Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 03:29 PM EDT

PDB ID	:	1UN9
Title	:	Crystal structure of the dihydroxyacetone kinase from C. freundii in complex with AMP-PNP and Mg2+
Authors	:	Siebold, C.; Arnold, I.; Garcia-Alles, L.F.; Baumann, U.; Erni, B.
Deposited on	:	2003-09-08
Resolution	:	3.10 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:

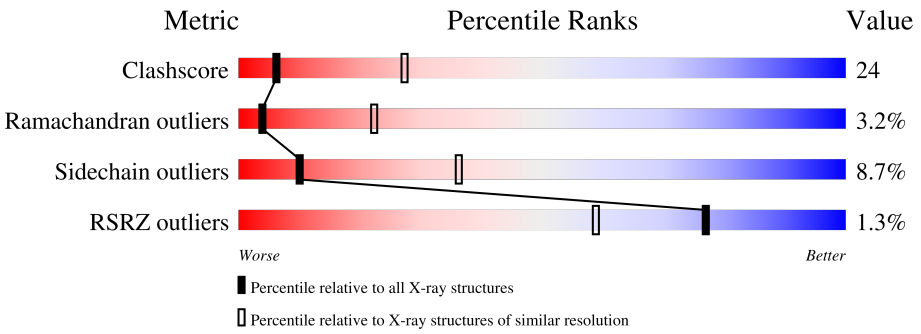
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	552	2% 56% 37%
1	B	552	% 56% 37%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7982 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.

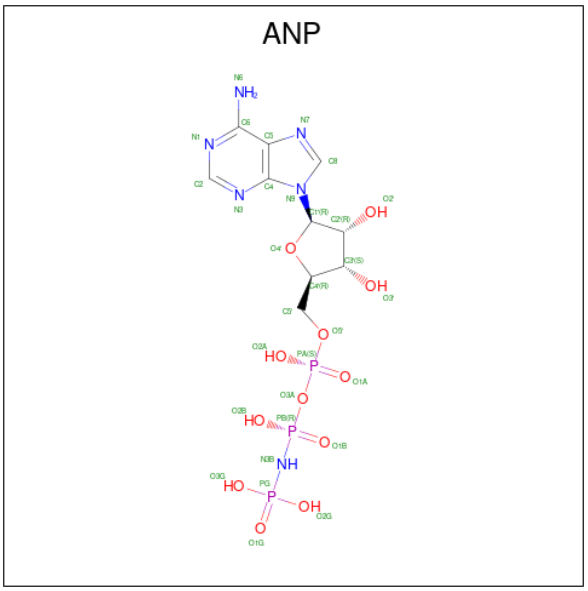
- Molecule 1 is a protein called DIHYDROXYACETONE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	3952	2481	692	761	18	0	0	0
1	B	537	3952	2481	692	761	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	MET	conflict	UNP P45510
A	538	ALA	ARG	conflict	UNP P45510
B	1	ALA	MET	conflict	UNP P45510
B	538	ALA	ARG	conflict	UNP P45510

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

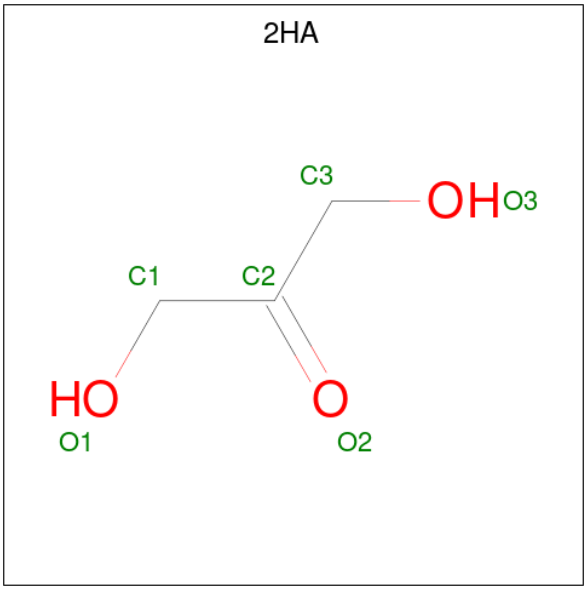


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0
2	B	1	31	10	6	12	3	0	0

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

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

- Molecule 4 is DIHYDROXYACETONE (three-letter code: 2HA) (formula: $C_3H_6O_3$).



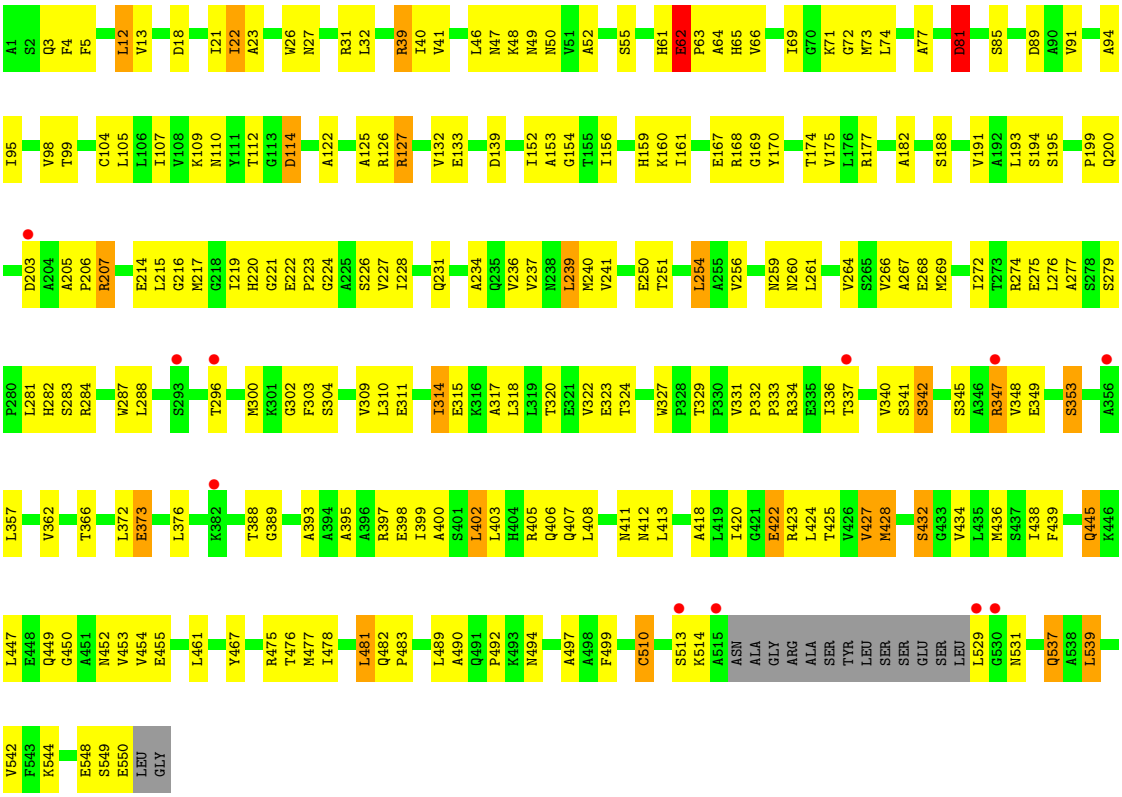
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0

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.

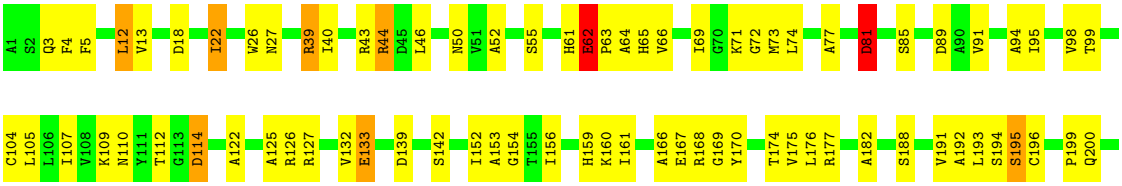
• Molecule 1: DIHYDROXYACETONE KINASE

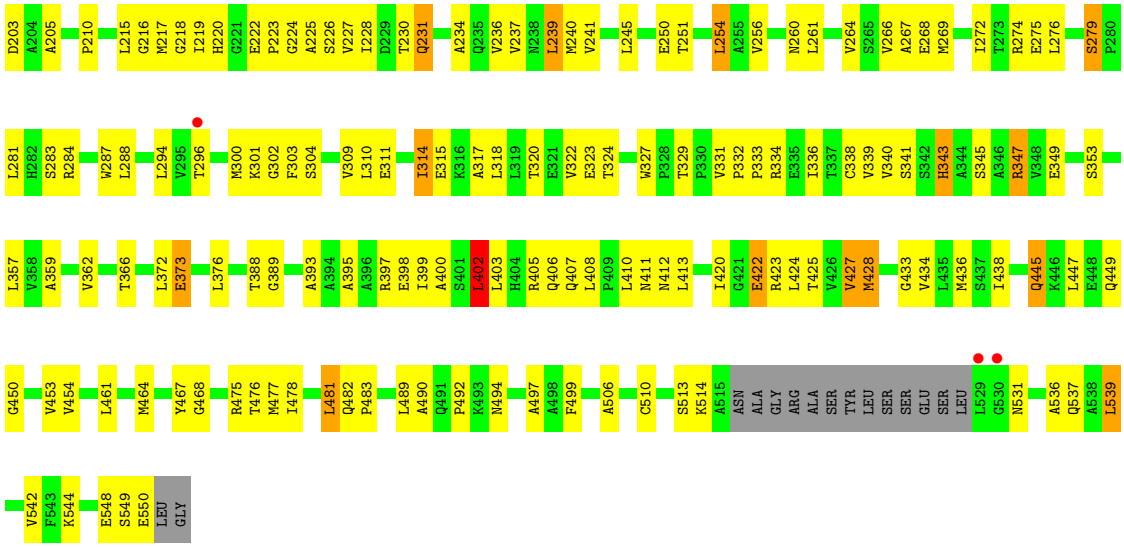
Chain A:



• Molecule 1: DIHYDROXYACETONE KINASE

Chain B:




D203 A204 A205 P210 L215 G216 M217 G218 I219 H220 G221 E222 P223 G224 A225 S226 V227 I228 D229 T230 Q231 A234 Q235 V236 V237 N238 L239 M240 V241 L245 E250 T251 L254 A255 V256 N260 L261 V264 S265 V266 A267 E268 M269 I272 T273 R274 E275 L276 S279 P280
L281 H282 S283 R284 W287 L288 L294 V295 T296 M300 K301 G302 F303 S304 V309 L310 E311 I314 E315 K316 A317 L318 L319 T320 E321 V322 E323 T324 W327 P328 T329 P330 V331 P332 P333 R334 E335 I336 T337 C338 V339 V340 S341 S342 H343 A344 S345 A346 R347 V348 E349 S353
L357 V358 A359 V362 T366 L372 E373 L376 T388 G389 A393 A394 A395 A396 R397 E398 I399 A400 S401 L402 L403 H404 R405 Q406 Q407 L408 P409 L410 N411 N412 L413 I420 G421 E422 R423 L424 T425 V426 V427 M428 G433 V434 L435 M436 S437 I438 Q445 K446 L447 E448 Q449
G450 V453 V454 L461 M464 Y467 G468 R475 T476 M477 I478 L481 Q482 P483 L489 A490 Q491 P492 K493 N494 A497 A498 F499 A506 C510 S513 K514 A515 ASN ALA GLY ARG ALA SER TYR LEU SER SER GLU SER LEU L529 G530 N531 A536 Q537 A538 L539
V542 F543 K544 E548 S549 E550 LEU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	100.79Å 124.87Å 236.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 39.21 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.1 (25.00-3.10) 93.7 (39.21-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , (Not available) 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: 2HA, 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	0.47	1/4015 (0.0%)	0.70	4/5459 (0.1%)
1	B	0.45	2/4015 (0.0%)	0.70	4/5459 (0.1%)
All	All	0.46	3/8030 (0.0%)	0.70	8/10918 (0.1%)

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	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	C-N	-5.88	1.23	1.34
1	B	210	PRO	N-CD	5.10	1.54	1.47
1	B	62	GLU	C-N	-5.06	1.24	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	GLU	N-CA-C	14.64	150.52	111.00
1	A	62	GLU	N-CA-C	14.60	150.42	111.00
1	B	62	GLU	C-N-CD	8.75	146.78	128.40
1	A	62	GLU	C-N-CA	-6.49	94.73	122.00
1	B	62	GLU	C-N-CA	-6.10	96.37	122.00
1	A	62	GLU	CB-CA-C	-5.65	99.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	GLU	N-CA-CB	-5.34	101.00	110.60
1	A	342	SER	CB-CA-C	5.02	119.64	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLU	Peptide
1	B	62	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3952	0	3978	209	1
1	B	3952	0	3978	205	0
2	A	31	0	13	5	0
2	B	31	0	13	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	6	0	6	1	0
4	B	6	0	6	1	0
All	All	7982	0	7994	390	1

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 24.

All (390) 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:133:GLU:HA	1:B:133:GLU:OE1	1.29	1.08
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.13	1.07
1:B:133:GLU:HG3	1:B:176:LEU:HD22	1.35	1.03
1:A:127:ARG:HH11	1:A:127:ARG:CG	1.74	0.99
1:A:348:VAL:HG23	1:B:127:ARG:HH22	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HG3	1:A:127:ARG:NH1	1.74	0.92
1:B:395:ALA:HB1	1:B:424:LEU:HD22	1.55	0.89
1:A:395:ALA:HB1	1:A:424:LEU:HD22	1.55	0.88
1:A:266:VAL:HG11	1:B:62:GLU:O	1.73	0.88
1:B:475:ARG:HH11	1:B:475:ARG:HB3	1.39	0.86
1:B:490:ALA:O	1:B:492:PRO:HD3	1.75	0.85
1:B:133:GLU:OE1	1:B:133:GLU:CA	2.18	0.84
1:A:475:ARG:HB3	1:A:475:ARG:HH11	1.41	0.83
1:B:424:LEU:O	1:B:428:MET:HG3	1.78	0.83
1:A:490:ALA:O	1:A:492:PRO:HD3	1.81	0.80
1:B:74:LEU:HD11	1:B:159:HIS:CD2	2.18	0.78
1:A:482:GLN:HB3	1:A:483:PRO:HD3	1.66	0.78
1:A:477:MET:HG2	2:A:1551:ANP:H8	1.66	0.78
1:B:398:GLU:HB2	1:B:427:VAL:HG11	1.65	0.77
1:B:362:VAL:O	1:B:366:THR:HG23	1.83	0.77
1:A:288:LEU:HG	1:A:333:PRO:HG3	1.68	0.76
1:B:482:GLN:HB3	1:B:483:PRO:HD3	1.66	0.76
1:A:398:GLU:HB2	1:A:427:VAL:HG11	1.67	0.75
1:A:74:LEU:HD11	1:A:159:HIS:CD2	2.22	0.75
1:A:362:VAL:O	1:A:366:THR:HG23	1.85	0.75
1:B:288:LEU:HG	1:B:333:PRO:HG3	1.68	0.75
1:A:65:HIS:HE1	1:A:109:LYS:HE3	1.52	0.74
1:A:272:ILE:HD13	1:A:303:PHE:CD2	2.22	0.74
1:B:264:VAL:HG11	1:B:269:MET:HE2	1.70	0.74
1:B:475:ARG:HB3	1:B:475:ARG:NH1	2.02	0.74
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.54	0.73
1:B:237:VAL:O	1:B:241:VAL:HG23	1.88	0.73
1:B:388:THR:HA	2:B:1551:ANP:O1A	1.89	0.73
1:A:237:VAL:O	1:A:241:VAL:HG23	1.88	0.73
1:B:272:ILE:HD13	1:B:303:PHE:CD2	2.24	0.72
1:A:266:VAL:CG1	1:B:62:GLU:O	2.37	0.71
1:A:475:ARG:HB3	1:A:475:ARG:NH1	2.04	0.71
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.55	0.71
1:A:250:GLU:HG3	1:A:251:THR:HG23	1.73	0.70
1:B:464:MET:HE2	2:B:1551:ANP:H2	1.73	0.70
1:B:250:GLU:HG3	1:B:251:THR:HG23	1.75	0.69
1:B:264:VAL:HG11	1:B:269:MET:CE	2.24	0.68
1:B:254:LEU:HA	1:B:310:LEU:HG	1.74	0.68
1:B:127:ARG:O	1:B:127:ARG:HG2	1.93	0.68
1:B:428:MET:SD	1:B:433:GLY:HA2	2.35	0.66
1:A:452:ASN:ND2	1:A:455:GLU:OE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HA	1:A:310:LEU:HG	1.77	0.66
1:B:276:LEU:O	1:B:279:SER:HB3	1.96	0.65
1:A:264:VAL:HG11	1:A:269:MET:HE2	1.79	0.65
1:B:72:GLY:HA3	1:B:322:VAL:HG12	1.78	0.65
1:A:395:ALA:HB2	1:A:428:MET:SD	2.37	0.65
1:A:267:ALA:HB2	1:B:62:GLU:OE1	1.96	0.65
1:A:264:VAL:HG11	1:A:269:MET:CE	2.27	0.65
1:A:160:LYS:HE3	1:A:318:LEU:O	1.96	0.64
1:B:43:ARG:NH2	1:B:71:LYS:HA	2.12	0.64
1:A:61:HIS:CE1	1:A:219:ILE:HG13	2.32	0.64
1:A:72:GLY:HA3	1:A:322:VAL:HG12	1.79	0.64
1:B:399:ILE:HD12	1:B:420:ILE:HG12	1.80	0.64
1:A:276:LEU:O	1:A:279:SER:HB3	1.96	0.63
1:A:399:ILE:HD12	1:A:420:ILE:HG12	1.80	0.63
1:B:160:LYS:HE3	1:B:318:LEU:O	1.98	0.63
1:B:261:LEU:HB2	1:B:302:GLY:O	1.99	0.63
1:A:65:HIS:CE1	1:A:109:LYS:HE3	2.33	0.62
1:A:499:PHE:CE1	1:A:544:LYS:HB2	2.34	0.62
1:B:26:TRP:CZ3	1:B:323:GLU:HG2	2.35	0.61
1:B:499:PHE:CE1	1:B:544:LYS:HB2	2.35	0.61
1:A:424:LEU:O	1:A:428:MET:HG3	1.99	0.61
1:B:126:ARG:HG3	1:B:126:ARG:NH1	2.14	0.61
1:B:61:HIS:CE1	1:B:219:ILE:HD12	2.36	0.61
1:B:61:HIS:HA	1:B:296:THR:O	2.01	0.60
1:A:418:ALA:HB1	1:B:127:ARG:NH1	2.16	0.60
1:A:256:VAL:HG11	1:A:276:LEU:HD11	1.83	0.60
1:B:256:VAL:HG11	1:B:276:LEU:HD11	1.83	0.60
1:B:481:LEU:HG	1:B:539:LEU:HD11	1.84	0.60
1:A:126:ARG:HG3	1:A:126:ARG:NH1	2.15	0.60
1:B:74:LEU:HD11	1:B:159:HIS:CG	2.36	0.60
1:B:109:LYS:NZ	4:B:1554:2HA:O1	2.34	0.60
1:B:13:VAL:HG11	1:B:39:ARG:HD3	1.82	0.60
1:A:395:ALA:HB2	1:A:428:MET:HG2	1.84	0.59
1:A:481:LEU:HG	1:A:539:LEU:HD11	1.83	0.59
1:A:46:LEU:HD11	1:A:98:VAL:HB	1.84	0.59
1:B:65:HIS:NE2	1:B:109:LYS:HE3	2.18	0.59
1:A:261:LEU:HG	1:A:300:MET:CE	2.33	0.59
1:A:13:VAL:HG11	1:A:39:ARG:HD3	1.84	0.58
1:A:261:LEU:HB2	1:A:302:GLY:O	2.03	0.58
1:A:272:ILE:HD13	1:A:303:PHE:CE2	2.38	0.58
1:B:454:VAL:HG12	1:B:489:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:SER:CB	1:A:411:ASN:HB2	2.33	0.58
1:A:74:LEU:HD11	1:A:159:HIS:CG	2.38	0.57
1:A:324:THR:OG1	1:A:327:TRP:HB3	2.04	0.57
1:B:353:SER:CB	1:B:411:ASN:HB2	2.34	0.57
1:B:261:LEU:HG	1:B:300:MET:CE	2.33	0.57
1:A:544:LYS:O	1:A:548:GLU:HG3	2.04	0.57
1:B:272:ILE:HD13	1:B:303:PHE:CE2	2.40	0.57
1:A:26:TRP:CZ3	1:A:323:GLU:HG2	2.40	0.57
1:A:310:LEU:HD13	1:A:315:GLU:OE1	2.04	0.57
1:B:152:ILE:HD11	1:B:188:SER:OG	2.05	0.57
1:B:310:LEU:HD22	1:B:315:GLU:HB2	1.85	0.57
1:B:544:LYS:O	1:B:548:GLU:HG3	2.05	0.57
1:A:476:THR:HG23	1:A:478:ILE:HB	1.86	0.56
1:A:152:ILE:HD11	1:A:188:SER:HB3	1.87	0.56
1:A:50:ASN:OD1	1:A:169:GLY:HA2	2.05	0.56
1:A:310:LEU:HD22	1:A:315:GLU:HB2	1.86	0.56
1:A:61:HIS:CE1	1:A:219:ILE:CG1	2.89	0.56
1:A:216:GLY:O	1:A:224:GLY:HA2	2.05	0.56
1:B:192:ALA:HB3	1:B:217:MET:CE	2.35	0.56
1:A:61:HIS:HA	1:A:296:THR:O	2.05	0.56
1:B:461:LEU:HD13	1:B:481:LEU:HD13	1.88	0.56
1:A:348:VAL:CG2	1:B:127:ARG:HH22	2.13	0.56
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.70	0.56
1:A:226:SER:OG	1:A:227:VAL:N	2.36	0.55
1:B:405:ARG:O	1:B:407:GLN:HG2	2.06	0.55
1:B:105:LEU:HD22	1:B:175:VAL:HG12	1.88	0.55
1:A:405:ARG:O	1:A:407:GLN:HG2	2.06	0.55
1:A:418:ALA:HB1	1:B:127:ARG:HH12	1.70	0.55
1:A:454:VAL:HG12	1:A:489:LEU:HD13	1.88	0.55
1:B:476:THR:HG23	1:B:478:ILE:HB	1.88	0.55
1:A:47:ASN:O	1:A:49:ASN:N	2.40	0.55
1:A:105:LEU:HD22	1:A:175:VAL:HG12	1.88	0.55
1:B:347:ARG:HA	1:B:422:GLU:OE2	2.07	0.55
1:A:107:ILE:HD12	1:A:159:HIS:HD2	1.72	0.55
1:B:192:ALA:HB3	1:B:217:MET:HE3	1.89	0.55
1:A:432:SER:HB2	2:A:1551:ANP:O2A	2.07	0.55
1:A:99:THR:HG23	1:A:104:CYS:HB3	1.88	0.54
1:B:43:ARG:HH22	1:B:71:LYS:HA	1.71	0.54
1:B:332:PRO:HG2	1:B:334:ARG:NH1	2.23	0.54
1:B:324:THR:OG1	1:B:327:TRP:HB3	2.08	0.54
1:A:18:ASP:O	1:A:22:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HA	1:A:159:HIS:HD1	1.73	0.54
1:B:177:ARG:HG2	1:B:177:ARG:HH11	1.73	0.54
1:A:395:ALA:HB2	1:A:428:MET:CG	2.38	0.54
1:B:261:LEU:HG	1:B:300:MET:HE2	1.89	0.54
1:A:481:LEU:HG	1:A:539:LEU:HD21	1.89	0.54
1:A:362:VAL:O	1:A:366:THR:CG2	2.54	0.53
1:A:274:ARG:O	1:A:274:ARG:HD3	2.08	0.53
1:B:46:LEU:HD11	1:B:98:VAL:HB	1.90	0.53
1:A:222:GLU:HB3	1:A:223:PRO:HD2	1.90	0.53
1:A:193:LEU:CB	1:B:3:GLN:HE21	2.22	0.53
1:A:347:ARG:HA	1:A:422:GLU:OE2	2.09	0.53
1:B:4:PHE:CZ	1:B:199:PRO:HG3	2.44	0.53
1:B:69:ILE:HD11	1:B:77:ALA:HB3	1.90	0.53
1:A:261:LEU:HG	1:A:300:MET:HE3	1.89	0.53
1:B:156:ILE:HA	1:B:159:HIS:ND1	2.24	0.53
1:B:362:VAL:O	1:B:366:THR:CG2	2.53	0.53
1:A:461:LEU:HD13	1:A:481:LEU:HD13	1.91	0.52
1:B:107:ILE:HD12	1:B:159:HIS:HD2	1.74	0.52
1:B:218:GLY:HA3	1:B:222:GLU:OE1	2.09	0.52
1:A:3:GLN:HE22	1:B:194:SER:HB3	1.75	0.52
1:B:99:THR:HG23	1:B:104:CYS:HB3	1.92	0.52
1:B:73:MET:SD	1:B:324:THR:HG21	2.49	0.52
1:B:254:LEU:HD12	1:B:284:ARG:O	2.09	0.52
1:B:310:LEU:HD13	1:B:315:GLU:OE1	2.08	0.52
1:A:260:ASN:HD22	1:A:269:MET:HG3	1.75	0.52
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.74	0.52
1:A:413:LEU:HB3	1:A:447:LEU:CD1	2.39	0.52
1:B:481:LEU:HG	1:B:539:LEU:HD21	1.92	0.52
1:A:156:ILE:HA	1:A:159:HIS:ND1	2.24	0.52
2:A:1551:ANP:O2B	2:A:1551:ANP:H5'2	2.10	0.52
1:A:332:PRO:HG2	1:A:334:ARG:NH1	2.25	0.52
1:A:5:PHE:CE2	1:B:193:LEU:HD21	2.45	0.51
1:A:207:ARG:HH22	1:A:217:MET:HG3	1.75	0.51
1:B:413:LEU:HB3	1:B:447:LEU:CD1	2.40	0.51
1:A:279:SER:C	1:A:281:LEU:H	2.13	0.51
1:A:397:ARG:HG3	1:A:397:ARG:HH11	1.74	0.51
1:A:477:MET:CG	2:A:1551:ANP:H8	2.38	0.51
1:B:403:LEU:HA	1:B:408:LEU:HD12	1.93	0.51
1:B:550:GLU:OE2	1:B:550:GLU:HA	2.10	0.51
1:A:61:HIS:CE1	1:A:219:ILE:HD12	2.46	0.51
1:A:403:LEU:HA	1:A:408:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:O	1:B:296:THR:HB	2.10	0.51
1:A:400:ALA:O	1:A:403:LEU:HB3	2.11	0.51
1:B:279:SER:C	1:B:281:LEU:H	2.13	0.51
1:B:50:ASN:HB3	1:B:166:ALA:O	2.10	0.51
1:A:91:VAL:O	1:A:95:ILE:HG13	2.10	0.51
1:A:261:LEU:O	1:A:296:THR:HB	2.11	0.51
1:B:91:VAL:O	1:B:95:ILE:HG13	2.10	0.50
1:A:127:ARG:CG	1:A:127:ARG:NH1	2.44	0.50
1:A:65:HIS:HE1	1:A:109:LYS:CE	2.23	0.50
1:A:69:ILE:HD11	1:A:77:ALA:HB3	1.94	0.50
1:A:161:ILE:HD13	1:A:317:ALA:HB3	1.94	0.50
1:A:269:MET:HE2	1:A:269:MET:HA	1.94	0.49
1:B:250:GLU:CG	1:B:251:THR:HG23	2.42	0.49
1:B:376:LEU:HB2	1:B:389:GLY:CA	2.43	0.49
1:A:329:THR:O	1:A:331:VAL:HG23	2.12	0.49
1:B:114:ASP:OD2	1:B:114:ASP:N	2.44	0.49
1:B:216:GLY:O	1:B:224:GLY:HA2	2.11	0.49
1:B:400:ALA:O	1:B:403:LEU:HB3	2.12	0.49
1:B:445:GLN:O	1:B:449:GLN:HG2	2.11	0.49
1:A:62:GLU:OE1	1:B:267:ALA:HB2	2.12	0.49
1:B:66:VAL:HA	1:B:69:ILE:CD1	2.42	0.49
1:B:336:ILE:HD12	1:B:336:ILE:O	2.12	0.49
1:A:62:GLU:O	1:B:266:VAL:CG1	2.60	0.49
1:A:376:LEU:HB2	1:A:389:GLY:CA	2.42	0.49
1:B:261:LEU:HD23	1:B:302:GLY:C	2.33	0.49
1:A:152:ILE:HD11	1:A:188:SER:CB	2.43	0.49
1:A:114:ASP:N	1:A:114:ASP:OD2	2.45	0.49
1:B:475:ARG:HH11	1:B:475:ARG:CB	2.18	0.49
1:A:73:MET:SD	1:A:324:THR:HG21	2.53	0.49
1:A:152:ILE:O	1:A:154:GLY:N	2.46	0.49
1:B:260:ASN:HD22	1:B:269:MET:HG3	1.77	0.49
1:B:274:ARG:O	1:B:274:ARG:HD3	2.13	0.49
1:A:22:ILE:HG22	1:A:22:ILE:O	2.12	0.49
1:B:397:ARG:HG3	1:B:397:ARG:HH11	1.77	0.49
1:A:168:ARG:HH22	1:A:320:THR:HG21	1.77	0.48
1:B:18:ASP:O	1:B:22:ILE:HG13	2.12	0.48
1:A:4:PHE:CZ	1:A:199:PRO:HG3	2.48	0.48
1:A:445:GLN:O	1:A:449:GLN:HG2	2.13	0.48
1:A:539:LEU:O	1:A:542:VAL:HB	2.13	0.48
1:B:329:THR:O	1:B:331:VAL:HG23	2.13	0.48
1:A:62:GLU:O	1:B:266:VAL:HG11	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:SER:HB2	1:B:114:ASP:OD2	2.12	0.48
1:B:168:ARG:HH22	1:B:320:THR:HG21	1.78	0.48
1:A:254:LEU:HD12	1:A:284:ARG:O	2.13	0.48
1:A:259:ASN:OD1	1:A:260:ASN:N	2.47	0.48
1:B:152:ILE:HD11	1:B:188:SER:CB	2.43	0.48
1:A:127:ARG:O	1:A:127:ARG:HG2	2.12	0.48
1:B:168:ARG:HH11	1:B:168:ARG:HG2	1.79	0.48
1:B:539:LEU:O	1:B:542:VAL:HB	2.13	0.48
1:A:61:HIS:HE1	1:A:219:ILE:HG13	1.77	0.48
1:A:66:VAL:HA	1:A:69:ILE:HD12	1.96	0.48
1:A:402:LEU:O	1:A:408:LEU:HG	2.14	0.48
1:A:550:GLU:HA	1:A:550:GLU:OE2	2.14	0.48
1:A:250:GLU:CG	1:A:251:THR:HG23	2.41	0.48
1:A:261:LEU:HD23	1:A:302:GLY:C	2.34	0.48
1:B:13:VAL:HG21	1:B:81:ASP:HA	1.95	0.48
1:B:513:SER:HB2	1:B:531:ASN:HB3	1.96	0.48
1:A:475:ARG:HH11	1:A:475:ARG:CB	2.20	0.48
1:A:269:MET:CE	1:A:269:MET:HA	2.44	0.47
1:B:22:ILE:O	1:B:22:ILE:HG22	2.14	0.47
1:B:40:ILE:HD13	1:B:94:ALA:HB2	1.95	0.47
1:A:40:ILE:HD13	1:A:94:ALA:HB2	1.96	0.47
1:A:64:ALA:HA	1:A:65:HIS:HA	1.59	0.47
1:A:69:ILE:HD11	1:A:77:ALA:CB	2.45	0.47
1:A:122:ALA:O	1:A:126:ARG:HG2	2.14	0.47
1:A:269:MET:HE1	1:A:272:ILE:HD12	1.96	0.47
1:B:222:GLU:HB3	1:B:223:PRO:HD2	1.97	0.47
1:B:287:TRP:CZ3	1:B:332:PRO:HD3	2.50	0.47
1:A:109:LYS:NZ	4:A:1554:2HA:O1	2.48	0.47
1:A:193:LEU:HB3	1:B:3:GLN:HE21	1.80	0.47
1:A:537:GLN:HA	1:A:537:GLN:HE21	1.79	0.47
1:A:513:SER:HB2	1:A:531:ASN:HB3	1.95	0.47
1:B:434:VAL:O	1:B:438:ILE:HG13	2.13	0.47
1:A:168:ARG:HB2	1:A:170:TYR:CD1	2.49	0.47
1:B:279:SER:C	1:B:281:LEU:N	2.69	0.47
1:B:269:MET:HE1	1:B:272:ILE:HD12	1.96	0.46
1:B:69:ILE:HD11	1:B:77:ALA:CB	2.45	0.46
1:B:490:ALA:C	1:B:492:PRO:HD3	2.36	0.46
1:A:336:ILE:O	1:A:336:ILE:HD12	2.15	0.46
1:B:477:MET:HB2	1:B:539:LEU:HD12	1.96	0.46
1:B:161:ILE:HD13	1:B:317:ALA:HB3	1.96	0.46
1:B:402:LEU:O	1:B:408:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:C	1:A:49:ASN:H	2.19	0.46
1:B:71:LYS:HG3	1:B:167:GLU:OE2	2.15	0.46
1:B:122:ALA:O	1:B:126:ARG:HG2	2.16	0.46
1:B:395:ALA:HB2	1:B:428:MET:HG2	1.97	0.46
1:A:482:GLN:HB3	1:A:483:PRO:CD	2.43	0.46
1:B:398:GLU:OE2	1:B:423:ARG:NH1	2.49	0.46
1:A:41:VAL:HG12	1:A:69:ILE:HD13	1.97	0.46
1:B:241:VAL:CG1	1:B:281:LEU:HB2	2.46	0.46
1:A:85:SER:HB2	1:A:114:ASP:OD2	2.15	0.46
1:A:228:ILE:HD13	1:A:239:LEU:HD23	1.98	0.46
1:B:193:LEU:HD12	1:B:301:LYS:HE2	1.97	0.45
1:A:3:GLN:HE21	1:B:193:LEU:CB	2.29	0.45
1:B:309:VAL:HG12	1:B:311:GLU:HG2	1.99	0.45
1:B:395:ALA:CB	1:B:424:LEU:HD22	2.39	0.45
1:A:279:SER:C	1:A:281:LEU:N	2.69	0.45
1:A:494:ASN:ND2	1:A:497:ALA:HB2	2.32	0.45
1:A:3:GLN:NE2	1:B:194:SER:HB3	2.31	0.45
1:B:168:ARG:HB2	1:B:170:TYR:CD1	2.50	0.45
1:B:226:SER:OG	1:B:227:VAL:N	2.48	0.45
1:B:269:MET:CE	1:B:269:MET:HA	2.46	0.45
1:A:139:ASP:OD1	1:A:139:ASP:N	2.49	0.45
1:A:398:GLU:OE2	1:A:423:ARG:NH1	2.49	0.45
1:B:152:ILE:O	1:B:154:GLY:N	2.50	0.45
1:A:277:ALA:O	1:A:282:HIS:HB2	2.17	0.45
1:B:353:SER:HB3	1:B:411:ASN:HB2	1.98	0.45
1:A:477:MET:HB2	1:A:539:LEU:HD12	1.98	0.45
1:B:264:VAL:HG21	1:B:269:MET:HE3	1.97	0.45
1:B:340:VAL:HG12	1:B:341:SER:N	2.32	0.45
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.31	0.45
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.73	0.45
1:A:65:HIS:CD2	1:A:159:HIS:HE1	2.35	0.44
1:A:182:ALA:HA	1:A:314:ILE:HD11	1.99	0.44
1:B:125:ALA:HB3	1:B:132:VAL:HG21	2.00	0.44
1:B:476:THR:CG2	1:B:478:ILE:HB	2.47	0.44
1:A:13:VAL:HG21	1:A:81:ASP:HA	1.98	0.44
1:A:241:VAL:CG1	1:A:281:LEU:HB2	2.48	0.44
1:B:343:HIS:O	1:B:343:HIS:CD2	2.70	0.44
1:A:26:TRP:O	1:A:27:ASN:C	2.55	0.44
1:A:264:VAL:HG21	1:A:269:MET:HE3	1.99	0.44
1:B:192:ALA:CB	1:B:217:MET:HE3	2.47	0.44
1:B:489:LEU:HD12	1:B:489:LEU:HA	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG12	1:A:311:GLU:HG2	2.00	0.44
1:B:52:ALA:O	1:B:104:CYS:HA	2.17	0.44
1:B:95:ILE:HG23	1:B:104:CYS:SG	2.58	0.44
1:A:337:THR:HG21	1:B:44:ARG:NH2	2.33	0.44
1:A:264:VAL:HG11	1:A:269:MET:HE3	2.00	0.43
1:A:287:TRP:CZ3	1:A:332:PRO:HD3	2.52	0.43
1:A:476:THR:CG2	1:A:478:ILE:HB	2.47	0.43
1:B:55:SER:O	1:B:77:ALA:HA	2.18	0.43
1:A:55:SER:O	1:A:77:ALA:HA	2.18	0.43
1:A:340:VAL:HG12	1:A:341:SER:N	2.33	0.43
1:A:194:SER:HB3	1:B:3:GLN:HE22	1.83	0.43
1:A:234:ALA:HA	1:A:275:GLU:OE1	2.18	0.43
1:A:207:ARG:NH1	1:A:214:GLU:OE1	2.42	0.43
1:B:182:ALA:HA	1:B:314:ILE:HD11	2.01	0.43
1:A:438:ILE:HD13	1:A:467:TYR:HD1	1.83	0.43
1:B:139:ASP:OD1	1:B:139:ASP:N	2.51	0.43
1:B:373:GLU:O	1:B:389:GLY:HA3	2.19	0.43
1:B:388:THR:CA	2:B:1551:ANP:O1A	2.62	0.43
1:A:397:ARG:HG3	1:A:397:ARG:NH1	2.34	0.43
1:A:236:VAL:O	1:A:240:MET:HG3	2.18	0.43
1:A:372:LEU:O	1:A:373:GLU:C	2.57	0.43
1:B:260:ASN:O	1:B:296:THR:HG22	2.19	0.43
1:B:372:LEU:O	1:B:373:GLU:C	2.56	0.43
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.91	0.43
1:B:372:LEU:HB3	1:B:376:LEU:HG	2.01	0.43
1:B:195:SER:OG	1:B:196:CYS:N	2.52	0.42
1:B:63:PRO:HD2	1:B:294:LEU:O	2.20	0.42
1:A:61:HIS:CE1	1:A:219:ILE:CD1	3.02	0.42
1:A:220:HIS:HB2	1:A:222:GLU:CD	2.40	0.42
1:A:264:VAL:HG12	1:A:268:GLU:HB2	2.01	0.42
1:B:132:VAL:HG12	1:B:133:GLU:N	2.35	0.42
1:B:261:LEU:HD13	1:B:261:LEU:HA	1.80	0.42
1:A:452:ASN:ND2	1:A:452:ASN:H	2.18	0.42
1:B:261:LEU:HG	1:B:300:MET:HE3	2.02	0.42
1:B:438:ILE:HD13	1:B:467:TYR:HD1	1.85	0.42
1:B:482:GLN:HB3	1:B:483:PRO:CD	2.43	0.42
1:A:52:ALA:O	1:A:104:CYS:HA	2.20	0.42
1:A:337:THR:HG21	1:B:44:ARG:HH21	1.83	0.42
1:B:26:TRP:O	1:B:27:ASN:C	2.58	0.42
1:B:234:ALA:HA	1:B:275:GLU:OE1	2.20	0.42
1:A:32:LEU:HD12	1:B:339:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:O	1:A:296:THR:HG22	2.19	0.42
1:A:269:MET:CE	1:A:272:ILE:HD12	2.50	0.42
1:A:353:SER:HB2	1:A:411:ASN:H	1.85	0.42
1:B:228:ILE:HD13	1:B:239:LEU:HD23	2.02	0.42
1:B:261:LEU:HD23	1:B:303:PHE:N	2.35	0.42
1:B:264:VAL:HG12	1:B:268:GLU:HB2	2.00	0.42
1:B:50:ASN:OD1	1:B:169:GLY:HA2	2.20	0.42
1:B:393:ALA:O	1:B:397:ARG:HG2	2.20	0.42
1:A:125:ALA:HB3	1:A:132:VAL:HG21	2.02	0.42
1:B:168:ARG:HG2	1:B:168:ARG:NH1	2.35	0.42
1:A:71:LYS:HG3	1:A:167:GLU:OE2	2.19	0.42
1:B:26:TRP:CH2	1:B:323:GLU:HG2	2.55	0.41
1:B:494:ASN:ND2	1:B:497:ALA:HB2	2.35	0.41
1:A:99:THR:CG2	1:A:104:CYS:HB3	2.48	0.41
1:A:261:LEU:HD13	1:A:261:LEU:HA	1.82	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.88	0.41
1:A:3:GLN:HE22	1:B:194:SER:CB	2.33	0.41
1:B:64:ALA:HA	1:B:65:HIS:HA	1.60	0.41
1:B:269:MET:HE2	1:B:269:MET:HA	2.02	0.41
1:A:221:GLY:O	1:A:222:GLU:C	2.59	0.41
1:A:422:GLU:O	1:A:422:GLU:HG2	2.21	0.41
1:B:4:PHE:CE1	1:B:199:PRO:HG3	2.55	0.41
1:B:142:SER:O	1:B:225:ALA:HB2	2.21	0.41
1:A:21:ILE:C	1:A:23:ALA:H	2.24	0.41
1:A:261:LEU:HG	1:A:300:MET:HE2	2.01	0.41
1:B:239:LEU:O	1:B:239:LEU:HD12	2.20	0.41
1:B:276:LEU:C	1:B:276:LEU:HD23	2.41	0.41
1:A:3:GLN:HE21	1:B:193:LEU:HB3	1.85	0.41
1:A:206:PRO:O	1:A:207:ARG:C	2.57	0.41
1:A:393:ALA:O	1:A:397:ARG:HG2	2.20	0.41
1:B:230:THR:OG1	1:B:231:GLN:N	2.53	0.41
1:B:413:LEU:HB3	1:B:447:LEU:HD13	2.02	0.41
1:A:193:LEU:HD21	1:B:5:PHE:CE2	2.56	0.41
1:B:152:ILE:HD11	1:B:188:SER:HB2	2.01	0.41
1:B:99:THR:CG2	1:B:104:CYS:HB3	2.51	0.41
1:A:72:GLY:HA3	1:A:322:VAL:CG1	2.48	0.41
1:A:132:VAL:HG12	1:A:133:GLU:N	2.36	0.41
1:A:309:VAL:CG1	1:A:311:GLU:HG2	2.51	0.41
1:A:372:LEU:HB3	1:A:376:LEU:HG	2.03	0.41
1:A:434:VAL:O	1:A:438:ILE:HG13	2.21	0.41
1:B:43:ARG:NH2	1:B:71:LYS:CA	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLY:HA3	1:B:322:VAL:CG1	2.48	0.41
1:B:220:HIS:HB2	1:B:222:GLU:CD	2.41	0.41
1:B:343:HIS:O	1:B:343:HIS:CG	2.74	0.41
1:B:468:GLY:O	2:B:1551:ANP:N6	2.54	0.41
1:B:309:VAL:CG1	1:B:311:GLU:HG2	2.51	0.41
1:B:506:ALA:HA	1:B:536:ALA:HB1	2.02	0.41
1:A:31:ARG:O	1:B:338:CYS:HA	2.20	0.40
1:A:95:ILE:HG23	1:A:104:CYS:SG	2.60	0.40
1:A:510:CYS:SG	1:A:529:LEU:HA	2.61	0.40
1:B:236:VAL:O	1:B:240:MET:HG3	2.21	0.40
1:B:359:ALA:HB2	1:B:410:LEU:HD13	2.03	0.40
1:A:259:ASN:HB3	1:A:304:SER:OG	2.21	0.40
1:A:388:THR:HA	2:A:1551:ANP:O1A	2.22	0.40
1:A:413:LEU:HB3	1:A:447:LEU:HD13	2.03	0.40
1:A:65:HIS:HD2	1:A:159:HIS:CE1	2.40	0.40
1:A:194:SER:HB3	1:B:3:GLN:NE2	2.37	0.40

All (1) 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:A:342:SER:CB	1:A:342:SER:CB[3_656]	2.08	0.12

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	533/552 (97%)	459 (86%)	56 (10%)	18 (3%)	3 21
1	B	533/552 (97%)	461 (86%)	56 (10%)	16 (3%)	4 23
All	All	1066/1104 (97%)	920 (86%)	112 (10%)	34 (3%)	4 22

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	153	ALA
1	B	62	GLU
1	B	153	ALA
1	A	48	LYS
1	A	81	ASP
1	A	203	ASP
1	A	283	SER
1	A	373	GLU
1	B	81	ASP
1	B	203	ASP
1	B	283	SER
1	B	373	GLU
1	B	549	SER
1	A	549	SER
1	B	110	ASN
1	A	110	ASN
1	A	195	SER
1	A	347	ARG
1	A	450	GLY
1	B	347	ARG
1	B	450	GLY
1	A	12	LEU
1	B	12	LEU
1	B	195	SER
1	A	22	ILE
1	A	439	PHE
1	B	402	LEU
1	A	205	ALA
1	A	314	ILE
1	B	205	ALA
1	B	314	ILE
1	A	63	PRO
1	B	22	ILE

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	414/425 (97%)	379 (92%)	35 (8%)	10 37
1	B	414/425 (97%)	377 (91%)	37 (9%)	9 34
All	All	828/850 (97%)	756 (91%)	72 (9%)	10 36

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

Mol	Chain	Res	Type
1	A	12	LEU
1	A	39	ARG
1	A	81	ASP
1	A	89	ASP
1	A	112	THR
1	A	114	ASP
1	A	127	ARG
1	A	174	THR
1	A	191	VAL
1	A	200	GLN
1	A	207	ARG
1	A	215	LEU
1	A	231	GLN
1	A	239	LEU
1	A	254	LEU
1	A	345	SER
1	A	349	GLU
1	A	353	SER
1	A	357	LEU
1	A	402	LEU
1	A	406	GLN
1	A	412	ASN
1	A	422	GLU
1	A	425	THR
1	A	427	VAL
1	A	428	MET
1	A	432	SER
1	A	436	MET
1	A	445	GLN
1	A	453	VAL
1	A	481	LEU
1	A	510	CYS
1	A	514	LYS
1	A	537	GLN

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Mol	Chain	Res	Type
1	A	539	LEU
1	B	12	LEU
1	B	39	ARG
1	B	44	ARG
1	B	62	GLU
1	B	81	ASP
1	B	89	ASP
1	B	112	THR
1	B	114	ASP
1	B	133	GLU
1	B	174	THR
1	B	191	VAL
1	B	200	GLN
1	B	215	LEU
1	B	231	GLN
1	B	239	LEU
1	B	254	LEU
1	B	279	SER
1	B	304	SER
1	B	343	HIS
1	B	345	SER
1	B	349	GLU
1	B	357	LEU
1	B	402	LEU
1	B	406	GLN
1	B	412	ASN
1	B	422	GLU
1	B	425	THR
1	B	427	VAL
1	B	428	MET
1	B	436	MET
1	B	445	GLN
1	B	453	VAL
1	B	481	LEU
1	B	510	CYS
1	B	514	LYS
1	B	537	GLN
1	B	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	65	HIS
1	A	96	GLN
1	A	146	ASN
1	A	159	HIS
1	A	406	GLN
1	A	412	ASN
1	A	445	GLN
1	A	537	GLN
1	B	3	GLN
1	B	146	ASN
1	B	159	HIS
1	B	343	HIS
1	B	406	GLN
1	B	412	ASN
1	B	445	GLN
1	B	537	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	2HA	A	1554	1	5,5,5	5.35	1 (20%)	4,5,5	5.35	2 (50%)
2	ANP	B	1551	3	29,33,33	2.96	7 (24%)	31,52,52	1.55	5 (16%)
4	2HA	B	1554	1	5,5,5	5.55	1 (20%)	4,5,5	4.97	2 (50%)
2	ANP	A	1551	3	29,33,33	2.94	7 (24%)	31,52,52	1.82	7 (22%)

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
4	2HA	A	1554	1	-	2/4/4/4	-
2	ANP	B	1551	3	-	3/14/38/38	0/3/3/3
4	2HA	B	1554	1	-	2/4/4/4	-
2	ANP	A	1551	3	-	4/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1554	2HA	O2-C2	12.28	1.43	1.21
4	A	1554	2HA	O2-C2	11.91	1.42	1.21
2	B	1551	ANP	PB-O1B	8.69	1.59	1.46
2	B	1551	ANP	PG-O1G	8.65	1.59	1.46
2	A	1551	ANP	PG-O1G	8.56	1.59	1.46
2	A	1551	ANP	PB-O1B	8.33	1.58	1.46
2	B	1551	ANP	C4-N3	5.93	1.43	1.35
2	A	1551	ANP	C4-N3	5.53	1.43	1.35
2	A	1551	ANP	PG-N3B	4.88	1.76	1.63
2	A	1551	ANP	PB-N3B	4.75	1.75	1.63
2	B	1551	ANP	PG-N3B	4.36	1.74	1.63
2	B	1551	ANP	PB-N3B	4.20	1.74	1.63
2	A	1551	ANP	PA-O1A	2.44	1.59	1.50
2	B	1551	ANP	PA-O1A	2.33	1.58	1.50
2	B	1551	ANP	C2-N3	2.05	1.35	1.32
2	A	1551	ANP	C2-N3	2.02	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1554	2HA	O2-C2-C3	-8.27	107.70	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1554	2HA	O2-C2-C3	-7.78	108.48	120.91
4	A	1554	2HA	O2-C2-C1	-7.24	109.34	120.91
4	B	1554	2HA	O2-C2-C1	-5.44	112.22	120.91
2	A	1551	ANP	C4'-O4'-C1'	-4.92	105.42	109.92
2	A	1551	ANP	O4'-C1'-N9	4.71	114.99	108.75
2	B	1551	ANP	C4-C5-N7	-3.69	105.44	109.34
2	B	1551	ANP	N3-C2-N1	-3.59	123.80	128.67
2	A	1551	ANP	N3-C2-N1	-3.34	124.14	128.67
2	B	1551	ANP	O1B-PB-N3B	-2.67	107.84	111.77
2	B	1551	ANP	C4'-O4'-C1'	2.56	112.27	109.92
2	A	1551	ANP	C4-C5-N7	-2.47	106.72	109.34
2	A	1551	ANP	O3A-PB-N3B	2.47	113.43	106.59
2	A	1551	ANP	O3G-PG-O1G	-2.24	107.82	113.45
2	B	1551	ANP	O3A-PB-N3B	2.22	112.75	106.59
2	A	1551	ANP	N6-C6-N1	2.04	122.70	118.33

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1551	ANP	PG-N3B-PB-O1B
2	A	1551	ANP	PA-O3A-PB-O2B
2	B	1551	ANP	PB-N3B-PG-O1G
4	A	1554	2HA	O1-C1-C2-O2
4	A	1554	2HA	O2-C2-C3-O3
4	B	1554	2HA	O1-C1-C2-O2
4	B	1554	2HA	O2-C2-C3-O3
2	A	1551	ANP	O4'-C4'-C5'-O5'
2	A	1551	ANP	C3'-C4'-C5'-O5'
2	B	1551	ANP	C3'-C4'-C5'-O5'
2	B	1551	ANP	O4'-C4'-C5'-O5'

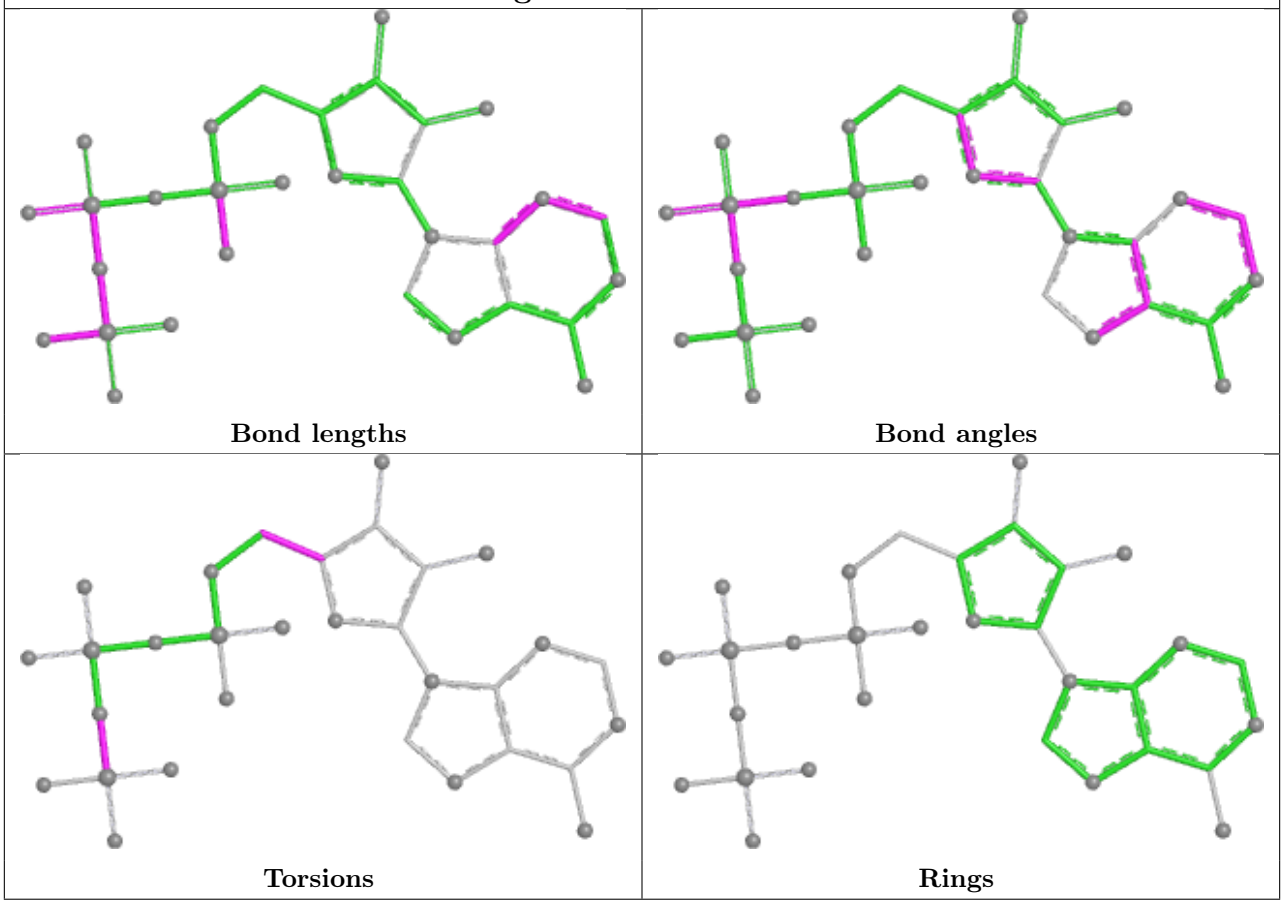
There are no ring outliers.

4 monomers are involved in 11 short contacts:

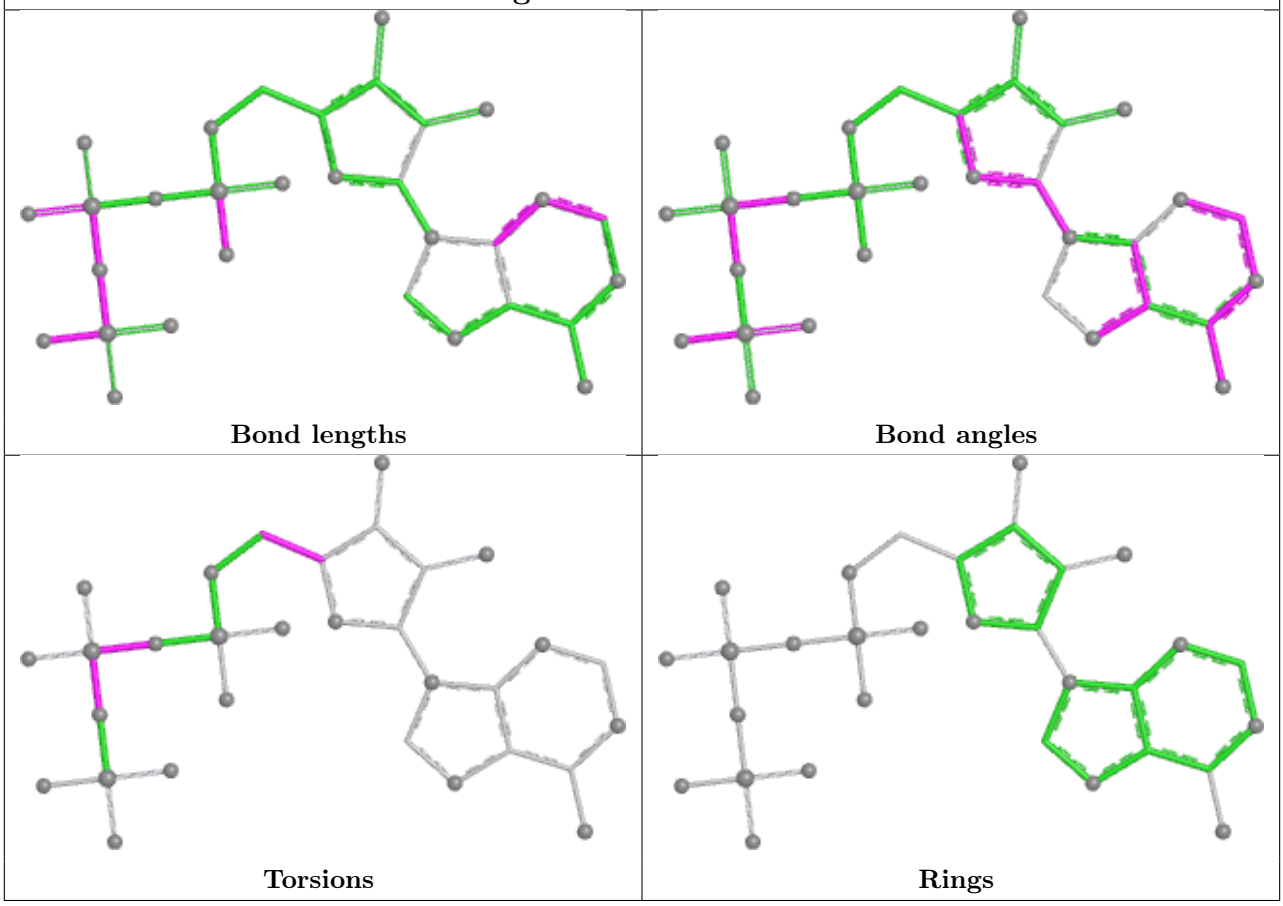
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1554	2HA	1	0
2	B	1551	ANP	4	0
4	B	1554	2HA	1	0
2	A	1551	ANP	5	0

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 1551



Ligand ANP A 1551



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	537/552 (97%)	-0.03	11 (2%)	65	44	14, 86, 114, 146	0
1	B	537/552 (97%)	-0.11	3 (0%)	89	78	14, 90, 113, 139	0
All	All	1074/1104 (97%)	-0.07	14 (1%)	77	59	14, 88, 114, 146	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	LEU	3.9
1	A	347	ARG	3.6
1	A	529	LEU	3.4
1	A	513	SER	3.2
1	B	530	GLY	3.1
1	A	530	GLY	2.9
1	A	293	SER	2.9
1	A	515	ALA	2.5
1	A	337	THR	2.3
1	A	356	ALA	2.2
1	A	296	THR	2.1
1	B	296	THR	2.1
1	A	382	LYS	2.1
1	A	203	ASP	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)

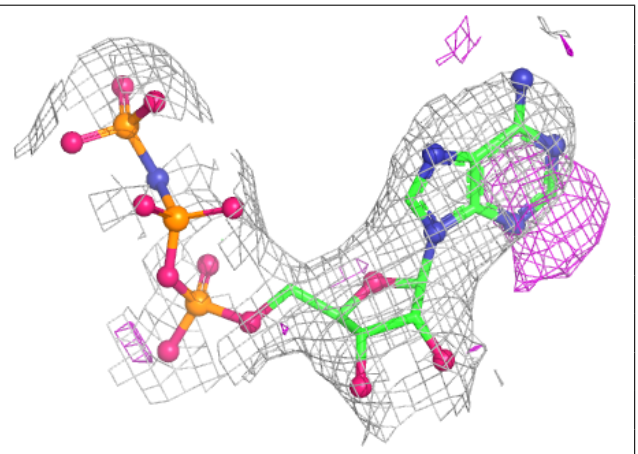
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

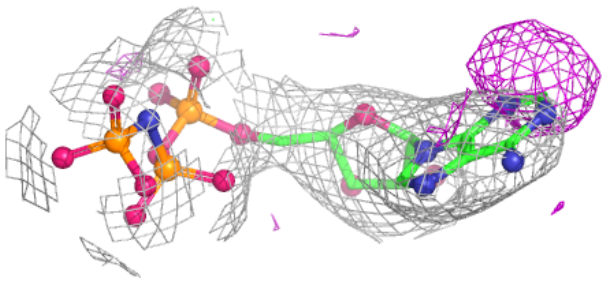
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1553	1/1	0.80	0.19	76,76,76,76	0
3	MG	B	1552	1/1	0.88	0.07	65,65,65,65	0
4	2HA	B	1554	6/6	0.93	0.18	12,16,16,17	0
2	ANP	B	1551	31/31	0.94	0.17	50,57,70,72	0
2	ANP	A	1551	31/31	0.94	0.14	59,64,77,79	0
4	2HA	A	1554	6/6	0.96	0.11	12,15,17,17	0
3	MG	A	1552	1/1	0.96	0.04	90,90,90,90	0
3	MG	B	1553	1/1	0.97	0.07	100,100,100,100	0

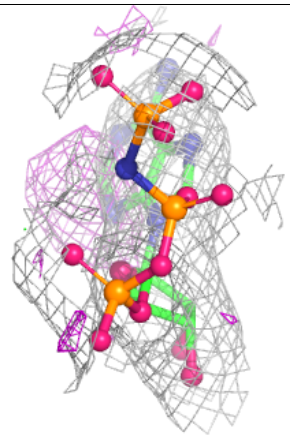
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 1551:

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

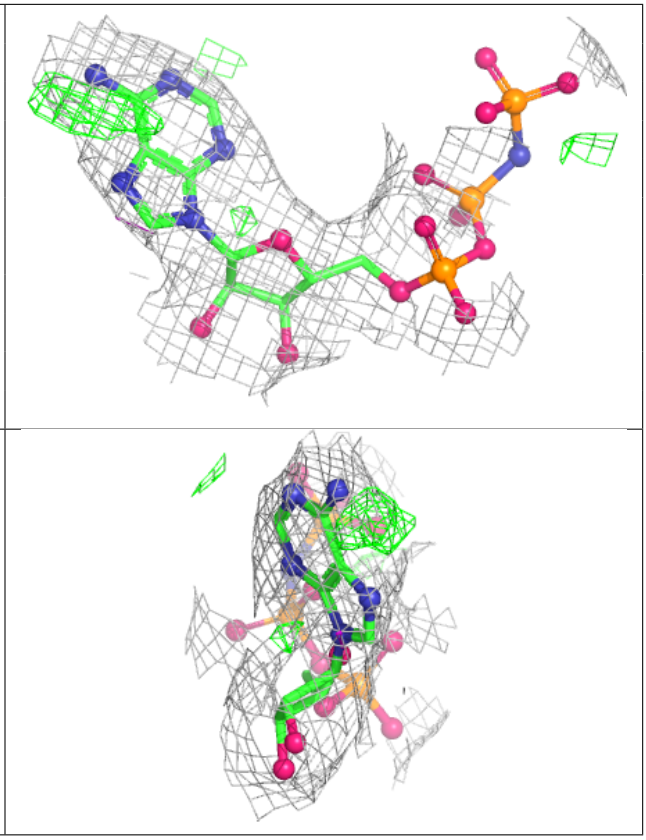






Electron density around ANP A 1551:

$2mF_o$-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.