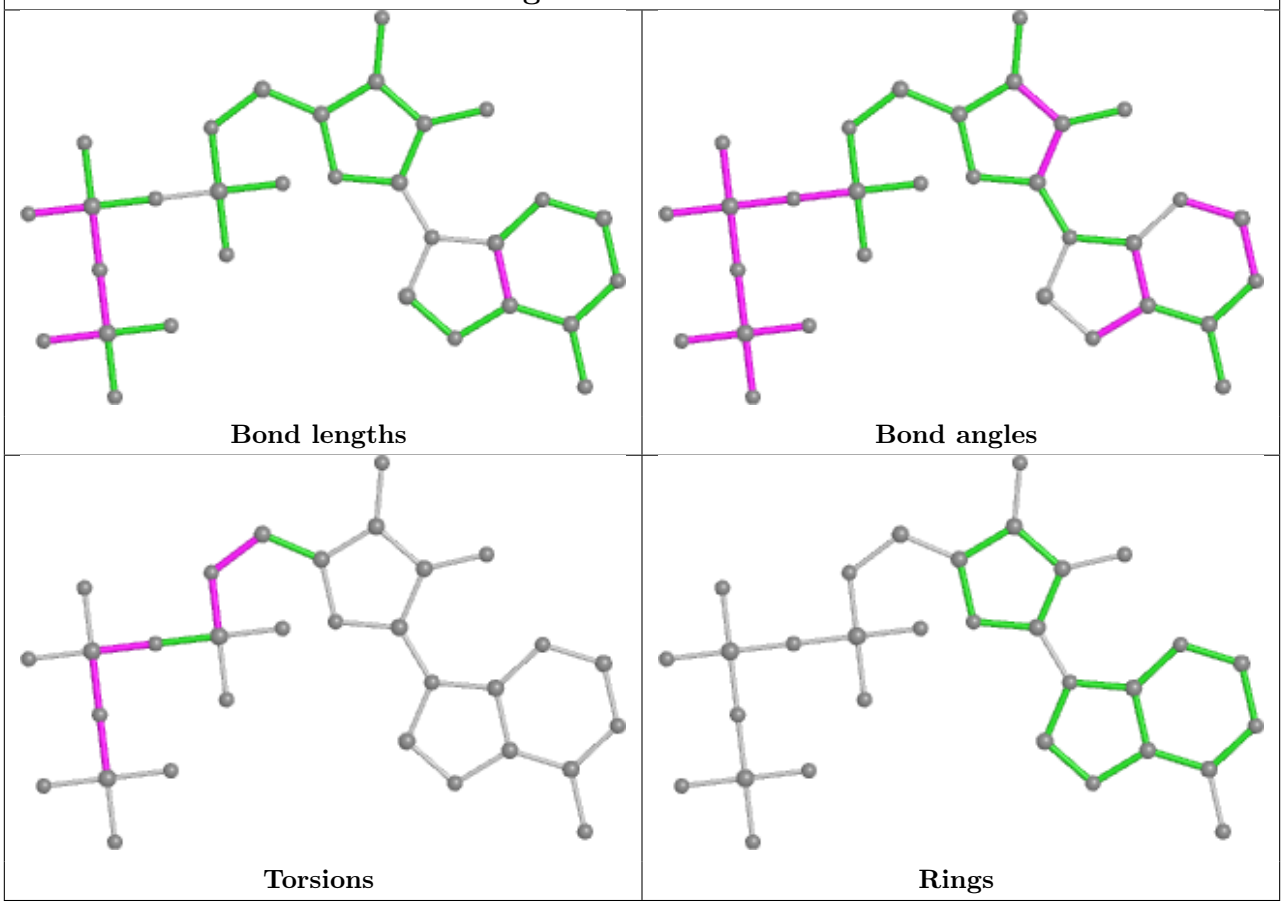
There are no ring outliers.

2 monomers are involved in 11 short contacts:

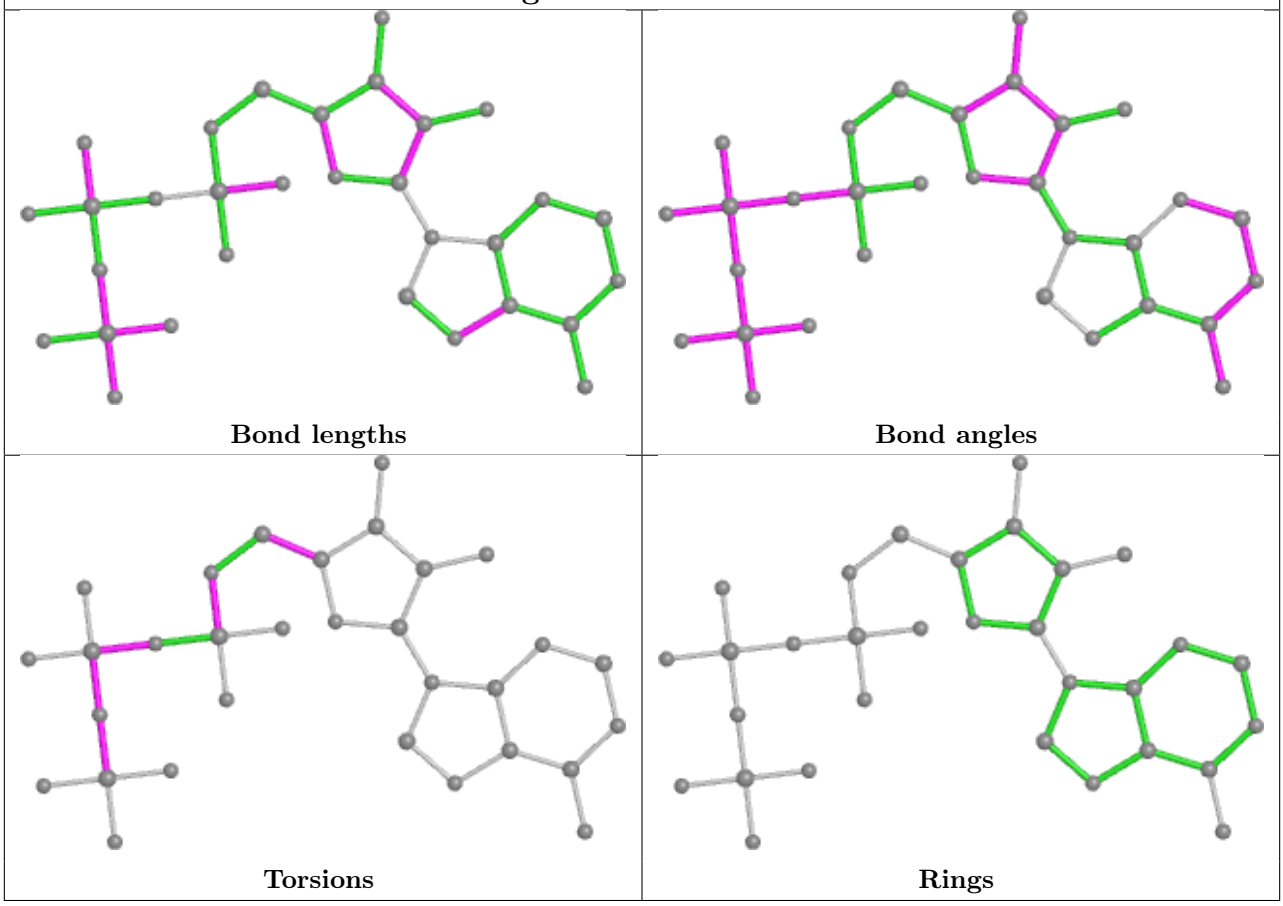
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ANP	7	0
2	A	701	ANP	4	0

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 701



Ligand ANP A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	577/680 (84%)	0.06	8 (1%)	75	48	26, 43, 72, 80	0
1	B	577/680 (84%)	-0.01	7 (1%)	79	53	26, 42, 74, 81	0
All	All	1154/1360 (84%)	0.03	15 (1%)	77	51	26, 42, 73, 81	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	5.3
1	A	70	ARG	4.8
1	A	427	LEU	3.1
1	B	114	VAL	3.0
1	B	72	LEU	3.0
1	B	617	ILE	2.7
1	A	97	PRO	2.6
1	A	428	VAL	2.6
1	B	68	GLU	2.6
1	A	214	LEU	2.3
1	A	69	LEU	2.3
1	B	492	SER	2.3
1	B	135	ILE	2.1
1	B	211	TYR	2.1
1	A	148	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

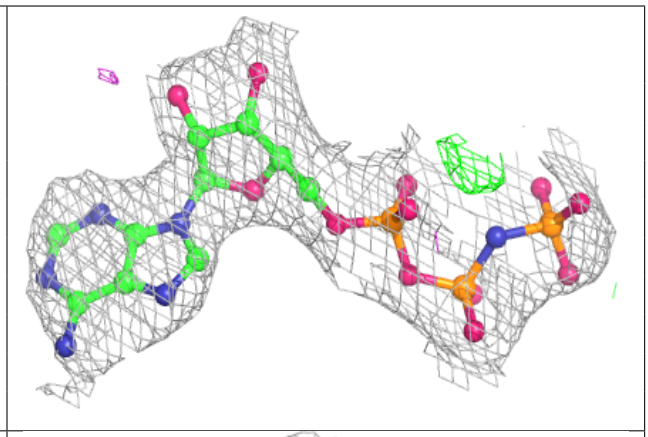
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

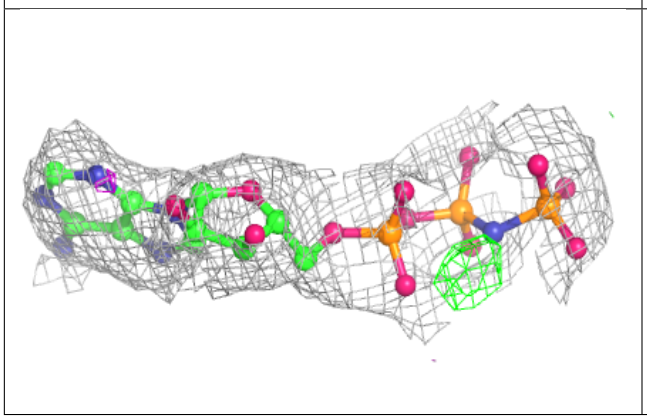
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	703	1/1	0.78	0.18	37,37,37,37	0
3	MG	A	702	1/1	0.91	0.09	45,45,45,45	0
2	ANP	B	701	31/31	0.93	0.18	36,37,40,40	0
2	ANP	A	701	31/31	0.95	0.17	36,40,44,45	0
3	MG	B	702	1/1	0.96	0.13	43,43,43,43	0
3	MG	A	703	1/1	0.97	0.16	79,79,79,79	0

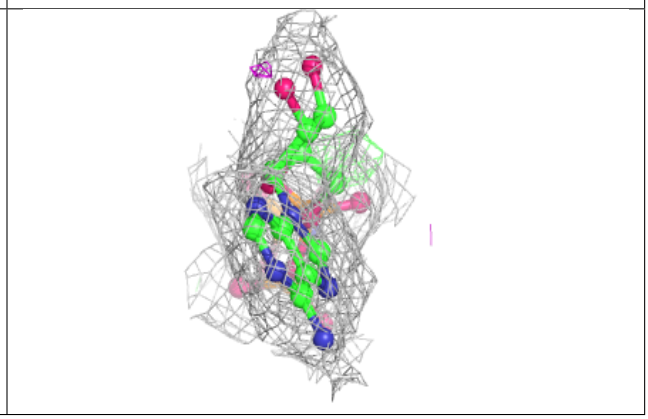
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

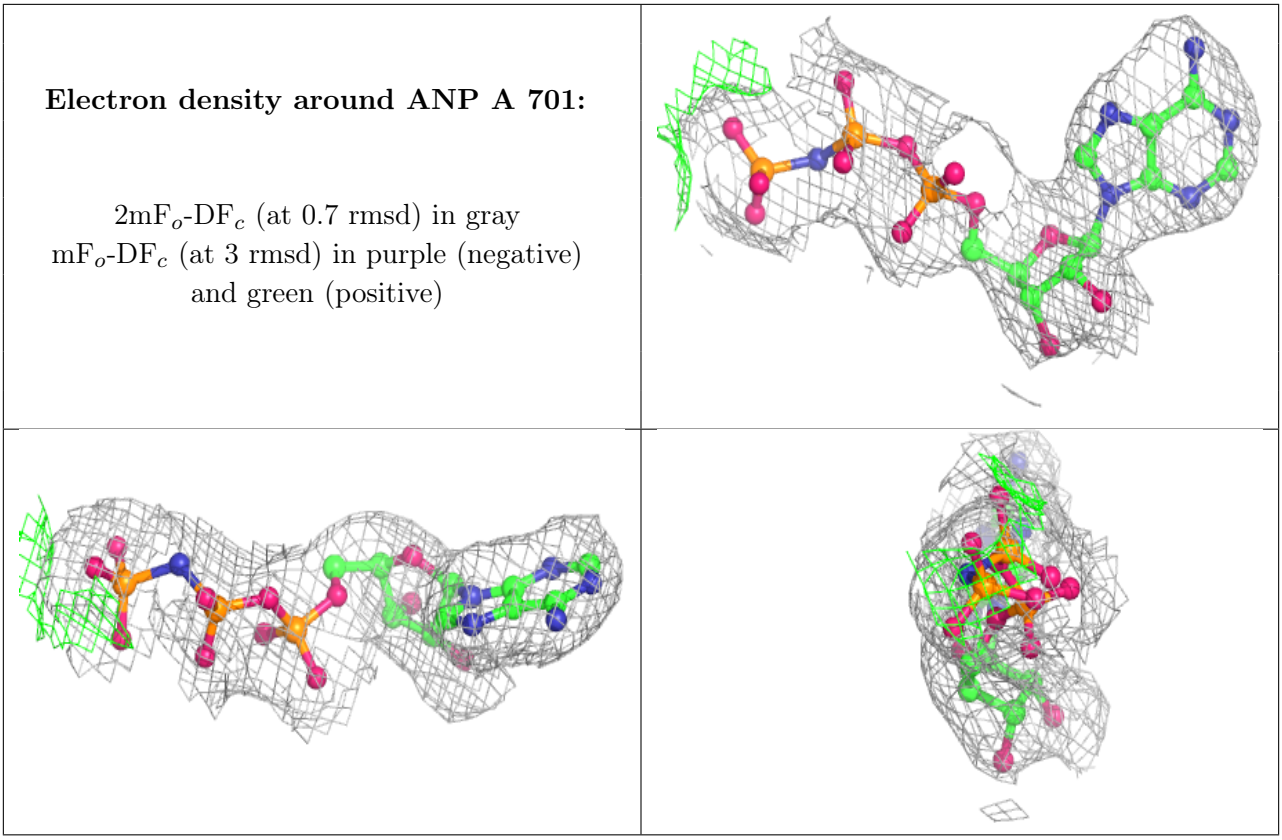






Electron density around ANP A 701:

$2mF_o$-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.