



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 1UN9 / pdb_00001un9
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

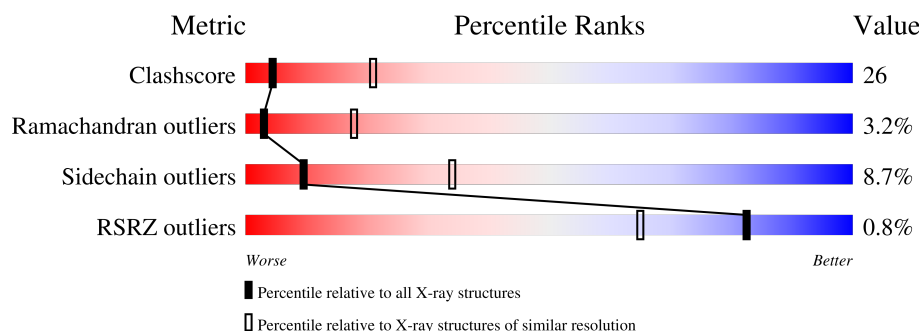
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	% 53% 39% 5% .
1	B	552	% 52% 40% . . .

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.

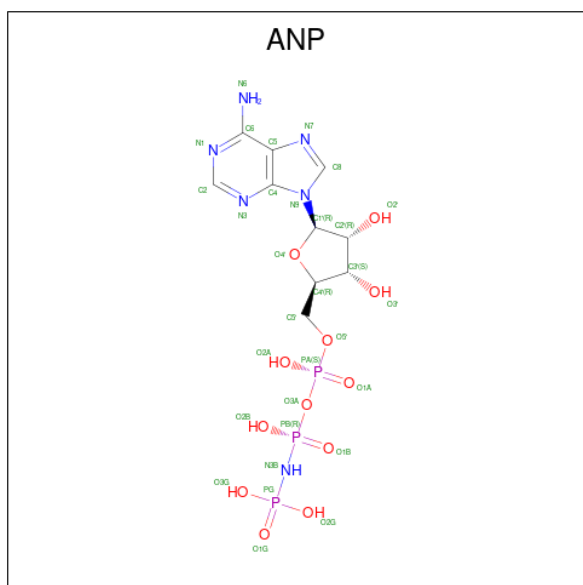
- Molecule 1 is a protein called DIHYDROXYACETONE KINASE.

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

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 (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

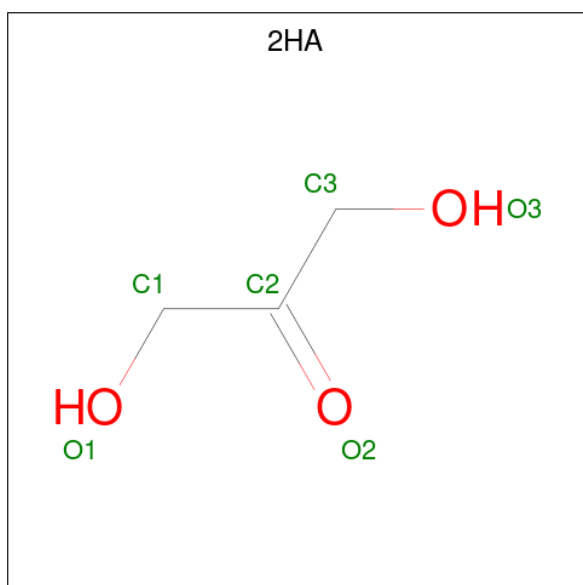


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is Dihydroxyacetone (CCD ID: 2HA) (formula: C₃H₆O₃).



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





4 Data and refinement statistics

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 25.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.1 (25.00-3.10) 93.5 (25.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 2HA

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	0.59	1/4015 (0.0%)	1.11	15/5459 (0.3%)
1	B	0.58	1/4015 (0.0%)	1.10	18/5459 (0.3%)
All	All	0.58	2/8030 (0.0%)	1.10	33/10918 (0.3%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	GLY	N-CA	5.22	1.51	1.45
1	B	210	PRO	N-CD	5.17	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLU	CA-C-N	-20.09	94.73	119.84
1	A	62	GLU	C-N-CA	-20.09	94.73	119.84
1	B	62	GLU	CA-C-N	-18.78	96.37	119.84
1	B	62	GLU	C-N-CA	-18.78	96.37	119.84
1	B	62	GLU	N-CA-C	18.42	150.52	109.81
1	A	62	GLU	N-CA-C	18.38	150.42	109.81
1	A	446	LYS	N-CA-C	-7.41	103.86	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	LYS	N-CA-C	-7.38	103.90	113.12
1	B	98	VAL	N-CA-C	7.12	120.00	113.10
1	A	98	VAL	N-CA-C	6.96	119.85	113.10
1	B	88	VAL	N-CA-C	-6.83	104.11	110.53
1	A	88	VAL	N-CA-C	-6.54	104.11	110.72
1	B	108	VAL	N-CA-C	5.91	117.09	108.53
1	B	74	LEU	N-CA-C	5.84	118.47	110.24
1	B	223	PRO	CB-CA-C	5.79	118.91	111.21
1	B	319	LEU	N-CA-C	5.72	119.08	111.75
1	A	108	VAL	N-CA-C	5.71	116.81	108.53
1	A	319	LEU	N-CA-C	5.71	119.06	111.75
1	A	62	GLU	CB-CA-C	-5.62	99.10	110.17
1	A	74	LEU	N-CA-C	5.40	117.86	110.24
1	A	79	CYS	N-CA-C	5.34	117.44	108.73
1	B	79	CYS	N-CA-C	5.33	117.42	108.73
1	B	62	GLU	C-N-CD	5.31	146.78	125.00
1	B	62	GLU	N-CA-CB	-5.27	101.00	110.37
1	B	429	GLY	N-CA-C	-5.22	104.57	112.41
1	A	220	HIS	CA-CB-CG	-5.19	108.61	113.80
1	B	491	GLN	CA-C-N	5.12	126.24	119.84
1	B	491	GLN	C-N-CA	5.12	126.24	119.84
1	B	70	GLY	N-CA-C	5.11	117.98	111.85
1	B	343	HIS	N-CA-C	5.05	116.92	108.23
1	A	205	ALA	CA-C-N	5.04	124.94	119.85
1	A	205	ALA	C-N-CA	5.04	124.94	119.85
1	A	343	HIS	N-CA-C	5.01	116.85	108.23

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 ⓘ

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	227	1
1	B	3952	0	3978	219	0
2	A	31	0	13	5	0
2	B	31	0	13	3	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	422	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 26.

All (422) 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
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:192:ALA:HB3	1:B:217:MET:HE2	1.56	0.86
1:A:264:VAL:HG11	1:A:269:MET:HE3	1.58	0.86
1:B:264:VAL:HG11	1:B:269:MET:HE3	1.57	0.86
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE2	1:A:269:MET:HA	1.68	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: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:269:MET:HE2	1:B:269:MET:HA	1.71	0.72
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:264:VAL:CG1	1:B:269:MET:HE3	2.21	0.69
1:B:261:LEU:HG	1:B:300:MET:HE2	1.74	0.69
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:A:264:VAL:CG1	1:A:269:MET:HE3	2.24	0.68
1:B:127:ARG:O	1:B:127:ARG:HG2	1.93	0.68
1:A:261:LEU:HG	1:A:300:MET:HE2	1.77	0.66
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:HB2	1:B:302:GLY:O	1.99	0.63
1:A:73:MET:HE1	1:A:327:TRP:CE3	2.34	0.62
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:269:MET:HE1	1:B:303:PHE:HB3	1.81	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:73:MET:HE1	1:B:327:TRP:CE3	2.35	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:A:269:MET:HE2	1:A:272:ILE:HD12	1.83	0.60
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:A:269:MET:HE1	1:A:303:PHE:HB3	1.82	0.59
1:B:65:HIS:NE2	1:B:109:LYS:HE3	2.18	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
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:A:261:LEU:HG	1:A:300:MET:CE	2.33	0.57
1:B:395:ALA:HB2	1:B:428:MET:HE3	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:CB	1:B:269:MET:HE3	2.35	0.57
1:B:261:LEU:HG	1:B:300:MET:CE	2.33	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:B:269:MET:HE2	1:B:272:ILE:HD12	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:A:61:HIS:HA	1:A:296:THR:O	2.05	0.56
1:A:279:SER:C	1:A:281:LEU:H	2.13	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:279:SER:C	1:B:281:LEU:H	2.13	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: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
1:B:261:LEU:HD23	1:B:302:GLY:C	2.33	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: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:464:MET:HE2	1:A:478:ILE:HD11	1.90	0.53
1:A:274:ARG:O	1:A:274:ARG:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD11	1:B:98:VAL:HB	1.90	0.53
1:B:192:ALA:HB3	1:B:217:MET:CE	2.35	0.53
1:A:264:VAL:CB	1:A:269:MET:HE3	2.38	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:B:464:MET:HE2	1:B:478:ILE:HD11	1.91	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:261:LEU:HD23	1:A:302:GLY:C	2.34	0.52
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:A:506:ALA:O	1:A:532:MET:HE2	2.09	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:477:MET:HE3	1:A:539:LEU:HD12	1.91	0.52
1:A:5:PHE:CE2	1:B:193:LEU:HD21	2.45	0.51
1:B:477:MET:HE3	1:B:539:LEU:HD12	1.90	0.51
1:A:207:ARG:HH22	1:A:217:MET:HG3	1.75	0.51
1:B:279:SER:C	1:B:281:LEU:N	2.69	0.51
1:B:413:LEU:HB3	1:B:447:LEU:CD1	2.40	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
1:B:261:LEU:O	1:B:296:THR:HB	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ALA:C	1:B:492:PRO:HD3	2.36	0.51
1:A:400:ALA:O	1:A:403:LEU:HB3	2.11	0.51
1:B:395:ALA:CB	1:B:428:MET:HE3	2.40	0.51
1:B:50:ASN:HB3	1:B:166:ALA:O	2.10	0.51
1:A:47:ASN:C	1:A:49:ASN:H	2.19	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:B:73:MET:HE3	1:B:160:LYS:HD2	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: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:73:MET:HE3	1:A:160:LYS:HD2	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:O	1:B:266:VAL:HG11	2.12	0.48
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:A:279:SER:C	1:A:281:LEU:N	2.69	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:26:TRP:O	1:A:27:ASN:C	2.55	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: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:372:LEU:O	1:A:373:GLU:C	2.57	0.47
1:B:372:LEU:O	1:B:373:GLU:C	2.56	0.47
1:B:506:ALA:O	1:B:532:MET:HE2	2.14	0.47
1:A:220:HIS:HB2	1:A:222:GLU:CD	2.40	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:B:26:TRP:O	1:B:27:ASN:C	2.58	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:69:ILE:HD11	1:B:77:ALA:CB	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:221:GLY:O	1:A:222:GLU:C	2.59	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:276:LEU:C	1:B:276:LEU:HD23	2.41	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:A:490:ALA:C	1:A:492:PRO:HD3	2.41	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:21:ILE:C	1:A:23:ALA:H	2.24	0.46
1:A:85:SER:HB2	1:A:114:ASP:OD2	2.15	0.46
1:A:206:PRO:O	1:A:207:ARG:C	2.57	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:B:220:HIS:HB2	1:B:222:GLU:CD	2.41	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: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: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:73:MET:HE3	1:B:160:LYS:CD	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:OD1	1:A:259:ASN:C	2.61	0.44
1:B:343:HIS:O	1:B:343:HIS:CD2	2.70	0.44
1:A:47:ASN:C	1:A:49:ASN:N	2.74	0.44
1:A:8:GLN:O	1:A:9:ARG:C	2.61	0.44
1:B:489:LEU:HD12	1:B:489:LEU:HA	1.67	0.44
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: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:B:464:MET:HE2	1:B:478:ILE:CD1	2.48	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:73:MET:HE3	1:A:160:LYS:CD	2.49	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:B:346:ALA:O	1:B:347:ARG:C	2.60	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:310:LEU:O	1:B:311:GLU:C	2.61	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:276:LEU:C	1:A:276:LEU:HD23	2.42	0.43
1:A:397:ARG:HG3	1:A:397:ARG:NH1	2.34	0.43
1:A:464:MET:HE2	1:A:478:ILE:CD1	2.48	0.43
1:B:8:GLN:O	1:B:9:ARG:C	2.61	0.43
1:A:236:VAL:O	1:A:240:MET:HG3	2.18	0.43
1:B:260:ASN:O	1:B:296:THR:HG22	2.19	0.43
1:A:7:ASN:CG	1:A:8:GLN:N	2.75	0.43
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.91	0.43
1:B:206:PRO:O	1:B:207:ARG:C	2.62	0.43
1:B:372:LEU:HB3	1:B:376:LEU:HG	2.01	0.43
1:A:274:ARG:HD3	1:A:274:ARG:C	2.44	0.42
1:B:21:ILE:C	1:B:23:ALA:H	2.27	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG12	1:A:268:GLU:HB2	2.01	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: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:310:LEU:O	1:A:311:GLU:C	2.62	0.42
1:A:337:THR:HG21	1:B:44:ARG:HH21	1.83	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
1:A:260:ASN:O	1:A:296:THR:HG22	2.19	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:A:346:ALA:O	1:A:347:ARG:C	2.62	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:A:154:GLY:O	1:A:155:THR:C	2.63	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:B:239:LEU:O	1:B:239:LEU:HD12	2.20	0.41
1:A:3:GLN:HE21	1:B:193:LEU:HB3	1.85	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:A:413:LEU:C	1:A:415:THR:N	2.78	0.41
1:B:132:VAL:HG12	1:B:133:GLU:N	2.35	0.41
1:B:152:ILE:HD11	1:B:188:SER:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:GLN:O	1:B:538:ALA:C	2.64	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:A:537:GLN:O	1:A:538:ALA:C	2.64	0.41
1:B:43:ARG:NH2	1:B:71:LYS:CA	2.82	0.41
1:B:72:GLY:HA3	1:B:322:VAL:CG1	2.48	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:A:448:GLU:C	1:A:450:GLY:H	2.29	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:B:401:SER:C	1:B:403:LEU:N	2.79	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:21:ILE:C	1:A:23:ALA:N	2.79	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

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	533/552 (97%)	459 (86%)	56 (10%)	18 (3%)	3	16
1	B	533/552 (97%)	461 (86%)	56 (10%)	16 (3%)	3	19
All	All	1066/1104 (97%)	920 (86%)	112 (10%)	34 (3%)	3	18

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	314	ILE
1	A	63	PRO
1	B	22	ILE

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	414/425 (97%)	378 (91%)	36 (9%)	9	34
1	B	414/425 (97%)	378 (91%)	36 (9%)	9	34
All	All	828/850 (97%)	756 (91%)	72 (9%)	9	34

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	239	LEU
1	A	244	LEU
1	A	254	LEU
1	A	261	LEU
1	A	345	SER
1	A	349	GLU
1	A	353	SER
1	A	357	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	402	LEU
1	A	406	GLN
1	A	422	GLU
1	A	423	ARG
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	459	THR
1	A	481	LEU
1	A	510	CYS
1	A	537	GLN
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	133	GLU
1	B	174	THR
1	B	191	VAL
1	B	200	GLN
1	B	215	LEU
1	B	239	LEU
1	B	244	LEU
1	B	254	LEU
1	B	261	LEU
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	422	GLU
1	B	423	ARG
1	B	425	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	427	VAL
1	B	428	MET
1	B	436	MET
1	B	445	GLN
1	B	453	VAL
1	B	459	THR
1	B	481	LEU
1	B	510	CYS
1	B	537	GLN
1	B	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	49	ASN
1	A	65	HIS
1	A	146	ASN
1	A	159	HIS
1	A	180	GLN
1	A	208	HIS
1	A	375	HIS
1	A	406	GLN
1	A	412	ASN
1	A	445	GLN
1	A	537	GLN
1	B	3	GLN
1	B	96	GLN
1	B	146	ASN
1	B	159	HIS
1	B	180	GLN
1	B	343	HIS
1	B	375	HIS
1	B	406	GLN
1	B	412	ASN
1	B	445	GLN
1	B	537	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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$
2	ANP	A	1551	3	33,33,33	2.91	11 (33%)	45,52,52	1.68	9 (20%)
4	2HA	B	1554	-	5,5,5	5.55	1 (20%)	4,5,5	4.97	2 (50%)
4	2HA	A	1554	-	5,5,5	5.35	1 (20%)	4,5,5	5.35	2 (50%)
2	ANP	B	1551	3	33,33,33	2.88	11 (33%)	45,52,52	1.83	11 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	1551	3	-	5/18/38/38	0/3/3/3
4	2HA	B	1554	-	-	2/4/4/4	-
4	2HA	A	1554	-	-	2/4/4/4	-
2	ANP	B	1551	3	-	3/18/38/38	0/3/3/3

All (24) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	4.94	1.43	1.34
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	A	1551	ANP	C4-N3	4.65	1.43	1.34
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	C5-C4	4.12	1.46	1.39
2	B	1551	ANP	C8-N7	3.32	1.38	1.31
2	B	1551	ANP	C5-C4	3.30	1.45	1.39
2	A	1551	ANP	C8-N7	3.27	1.38	1.31
2	A	1551	ANP	C4-N9	-2.68	1.32	1.37
2	A	1551	ANP	C5-N7	-2.68	1.34	1.39
2	B	1551	ANP	C5-C6	2.64	1.48	1.41
2	B	1551	ANP	C5-N7	-2.63	1.34	1.39
2	B	1551	ANP	C4-N9	-2.51	1.32	1.37
2	A	1551	ANP	PA-O1A	2.44	1.59	1.50
2	A	1551	ANP	C5-C6	2.35	1.47	1.41
2	B	1551	ANP	PA-O1A	2.33	1.58	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1554	2HA	O2-C2-C3	-8.27	107.70	120.91
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	B	1551	ANP	C5-C4-N9	4.57	110.79	105.81
2	B	1551	ANP	C4-C5-N7	-4.50	105.44	110.58
2	B	1551	ANP	C5-C4-N3	-3.97	121.25	126.72
2	A	1551	ANP	C5-C4-N9	3.96	110.12	105.81
2	B	1551	ANP	C6-C5-N7	3.76	139.35	132.09
2	A	1551	ANP	O4'-C1'-N9	3.59	114.99	108.09
2	A	1551	ANP	C4-C5-N7	-3.37	106.72	110.58
2	A	1551	ANP	C5-C4-N3	-3.23	122.27	126.72
2	B	1551	ANP	N3-C2-N1	-3.16	123.80	128.58
2	A	1551	ANP	N3-C2-N1	-2.94	124.14	128.58
2	A	1551	ANP	C2-N1-C6	2.86	123.42	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1551	ANP	C6-C5-N7	2.85	137.58	132.09
2	B	1551	ANP	O1B-PB-N3B	-2.67	107.84	111.77
2	B	1551	ANP	C3'-C2'-C1'	2.64	106.46	101.46
2	A	1551	ANP	O3A-PB-N3B	2.47	113.43	106.59
2	B	1551	ANP	C2-N3-C4	2.45	117.82	111.83
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	B	1551	ANP	C2-N1-C6	2.02	122.05	118.73
2	B	1551	ANP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (12) 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'
2	A	1551	ANP	O4'-C1'-N9-C8

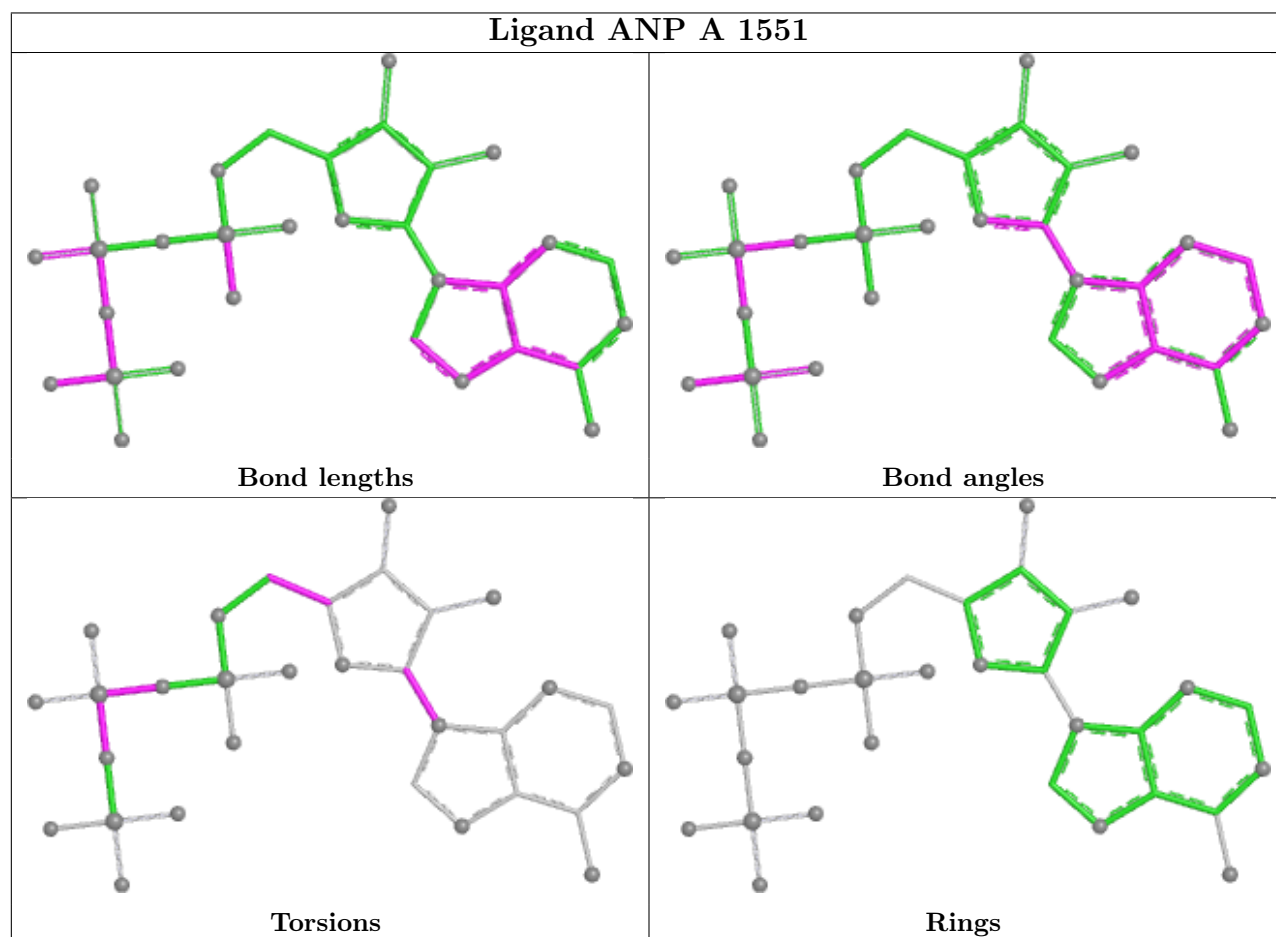
There are no ring outliers.

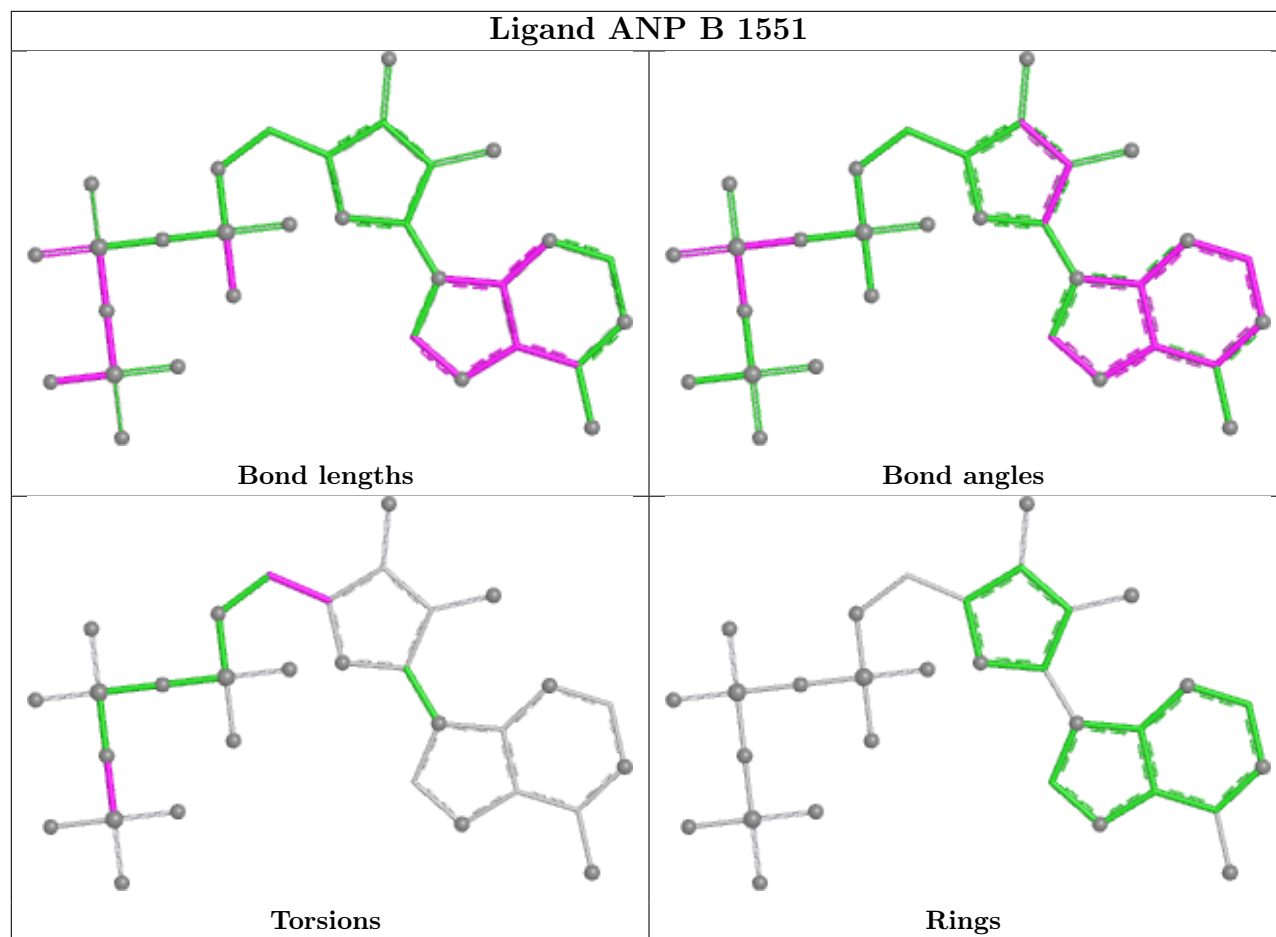
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1551	ANP	5	0
4	B	1554	2HA	1	0
4	A	1554	2HA	1	0
2	B	1551	ANP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.09	5 (0%)	81 63	14, 86, 114, 146	0
1	B	537/552 (97%)	0.17	4 (0%)	84 68	14, 90, 113, 139	0
All	All	1074/1104 (97%)	0.13	9 (0%)	82 65	14, 88, 114, 146	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	GLY	3.3
1	B	70	GLY	3.2
1	A	70	GLY	2.6
1	A	529	LEU	2.6
1	A	62	GLU	2.5
1	A	219	ILE	2.4
1	B	68	PHE	2.4
1	A	453	VAL	2.1
1	B	66	VAL	2.1

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 oligosaccharides in this entry.

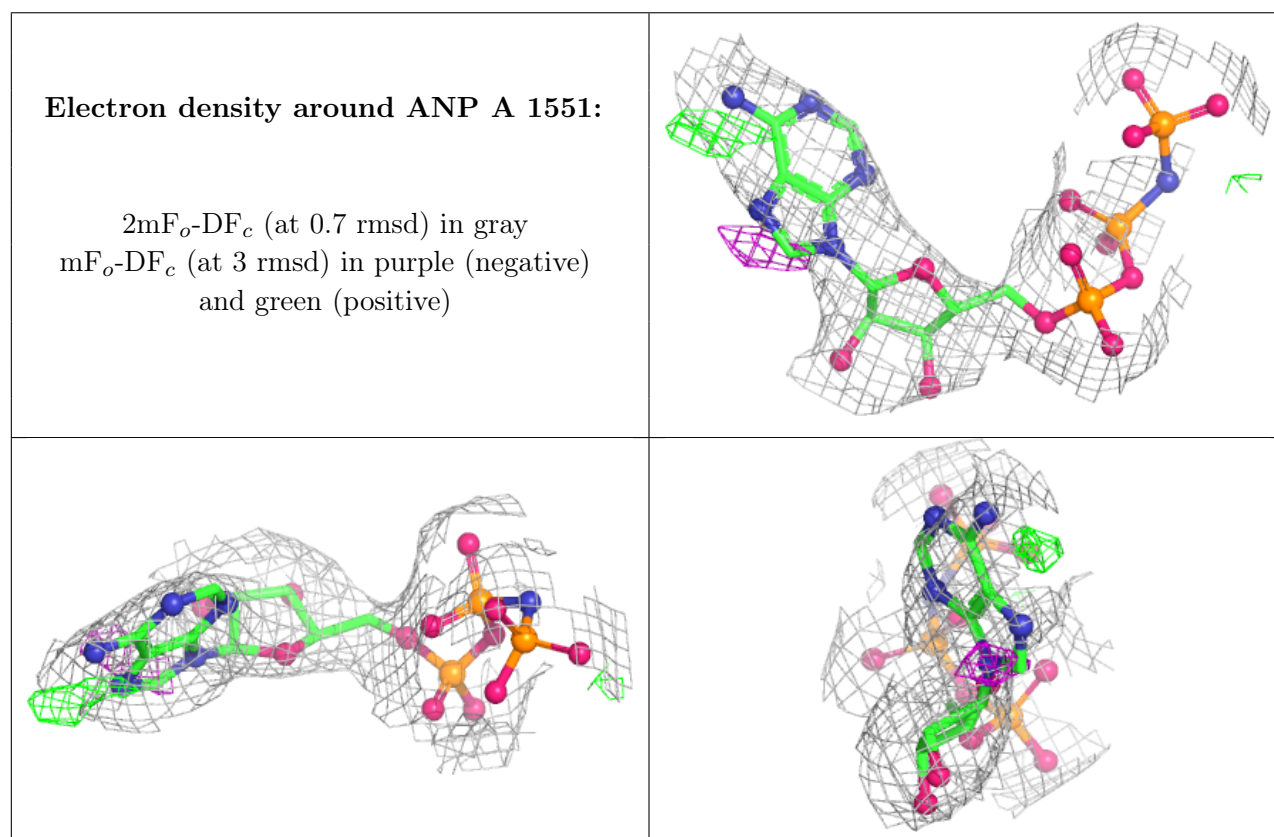
6.4 Ligands [i](#)

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.

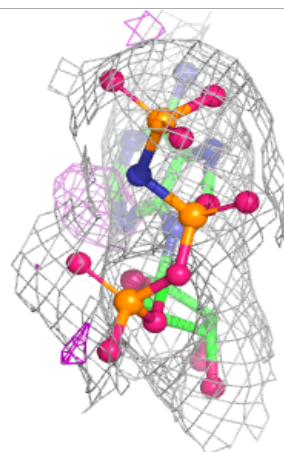
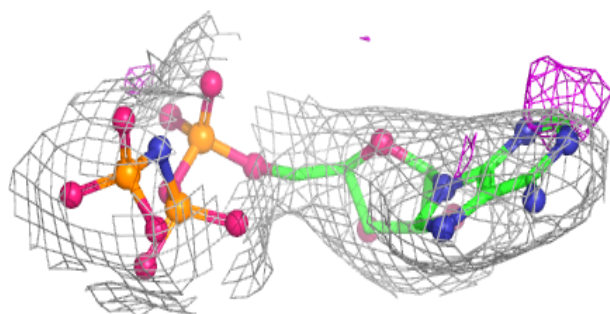
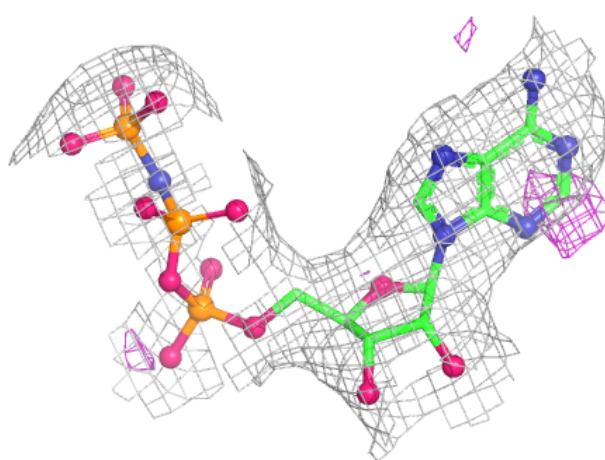
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	1553	1/1	0.77	0.09	76,76,76,76	0
3	MG	B	1553	1/1	0.89	0.10	100,100,100,100	0
4	2HA	B	1554	6/6	0.90	0.13	12,16,16,17	0
2	ANP	A	1551	31/31	0.92	0.09	59,64,77,79	0
4	2HA	A	1554	6/6	0.93	0.12	12,15,17,17	0
3	MG	A	1552	1/1	0.93	0.05	90,90,90,90	0
2	ANP	B	1551	31/31	0.94	0.07	50,57,70,72	0
3	MG	B	1552	1/1	0.99	0.05	65,65,65,65	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)



6.5 Other polymers [i](#)

There are no such residues in this entry.