Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:51 pm BST

PDB ID	:	2ZPA
Title	:	Crystal Structure of tRNA(Met) Cytidine Acetyltransferase
Authors	:	Chimnaronk, S.; Manita, T.; Yao, M.; Tanaka, I.
Deposited on	:	2008-07-08
Resolution	:	2.35 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 following versions of software and data (see references ⓘ) were used in the production of this report:

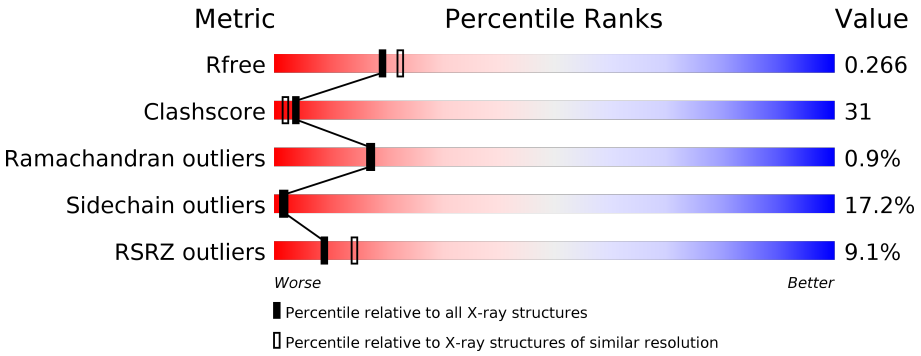
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	671	4% 61% 29% 8%
1	B	671	14% 48% 38% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACO	A	700	X	-	-	-
2	ACO	B	701	X	-	-	-

2 Entry composition

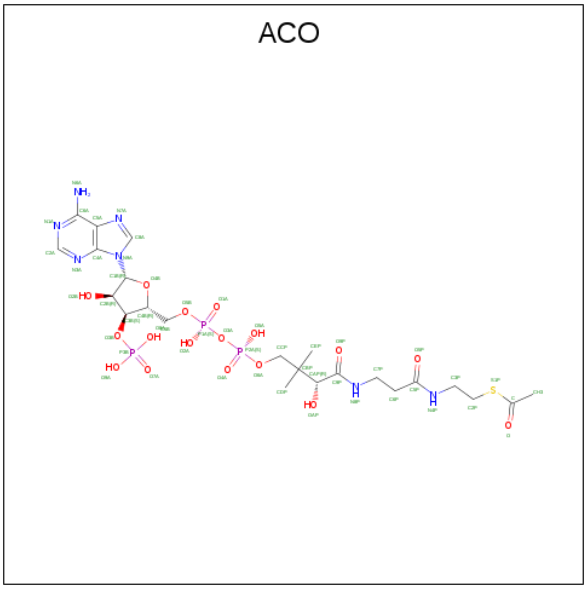
There are 5 unique types of molecules in this entry. The entry contains 10891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein ypfI.

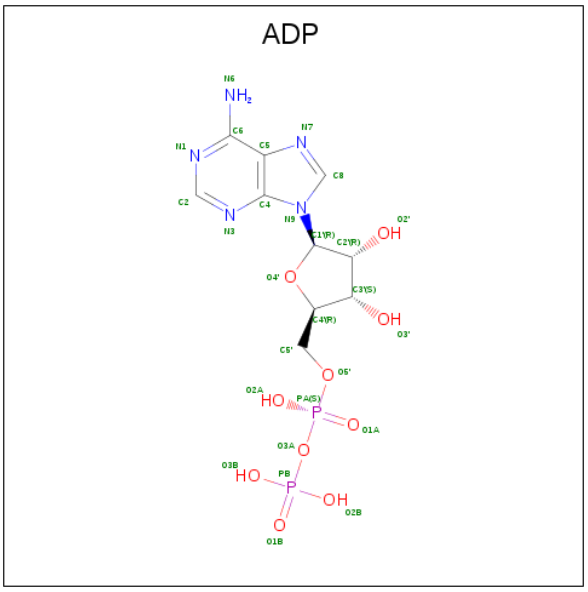
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	Se	0	0	0
			5189	3291	951	929	8	10			
1	B	662	Total	C	N	O	S	Se	0	0	0
			5218	3309	955	935	8	11			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



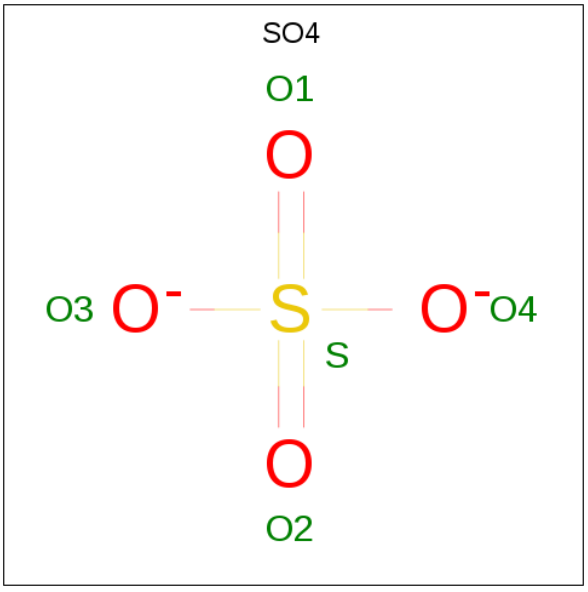
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 5 is water.

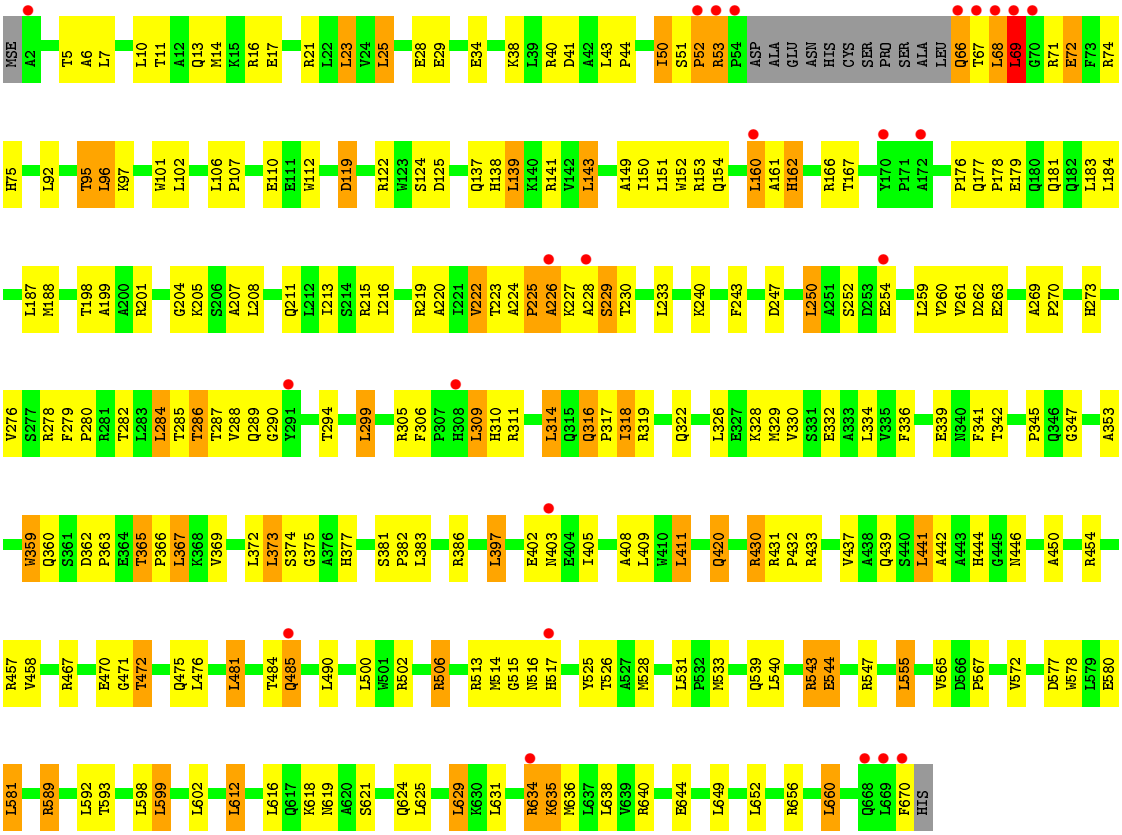
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	B	126	Total O 126 126	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

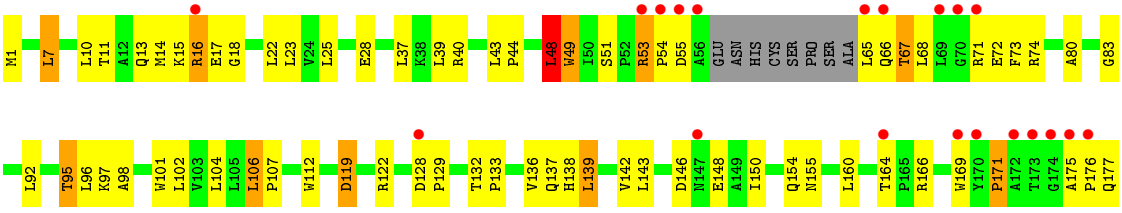
- Molecule 1: Uncharacterized protein ypfI

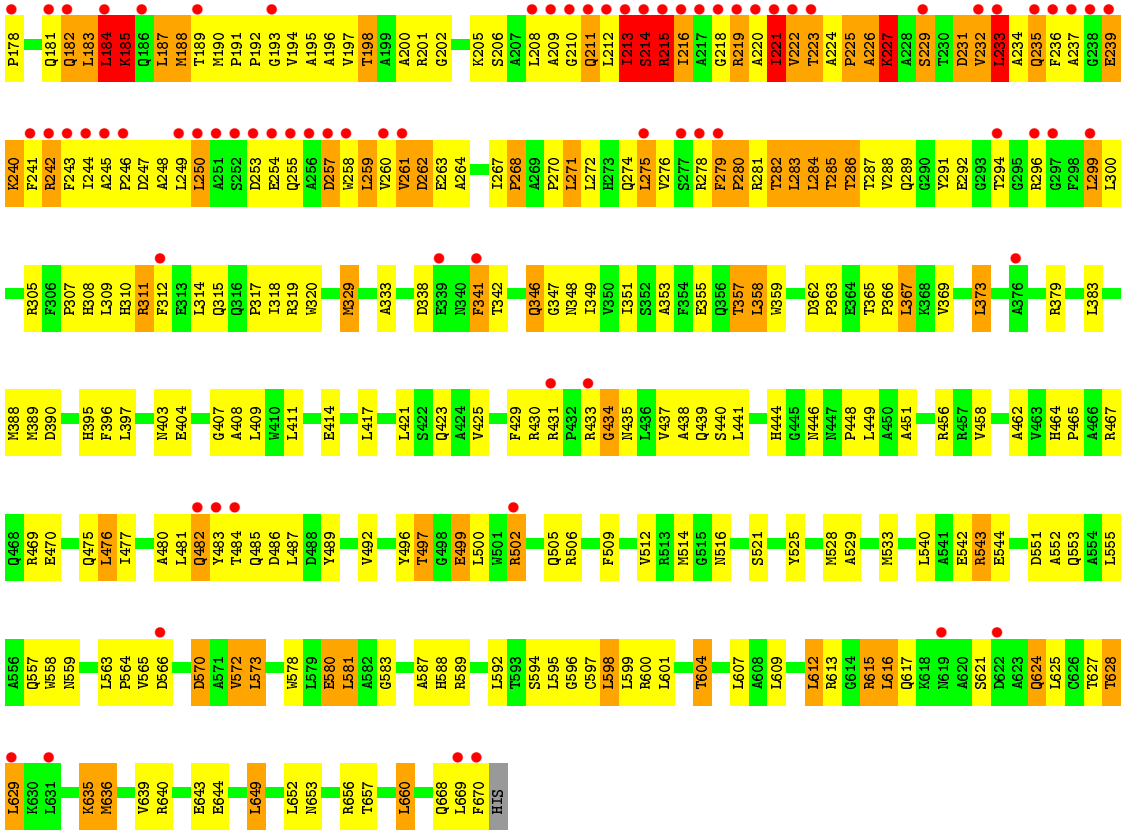
Chain A:



- Molecule 1: Uncharacterized protein ypfI

Chain B:




P178 Q181 Q182 L183 L184 K185 Q186 L187 M188 T189 M190 P191 P192 G193 V194 A195 A196 V197 T198 A199 A200 R201 G202 K205 S206 A207 L208 A209 G210 Q211 L212 I213 S214 R215 I216 A217 G218 R219 A220 I221 V222 T223 A224 P225 A226 K227 A228 S229 T230 D231 V232 L233 A234 Q235 F236 A237 G238 E239
K240 F241 R242 F243 I244 A245 P246 D247 A248 L249 L250 A251 S252 D253 E254 Q255 A256 D257 W258 L259 V260 V261 D262 E263 A264 I267 P268 A269 P270 L271 L272 H273 Q274 L275 V276 S277 R278 F279 P280 R281 T282 L283 L284 T285 T286 T287 V288 Q289 G290 Y291 E292 G293 T294 G295 R296 G297 F298 L299 L300
R305 F306 P307 H308 L309 H310 R311 F312 E313 L314 Q315 Q316 P317 I318 R319 W320 M329 A333 D338 E339 N340 F341 T342 Q346 G347 N348 I349 V350 I351 S352 A353 F354 E355 Q356 T357 L358 W359 D362 P363 E364 T365 P366 L367 K368 V369 L373 A376 R379 L383
M388 M389 D390 H395 F396 L397 N403 E404 G407 A408 L409 W410 L411 E414 L417 L421 S422 Q423 A424 V425 F429 R430 R431 P432 R433 G434 N435 L436 V437 A438 Q439 S440 L441 H444 G445 N446 W447 P448 L449 A450 A451 R456 R457 V458 A462 V463 H464 P465 A466 R467
Q468 R469 E470 Q475 L476 I477 A480 L481 Q482 Y483 T484 Q485 D486 L487 D488 Y489 V492 Y496 T497 G498 E499 L500 W501 R502 Q505 R506 F509 V512 R513 M514 G515 N516 S521 Y525 M528 A529 M533 L540 A541 E542 R543 E544 D551 A552 Q553 A554 L555
A556 Q557 W558 N559 L563 P564 V565 D566 D570 A571 V572 L573 W578 L579 E580 L581 A582 G583 A587 H588 R589 L592 T593 S594 L595 G596 C597 L598 L599 R600 L601 T604 L607 A608 L609 L612 R613 G614 R615 L616 Q617 K618 N619 A620 S621 D622 A623 Q624 L625 G626 T627 T628
L629 K630 L631 K635 M636 V639 R640 E643 E644 L649 L652 N653 R656 T657 L660 Q668 L669 F670 HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.30Å 100.99Å 263.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 40.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-2.35) 96.3 (40.99-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.274 0.226 , 0.266	Depositor DCC
R_{free} test set	5085 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10891	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, SO4, ADP

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	0.48	0/5306	0.77	7/7197 (0.1%)
1	B	0.49	2/5335 (0.0%)	0.82	16/7236 (0.2%)
All	All	0.48	2/10641 (0.0%)	0.79	23/14433 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLN	C-N	5.74	1.47	1.34
1	B	617	GLN	N-CA	5.51	1.57	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ARG	CD-NE-CZ	14.20	143.47	123.60
1	A	66	GLN	C-N-CA	-10.02	96.65	121.70
1	B	49	TRP	N-CA-CB	9.03	126.86	110.60
1	B	187	LEU	N-CA-C	-8.68	87.57	111.00
1	A	226	ALA	N-CA-C	-8.12	89.08	111.00
1	B	213	ILE	C-N-CA	-7.18	103.76	121.70
1	A	52	PRO	CA-N-CD	-6.68	102.15	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	LEU	C-N-CA	6.47	137.88	121.70
1	B	226	ALA	N-CA-C	-6.12	94.48	111.00
1	B	213	ILE	CA-C-N	6.10	130.62	117.20
1	B	270	PRO	CA-N-CD	-5.87	103.29	111.50
1	A	52	PRO	N-CA-C	5.80	127.17	112.10
1	B	434	GLY	N-CA-C	-5.79	98.62	113.10
1	A	397	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	66	GLN	CA-C-N	5.53	129.37	117.20
1	B	185	LYS	C-N-CA	-5.43	108.12	121.70
1	B	227	LYS	N-CA-C	5.40	125.57	111.00
1	B	54	PRO	N-CA-C	-5.28	98.36	112.10
1	B	214	SER	CA-C-N	5.28	128.82	117.20
1	B	171	PRO	CA-N-CD	-5.26	104.14	111.50
1	B	617	GLN	N-CA-CB	-5.24	101.16	110.60
1	B	270	PRO	CA-C-N	-5.23	105.69	117.20
1	B	669	LEU	CB-CA-C	-5.08	100.55	110.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	TRP	Mainchain
1	B	48	LEU	Peptide
1	B	656	ARG	Sidechain

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	5189	0	5151	230	0
1	B	5218	0	5183	413	0
2	A	51	0	30	3	0
2	B	51	0	33	7	0
3	A	27	0	12	2	0
4	B	5	0	0	1	0
5	A	224	0	0	13	0
5	B	126	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10891	0	10409	643	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 31.

All (643) 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:A:67:THR:CG2	1:A:71:ARG:HD3	1.36	1.51
1:B:185:LYS:HG3	1:B:215:ARG:NH2	1.51	1.25
1:B:274:GLN:HB3	1:B:278:ARG:NH2	1.62	1.14
1:B:221:ILE:HG23	1:B:259:LEU:HA	1.34	1.08
1:B:215:ARG:NH1	1:B:215:ARG:HG3	1.60	1.08
1:A:506:ARG:NH1	1:A:506:ARG:HG3	1.52	1.08
1:A:67:THR:CG2	1:A:71:ARG:CD	2.31	1.07
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.08	1.07
1:A:250:LEU:HD13	1:A:278:ARG:HH22	1.18	1.07
1:B:185:LYS:CG	1:B:215:ARG:HH21	1.66	1.06
1:B:11:THR:HA	1:B:14:MSE:HE3	1.10	1.05
1:B:184:LEU:HD11	1:B:211:GLN:HG2	1.38	1.04
1:A:506:ARG:CG	1:A:506:ARG:HH11	1.70	1.04
1:B:214:SER:HB2	1:B:240:LYS:HG3	1.38	1.04
1:A:67:THR:HG21	1:A:71:ARG:CD	1.89	1.03
1:B:185:LYS:HB2	1:B:215:ARG:HE	1.21	1.03
1:A:506:ARG:HG3	1:A:506:ARG:HH11	0.89	1.02
1:B:10:LEU:HG	1:B:14:MSE:HE2	1.41	1.00
1:A:11:THR:HA	1:A:14:MSE:HE2	1.03	1.00
1:A:514:MSE:HE2	1:A:525:TYR:HB3	1.43	1.00
1:B:192:PRO:HA	1:B:281:ARG:HG2	1.43	1.00
1:B:458:VAL:HB	1:B:492:VAL:HG22	1.43	0.98
1:A:67:THR:HG22	1:A:67:THR:O	1.63	0.98
1:B:484:THR:HG23	1:B:533:MSE:HE1	1.44	0.97
1:B:612:LEU:O	1:B:616:LEU:HD12	1.64	0.97
1:B:359:TRP:CZ3	1:B:367:LEU:HD13	2.00	0.96
1:A:67:THR:HG21	1:A:71:ARG:HD3	0.99	0.96
1:B:497:THR:HG22	1:B:500:LEU:H	1.27	0.96
1:B:11:THR:CA	1:B:14:MSE:HE3	1.95	0.96
1:B:213:ILE:CG2	1:B:237:ALA:HB1	1.96	0.95
1:B:185:LYS:CB	1:B:215:ARG:HE	1.81	0.94
1:A:11:THR:HA	1:A:14:MSE:CE	1.98	0.93
1:A:514:MSE:HE2	1:A:525:TYR:CB	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:HB3	1:B:278:ARG:HH22	1.29	0.92
1:B:264:ALA:CB	1:B:284:LEU:HD11	1.99	0.91
1:B:184:LEU:HD11	1:B:211:GLN:CG	2.01	0.91
1:B:274:GLN:CB	1:B:278:ARG:HH22	1.84	0.90
1:A:250:LEU:HD22	1:A:278:ARG:HH21	1.36	0.90
1:B:264:ALA:HB3	1:B:284:LEU:HD11	1.54	0.89
1:B:346:GLN:HE21	1:B:346:GLN:HA	1.38	0.88
1:B:500:LEU:HD21	2:B:701:ACO:H21	1.55	0.88
2:A:700:ACO:H8A	2:A:700:ACO:O5B	1.73	0.88
1:B:223:THR:HG23	1:B:246:PRO:HD3	1.56	0.87
1:B:359:TRP:HZ3	1:B:367:LEU:HD13	1.36	0.87
1:A:11:THR:CA	1:A:14:MSE:HE2	1.98	0.87
1:B:274:GLN:CB	1:B:278:ARG:NH2	2.38	0.87
1:B:185:LYS:HB2	1:B:215:ARG:NE	1.90	0.86
1:A:226:ALA:HA	5:A:821:HOH:O	1.74	0.86
1:A:67:THR:HG23	1:A:71:ARG:HD3	1.55	0.85
1:B:430:ARG:HH11	1:B:670:PHE:HE1	1.24	0.85
1:B:214:SER:CB	1:B:240:LYS:HG3	2.05	0.85
1:B:365:THR:HB	1:B:366:PRO:HD3	1.55	0.85
1:B:215:ARG:NH1	1:B:215:ARG:O	2.10	0.85
1:B:262:ASP:HA	1:B:285:THR:HG23	1.59	0.84
1:B:289:GLN:CG	1:B:296:ARG:HH11	1.91	0.84
1:B:185:LYS:HG3	1:B:215:ARG:HH21	0.74	0.84
1:B:573:LEU:HD22	1:B:604:THR:HG21	1.60	0.83
1:B:311:ARG:HG3	1:B:311:ARG:HH11	1.43	0.83
1:B:11:THR:HA	1:B:14:MSE:CE	2.03	0.83
1:A:250:LEU:HD22	1:A:278:ARG:NH2	1.94	0.83
1:A:634:ARG:NH1	1:A:638:LEU:HB2	1.93	0.82
1:B:178:PRO:O	1:B:182:GLN:HG3	1.80	0.82
1:A:621:SER:OG	1:A:624:GLN:HG3	1.80	0.80
1:A:289:GLN:HG3	1:A:290:GLY:H	1.45	0.80
1:A:198:THR:HG21	1:A:311:ARG:HH21	1.47	0.80
1:B:7:LEU:HD13	1:B:160:LEU:CD2	2.12	0.80
1:A:471:GLY:O	1:A:475:GLN:HG3	1.81	0.80
1:B:244:ILE:HD11	1:B:248:ALA:HB3	1.64	0.80
1:A:250:LEU:HA	1:A:278:ARG:NH2	1.97	0.79
1:B:68:LEU:HG	1:B:71:ARG:HH12	1.46	0.79
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.40	0.79
1:B:497:THR:HG23	1:B:499:GLU:HG3	1.64	0.79
1:B:262:ASP:HA	1:B:285:THR:CG2	2.12	0.79
1:A:67:THR:HG22	1:A:71:ARG:HD3	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HB3	1:B:282:THR:HG23	1.65	0.79
1:B:215:ARG:HH11	1:B:215:ARG:C	1.87	0.79
1:A:441:LEU:HD13	1:A:528:MSE:HE1	1.63	0.78
1:B:214:SER:C	1:B:216:ILE:H	1.87	0.78
1:B:212:LEU:H	1:B:212:LEU:HD12	1.47	0.78
1:B:497:THR:HG22	1:B:500:LEU:N	1.99	0.78
1:B:183:LEU:O	1:B:183:LEU:HD22	1.83	0.77
1:A:359:TRP:HZ3	1:A:367:LEU:HD13	1.48	0.77
1:B:7:LEU:HD13	1:B:160:LEU:HD22	1.66	0.77
1:B:190:MSE:HE2	1:B:258:TRP:CH2	2.19	0.77
1:B:213:ILE:HB	1:B:237:ALA:CB	2.14	0.77
1:B:215:ARG:CG	1:B:215:ARG:O	2.32	0.77
1:B:329:MSE:HE2	1:B:333:ALA:HB2	1.67	0.77
1:B:185:LYS:CE	1:B:189:THR:HA	2.15	0.77
1:A:634:ARG:HD3	1:A:634:ARG:O	1.85	0.76
1:B:215:ARG:NH1	1:B:216:ILE:HA	2.00	0.76
1:B:213:ILE:CB	1:B:237:ALA:HB1	2.15	0.76
1:B:275:LEU:CD2	1:B:279:PHE:HE2	2.00	0.75
1:B:213:ILE:HB	1:B:237:ALA:HB1	1.66	0.75
1:B:184:LEU:HD11	1:B:211:GLN:HB3	1.68	0.74
1:A:250:LEU:HD13	1:A:278:ARG:NH2	2.00	0.74
1:A:160:LEU:HD22	1:A:161:ALA:O	1.87	0.74
1:A:634:ARG:HD2	5:A:913:HOH:O	1.88	0.74
1:B:318:ILE:HD11	5:B:1017:HOH:O	1.87	0.74
1:B:215:ARG:HG3	1:B:215:ARG:O	1.87	0.73
1:B:624:GLN:O	1:B:628:THR:HG22	1.88	0.73
1:A:228:ALA:O	1:A:229:SER:C	2.26	0.73
1:B:188:MSE:HE1	1:B:283:LEU:HG	1.71	0.73
1:B:250:LEU:HD21	1:B:271:LEU:HD21	1.69	0.73
1:B:289:GLN:CD	1:B:296:ARG:HH11	1.91	0.73
1:B:214:SER:HB2	1:B:240:LYS:HZ3	1.51	0.73
1:B:309:LEU:HD23	1:B:310:HIS:N	2.03	0.72
1:B:184:LEU:HD11	1:B:211:GLN:CB	2.19	0.72
1:B:221:ILE:CG2	1:B:259:LEU:HA	2.18	0.72
1:B:215:ARG:CG	1:B:215:ARG:HH11	1.88	0.72
1:B:213:ILE:O	1:B:216:ILE:HG22	1.90	0.72
1:B:209:ALA:CB	1:B:233:LEU:HD21	2.20	0.72
1:B:231:ASP:O	1:B:235:GLN:HB3	1.91	0.71
1:A:437:VAL:HG13	1:A:528:MSE:HE3	1.73	0.71
1:B:636:MSE:HG2	5:B:980:HOH:O	1.88	0.71
1:B:240:LYS:HD3	1:B:240:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HD3	1:A:230:THR:HG21	1.72	0.71
1:B:185:LYS:HG3	1:B:215:ARG:CZ	2.21	0.70
1:B:268:PRO:HD3	1:B:521:SER:O	1.90	0.70
1:A:386:ARG:NH1	5:A:957:HOH:O	2.23	0.70
1:A:28:GLU:HG3	1:A:154:GLN:OE1	1.91	0.70
1:B:138:HIS:HB2	1:B:389:MSE:HE1	1.74	0.70
1:B:581:LEU:HD13	1:B:597:CYS:SG	2.32	0.69
1:B:373:LEU:HD13	1:B:408:ALA:HB3	1.74	0.69
1:A:67:THR:CG2	1:A:67:THR:O	2.37	0.69
1:A:506:ARG:CG	1:A:506:ARG:NH1	2.35	0.69
1:B:435:ASN:O	1:B:439:GLN:HG2	1.92	0.69
1:B:497:THR:CG2	1:B:500:LEU:H	2.02	0.69
1:B:215:ARG:HH12	1:B:216:ILE:HA	1.57	0.69
1:B:185:LYS:HE3	1:B:189:THR:HA	1.73	0.68
1:B:275:LEU:CD2	1:B:279:PHE:CE2	2.76	0.68
1:B:188:MSE:HE3	1:B:258:TRP:HZ2	1.58	0.68
1:B:213:ILE:HG21	1:B:237:ALA:HB1	1.75	0.68
1:B:221:ILE:O	1:B:260:VAL:HG22	1.92	0.68
1:B:222:VAL:HG13	1:B:242:ARG:O	1.94	0.67
1:B:244:ILE:HD11	1:B:248:ALA:CB	2.24	0.67
1:A:207:ALA:O	1:A:211:GLN:HG3	1.95	0.67
1:A:347:GLY:O	1:A:467:ARG:NH1	2.22	0.67
1:B:221:ILE:HD13	1:B:259:LEU:HG	1.74	0.67
1:B:347:GLY:O	1:B:467:ARG:NH1	2.28	0.67
1:B:240:LYS:HD3	1:B:240:LYS:H	1.60	0.67
1:A:263:GLU:OE2	1:A:287:THR:HG23	1.95	0.67
1:B:279:PHE:CD2	1:B:279:PHE:N	2.63	0.67
1:A:402:GLU:C	1:A:403:ASN:HD22	1.99	0.66
1:B:469:ARG:NE	2:B:701:ACO:O2B	2.28	0.66
1:B:184:LEU:O	1:B:212:LEU:HD21	1.93	0.66
1:B:607:LEU:O	1:B:613:ARG:NH1	2.27	0.66
1:B:259:LEU:O	1:B:282:THR:HA	1.95	0.66
1:B:209:ALA:C	1:B:233:LEU:HD21	2.17	0.66
1:B:484:THR:CG2	1:B:533:MSE:HE1	2.21	0.66
1:B:209:ALA:HB3	1:B:233:LEU:CD2	2.25	0.66
1:B:184:LEU:CD1	1:B:211:GLN:HG2	2.21	0.65
1:A:204:GLY:HA2	3:A:800:ADP:O1A	1.96	0.65
1:B:185:LYS:HD3	1:B:189:THR:HA	1.77	0.65
1:B:373:LEU:CD1	1:B:408:ALA:HB3	2.27	0.65
1:A:286:THR:HG21	1:A:299:LEU:HD11	1.79	0.65
1:B:259:LEU:HD23	1:B:260:VAL:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HG3	1:A:430:ARG:HH11	1.62	0.65
1:B:349:ILE:O	1:B:349:ILE:HD12	1.97	0.65
1:B:213:ILE:HD12	1:B:220:ALA:HB3	1.78	0.64
1:B:235:GLN:HG2	1:B:235:GLN:O	1.96	0.64
1:B:14:MSE:HE1	1:B:101:TRP:CZ2	2.32	0.64
1:B:263:GLU:OE1	1:B:286:THR:HA	1.97	0.64
1:B:259:LEU:HD11	1:B:275:LEU:HD13	1.79	0.64
1:B:188:MSE:HE1	1:B:283:LEU:CD2	2.28	0.64
1:B:14:MSE:HE1	1:B:101:TRP:CE2	2.33	0.64
1:B:512:VAL:HG13	1:B:544:GLU:HB3	1.80	0.64
1:B:221:ILE:CD1	1:B:259:LEU:HG	2.29	0.63
1:B:104:LEU:HG	1:B:106:LEU:HD13	1.79	0.63
1:B:214:SER:HB2	1:B:240:LYS:CG	2.22	0.63
1:A:199:ALA:HB3	1:A:205:LYS:HD3	1.80	0.63
1:A:359:TRP:CZ2	1:A:366:PRO:HB2	2.34	0.63
1:A:472:THR:HG23	5:A:887:HOH:O	1.99	0.63
1:B:51:SER:O	1:B:53:ARG:N	2.32	0.63
1:A:10:LEU:HD22	1:A:160:LEU:HD21	1.81	0.63
1:B:128:ASP:HB3	1:B:129:PRO:HD2	1.78	0.62
1:A:17:GLU:HB3	1:A:166:ARG:HG3	1.80	0.62
1:A:72:GLU:HG2	1:A:319:ARG:HH12	1.65	0.62
1:B:28:GLU:HB3	5:B:1006:HOH:O	1.99	0.62
1:A:96:LEU:HD21	1:A:102:LEU:HD23	1.80	0.62
1:B:264:ALA:HB2	1:B:284:LEU:HD11	1.79	0.62
1:B:208:LEU:C	1:B:208:LEU:HD13	2.20	0.62
1:B:223:THR:HA	1:B:243:PHE:CE1	2.34	0.62
1:B:279:PHE:HB3	1:B:280:PRO:HD2	1.82	0.62
1:B:196:ALA:CB	1:B:309:LEU:HD21	2.30	0.62
1:A:437:VAL:O	1:A:441:LEU:HD22	2.00	0.61
1:B:259:LEU:HB3	1:B:282:THR:CG2	2.30	0.61
1:B:67:THR:C	1:B:68:LEU:HD12	2.20	0.61
1:B:44:PRO:HA	5:B:968:HOH:O	2.00	0.61
1:A:227:LYS:HD3	1:A:230:THR:CG2	2.29	0.61
1:B:275:LEU:HD23	1:B:279:PHE:HE2	1.65	0.61
1:B:250:LEU:HD21	1:B:271:LEU:CD2	2.31	0.61
1:B:311:ARG:HH11	1:B:311:ARG:CG	2.10	0.61
1:A:188:MSE:HE1	1:A:215:ARG:O	2.01	0.61
1:A:44:PRO:HA	5:A:1013:HOH:O	1.98	0.61
1:B:292:GLU:N	1:B:292:GLU:OE2	2.34	0.61
1:B:482:GLN:HA	1:B:482:GLN:OE1	1.99	0.61
1:A:635:LYS:H	1:A:635:LYS:CD	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:HIS:CB	1:B:389:MSE:HE1	2.31	0.60
1:B:351:ILE:HD12	1:B:476:LEU:HD13	1.81	0.60
1:A:280:PRO:HD3	5:A:1004:HOH:O	2.01	0.60
1:B:214:SER:C	1:B:216:ILE:N	2.49	0.60
1:B:403:ASN:O	1:B:404:GLU:HG2	2.01	0.60
1:A:437:VAL:HG13	1:A:528:MSE:CE	2.31	0.60
1:B:48:LEU:HG	1:B:49:TRP:N	2.08	0.60
1:B:296:ARG:NH2	1:B:341:PHE:CE2	2.68	0.60
1:B:497:THR:CG2	1:B:499:GLU:HG3	2.29	0.60
1:B:621:SER:O	1:B:625:LEU:HD22	2.01	0.60
1:A:250:LEU:HA	1:A:278:ARG:HH21	1.65	0.60
1:A:372:LEU:HD22	1:A:405:ILE:HG22	1.83	0.60
1:A:539:GLN:O	1:A:543:ARG:HB2	2.01	0.60
1:B:214:SER:HB2	1:B:240:LYS:NZ	2.16	0.60
1:B:215:ARG:HH12	1:B:216:ILE:CA	2.15	0.60
1:B:209:ALA:HB3	1:B:233:LEU:HD21	1.84	0.60
1:B:359:TRP:HZ3	1:B:367:LEU:CD1	2.11	0.60
1:B:506:ARG:HG3	1:B:506:ARG:HH11	1.67	0.60
1:B:649:LEU:HB3	1:B:657:THR:HG21	1.82	0.60
1:B:249:LEU:HD13	1:B:249:LEU:C	2.21	0.60
1:B:430:ARG:NH1	1:B:670:PHE:HE1	1.95	0.60
1:B:185:LYS:CD	1:B:189:THR:HA	2.32	0.60
1:B:600:ARG:O	1:B:604:THR:HG22	2.01	0.60
1:A:373:LEU:CD1	1:A:408:ALA:HB3	2.32	0.59
1:B:215:ARG:NH1	1:B:216:ILE:CA	2.65	0.59
1:B:276:VAL:HG12	1:B:276:VAL:O	2.01	0.59
1:B:200:ALA:HA	1:B:288:VAL:O	2.02	0.59
1:B:341:PHE:CD1	1:B:342:THR:N	2.70	0.59
1:B:258:TRP:HA	1:B:281:ARG:O	2.02	0.59
1:B:264:ALA:HB3	1:B:284:LEU:CD1	2.30	0.59
1:A:359:TRP:CZ3	1:A:367:LEU:HD13	2.35	0.59
1:A:481:LEU:HD12	1:A:533:MSE:HE3	1.85	0.59
1:B:225:PRO:O	1:B:227:LYS:N	2.35	0.59
1:B:244:ILE:CG2	1:B:249:LEU:HD23	2.32	0.59
1:B:437:VAL:HG13	1:B:528:MSE:HE3	1.85	0.59
1:A:67:THR:HG22	1:A:71:ARG:HB2	1.85	0.59
1:B:80:ALA:HA	1:B:83:GLY:O	2.02	0.59
1:B:639:VAL:O	1:B:643:GLU:HG3	2.02	0.59
1:A:635:LYS:HD2	5:A:822:HOH:O	2.03	0.58
1:B:222:VAL:HB	1:B:260:VAL:CG2	2.31	0.58
1:B:188:MSE:HE1	1:B:283:LEU:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:HG3	1:B:267:ILE:HG13	1.86	0.58
1:A:514:MSE:HE2	1:A:525:TYR:HB2	1.83	0.58
1:B:184:LEU:HD23	1:B:212:LEU:HG	1.85	0.58
1:B:635:LYS:O	1:B:639:VAL:HG23	2.04	0.58
1:A:629:LEU:HB3	1:A:631:LEU:CD2	2.34	0.58
1:B:261:VAL:HG22	1:B:264:ALA:HB2	1.85	0.58
1:B:467:ARG:HD2	1:B:470:GLU:OE2	2.04	0.58
1:B:670:PHE:CD1	1:B:670:PHE:C	2.77	0.58
1:B:261:VAL:CG2	1:B:264:ALA:HB2	2.34	0.57
1:B:296:ARG:NH2	1:B:341:PHE:CZ	2.71	0.57
1:B:484:THR:O	1:B:485:GLN:HG3	2.03	0.57
1:A:68:LEU:HD12	1:A:68:LEU:H	1.69	0.57
1:B:214:SER:O	1:B:216:ILE:N	2.37	0.57
1:B:396:PHE:O	1:B:397:LEU:HD22	2.04	0.57
1:A:420:GLN:CD	1:A:420:GLN:H	2.07	0.57
1:A:69:LEU:HD11	1:A:71:ARG:HD2	1.85	0.57
1:B:195:ALA:HB1	1:B:312:PHE:HE2	1.68	0.57
1:B:222:VAL:HA	1:B:260:VAL:O	2.04	0.57
1:B:274:GLN:C	1:B:278:ARG:HH21	2.07	0.57
1:B:222:VAL:CG1	1:B:242:ARG:O	2.52	0.57
1:B:359:TRP:CH2	1:B:367:LEU:HD13	2.38	0.57
1:B:194:VAL:HG13	1:B:282:THR:OG1	2.05	0.56
1:B:244:ILE:HG23	1:B:249:LEU:HD23	1.86	0.56
1:A:50:ILE:HG21	1:A:92:LEU:HD22	1.86	0.56
1:B:259:LEU:HD23	1:B:260:VAL:H	1.68	0.56
1:A:14:MSE:HE1	1:A:101:TRP:NE1	2.20	0.56
1:A:176:PRO:HG2	1:A:181:GLN:NE2	2.20	0.56
1:B:189:THR:OG1	1:B:189:THR:O	2.22	0.56
1:B:594:SER:O	1:B:598:LEU:HB2	2.05	0.56
1:B:185:LYS:HA	1:B:188:MSE:HB3	1.86	0.56
1:A:345:PRO:HG2	1:A:467:ARG:HG3	1.88	0.56
1:A:619:ASN:HB3	5:A:990:HOH:O	2.05	0.56
1:A:67:THR:HG21	1:A:71:ARG:HH11	1.70	0.56
1:A:634:ARG:HH11	1:A:638:LEU:HB2	1.67	0.56
1:B:132:THR:HB	1:B:390:ASP:OD2	2.06	0.56
1:A:516:ASN:HD21	1:A:555:LEU:HD12	1.71	0.56
1:B:341:PHE:CE1	1:B:342:THR:HG23	2.41	0.56
1:B:190:MSE:C	1:B:191:PRO:O	2.41	0.55
1:B:13:GLN:O	1:B:17:GLU:HG3	2.05	0.55
1:B:245:ALA:HB1	1:B:246:PRO:HD2	1.89	0.55
1:B:363:PRO:O	1:B:367:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:O	1:A:17:GLU:HG3	2.06	0.55
1:A:282:THR:HG22	1:A:284:LEU:HD13	1.89	0.55
1:A:213:ILE:HG23	1:A:220:ALA:HB3	1.88	0.55
1:B:246:PRO:O	1:B:249:LEU:HB3	2.06	0.55
1:A:25:LEU:HD12	1:A:152:TRP:HB3	1.87	0.55
1:A:309:LEU:HD13	1:A:310:HIS:N	2.21	0.55
1:A:318:ILE:HD12	1:A:318:ILE:O	2.07	0.55
1:A:430:ARG:HG3	1:A:430:ARG:NH1	2.21	0.55
1:B:257:ASP:O	1:B:280:PRO:HG2	2.07	0.55
1:B:68:LEU:HD12	1:B:68:LEU:N	2.22	0.55
1:B:551:ASP:OD2	1:B:596:GLY:HA3	2.06	0.54
1:A:382:PRO:O	1:A:386:ARG:HG2	2.06	0.54
1:B:469:ARG:HD3	2:B:701:ACO:C8A	2.37	0.54
1:B:190:MSE:SE	1:B:310:HIS:HD2	2.40	0.54
1:A:223:THR:HG22	1:A:261:VAL:HG22	1.89	0.54
1:A:369:VAL:HG12	1:A:373:LEU:HD22	1.90	0.54
1:A:66:GLN:HB3	1:A:68:LEU:HD12	1.88	0.54
1:A:629:LEU:HB3	1:A:631:LEU:HD21	1.89	0.54
1:B:92:LEU:O	1:B:95:THR:HG22	2.07	0.54
1:B:423:GLN:HE21	1:B:449:LEU:HD11	1.73	0.54
1:B:506:ARG:NE	1:B:506:ARG:HA	2.22	0.54
1:B:274:GLN:CA	1:B:278:ARG:NH2	2.70	0.54
1:B:500:LEU:CD2	2:B:701:ACO:H21	2.35	0.54
1:A:247:ASP:HB2	5:A:989:HOH:O	2.08	0.54
1:A:634:ARG:HD3	1:A:634:ARG:C	2.28	0.54
1:A:110:GLU:OE2	1:A:153:ARG:NH2	2.42	0.53
1:B:14:MSE:HE1	1:B:101:TRP:NE1	2.24	0.53
1:B:107:PRO:HB3	5:B:927:HOH:O	2.08	0.53
1:B:139:LEU:O	1:B:143:LEU:HG	2.08	0.53
1:B:467:ARG:NH2	1:B:470:GLU:OE1	2.41	0.53
1:B:72:GLU:HB2	1:B:97:LYS:HG3	1.90	0.53
1:A:373:LEU:HD13	1:A:408:ALA:HB3	1.89	0.53
1:B:506:ARG:NH1	1:B:506:ARG:HG3	2.24	0.53
1:B:213:ILE:HB	1:B:237:ALA:HB2	1.88	0.53
1:A:502:ARG:HH22	1:B:1:MSE:N	2.06	0.53
1:A:67:THR:HA	1:A:69:LEU:HD21	1.90	0.53
1:B:195:ALA:O	1:B:284:LEU:N	2.38	0.53
1:A:216:ILE:O	1:A:240:LYS:NZ	2.42	0.53
1:A:444:HIS:HD2	1:A:593:THR:OG1	1.91	0.53
1:B:259:LEU:CD2	1:B:260:VAL:N	2.72	0.53
1:B:299:LEU:HD13	1:B:299:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG12	1:B:222:VAL:N	2.24	0.53
1:B:358:LEU:HD13	1:B:362:ASP:HB3	1.91	0.53
1:B:72:GLU:HB2	1:B:97:LYS:CG	2.38	0.53
1:B:294:THR:HG21	1:B:299:LEU:HD23	1.89	0.53
1:A:198:THR:HG21	1:A:311:ARG:NH2	2.21	0.53
1:A:502:ARG:NH2	1:B:1:MSE:N	2.57	0.53
1:B:7:LEU:HD13	1:B:160:LEU:HD21	1.89	0.53
1:B:220:ALA:C	1:B:221:ILE:HG22	2.29	0.53
1:A:635:LYS:H	1:A:635:LYS:HD2	1.74	0.52
1:B:202:GLY:O	1:B:317:PRO:HA	2.10	0.52
1:A:250:LEU:CA	1:A:278:ARG:NH2	2.72	0.52
1:B:215:ARG:CD	1:B:215:ARG:O	2.58	0.52
1:B:649:LEU:HB3	1:B:657:THR:CG2	2.39	0.52
1:A:289:GLN:HG3	1:A:290:GLY:N	2.21	0.52
1:B:311:ARG:NH1	1:B:311:ARG:CG	2.72	0.52
1:A:162:HIS:N	1:A:162:HIS:ND1	2.56	0.52
1:B:198:THR:HB	1:B:286:THR:HG22	1.92	0.52
1:A:34:GLU:O	1:A:38:LYS:HG3	2.10	0.52
1:B:176:PRO:HB3	1:B:211:GLN:OE1	2.09	0.52
1:B:209:ALA:C	1:B:233:LEU:CD2	2.79	0.52
1:B:249:LEU:CD1	1:B:275:LEU:HG	2.40	0.52
1:A:139:LEU:O	1:A:143:LEU:HB2	2.10	0.51
1:A:68:LEU:HD13	1:A:68:LEU:O	2.09	0.51
1:A:402:GLU:C	1:A:403:ASN:ND2	2.63	0.51
1:A:514:MSE:HE3	1:A:526:THR:O	2.10	0.51
1:B:16:ARG:HH21	1:B:16:ARG:HG2	1.75	0.51
1:B:583:GLY:O	1:B:587:ALA:HB3	2.11	0.51
1:A:23:LEU:CD1	1:A:25:LEU:HD13	2.40	0.51
1:A:177:GLN:HB3	1:A:178:PRO:HD2	1.93	0.51
1:A:67:THR:HG21	1:A:71:ARG:NH1	2.26	0.51
1:B:395:HIS:NE2	1:B:456:ARG:NH2	2.58	0.51
1:A:289:GLN:CG	1:A:290:GLY:H	2.22	0.51
1:A:484:THR:HG22	1:A:485:GLN:N	2.25	0.51
1:B:175:ALA:HB1	1:B:176:PRO:HD2	1.93	0.51
1:B:512:VAL:HG13	1:B:544:GLU:CB	2.41	0.51
1:A:328:LYS:O	1:A:332:GLU:HG3	2.10	0.50
1:B:196:ALA:HB3	1:B:309:LEU:HD21	1.94	0.50
1:B:341:PHE:HD1	1:B:342:THR:H	1.60	0.50
1:B:489:TYR:HA	1:B:533:MSE:HG3	1.92	0.50
1:A:513:ARG:NH2	5:A:961:HOH:O	2.43	0.50
1:B:205:LYS:O	1:B:208:LEU:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:HG11	1:B:241:PHE:CD1	2.46	0.50
1:A:437:VAL:HG23	1:A:457:ARG:HD3	1.93	0.50
1:A:636:MSE:HG3	5:A:803:HOH:O	2.11	0.50
1:A:442:ALA:O	1:A:589:ARG:NH2	2.45	0.50
1:B:223:THR:HG23	1:B:224:ALA:N	2.26	0.50
1:B:621:SER:OG	1:B:624:GLN:HB2	2.11	0.50
1:A:23:LEU:HD22	1:A:150:ILE:HB	1.93	0.50
1:B:552:ALA:HA	1:B:563:LEU:HD22	1.93	0.50
1:B:250:LEU:O	1:B:250:LEU:CD1	2.60	0.49
1:B:262:ASP:OD1	1:B:285:THR:HG21	2.12	0.49
1:B:485:GLN:O	1:B:486:ASP:HB3	2.12	0.49
1:B:486:ASP:O	1:B:486:ASP:OD1	2.30	0.49
1:A:252:SER:HB2	1:A:254:GLU:OE2	2.12	0.49
1:A:467:ARG:HA	1:A:470:GLU:OE2	2.12	0.49
1:B:184:LEU:CD1	1:B:211:GLN:HB3	2.39	0.49
1:B:185:LYS:CG	1:B:215:ARG:HE	2.25	0.49
1:B:112:TRP:CD2	1:B:136:VAL:HG13	2.47	0.49
1:B:222:VAL:HG11	1:B:241:PHE:CE1	2.46	0.49
1:A:72:GLU:HG2	1:A:319:ARG:NH1	2.27	0.49
1:B:119:ASP:OD2	1:B:122:ARG:NH1	2.45	0.49
1:B:201:ARG:NH1	1:B:291:TYR:O	2.45	0.49
1:A:500:LEU:HD21	2:A:700:ACO:H22	1.94	0.49
1:B:205:LYS:HE3	1:B:287:THR:OG1	2.13	0.49
1:A:119:ASP:OD2	1:A:122:ARG:NH1	2.46	0.49
1:A:437:VAL:HG12	1:A:441:LEU:HD22	1.95	0.49
1:A:446:ASN:ND2	1:A:580:GLU:HG3	2.28	0.49
1:B:169:TRP:CZ3	1:B:171:PRO:HD3	2.47	0.49
1:B:525:TYR:CE2	1:B:559:ASN:HB3	2.48	0.49
1:A:397:LEU:HB2	1:A:409:LEU:HB3	1.95	0.48
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.18	0.48
1:A:23:LEU:HD11	1:A:25:LEU:HD13	1.95	0.48
1:A:318:ILE:HG12	3:A:800:ADP:O4'	2.12	0.48
1:B:206:SER:O	1:B:233:LEU:HD22	2.13	0.48
1:A:345:PRO:HG2	1:A:467:ARG:CG	2.43	0.48
1:A:69:LEU:HD23	1:A:69:LEU:N	2.28	0.48
1:B:188:MSE:CE	1:B:258:TRP:HZ2	2.25	0.48
1:A:68:LEU:HD13	1:A:68:LEU:C	2.33	0.48
1:B:555:LEU:HD23	1:B:563:LEU:HD21	1.96	0.48
1:A:179:GLU:OE1	1:A:316:GLN:HB2	2.13	0.48
1:A:96:LEU:CD2	1:A:102:LEU:HD23	2.44	0.48
1:B:225:PRO:O	1:B:226:ALA:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:TRP:CZ3	1:B:367:LEU:CD1	2.84	0.48
1:B:502:ARG:HA	1:B:505:GLN:HB3	1.96	0.48
1:A:670:PHE:N	1:A:670:PHE:CD2	2.79	0.48
1:A:306:PHE:CB	1:A:309:LEU:HD23	2.44	0.47
1:A:353:ALA:HB2	1:A:397:LEU:HD13	1.95	0.47
1:B:132:THR:O	1:B:132:THR:OG1	2.30	0.47
1:A:502:ARG:NH2	1:B:1:MSE:H2	2.11	0.47
1:A:250:LEU:CD1	1:A:278:ARG:HH22	2.07	0.47
1:A:106:LEU:HB3	1:A:107:PRO:HD2	1.96	0.47
1:A:50:ILE:CG2	1:A:92:LEU:HD22	2.45	0.47
1:B:279:PHE:HD2	1:B:279:PHE:H	1.62	0.47
1:B:407:GLY:HA2	1:B:462:ALA:O	2.13	0.47
1:A:359:TRP:CE2	1:A:366:PRO:HB2	2.50	0.47
1:B:196:ALA:HB2	1:B:309:LEU:HD21	1.97	0.47
1:B:640:ARG:O	1:B:644:GLU:HG3	2.14	0.47
1:B:10:LEU:HD23	1:B:160:LEU:HD21	1.95	0.47
1:A:454:ARG:NH2	5:A:880:HOH:O	2.47	0.47
1:B:223:THR:CG2	1:B:224:ALA:N	2.78	0.47
1:B:18:GLY:HA2	1:B:98:ALA:HB1	1.96	0.47
1:B:233:LEU:C	1:B:233:LEU:HD13	2.35	0.47
1:B:581:LEU:CD1	1:B:597:CYS:SG	3.03	0.47
1:B:215:ARG:HD2	1:B:215:ARG:O	2.14	0.46
1:B:222:VAL:HG22	1:B:243:PHE:HD1	1.79	0.46
1:B:496:TYR:CD1	1:B:514:MSE:HE1	2.49	0.46
1:B:244:ILE:O	1:B:244:ILE:HG23	2.16	0.46
1:A:289:GLN:HG2	1:A:336:PHE:O	2.14	0.46
1:B:229:SER:HB3	1:B:231:ASP:OD1	2.15	0.46
1:B:184:LEU:HD21	1:B:211:GLN:HB3	1.97	0.46
1:B:506:ARG:NH2	2:B:701:ACO:O9A	2.48	0.46
1:A:506:ARG:NH1	2:A:700:ACO:P3B	2.89	0.46
1:A:68:LEU:HD12	1:A:68:LEU:N	2.31	0.46
1:B:10:LEU:C	1:B:14:MSE:HE2	2.36	0.46
1:B:310:HIS:HB3	1:B:312:PHE:CZ	2.51	0.46
1:A:184:LEU:HD13	1:A:208:LEU:HD12	1.97	0.46
1:B:154:GLN:O	1:B:155:ASN:HB2	2.15	0.46
1:A:369:VAL:HG13	1:A:408:ALA:HB1	1.98	0.46
1:B:222:VAL:HB	1:B:260:VAL:HG22	1.97	0.46
1:B:249:LEU:HD11	1:B:275:LEU:HG	1.98	0.46
1:A:6:ALA:HB1	1:A:160:LEU:HD12	1.98	0.46
1:B:319:ARG:HB2	1:B:320:TRP:CE3	2.51	0.46
1:A:259:LEU:HB2	1:A:279:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:O	1:B:257:ASP:OD1	2.34	0.46
1:B:435:ASN:HB3	1:B:438:ALA:HB3	1.96	0.46
1:B:214:SER:CB	1:B:240:LYS:HZ3	2.26	0.45
1:A:183:LEU:HD22	1:A:314:LEU:HD13	1.98	0.45
1:A:341:PHE:CZ	1:A:375:GLY:HA3	2.51	0.45
1:A:634:ARG:HH12	1:A:638:LEU:HD13	1.81	0.45
1:B:213:ILE:HG23	1:B:240:LYS:HB2	1.98	0.45
1:B:240:LYS:H	1:B:240:LYS:CD	2.17	0.45
1:B:279:PHE:HB3	1:B:280:PRO:CD	2.45	0.45
1:B:397:LEU:HB2	1:B:409:LEU:HB3	1.98	0.45
1:A:660:LEU:HD12	1:A:660:LEU:HA	1.67	0.45
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.71	0.45
1:B:566:ASP:HB3	5:B:997:HOH:O	2.16	0.45
1:B:10:LEU:O	1:B:14:MSE:HG3	2.16	0.45
1:B:480:ALA:O	1:B:484:THR:CG2	2.64	0.45
1:A:149:ALA:O	1:A:151:LEU:HD22	2.16	0.45
1:A:437:VAL:HG12	1:A:441:LEU:CD2	2.47	0.45
1:B:208:LEU:CD1	1:B:208:LEU:C	2.85	0.45
1:B:193:GLY:O	1:B:281:ARG:HA	2.17	0.45
1:A:329:MSE:HB3	1:A:329:MSE:HE3	1.93	0.45
1:B:213:ILE:HG22	1:B:237:ALA:HB1	1.92	0.45
1:B:122:ARG:NH2	1:B:383:LEU:HD11	2.31	0.45
1:B:216:ILE:HD13	1:B:218:GLY:H	1.82	0.45
1:B:477:ILE:O	1:B:481:LEU:HD23	2.17	0.45
1:B:555:LEU:HD12	1:B:595:LEU:HD23	1.99	0.45
1:B:132:THR:HA	1:B:390:ASP:CG	2.37	0.44
1:A:306:PHE:HB2	1:A:309:LEU:HD23	1.99	0.44
1:A:69:LEU:CD1	1:A:71:ARG:HD2	2.47	0.44
1:B:263:GLU:H	1:B:285:THR:HG23	1.82	0.44
1:B:583:GLY:HA3	1:B:589:ARG:HD2	1.99	0.44
1:A:262:ASP:HB2	1:A:285:THR:OG1	2.18	0.44
1:A:432:PRO:HG2	1:A:439:GLN:OE1	2.17	0.44
1:B:17:GLU:HB3	1:B:166:ARG:HB2	1.99	0.44
1:B:259:LEU:HD13	1:B:282:THR:CG2	2.46	0.44
1:B:464:HIS:ND1	1:B:465:PRO:HD2	2.32	0.44
1:B:581:LEU:HG	1:B:601:LEU:HD22	1.99	0.44
2:B:701:ACO:N8P	2:B:701:ACO:H131	2.32	0.44
1:B:213:ILE:CD1	1:B:220:ALA:CB	2.95	0.44
1:B:250:LEU:O	1:B:250:LEU:HD12	2.17	0.44
1:B:578:TRP:HZ3	1:B:657:THR:CG2	2.30	0.44
1:B:71:ARG:NH2	1:B:73:PHE:CZ	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:O	1:A:230:THR:N	2.50	0.44
1:B:446:ASN:HA	1:B:580:GLU:OE2	2.18	0.44
1:B:215:ARG:HH12	1:B:216:ILE:CB	2.31	0.44
1:B:369:VAL:HG12	1:B:373:LEU:HD22	2.00	0.44
1:A:151:LEU:N	1:A:151:LEU:HD22	2.33	0.44
1:A:199:ALA:C	1:A:288:VAL:HG12	2.38	0.44
1:A:441:LEU:HD13	1:A:528:MSE:CE	2.41	0.44
1:B:188:MSE:HE1	1:B:283:LEU:HD23	1.99	0.44
1:B:239:GLU:C	1:B:241:PHE:N	2.71	0.44
1:B:542:GLU:HG3	1:B:543:ARG:N	2.33	0.44
1:A:92:LEU:HD23	1:A:102:LEU:HD21	1.99	0.44
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.80	0.44
1:A:289:GLN:NE2	1:A:374:SER:OG	2.49	0.43
1:B:209:ALA:HB3	1:B:233:LEU:HD23	1.97	0.43
1:B:216:ILE:HG23	1:B:218:GLY:O	2.17	0.43
1:B:213:ILE:CD1	1:B:220:ALA:HB3	2.45	0.43
1:B:264:ALA:CB	1:B:284:LEU:CD1	2.86	0.43
1:B:481:LEU:HA	1:B:484:THR:HG22	1.99	0.43
1:A:252:SER:OG	1:A:254:GLU:HG2	2.18	0.43
1:A:250:LEU:CD2	1:A:278:ARG:NH2	2.75	0.43
1:A:506:ARG:HA	1:A:506:ARG:HD2	1.11	0.43
1:A:74:ARG:O	1:A:75:HIS:HB2	2.18	0.43
1:B:649:LEU:C	1:B:657:THR:HG21	2.38	0.43
1:B:138:HIS:HB2	1:B:389:MSE:CE	2.47	0.43
1:B:16:ARG:HH21	1:B:16:ARG:CG	2.32	0.43
1:B:177:GLN:HB3	1:B:178:PRO:HD2	2.01	0.43
1:B:185:LYS:HD3	1:B:189:THR:CA	2.48	0.43
1:A:329:MSE:HE3	1:A:330:VAL:HG23	2.01	0.43
1:A:362:ASP:OD1	1:A:365:THR:CG2	2.66	0.43
1:B:212:LEU:HD12	1:B:212:LEU:N	2.23	0.43
1:B:249:LEU:HD11	1:B:275:LEU:CG	2.48	0.43
1:A:92:LEU:O	1:A:95:THR:HG22	2.19	0.43
1:B:192:PRO:HB3	1:B:280:PRO:HB2	2.00	0.43
1:B:355:GLU:HB2	1:B:357:THR:HG23	2.01	0.43
1:A:199:ALA:O	1:A:287:THR:HA	2.18	0.43
1:A:314:LEU:HA	1:A:314:LEU:HD12	1.88	0.43
1:A:373:LEU:HD11	1:A:408:ALA:HB3	2.00	0.43
1:B:185:LYS:HG3	1:B:215:ARG:NE	2.34	0.43
1:B:346:GLN:HE21	1:B:346:GLN:CA	2.12	0.43
1:A:122:ARG:HH21	1:A:383:LEU:HD11	1.83	0.43
1:A:10:LEU:O	1:A:14:MSE:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:51:SER:N	2.33	0.43
1:A:612:LEU:HD22	1:A:644:GLU:HB2	2.01	0.43
1:B:485:GLN:O	1:B:486:ASP:CB	2.66	0.43
1:A:273:HIS:NE2	1:A:305:ARG:HB3	2.33	0.43
1:A:326:LEU:HD12	1:A:329:MSE:CE	2.49	0.43
1:A:411:LEU:HD12	1:A:458:VAL:HA	2.01	0.43
1:B:181:GLN:OE1	1:B:181:GLN:HA	2.19	0.43
1:B:234:ALA:HB2	1:B:241:PHE:CD1	2.53	0.43
1:B:509:PHE:HB3	1:B:529:ALA:HB1	2.00	0.43
1:B:516:ASN:HB2	1:B:592:LEU:HD23	2.01	0.43
1:A:577:ASP:O	1:A:581:LEU:HD22	2.19	0.43
1:B:307:PRO:O	1:B:308:HIS:HB2	2.17	0.43
1:A:184:LEU:HD13	1:A:208:LEU:CD1	2.49	0.42
1:A:262:ASP:HA	1:A:285:THR:OG1	2.19	0.42
1:A:53:ARG:HB3	1:A:53:ARG:HE	1.45	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD13	1.64	0.42
1:A:67:THR:CG2	1:A:71:ARG:HH11	2.32	0.42
1:B:210:GLY:N	1:B:233:LEU:HD22	2.34	0.42
1:B:245:ALA:O	1:B:249:LEU:CB	2.67	0.42
1:B:353:ALA:HB2	1:B:397:LEU:HD13	2.00	0.42
1:A:317:PRO:HD2	1:A:322:GLN:HB2	2.01	0.42
1:A:339:GLU:O	1:A:342:THR:HB	2.20	0.42
1:B:489:TYR:C	1:B:489:TYR:CD1	2.92	0.42
1:B:242:ARG:HD3	1:B:243:PHE:N	2.34	0.42
1:B:578:TRP:HZ3	1:B:657:THR:HG22	1.85	0.42
1:A:276:VAL:HG22	1:A:282:THR:HG21	2.01	0.42
1:B:355:GLU:OE1	1:B:395:HIS:ND1	2.46	0.42
1:A:92:LEU:CD2	1:A:102:LEU:HD21	2.49	0.42
1:B:496:TYR:OH	1:B:564:PRO:HG3	2.19	0.42
1:A:224:ALA:HB1	1:A:225:PRO:HD2	2.02	0.42
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.93	0.42
1:A:540:LEU:O	1:A:544:GLU:HB2	2.20	0.42
1:B:184:LEU:CG	1:B:211:GLN:HB3	2.49	0.42
1:B:184:LEU:CD1	1:B:211:GLN:CG	2.87	0.42
1:B:355:GLU:O	1:B:358:LEU:HB2	2.20	0.42
1:B:395:HIS:CD2	1:B:456:ARG:CZ	3.02	0.42
1:B:553:GLN:O	1:B:557:GLN:HG3	2.19	0.42
1:A:565:VAL:O	1:A:567:PRO:HD3	2.20	0.42
1:B:101:TRP:CH2	1:B:150:ILE:HG13	2.54	0.42
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.93	0.42
1:B:612:LEU:C	1:B:616:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HA	1:B:629:LEU:HD13	1.88	0.42
1:B:232:VAL:HB	1:B:233:LEU:H	1.32	0.42
1:B:421:LEU:O	1:B:425:VAL:HG23	2.20	0.42
1:A:441:LEU:HB3	1:A:450:ALA:HB1	2.02	0.42
1:B:440:SER:OG	1:B:444:HIS:HD2	2.02	0.42
1:B:581:LEU:HD12	1:B:581:LEU:HA	1.84	0.42
1:A:13:GLN:HG3	1:A:16:ARG:HH21	1.84	0.41
1:A:40:ARG:HG3	1:A:41:ASP:N	2.35	0.41
1:B:11:THR:CA	1:B:14:MSE:CE	2.80	0.41
1:B:429:PHE:CD1	1:B:668:GLN:HA	2.54	0.41
1:B:609:LEU:HD22	1:B:644:GLU:HB3	2.02	0.41
1:A:227:LYS:O	1:A:228:ALA:C	2.58	0.41
1:B:51:SER:CB	5:B:1004:HOH:O	2.67	0.41
1:B:570:ASP:OD2	1:B:572:VAL:HG12	2.20	0.41
1:A:269:ALA:N	1:A:270:PRO:HD2	2.36	0.41
1:B:146:ASP:OD2	1:B:148:GLU:HB2	2.20	0.41
1:B:148:GLU:OE2	1:B:166:ARG:NH2	2.54	0.41
1:B:53:ARG:O	1:B:55:ASP:OD1	2.37	0.41
1:B:660:LEU:CD1	5:B:1020:HOH:O	2.69	0.41
1:A:106:LEU:HD13	1:A:112:TRP:CH2	2.54	0.41
1:B:244:ILE:O	1:B:249:LEU:HB2	2.20	0.41
1:B:317:PRO:HG2	1:B:320:TRP:O	2.20	0.41
1:B:429:PHE:CE2	1:B:588:HIS:HD2	2.38	0.41
1:A:102:LEU:C	1:A:102:LEU:HD13	2.41	0.41
1:A:124:SER:O	1:A:125:ASP:HB2	2.20	0.41
1:A:233:LEU:HD23	1:A:233:LEU:O	2.21	0.41
1:A:7:LEU:HA	1:A:7:LEU:HD12	1.91	0.41
1:B:221:ILE:CG1	1:B:222:VAL:N	2.84	0.41
1:B:65:LEU:O	1:B:66:GLN:HG2	2.21	0.41
1:A:69:LEU:HG	1:A:71:ARG:HG3	2.02	0.41
1:B:329:MSE:HE2	1:B:333:ALA:CB	2.45	0.41
1:B:434:GLY:O	1:B:439:GLN:NE2	2.51	0.41
1:B:499:GLU:O	1:B:500:LEU:C	2.55	0.41
1:A:294:THR:OG1	1:A:299:LEU:CD2	2.68	0.41
1:B:388:MSE:HG3	1:B:396:PHE:CE1	2.56	0.41
1:B:476:LEU:HD12	1:B:476:LEU:HA	1.90	0.41
1:A:362:ASP:O	1:A:366:PRO:HD2	2.20	0.41
1:A:578:TRP:CZ3	1:A:656:ARG:HG2	2.55	0.41
1:A:629:LEU:CB	1:A:631:LEU:CD2	2.99	0.41
1:B:133:PRO:O	1:B:137:GLN:HG3	2.20	0.41
1:B:195:ALA:HB3	1:B:283:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLY:N	4:B:801:SO4:O2	2.54	0.41
1:A:514:MSE:HE3	1:A:515:GLY:H	1.85	0.41
1:B:208:LEU:O	1:B:211:GLN:HB2	2.21	0.41
1:B:197:VAL:HG12	1:B:312:PHE:HB2	2.02	0.41
1:B:414:GLU:HG2	1:B:435:ASN:HA	2.02	0.41
1:B:74:ARG:HB2	1:B:74:ARG:NH2	2.36	0.41
1:A:543:ARG:NH1	1:A:543:ARG:HG2	2.36	0.41
1:B:10:LEU:HG	1:B:14:MSE:CE	2.31	0.41
1:B:15:LYS:HE3	1:B:74:ARG:HH11	1.85	0.41
1:B:215:ARG:NH1	1:B:215:ARG:C	2.63	0.41
1:B:409:LEU:HG	1:B:411:LEU:HD22	2.02	0.41
1:B:417:LEU:HD22	1:B:451:ALA:HB1	2.01	0.41
1:A:137:GLN:O	1:A:141:ARG:HG3	2.20	0.41
1:A:176:PRO:HG2	1:A:181:GLN:HE21	1.86	0.41
1:B:363:PRO:O	1:B:366:PRO:HD2	2.20	0.41
1:B:365:THR:HB	1:B:366:PRO:CD	2.39	0.41
1:A:138:HIS:HA	1:A:141:ARG:NH1	2.36	0.40
1:A:205:LYS:CE	1:A:287:THR:HG22	2.50	0.40
1:B:274:GLN:CG	1:B:278:ARG:HH22	2.31	0.40
1:B:274:GLN:HB3	1:B:278:ARG:HH21	1.70	0.40
1:B:653:ASN:O	1:B:657:THR:HG23	2.20	0.40
1:A:122:ARG:NH2	1:A:383:LEU:HD11	2.36	0.40
1:A:222:VAL:HA	1:A:260:VAL:O	2.21	0.40
1:B:7:LEU:CD1	1:B:160:LEU:HD22	2.44	0.40
1:B:249:LEU:HD11	1:B:275:LEU:HD21	2.02	0.40
1:A:184:LEU:HD12	1:A:184:LEU:HA	1.88	0.40
1:A:222:VAL:HG22	1:A:243:PHE:HD2	1.86	0.40
1:B:558:TRP:HH2	1:B:615:ARG:NH1	2.19	0.40
2:B:701:ACO:HN8	2:B:701:ACO:H131	1.87	0.40
1:B:73:PHE:CD1	1:B:73:PHE:N	2.90	0.40
1:A:363:PRO:O	1:A:367:LEU:HB2	2.21	0.40
1:A:484:THR:CG2	1:A:485:GLN:N	2.84	0.40
1:A:547:ARG:HD2	5:A:1012:HOH:O	2.22	0.40
1:A:599:LEU:HD11	1:A:616:LEU:HB3	2.03	0.40
1:B:274:GLN:C	1:B:278:ARG:NH2	2.74	0.40
1:B:446:ASN:O	1:B:448:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	654/671 (98%)	633 (97%)	18 (3%)	3 (0%)	29 32
1	B	658/671 (98%)	605 (92%)	44 (7%)	9 (1%)	11 9
All	All	1312/1342 (98%)	1238 (94%)	62 (5%)	12 (1%)	17 17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	LEU
1	B	227	LYS
1	B	215	ARG
1	B	232	VAL
1	A	225	PRO
1	B	280	PRO
1	A	229	SER
1	B	213	ILE
1	B	225	PRO
1	B	221	ILE
1	B	233	LEU
1	A	69	LEU

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
1	A	532/532 (100%)	460 (86%)	72 (14%)	4 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	535/532 (101%)	424 (79%)	111 (21%)	1 1
All	All	1067/1064 (100%)	884 (83%)	183 (17%)	2 1

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	21	ARG
1	A	23	LEU
1	A	25	LEU
1	A	29	GLU
1	A	43	LEU
1	A	50	ILE
1	A	52	PRO
1	A	53	ARG
1	A	68	LEU
1	A	69	LEU
1	A	72	GLU
1	A	95	THR
1	A	96	LEU
1	A	97	LYS
1	A	119	ASP
1	A	139	LEU
1	A	143	LEU
1	A	160	LEU
1	A	162	HIS
1	A	167	THR
1	A	187	LEU
1	A	219	ARG
1	A	222	VAL
1	A	250	LEU
1	A	284	LEU
1	A	286	THR
1	A	299	LEU
1	A	309	LEU
1	A	314	LEU
1	A	316	GLN
1	A	318	ILE
1	A	334	LEU
1	A	360	GLN
1	A	365	THR
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	377	HIS
1	A	381	SER
1	A	411	LEU
1	A	420	GLN
1	A	430	ARG
1	A	431	ARG
1	A	433	ARG
1	A	441	LEU
1	A	472	THR
1	A	476	LEU
1	A	481	LEU
1	A	485	GLN
1	A	506	ARG
1	A	517	HIS
1	A	531	LEU
1	A	543	ARG
1	A	544	GLU
1	A	555	LEU
1	A	572	VAL
1	A	581	LEU
1	A	589	ARG
1	A	592	LEU
1	A	598	LEU
1	A	599	LEU
1	A	602	LEU
1	A	612	LEU
1	A	618	LYS
1	A	625	LEU
1	A	629	LEU
1	A	634	ARG
1	A	635	LYS
1	A	640	ARG
1	A	649	LEU
1	A	652	LEU
1	A	660	LEU
1	B	7	LEU
1	B	16	ARG
1	B	22	LEU
1	B	23	LEU
1	B	25	LEU
1	B	37	LEU

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	40	ARG
1	B	43	LEU
1	B	48	LEU
1	B	53	ARG
1	B	67	THR
1	B	95	THR
1	B	96	LEU
1	B	102	LEU
1	B	106	LEU
1	B	119	ASP
1	B	139	LEU
1	B	142	VAL
1	B	164	THR
1	B	183	LEU
1	B	184	LEU
1	B	185	LYS
1	B	187	LEU
1	B	188	MSE
1	B	198	THR
1	B	211	GLN
1	B	213	ILE
1	B	214	SER
1	B	215	ARG
1	B	216	ILE
1	B	219	ARG
1	B	221	ILE
1	B	222	VAL
1	B	223	THR
1	B	229	SER
1	B	231	ASP
1	B	233	LEU
1	B	235	GLN
1	B	236	PHE
1	B	239	GLU
1	B	240	LYS
1	B	242	ARG
1	B	247	ASP
1	B	250	LEU
1	B	253	ASP
1	B	254	GLU
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	257	ASP
1	B	259	LEU
1	B	261	VAL
1	B	262	ASP
1	B	268	PRO
1	B	271	LEU
1	B	272	LEU
1	B	275	LEU
1	B	279	PHE
1	B	282	THR
1	B	283	LEU
1	B	284	LEU
1	B	285	THR
1	B	286	THR
1	B	299	LEU
1	B	300	LEU
1	B	305	ARG
1	B	311	ARG
1	B	315	GLN
1	B	329	MSE
1	B	338	ASP
1	B	341	PHE
1	B	346	GLN
1	B	348	ASN
1	B	357	THR
1	B	358	LEU
1	B	367	LEU
1	B	373	LEU
1	B	379	ARG
1	B	431	ARG
1	B	433	ARG
1	B	441	LEU
1	B	475	GLN
1	B	476	LEU
1	B	482	GLN
1	B	483	TYR
1	B	487	LEU
1	B	497	THR
1	B	499	GLU
1	B	502	ARG
1	B	540	LEU
1	B	543	ARG

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Mol	Chain	Res	Type
1	B	565	VAL
1	B	570	ASP
1	B	572	VAL
1	B	573	LEU
1	B	580	GLU
1	B	581	LEU
1	B	598	LEU
1	B	599	LEU
1	B	604	THR
1	B	612	LEU
1	B	615	ARG
1	B	616	LEU
1	B	624	GLN
1	B	627	THR
1	B	628	THR
1	B	629	LEU
1	B	635	LYS
1	B	636	MSE
1	B	649	LEU
1	B	652	LEU
1	B	660	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	114	ASN
1	A	115	GLN
1	A	134	HIS
1	A	137	GLN
1	A	181	GLN
1	A	255	GLN
1	A	274	GLN
1	A	322	GLN
1	A	348	ASN
1	A	403	ASN
1	A	423	GLN
1	A	444	HIS
1	A	505	GLN
1	A	516	ASN
1	A	569	ASN
1	A	668	GLN

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Mol	Chain	Res	Type
1	B	35	HIS
1	B	82	HIS
1	B	115	GLN
1	B	134	HIS
1	B	155	ASN
1	B	177	GLN
1	B	182	GLN
1	B	273	HIS
1	B	310	HIS
1	B	315	GLN
1	B	346	GLN
1	B	371	GLN
1	B	419	GLN
1	B	423	GLN
1	B	444	HIS
1	B	446	ASN
1	B	588	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.15	0
2	ACO	A	700	-	45,53,53	3.64	15 (33%)	56,79,79	5.64	32 (57%)
3	ADP	A	800	-	24,29,29	1.28	2 (8%)	29,45,45	1.80	3 (10%)
2	ACO	B	701	-	45,53,53	2.80	15 (33%)	56,79,79	4.77	22 (39%)

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	ACO	A	700	-	1/1/12/14	16/47/67/67	0/3/3/3
3	ADP	A	800	-	-	6/12/32/32	0/3/3/3
2	ACO	B	701	-	1/1/12/14	13/47/67/67	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ACO	O5P-C5P	17.07	1.58	1.23
2	B	701	ACO	O5P-C5P	7.99	1.39	1.23
2	A	700	ACO	O9P-C9P	7.05	1.37	1.23
2	A	700	ACO	CH3-C	-6.23	1.25	1.50
2	A	700	ACO	C5P-N4P	6.12	1.47	1.33
2	B	701	ACO	C5P-N4P	5.40	1.45	1.33
2	A	700	ACO	C2A-N1A	5.10	1.43	1.33
2	B	701	ACO	CH3-C	-5.10	1.30	1.50
2	A	700	ACO	C2A-N3A	4.96	1.40	1.32
2	B	701	ACO	C2A-N1A	4.92	1.43	1.33
2	B	701	ACO	O9P-C9P	4.88	1.33	1.23
2	B	701	ACO	C2B-C1B	-4.75	1.46	1.53
2	B	701	ACO	C6P-C5P	4.68	1.60	1.51
2	A	700	ACO	O4B-C1B	4.37	1.47	1.41
2	B	701	ACO	P3B-O3B	4.35	1.67	1.59
2	B	701	ACO	O4B-C4B	4.34	1.54	1.45
2	A	700	ACO	P3B-O3B	4.31	1.67	1.59
2	B	701	ACO	P3B-O7A	3.83	1.62	1.50
2	B	701	ACO	O4B-C1B	3.61	1.46	1.41
3	A	800	ADP	O4'-C1'	3.45	1.45	1.41
2	B	701	ACO	C2A-N3A	3.44	1.37	1.32
2	A	700	ACO	C5A-C4A	3.35	1.49	1.40
2	A	700	ACO	C6A-C5A	3.23	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ADP	C8-N7	-2.88	1.29	1.34
2	B	701	ACO	C6A-C5A	2.86	1.53	1.43
2	B	701	ACO	OAP-CAP	-2.72	1.37	1.42
2	A	700	ACO	O4B-C4B	2.69	1.51	1.45
2	A	700	ACO	OAP-CAP	2.64	1.47	1.42
2	A	700	ACO	P3B-O7A	2.58	1.58	1.50
2	B	701	ACO	C4A-N3A	2.23	1.38	1.35
2	A	700	ACO	C6P-C5P	2.10	1.55	1.51
2	A	700	ACO	CDP-CBP	2.07	1.58	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	ACO	C2P-C3P-N4P	16.37	146.81	112.42
2	A	700	ACO	O5P-C5P-C6P	-15.23	94.17	122.02
2	A	700	ACO	CEP-CBP-CAP	15.17	135.13	108.82
2	B	701	ACO	O5P-C5P-C6P	-15.10	94.41	122.02
2	B	701	ACO	C2P-C3P-N4P	14.05	141.94	112.42
2	B	701	ACO	O5P-C5P-N4P	-14.02	96.56	123.01
2	A	700	ACO	CEP-CBP-CDP	-12.12	84.46	109.17
2	A	700	ACO	O5P-C5P-N4P	-11.06	102.14	123.01
2	A	700	ACO	CAP-C9P-N8P	-10.91	94.86	116.58
2	A	700	ACO	O6A-CCP-CBP	10.15	126.86	110.55
2	A	700	ACO	O2B-C2B-C1B	9.50	145.94	110.85
2	B	701	ACO	O6A-CCP-CBP	8.28	123.85	110.55
2	B	701	ACO	C1B-N9A-C4A	-8.12	112.38	126.64
2	B	701	ACO	O2B-C2B-C1B	8.07	140.67	110.85
2	A	700	ACO	C3P-N4P-C5P	-7.81	108.34	122.84
2	B	701	ACO	CAP-C9P-N8P	-7.49	101.67	116.58
2	B	701	ACO	CEP-CBP-CAP	7.49	121.80	108.82
2	B	701	ACO	C6P-C5P-N4P	6.92	128.08	116.42
2	A	700	ACO	O9P-C9P-CAP	6.80	141.80	121.06
2	A	700	ACO	C2P-S1P-C	6.63	136.55	101.68
2	B	701	ACO	C2P-S1P-C	6.61	136.45	101.68
3	A	800	ADP	PA-O3A-PB	-6.45	110.69	132.83
2	A	700	ACO	CDP-CBP-CAP	-6.26	97.97	108.82
2	A	700	ACO	C6P-C7P-N8P	-5.58	100.64	111.90
2	A	700	ACO	CDP-CBP-CCP	5.48	117.17	108.23
2	B	701	ACO	CEP-CBP-CCP	-5.39	99.44	108.23
2	B	701	ACO	CDP-CBP-CAP	-5.30	99.64	108.82
2	B	701	ACO	C7P-N8P-C9P	5.25	131.95	122.59
2	A	700	ACO	C7P-N8P-C9P	4.93	131.38	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	ACO	OAP-CAP-CBP	4.87	121.72	110.25
2	B	701	ACO	O9P-C9P-CAP	4.85	135.87	121.06
2	B	701	ACO	O3B-C3B-C2B	4.75	128.89	111.68
3	A	800	ADP	N3-C2-N1	-4.52	121.62	128.68
2	A	700	ACO	C7P-C6P-C5P	-4.33	105.15	112.36
2	B	701	ACO	C3P-N4P-C5P	4.21	130.66	122.84
2	A	700	ACO	P1A-O5B-C5B	-3.72	99.85	121.68
2	A	700	ACO	O4B-C4B-C5B	-3.59	97.56	109.37
2	B	701	ACO	C7P-C6P-C5P	-3.56	106.44	112.36
2	A	700	ACO	O-C-S1P	-3.44	107.33	122.60
2	B	701	ACO	O-C-S1P	-3.41	107.47	122.60
2	B	701	ACO	O4B-C4B-C5B	3.37	120.47	109.37
2	A	700	ACO	C1B-N9A-C4A	3.22	132.31	126.64
2	A	700	ACO	C6P-C5P-N4P	3.05	121.56	116.42
2	A	700	ACO	CEP-CBP-CCP	-2.99	103.35	108.23
2	A	700	ACO	OAP-CAP-C9P	2.89	123.32	109.42
2	A	700	ACO	O4B-C1B-C2B	-2.69	103.00	106.93
2	A	700	ACO	O2A-P1A-O5B	2.63	119.98	107.75
2	B	701	ACO	CDP-CBP-CCP	2.63	112.52	108.23
2	A	700	ACO	O5B-C5B-C4B	2.59	117.92	108.99
2	A	700	ACO	C5B-C4B-C3B	-2.52	106.04	114.40
3	A	800	ADP	O2A-PA-O1A	-2.45	100.11	112.24
2	B	701	ACO	C4A-C5A-N7A	2.40	111.90	109.40
2	B	701	ACO	C3B-C2B-C1B	2.35	105.09	99.89
2	A	700	ACO	C4A-C5A-N7A	2.34	111.84	109.40
2	A	700	ACO	C3B-C2B-C1B	2.26	104.90	99.89
2	A	700	ACO	C5A-C6A-N1A	-2.17	115.44	120.35
2	A	700	ACO	P2A-O6A-CCP	2.09	133.62	121.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	700	ACO	C2B
2	B	701	ACO	C2B

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ACO	O4B-C4B-C5B-O5B
2	A	700	ACO	C5B-O5B-P1A-O3A
2	A	700	ACO	C9P-CAP-CBP-CCP
2	A	700	ACO	C9P-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
2	A	700	ACO	C9P-CAP-CBP-CEP
2	A	700	ACO	N8P-C9P-CAP-OAP
2	A	700	ACO	S1P-C2P-C3P-N4P
3	A	800	ADP	C5'-O5'-PA-O1A
3	A	800	ADP	C5'-O5'-PA-O3A
3	A	800	ADP	O4'-C4'-C5'-O5'
2	B	701	ACO	O4B-C4B-C5B-O5B
2	B	701	ACO	C5B-O5B-P1A-O1A
2	B	701	ACO	C5B-O5B-P1A-O3A
2	B	701	ACO	N8P-C9P-CAP-OAP
2	B	701	ACO	O5P-C5P-N4P-C3P
2	B	701	ACO	C3P-C2P-S1P-C
2	B	701	ACO	CH3-C-S1P-C2P
2	A	700	ACO	O5P-C5P-N4P-C3P
2	A	700	ACO	C3B-C4B-C5B-O5B
3	A	800	ADP	C3'-C4'-C5'-O5'
2	B	701	ACO	C3B-C4B-C5B-O5B
2	A	700	ACO	C6P-C7P-N8P-C9P
2	A	700	ACO	CEP-CBP-CCP-O6A
2	A	700	ACO	CH3-C-S1P-C2P
2	A	700	ACO	O9P-C9P-CAP-OAP
2	B	701	ACO	O9P-C9P-CAP-OAP
2	B	701	ACO	C6P-C7P-N8P-C9P
2	B	701	ACO	C9P-CAP-CBP-CEP
2	A	700	ACO	C3B-O3B-P3B-O8A
3	A	800	ADP	PB-O3A-PA-O2A
2	A	700	ACO	C5B-O5B-P1A-O1A
2	B	701	ACO	C9P-CAP-CBP-CCP
2	A	700	ACO	C6P-C5P-N4P-C3P
2	B	701	ACO	C3B-O3B-P3B-O9A
3	A	800	ADP	PB-O3A-PA-O1A

There are no ring outliers.

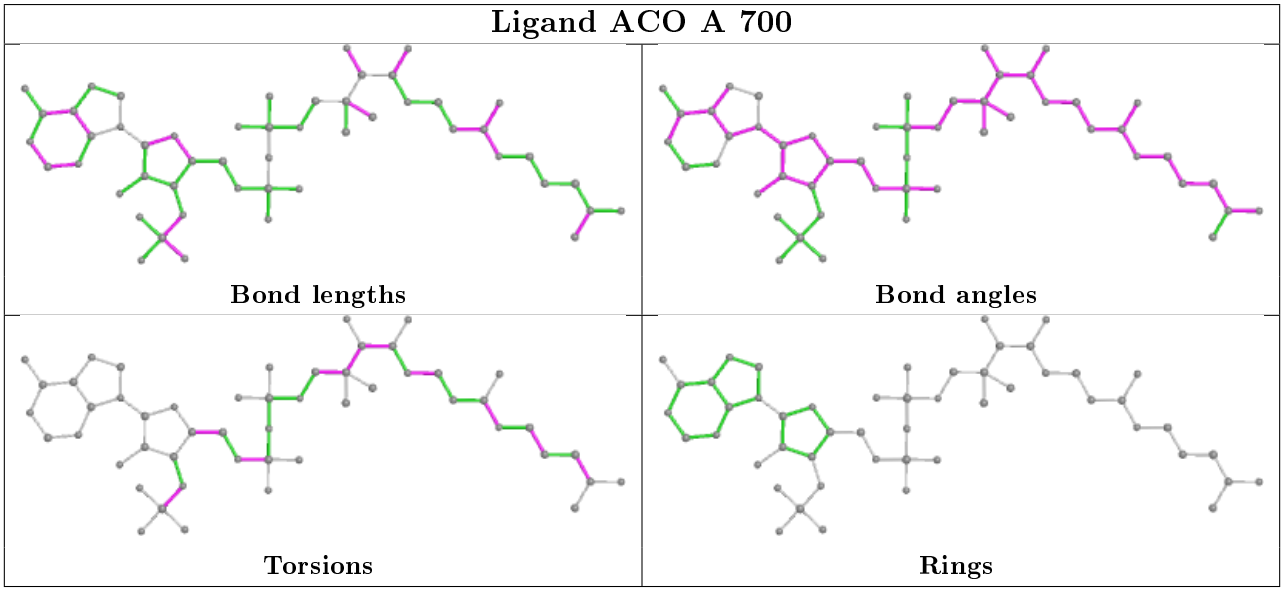
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	SO4	1	0
2	A	700	ACO	3	0
3	A	800	ADP	2	0
2	B	701	ACO	7	0

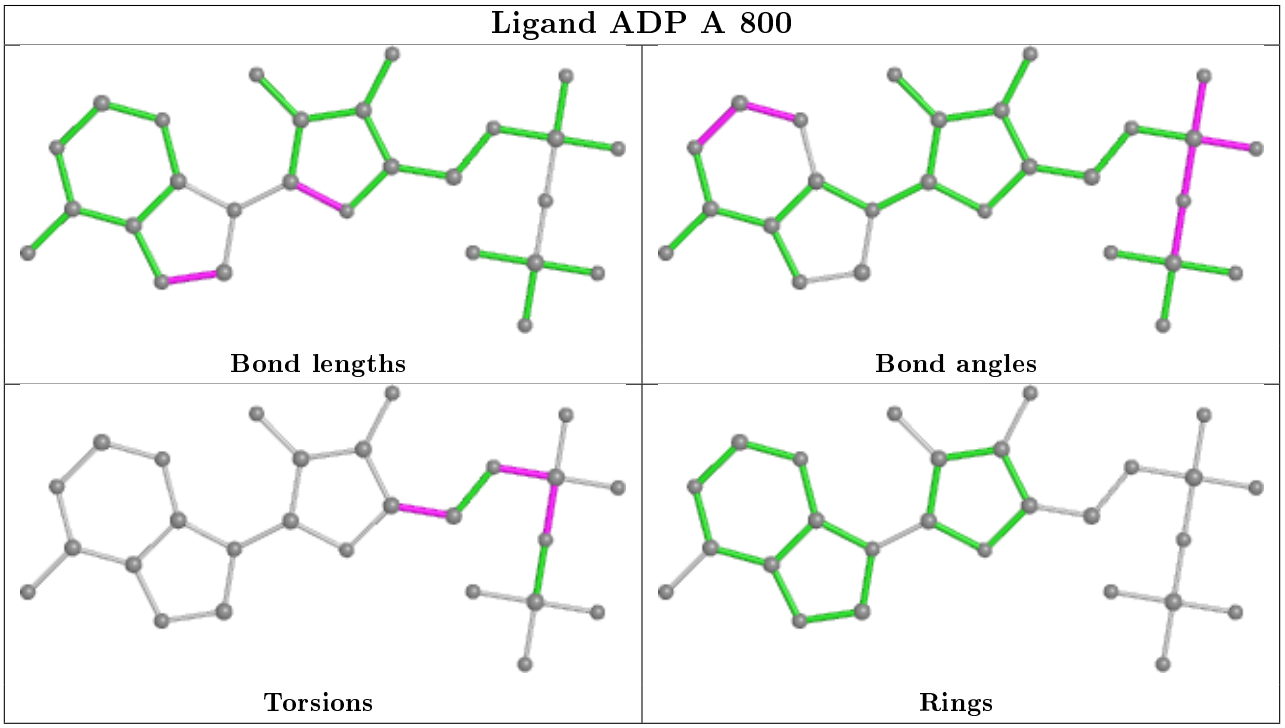
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

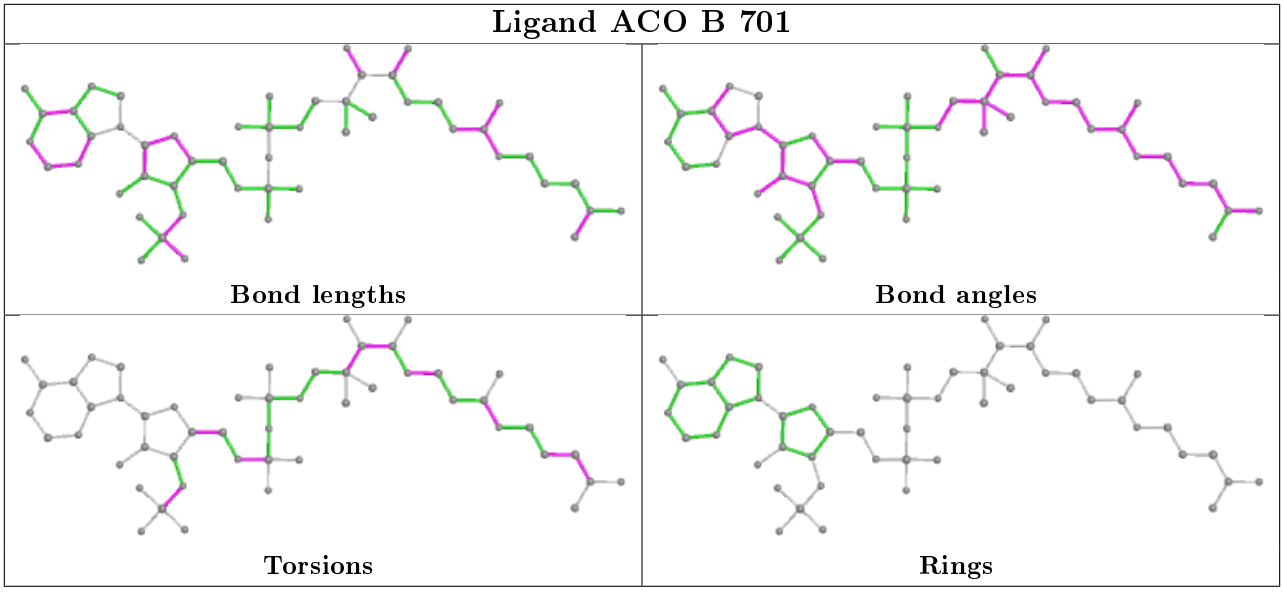
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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 ACO A 700



Ligand ADP A 800





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	648/671 (96%)	0.24	24 (3%) 41 54	18, 35, 62, 90	0
1	B	651/671 (97%)	0.95	94 (14%) 2 4	22, 49, 99, 100	0
All	All	1299/1342 (96%)	0.59	118 (9%) 9 14	18, 42, 95, 100	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	ILE	10.6
1	B	54	PRO	9.7
1	B	244	ILE	9.5
1	B	216	ILE	8.2
1	A	54	PRO	8.2
1	B	241	PHE	7.9
1	B	238	GLY	7.8
1	B	243	PHE	7.0
1	B	184	LEU	6.9
1	B	251	ALA	6.8
1	B	213	ILE	6.8
1	B	55	ASP	6.7
1	B	220	ALA	6.6
1	B	233	LEU	6.4
1	B	173	THR	6.4
1	B	212	LEU	6.0
1	B	219	ARG	5.8
1	B	53	ARG	5.8
1	B	209	ALA	5.6
1	B	237	ALA	5.5
1	B	483	TYR	5.3
1	B	242	ARG	5.3
1	B	217	ALA	5.3
1	A	670	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	ARG	5.1
1	B	255	GLN	5.1
1	B	482	GLN	5.0
1	B	275	LEU	4.8
1	B	236	PHE	4.7
1	B	484	THR	4.7
1	B	56	ALA	4.5
1	B	172	ALA	4.4
1	B	502	ARG	4.3
1	B	256	ALA	4.3
1	B	341	PHE	4.3
1	B	670	PHE	4.3
1	A	70	GLY	4.3
1	B	257	ASP	4.1
1	B	250	LEU	4.1
1	A	69	LEU	4.1
1	B	258	TRP	4.0
1	B	186	GLN	4.0
1	B	252	SER	4.0
1	B	312	PHE	4.0
1	B	214	SER	4.0
1	B	175	ALA	3.9
1	B	69	LEU	3.7
1	B	246	PRO	3.7
1	B	170	TYR	3.7
1	B	223	THR	3.7
1	B	65	LEU	3.6
1	B	211	GLN	3.6
1	B	277	SER	3.6
1	B	254	GLU	3.5
1	B	279	PHE	3.5
1	B	189	THR	3.5
1	B	229	SER	3.3
1	B	232	VAL	3.3
1	A	67	THR	3.3
1	A	2	ALA	3.2
1	B	174	GLY	3.2
1	B	249	LEU	3.2
1	A	403	ASN	3.2
1	B	181	GLN	3.2
1	B	631	LEU	3.1
1	B	235	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	GLN	3.0
1	B	619	ASN	3.0
1	A	291	TYR	3.0
1	B	433	ARG	3.0
1	B	208	LEU	2.9
1	B	218	GLY	2.9
1	B	253	ASP	2.8
1	B	71	ARG	2.8
1	A	668	GLN	2.7
1	B	147	ASN	2.7
1	B	178	PRO	2.7
1	B	339	GLU	2.7
1	A	172	ALA	2.6
1	B	376	ALA	2.6
1	B	239	GLU	2.6
1	B	669	LEU	2.5
1	B	193	GLY	2.5
1	B	299	LEU	2.5
1	B	261	VAL	2.5
1	A	308	HIS	2.5
1	A	228	ALA	2.5
1	A	52	PRO	2.5
1	B	164	THR	2.4
1	B	297	GLY	2.4
1	A	254	GLU	2.4
1	A	160	LEU	2.4
1	B	222	VAL	2.4
1	B	245	ALA	2.4
1	A	66	GLN	2.4
1	B	169	TRP	2.4
1	B	70	GLY	2.4
1	B	176	PRO	2.3
1	B	622	ASP	2.3
1	B	629	LEU	2.3
1	B	566	ASP	2.3
1	A	170	TYR	2.3
1	B	16	ARG	2.2
1	B	431	ARG	2.2
1	A	485	GLN	2.2
1	B	260	VAL	2.1
1	A	634	ARG	2.1
1	B	294	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	53	ARG	2.1
1	B	215	ARG	2.1
1	A	68	LEU	2.1
1	A	517	HIS	2.1
1	B	296	ARG	2.1
1	B	210	GLY	2.1
1	A	226	ALA	2.0
1	B	128	ASP	2.0
1	A	669	LEU	2.0
1	B	66	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

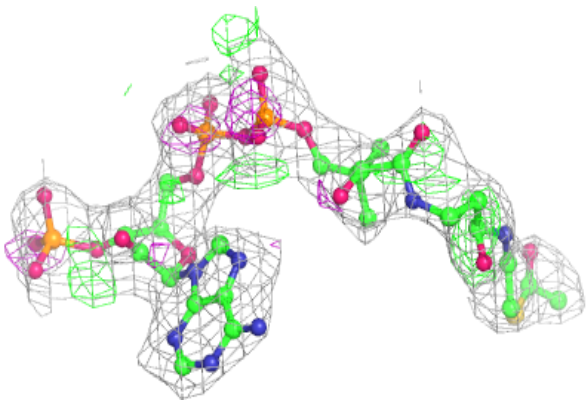
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

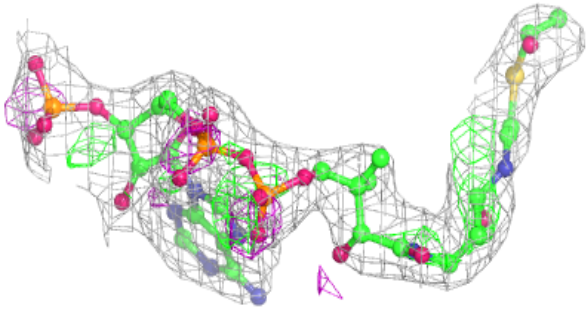
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	B	701	51/51	0.86	0.23	24,50,93,95	0
2	ACO	A	700	51/51	0.87	0.25	18,66,88,89	0
4	SO4	B	801	5/5	0.91	0.15	77,78,78,79	0
3	ADP	A	800	27/27	0.94	0.15	29,38,39,43	0

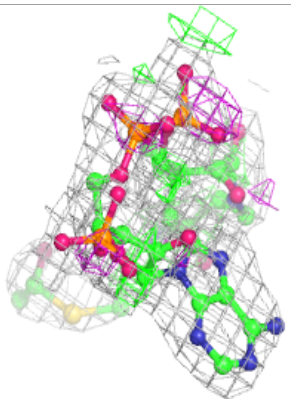
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO 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)

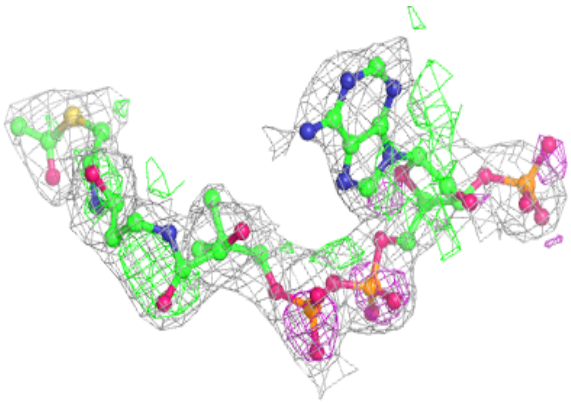


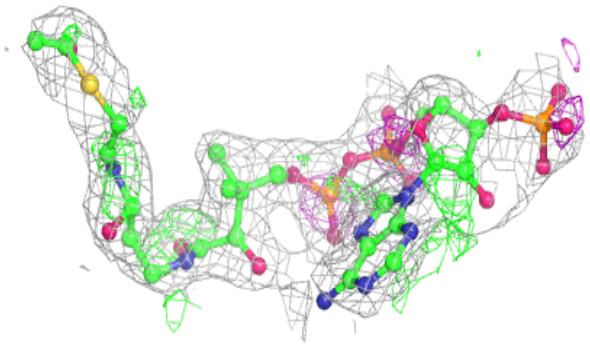


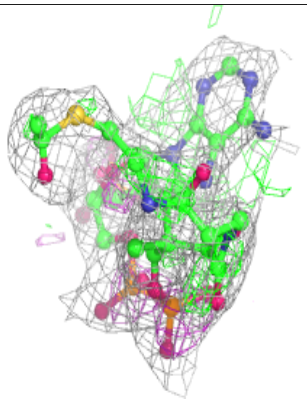


Electron density around ACO A 700:

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

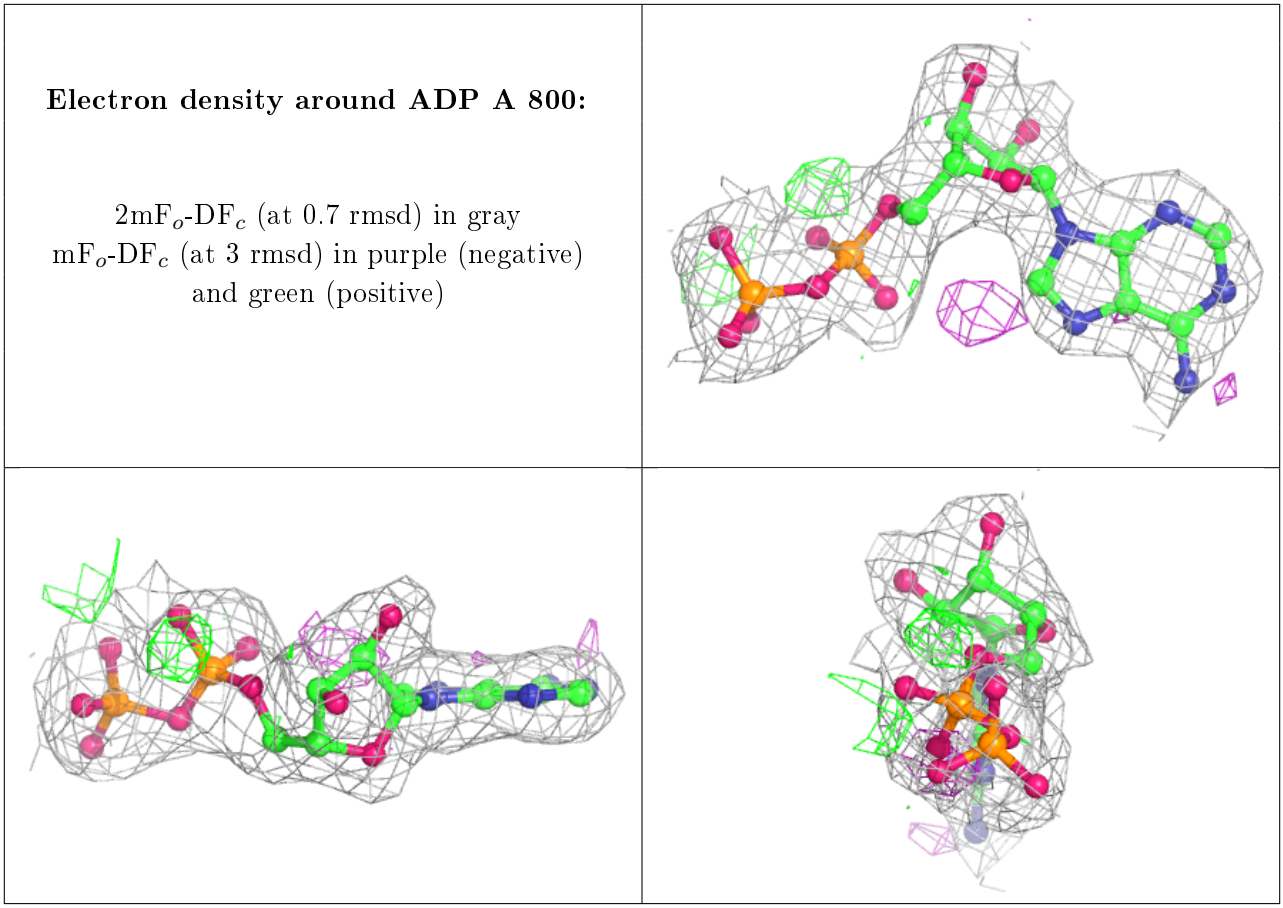






Electron density around ADP A 800:

$2mF_o$-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

There are no such residues in this entry.