



## Full wwPDB X-ray Structure Validation Report

Dec 8, 2023 – 03:27 am GMT

PDB ID : 2VWB  
Title : Structure of the archaeal Kae1-Bud32 fusion protein MJ1130: a model for the eukaryotic EKC-KEOPS subcomplex involved in transcription and telomere homeostasis.  
Authors : Hecker, A.; Lopreiato, R.; Graille, M.; Collinet, B.; Forterre, P.; Domenico, L.; van Tilbeurgh, H.  
Deposited on : 2008-06-20  
Resolution : 3.05 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](mailto: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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

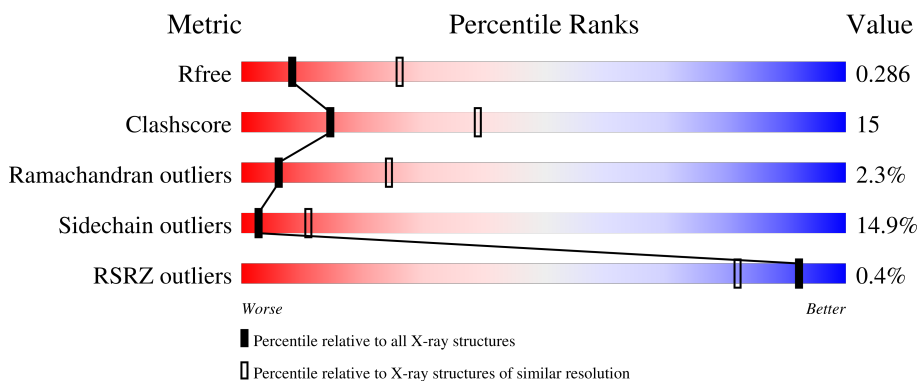
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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  $\geq 3$ , 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	535	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 62%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 62%; width: 30%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 92%; width: 5%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 97%; width: 5%; height: 10px; background-color: grey;"></div> </div> </div>
1	B	535	<div style="display: flex; align-items: center;"> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 56%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 56%; width: 33%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 89%; width: 6%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 95%; width: 5%; height: 10px; background-color: grey;"></div> </div> </div>

## 2 Entry composition [i](#)

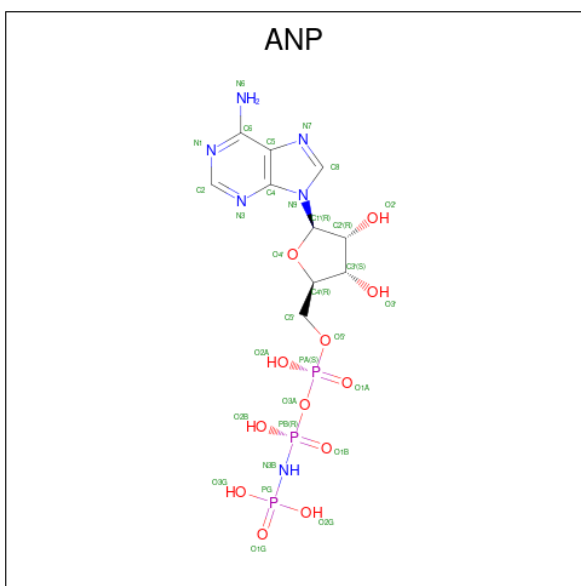
There are 2 unique types of molecules in this entry. The entry contains 8210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	Total 4125	C 2636	N 698	O 770	S 21	0	0	0
1	B	507	Total 4023	C 2568	N 680	O 754	S 21	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

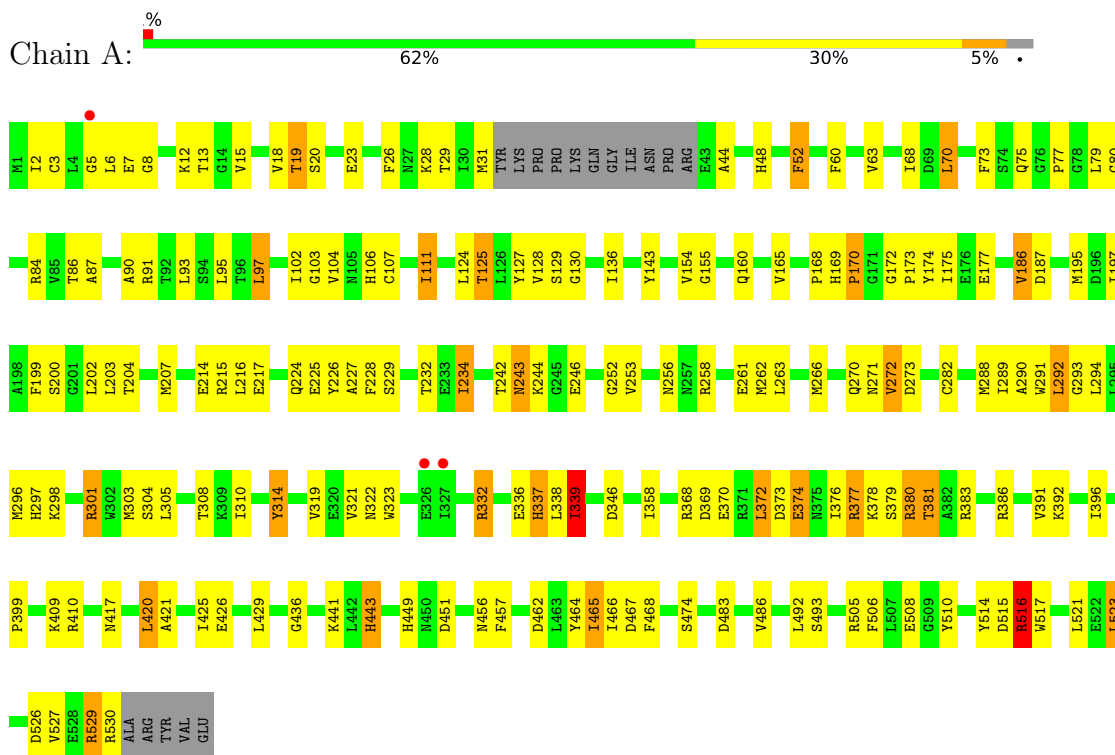


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

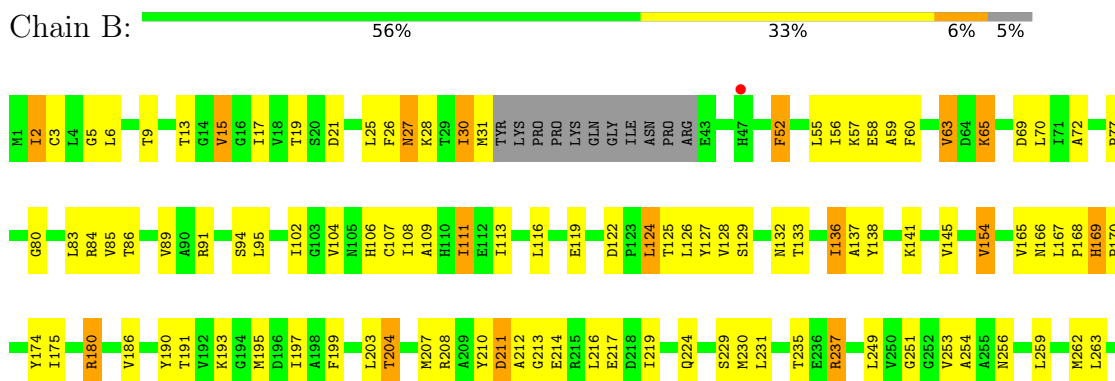
### 3 Residue-property plots [i](#)

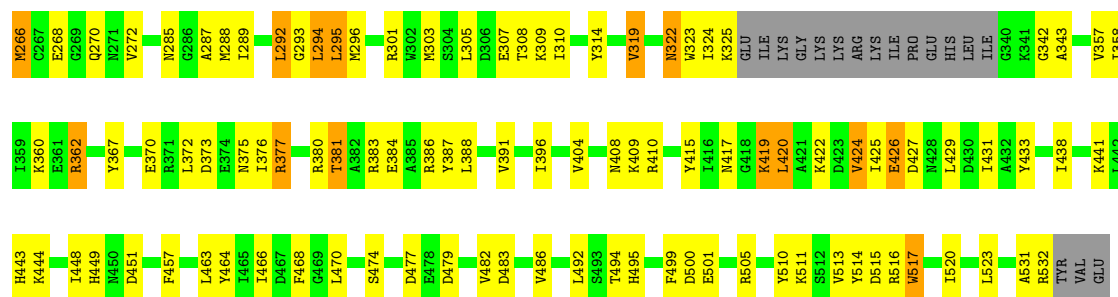
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE



#### • Molecule 1: PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.42Å 148.95Å 65.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.05 19.95 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.95-3.05) 94.4 (19.95-3.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.04Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.301 0.210 , 0.286	Depositor DCC
$R_{free}$ test set	1319 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.010 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/4199	0.70	1/5660 (0.0%)
1	B	0.54	0/4094	0.72	1/5520 (0.0%)
All	All	0.54	0/8293	0.71	2/11180 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	124	LEU	CA-CB-CG	5.87	128.80	115.30
1	B	124	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	HIS	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	4125	0	4181	122	0
1	B	4023	0	4060	131	0
2	A	31	0	13	2	0
2	B	31	0	13	1	0
All	All	8210	0	8267	252	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 15.

All (252) 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:516:ARG:HH11	1:A:516:ARG:HG2	1.13	1.13
1:B:104:VAL:HG13	1:B:292:LEU:HD12	1.34	1.08
1:A:242:THR:HG21	1:A:244:LYS:HG2	1.37	1.06
1:A:242:THR:CG2	1:A:244:LYS:HG2	1.90	1.01
1:A:107:CYS:HG	1:A:127:TYR:HE2	1.09	0.99
1:B:449:HIS:HD2	1:B:451:ASP:H	1.12	0.93
1:B:108:ILE:HD12	1:B:319:VAL:HG11	1.50	0.91
1:A:516:ARG:HG2	1:A:516:ARG:NH1	1.76	0.88
1:B:108:ILE:CD1	1:B:319:VAL:HG11	2.04	0.87
1:B:107:CYS:HG	1:B:127:TYR:HE2	0.84	0.84
1:B:285:ASN:ND2	1:B:288:MET:H	1.74	0.84
1:A:449:HIS:HE1	1:A:467:ASP:O	1.59	0.84
1:B:107:CYS:SG	1:B:127:TYR:HE2	2.02	0.82
1:B:377:ARG:O	1:B:381:THR:HG23	1.80	0.81
1:A:242:THR:HG21	1:A:244:LYS:CG	2.12	0.79
1:A:104:VAL:HG13	1:A:292:LEU:HD12	1.64	0.79
1:B:104:VAL:HG13	1:B:292:LEU:CD1	2.12	0.78
1:B:107:CYS:SG	1:B:127:TYR:CE2	2.75	0.77
1:B:128:VAL:O	1:B:251:GLY:HA3	1.83	0.77
1:B:195:MET:SD	1:B:237:ARG:HD2	2.26	0.76
1:B:449:HIS:CD2	1:B:451:ASP:H	2.02	0.75
1:B:104:VAL:HG22	1:B:296:MET:CE	2.16	0.75
1:A:258:ARG:HH21	1:A:261:GLU:HG2	1.51	0.74
1:A:516:ARG:HH11	1:A:516:ARG:CG	1.96	0.74
1:B:433:TYR:HB2	1:B:505:ARG:HG3	1.70	0.74
1:B:104:VAL:HG22	1:B:296:MET:HE1	1.68	0.73
1:A:195:MET:O	1:A:234:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:HD21	1:B:288:MET:H	1.37	0.73
1:A:129:SER:HA	1:A:253:VAL:HG23	1.72	0.72
1:B:104:VAL:CG1	1:B:292:LEU:HD12	2.17	0.72
1:A:87:ALA:HB2	1:A:310:ILE:HD11	1.73	0.71
1:A:336:GLU:O	1:A:338:LEU:N	2.21	0.71
1:B:449:HIS:HD2	1:B:451:ASP:N	1.88	0.71
1:B:477:ASP:OD1	1:B:516:ARG:NH1	2.23	0.70
1:A:449:HIS:HD2	1:A:451:ASP:H	1.39	0.70
1:B:193:LYS:HZ3	1:B:482:VAL:HG21	1.56	0.70
1:B:154:VAL:HG13	1:B:199:PHE:CZ	2.27	0.69
1:A:456:ASN:ND2	1:A:467:ASP:HB3	2.08	0.69
1:A:168:PRO:HB2	1:A:174:TYR:CE1	2.28	0.69
1:A:106:HIS:NE2	2:A:1531:ANP:O1G	2.21	0.69
1:B:52:PHE:O	1:B:56:ILE:HG13	1.93	0.68
1:B:193:LYS:NZ	1:B:482:VAL:HG21	2.09	0.67
1:A:242:THR:HG22	1:A:244:LYS:HG2	1.76	0.67
1:B:77:PRO:HD2	1:B:106:HIS:HB3	1.75	0.66
1:A:243:ASN:HD22	1:A:243:ASN:H	1.44	0.65
1:B:136:ILE:HG22	1:B:145:VAL:HA	1.79	0.65
1:A:373:ASP:O	1:A:377:ARG:HG2	1.97	0.65
1:A:380:ARG:HH21	1:A:380:ARG:CG	2.10	0.65
1:B:91:ARG:NH1	1:B:308:THR:O	2.30	0.65
1:B:17:ILE:HD11	1:B:59:ALA:HB1	1.78	0.64
1:B:95:LEU:HD21	1:B:305:LEU:HD11	1.79	0.64
1:A:107:CYS:SG	1:A:127:TYR:HE2	2.17	0.64
1:A:229:SER:HA	1:A:262:MET:HE3	1.80	0.63
1:B:531:ALA:O	1:B:532:ARG:HB2	1.98	0.63
1:A:457:PHE:CE1	1:A:465:ILE:HG23	2.34	0.63
1:A:336:GLU:C	1:A:338:LEU:H	2.03	0.62
1:A:372:LEU:HD22	1:A:376:ILE:HD11	1.79	0.62
1:A:172:GLY:O	1:A:175:ILE:HG13	1.99	0.62
1:A:374:GLU:O	1:A:378:LYS:HB2	1.99	0.62
1:B:19:THR:HG22	1:B:21:ASP:H	1.64	0.62
1:B:180:ARG:HB2	1:B:180:ARG:HH11	1.65	0.62
1:B:441:LYS:HG3	1:B:513:VAL:HG11	1.81	0.62
1:A:449:HIS:CE1	1:A:467:ASP:O	2.49	0.61
1:A:204:THR:HA	1:A:207:MET:HE2	1.82	0.61
1:A:271:ASN:HB2	1:B:307:GLU:OE1	2.01	0.61
1:B:169:HIS:O	1:B:169:HIS:ND1	2.33	0.61
1:A:252:GLY:HA3	2:A:1531:ANP:O5'	2.02	0.60
1:A:232:THR:OG1	1:A:262:MET:HE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:MET:HA	1:B:307:GLU:OE2	2.01	0.60
1:B:408:ASN:HB3	1:B:410:ARG:HE	1.64	0.60
1:A:232:THR:OG1	1:A:262:MET:CE	2.50	0.59
1:A:246:GLU:HA	1:A:272:VAL:HG23	1.84	0.58
1:B:429:LEU:HD23	1:B:505:ARG:NH2	2.18	0.58
1:A:70:LEU:HD11	1:A:297:HIS:CG	2.39	0.58
1:A:483:ASP:O	1:A:486:VAL:HG22	2.03	0.58
1:A:391:VAL:HG11	1:A:465:ILE:HD11	1.86	0.57
1:A:19:THR:OG1	1:A:23:GLU:HB3	2.04	0.57
1:B:108:ILE:CD1	1:B:319:VAL:CG1	2.78	0.57
1:B:322:ASN:HD22	1:B:323:TRP:HE3	1.52	0.57
1:B:109:ALA:O	1:B:288:MET:HB2	2.05	0.56
1:B:214:GLU:HB3	1:B:219:ILE:HD11	1.87	0.56
1:A:175:ILE:CD1	1:A:224:GLN:HE21	2.17	0.56
1:A:165:VAL:HG12	1:A:165:VAL:O	2.05	0.56
1:B:322:ASN:ND2	1:B:323:TRP:HE3	2.04	0.55
1:B:373:ASP:O	1:B:377:ARG:HG3	2.06	0.55
1:B:102:ILE:HG22	1:B:303:MET:HG3	1.88	0.55
1:A:52:PHE:CZ	1:A:86:THR:HG23	2.41	0.55
1:A:73:PHE:HZ	1:A:308:THR:HB	1.71	0.55
1:B:415:TYR:HE2	1:B:417:ASN:HD22	1.54	0.55
1:B:391:VAL:HG13	1:B:396:ILE:HB	1.89	0.54
1:B:249:LEU:HD21	1:B:254:ALA:HA	1.90	0.54
1:B:457:PHE:HB3	1:B:463:LEU:HD11	1.89	0.54
1:A:443:HIS:HD2	1:A:510:TYR:OH	1.90	0.54
1:A:288:MET:HG3	1:A:289:ILE:HD12	1.90	0.54
1:B:124:LEU:HA	1:B:137:ALA:HB2	1.90	0.54
1:A:523:LEU:O	1:A:527:VAL:HG23	2.07	0.54
1:B:107:CYS:O	1:B:111:ILE:HG23	2.08	0.53
1:A:60:PHE:HA	1:A:63:VAL:O	2.09	0.53
1:B:285:ASN:HD21	1:B:288:MET:N	2.03	0.53
1:B:60:PHE:HA	1:B:63:VAL:O	2.08	0.53
1:A:229:SER:HA	1:A:262:MET:CE	2.37	0.53
1:B:127:TYR:CE2	1:B:132:ASN:ND2	2.77	0.52
1:B:373:ASP:O	1:B:377:ARG:CG	2.57	0.52
1:A:215:ARG:NH1	1:A:217:GLU:HB2	2.24	0.52
1:A:396:ILE:HD11	1:A:441:LYS:HB2	1.92	0.52
1:A:380:ARG:HH21	1:A:380:ARG:HG3	1.74	0.52
1:A:102:ILE:HD11	1:A:293:GLY:HA2	1.92	0.52
1:A:242:THR:O	1:A:332:ARG:NH2	2.43	0.52
1:B:3:CYS:HB3	1:B:294:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HB3	1:B:310:ILE:HD12	1.92	0.51
1:B:108:ILE:HD11	1:B:319:VAL:CG1	2.39	0.51
1:B:126:LEU:HD13	1:B:235:THR:OG1	2.11	0.51
1:B:443:HIS:HD2	1:B:510:TYR:OH	1.93	0.51
1:B:26:PHE:O	1:B:27:ASN:HB3	2.10	0.51
1:B:420:LEU:HD13	1:B:422:LYS:HB3	1.92	0.51
1:B:168:PRO:HB2	1:B:170:PRO:HD2	1.92	0.51
1:B:165:VAL:HG13	1:B:210:TYR:CZ	2.46	0.51
1:B:106:HIS:NE2	2:B:1533:ANP:O1G	2.43	0.50
1:B:204:THR:HA	1:B:207:MET:HE2	1.93	0.50
1:B:457:PHE:HA	1:B:464:TYR:O	2.11	0.50
1:A:160:GLN:NE2	1:A:203:LEU:HD21	2.27	0.50
1:B:285:ASN:ND2	1:B:288:MET:N	2.52	0.50
1:A:232:THR:HG23	1:A:263:LEU:HD23	1.93	0.50
1:A:44:ALA:O	1:A:48:HIS:HD2	1.95	0.50
1:A:12:LYS:HG3	1:A:31:MET:HG2	1.94	0.49
1:A:338:LEU:HG	1:A:339:ILE:HD12	1.93	0.49
1:A:7:GLU:HB2	1:A:289:ILE:HD13	1.94	0.49
1:B:224:GLN:HE22	1:B:256:ASN:ND2	2.09	0.49
1:A:294:LEU:O	1:A:298:LYS:HB2	2.12	0.49
1:A:130:GLY:HA2	1:A:155:GLY:HA3	1.94	0.49
1:B:211:ASP:C	1:B:213:GLY:H	2.16	0.49
1:A:102:ILE:HG22	1:A:303:MET:HB2	1.94	0.49
1:A:111:ILE:HD11	1:A:143:TYR:OH	2.13	0.49
1:A:73:PHE:CZ	1:A:308:THR:HB	2.48	0.48
1:B:113:ILE:HD13	1:B:288:MET:HA	1.95	0.48
1:B:449:HIS:O	1:B:483:ASP:OD2	2.31	0.48
1:A:77:PRO:HD2	1:A:106:HIS:HB3	1.95	0.48
1:A:186:VAL:HG11	1:A:214:GLU:HG2	1.95	0.48
1:A:301:ARG:HH12	1:A:322:ASN:ND2	2.11	0.48
1:A:436:GLY:HA2	1:A:506:PHE:CE1	2.49	0.48
1:A:104:VAL:HG13	1:A:292:LEU:CD1	2.40	0.47
1:B:126:LEU:HD11	1:B:231:LEU:HD22	1.95	0.47
1:B:448:ILE:HG12	1:B:479:ASP:HB3	1.95	0.47
1:B:190:TYR:CE1	1:B:230:MET:HG3	2.49	0.47
1:B:377:ARG:HB2	1:B:409:LYS:HG2	1.97	0.47
1:A:242:THR:HG22	1:A:243:ASN:N	2.29	0.47
1:A:377:ARG:HB2	1:A:409:LYS:HG2	1.96	0.47
1:A:75:GLN:NE2	1:A:103:GLY:HA3	2.28	0.47
1:A:225:GLU:HB3	1:A:372:LEU:HD12	1.97	0.47
1:A:368:ARG:HG3	1:A:373:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HD2	1:B:58:GLU:OE1	2.15	0.47
1:B:126:LEU:HD23	1:B:249:LEU:HD13	1.95	0.47
1:B:128:VAL:HG23	1:B:253:VAL:HB	1.96	0.47
1:B:362:ARG:HD2	1:B:381:THR:HG22	1.96	0.47
1:B:5:GLY:HA2	1:B:72:ALA:O	2.15	0.47
1:B:511:LYS:HG2	1:B:517:TRP:CD2	2.50	0.47
1:B:342:GLY:O	1:B:343:ALA:HB3	2.15	0.47
1:B:375:ASN:N	1:B:375:ASN:HD22	2.13	0.47
1:A:102:ILE:HD11	1:A:293:GLY:CA	2.45	0.46
1:B:52:PHE:CZ	1:B:86:THR:HG23	2.50	0.46
1:A:170:PRO:O	1:A:173:PRO:HD2	2.15	0.46
1:B:91:ARG:HD2	1:B:308:THR:OG1	2.16	0.46
1:B:203:LEU:O	1:B:207:MET:HG3	2.16	0.46
1:A:336:GLU:C	1:A:338:LEU:N	2.68	0.46
1:B:396:ILE:HG23	1:B:438:ILE:HG12	1.97	0.46
1:A:95:LEU:C	1:A:97:LEU:H	2.20	0.45
1:B:285:ASN:HD22	1:B:287:ALA:HB3	1.82	0.45
1:A:87:ALA:O	1:A:91:ARG:HB2	2.17	0.45
1:A:380:ARG:CG	1:A:380:ARG:NH2	2.77	0.45
1:B:84:ARG:HH22	1:B:309:LYS:NZ	2.13	0.45
1:A:199:PHE:O	1:A:200:SER:C	2.55	0.45
1:B:288:MET:HG3	1:B:289:ILE:HD12	1.98	0.45
1:A:379:SER:O	1:A:383:ARG:HG3	2.16	0.45
1:A:420:LEU:O	1:A:421:ALA:C	2.55	0.45
1:A:52:PHE:HZ	1:A:86:THR:HG23	1.81	0.45
1:A:321:VAL:HA	1:A:323:TRP:CZ3	2.51	0.45
1:B:180:ARG:HB2	1:B:180:ARG:NH1	2.32	0.45
1:B:424:VAL:HG23	1:B:431:ILE:HD13	1.98	0.45
1:A:165:VAL:O	1:A:165:VAL:CG1	2.65	0.45
1:B:65:LYS:H	1:B:65:LYS:HG2	1.56	0.45
1:A:292:LEU:HD13	1:A:296:MET:HE2	1.98	0.45
1:A:339:ILE:H	1:A:339:ILE:HG13	1.44	0.45
1:B:85:VAL:O	1:B:89:VAL:HG23	2.17	0.45
1:B:2:ILE:HD11	1:B:17:ILE:CG2	2.47	0.44
1:B:169:HIS:N	1:B:170:PRO:CD	2.80	0.44
1:B:384:GLU:O	1:B:388:LEU:HG	2.17	0.44
1:B:429:LEU:HD23	1:B:505:ARG:HH21	1.83	0.44
1:B:444:LYS:HA	1:B:514:TYR:CE2	2.53	0.44
1:B:266:MET:HB2	1:B:367:TYR:CD1	2.53	0.44
1:B:154:VAL:HG13	1:B:199:PHE:CE2	2.53	0.44
1:A:224:GLN:HE22	1:A:256:ASN:HD21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:HB3	1:A:262:MET:HE2	1.76	0.44
1:A:301:ARG:NH1	1:A:322:ASN:ND2	2.65	0.44
1:A:409:LYS:HD2	1:A:409:LYS:N	2.33	0.44
1:B:270:GLN:HE22	1:B:342:GLY:H	1.66	0.44
1:B:482:VAL:O	1:B:486:VAL:HG13	2.17	0.43
1:B:516:ARG:O	1:B:520:ILE:HD12	2.17	0.43
1:A:6:LEU:HD22	1:A:90:ALA:HB2	1.99	0.43
1:A:243:ASN:HD22	1:A:243:ASN:N	2.13	0.43
1:B:295:LEU:HD12	1:B:323:TRP:HB2	2.00	0.43
1:B:448:ILE:HD13	1:B:474:SER:HB3	2.00	0.43
1:A:204:THR:HA	1:A:207:MET:CE	2.46	0.43
1:A:18:VAL:HG22	1:A:290:ALA:HB1	2.00	0.43
1:B:128:VAL:HG12	1:B:133:THR:HG23	2.00	0.43
1:B:229:SER:HA	1:B:262:MET:CE	2.48	0.43
1:B:511:LYS:HG2	1:B:517:TRP:CG	2.53	0.43
1:A:104:VAL:HG22	1:A:296:MET:CE	2.48	0.43
1:A:111:ILE:HB	1:A:125:THR:HG21	1.99	0.43
1:B:262:MET:CE	1:B:367:TYR:CD2	3.02	0.43
1:B:383:ARG:O	1:B:387:TYR:HD2	2.01	0.43
1:B:494:THR:C	1:B:495:HIS:CD2	2.92	0.43
1:B:293:GLY:O	1:B:294:LEU:C	2.56	0.43
1:A:381:THR:HG21	1:A:409:LYS:O	2.19	0.43
1:A:457:PHE:HA	1:A:464:TYR:O	2.19	0.43
1:A:175:ILE:HD12	1:A:224:GLN:NE2	2.34	0.42
1:A:70:LEU:HD11	1:A:297:HIS:CD2	2.53	0.42
1:A:200:SER:O	1:A:204:THR:HG23	2.19	0.42
1:A:457:PHE:HE1	1:A:465:ILE:HG23	1.82	0.42
1:B:186:VAL:HG11	1:B:214:GLU:HG2	2.01	0.42
1:A:102:ILE:HD12	1:A:296:MET:HE3	2.00	0.42
1:B:425:ILE:HG23	1:B:426:GLU:N	2.34	0.42
1:B:133:THR:CG2	1:B:231:LEU:HD21	2.49	0.42
1:B:259:LEU:HG	1:B:263:LEU:HD12	2.01	0.42
1:B:167:LEU:HD22	1:B:174:TYR:HB3	2.02	0.42
1:A:380:ARG:HG3	1:A:380:ARG:NH2	2.34	0.42
1:B:449:HIS:CD2	1:B:451:ASP:N	2.75	0.42
1:A:392:LYS:NZ	1:A:399:PRO:O	2.53	0.42
1:A:224:GLN:O	1:A:225:GLU:C	2.56	0.41
1:A:526:ASP:HB3	1:A:530:ARG:HH21	1.85	0.41
1:B:3:CYS:HB3	1:B:294:LEU:CD2	2.49	0.41
1:A:215:ARG:HH12	1:A:217:GLU:HB2	1.84	0.41
1:A:443:HIS:CD2	1:A:510:TYR:OH	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG23	1:B:55:LEU:HD21	2.01	0.41
1:B:129:SER:HA	1:B:253:VAL:HG23	2.01	0.41
1:B:419:LYS:H	1:B:419:LYS:HG2	1.75	0.41
1:A:228:PHE:O	1:A:262:MET:HE1	2.20	0.41
1:A:253:VAL:O	1:A:253:VAL:HG12	2.19	0.41
1:A:465:ILE:H	1:A:465:ILE:HG13	1.52	0.41
1:B:9:THR:HG1	1:B:106:HIS:CD2	2.38	0.41
1:B:383:ARG:O	1:B:387:TYR:CD2	2.73	0.41
1:B:451:ASP:HB2	1:B:470:LEU:HD12	2.02	0.41
1:A:226:TYR:O	1:A:227:ALA:C	2.59	0.41
1:B:229:SER:HA	1:B:262:MET:HE1	2.01	0.41
1:A:5:GLY:O	1:A:15:VAL:HA	2.21	0.41
1:A:449:HIS:HD2	1:A:451:ASP:N	2.13	0.41
1:A:26:PHE:CZ	1:A:28:LYS:HB2	2.56	0.40
1:B:6:LEU:HG	1:B:15:VAL:HG12	2.02	0.40
1:B:360:LYS:O	1:B:410:ARG:HA	2.22	0.40
1:A:60:PHE:HE1	1:A:68:ILE:HD12	1.86	0.40
1:B:138:TYR:OH	1:B:141:LYS:HA	2.22	0.40
1:A:377:ARG:HG2	1:A:377:ARG:H	1.65	0.40
1:A:372:LEU:HD22	1:A:376:ILE:CD1	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	515/535 (96%)	454 (88%)	51 (10%)	10 (2%)	<b>8</b> 29
1	B	501/535 (94%)	425 (85%)	63 (13%)	13 (3%)	<b>5</b> 22
All	All	1016/1070 (95%)	879 (86%)	114 (11%)	23 (2%)	<b>6</b> 24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	337	HIS
1	A	339	ILE
1	B	166	ASN
1	A	80	GLY
1	A	314	TYR
1	A	529	ARG
1	B	27	ASN
1	B	80	GLY
1	B	427	ASP
1	B	25	LEU
1	B	212	ALA
1	B	217	GLU
1	B	499	PHE
1	A	177	GLU
1	A	516	ARG
1	B	208	ARG
1	A	425	ILE
1	B	500	ASP
1	B	515	ASP
1	A	8	GLY
1	B	169	HIS
1	B	376	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	443/457 (97%)	372 (84%)	71 (16%)	2	9
1	B	431/457 (94%)	372 (86%)	59 (14%)	3	14
All	All	874/914 (96%)	744 (85%)	130 (15%)	3	11

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	3	CYS
1	A	13	THR
1	A	19	THR
1	A	20	SER
1	A	29	THR
1	A	52	PHE
1	A	70	LEU
1	A	79	LEU
1	A	84	ARG
1	A	93	LEU
1	A	97	LEU
1	A	111	ILE
1	A	125	THR
1	A	128	VAL
1	A	136	ILE
1	A	154	VAL
1	A	186	VAL
1	A	187	ASP
1	A	197	ILE
1	A	202	LEU
1	A	216	LEU
1	A	234	ILE
1	A	243	ASN
1	A	266	MET
1	A	270	GLN
1	A	272	VAL
1	A	273	ASP
1	A	282	CYS
1	A	291	TRP
1	A	292	LEU
1	A	301	ARG
1	A	304	SER
1	A	305	LEU
1	A	314	TYR
1	A	319	VAL
1	A	332	ARG
1	A	337	HIS
1	A	339	ILE
1	A	346	ASP
1	A	358	ILE
1	A	369	ASP
1	A	370	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	372	LEU
1	A	374	GLU
1	A	377	ARG
1	A	380	ARG
1	A	381	THR
1	A	386	ARG
1	A	410	ARG
1	A	417	ASN
1	A	420	LEU
1	A	426	GLU
1	A	429	LEU
1	A	443	HIS
1	A	462	ASP
1	A	465	ILE
1	A	466	ILE
1	A	468	PHE
1	A	474	SER
1	A	492	LEU
1	A	493	SER
1	A	505	ARG
1	A	508	GLU
1	A	514	TYR
1	A	515	ASP
1	A	516	ARG
1	A	517	TRP
1	A	521	LEU
1	A	523	LEU
1	A	529	ARG
1	B	2	ILE
1	B	13	THR
1	B	15	VAL
1	B	30	ILE
1	B	31	MET
1	B	52	PHE
1	B	57	LYS
1	B	63	VAL
1	B	65	LYS
1	B	69	ASP
1	B	70	LEU
1	B	94	SER
1	B	111	ILE
1	B	116	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	119	GLU
1	B	122	ASP
1	B	125	THR
1	B	136	ILE
1	B	154	VAL
1	B	175	ILE
1	B	180	ARG
1	B	191	THR
1	B	197	ILE
1	B	204	THR
1	B	211	ASP
1	B	216	LEU
1	B	237	ARG
1	B	266	MET
1	B	268	GLU
1	B	272	VAL
1	B	292	LEU
1	B	294	LEU
1	B	295	LEU
1	B	301	ARG
1	B	314	TYR
1	B	319	VAL
1	B	322	ASN
1	B	324	ILE
1	B	325	LYS
1	B	357	VAL
1	B	358	ILE
1	B	362	ARG
1	B	370	GLU
1	B	372	LEU
1	B	377	ARG
1	B	380	ARG
1	B	381	THR
1	B	386	ARG
1	B	404	VAL
1	B	419	LYS
1	B	420	LEU
1	B	424	VAL
1	B	426	GLU
1	B	466	ILE
1	B	468	PHE
1	B	492	LEU

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Mol	Chain	Res	Type
1	B	501	GLU
1	B	517	TRP
1	B	523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	75	GLN
1	A	160	GLN
1	A	224	GLN
1	A	241	HIS
1	A	243	ASN
1	A	285	ASN
1	A	322	ASN
1	A	375	ASN
1	A	417	ASN
1	A	443	HIS
1	A	449	HIS
1	A	456	ASN
1	B	160	GLN
1	B	224	GLN
1	B	270	GLN
1	B	271	ASN
1	B	285	ASN
1	B	297	HIS
1	B	313	ASN
1	B	322	ASN
1	B	375	ASN
1	B	408	ASN
1	B	417	ASN
1	B	443	HIS
1	B	449	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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
2	ANP	B	1533	-	29,33,33	2.00	7 (24%)	31,52,52	1.64	6 (19%)
2	ANP	A	1531	-	29,33,33	1.90	5 (17%)	31,52,52	1.75	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	B	1533	-	-	4/14/38/38	0/3/3/3
2	ANP	A	1531	-	-	1/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1533	ANP	PG-N3B	5.30	1.77	1.63
2	A	1531	ANP	PG-N3B	5.19	1.76	1.63
2	B	1533	ANP	PB-N3B	5.11	1.76	1.63
2	A	1531	ANP	PB-N3B	5.04	1.76	1.63
2	B	1533	ANP	PB-O1B	3.76	1.52	1.46
2	A	1531	ANP	PB-O1B	3.50	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1533	ANP	PG-O1G	3.13	1.51	1.46
2	A	1531	ANP	PG-O1G	3.04	1.51	1.46
2	B	1533	ANP	C5-C4	2.65	1.48	1.40
2	A	1531	ANP	C5-C4	2.47	1.47	1.40
2	B	1533	ANP	PB-O3A	2.25	1.61	1.59
2	B	1533	ANP	C2-N3	2.13	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1531	ANP	O2B-PB-O1B	4.15	118.63	109.92
2	B	1533	ANP	O2G-PG-O3G	3.76	117.65	107.64
2	A	1531	ANP	O2G-PG-O3G	3.68	117.44	107.64
2	B	1533	ANP	O2B-PB-O1B	3.34	116.93	109.92
2	A	1531	ANP	N3-C2-N1	-3.34	123.46	128.68
2	B	1533	ANP	N3-C2-N1	-3.25	123.60	128.68
2	A	1531	ANP	PB-O3A-PA	-3.07	121.80	132.62
2	A	1531	ANP	O1G-PG-N3B	-2.84	107.58	111.77
2	B	1533	ANP	O1G-PG-N3B	-2.77	107.69	111.77
2	B	1533	ANP	C4-C5-N7	-2.75	106.53	109.40
2	B	1533	ANP	PB-O3A-PA	-2.52	123.74	132.62
2	A	1531	ANP	C4-C5-N7	-2.30	107.00	109.40
2	A	1531	ANP	C3'-C2'-C1'	2.24	104.36	100.98
2	A	1531	ANP	O3G-PG-O1G	-2.24	107.82	113.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

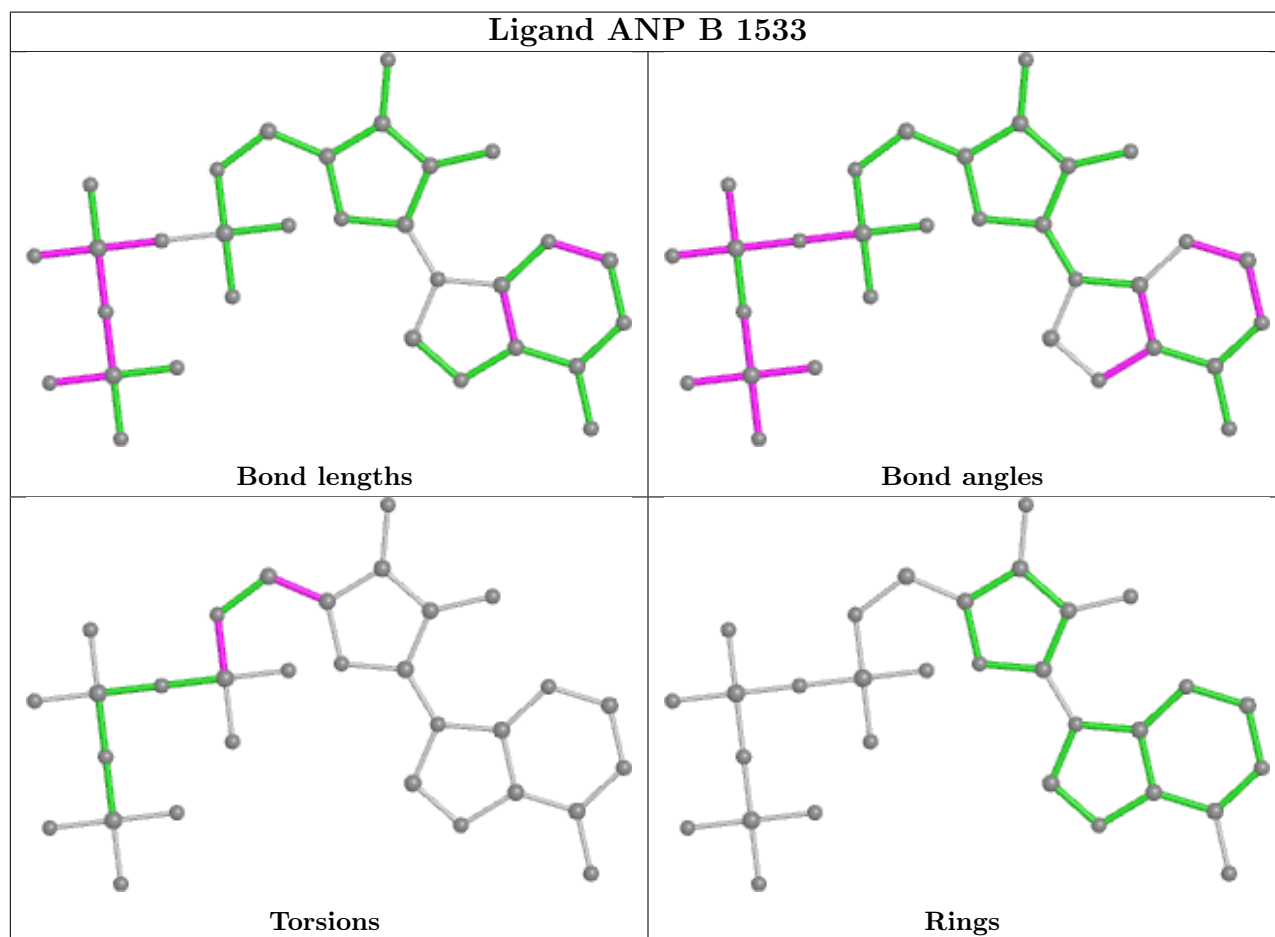
Mol	Chain	Res	Type	Atoms
2	A	1531	ANP	PG-N3B-PB-O3A
2	B	1533	ANP	C5'-O5'-PA-O1A
2	B	1533	ANP	C3'-C4'-C5'-O5'
2	B	1533	ANP	O4'-C4'-C5'-O5'
2	B	1533	ANP	C5'-O5'-PA-O3A

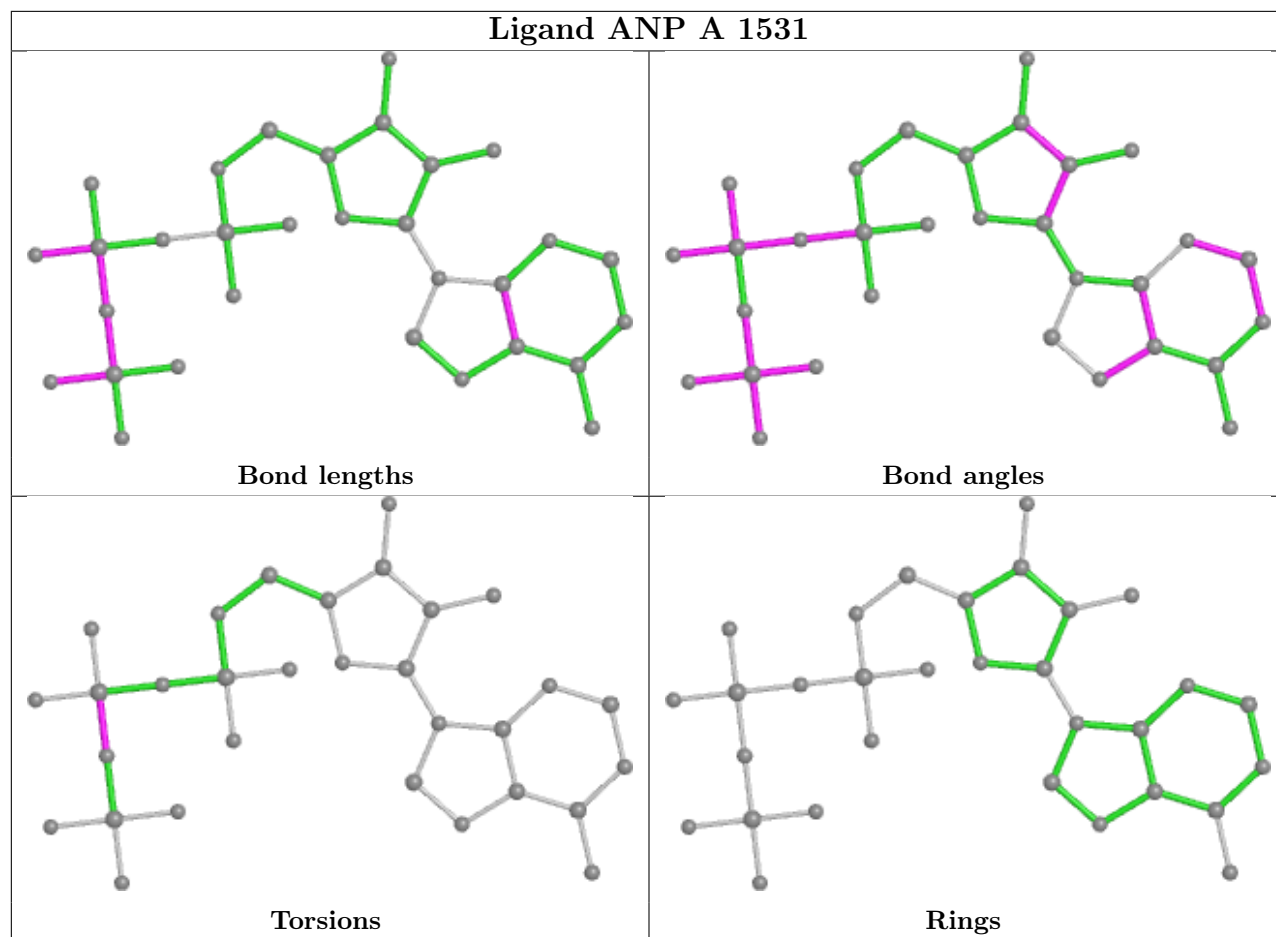
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1533	ANP	1	0
2	A	1531	ANP	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/535 (97%)	-0.33	3 (0%) 89 76	34, 56, 85, 107	0
1	B	507/535 (94%)	-0.34	1 (0%) 95 89	35, 60, 93, 112	0
All	All	1026/1070 (95%)	-0.33	4 (0%) 92 82	34, 58, 90, 112	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	2.8
1	A	326	GLU	2.4
1	B	47	HIS	2.2
1	A	327	ILE	2.2

### 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, 95<sup>th</sup> 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.

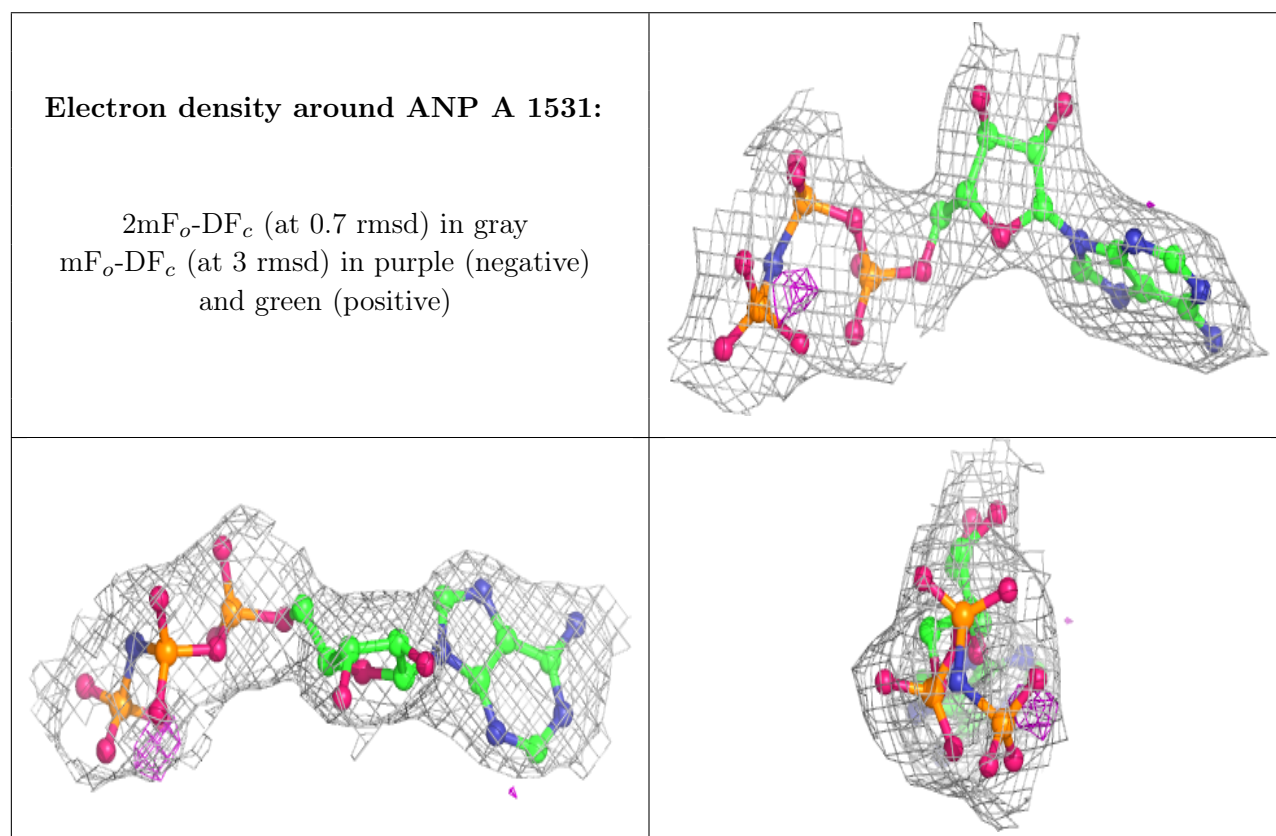
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ANP	A	1531	31/31	0.96	0.13	43,45,74,74	0

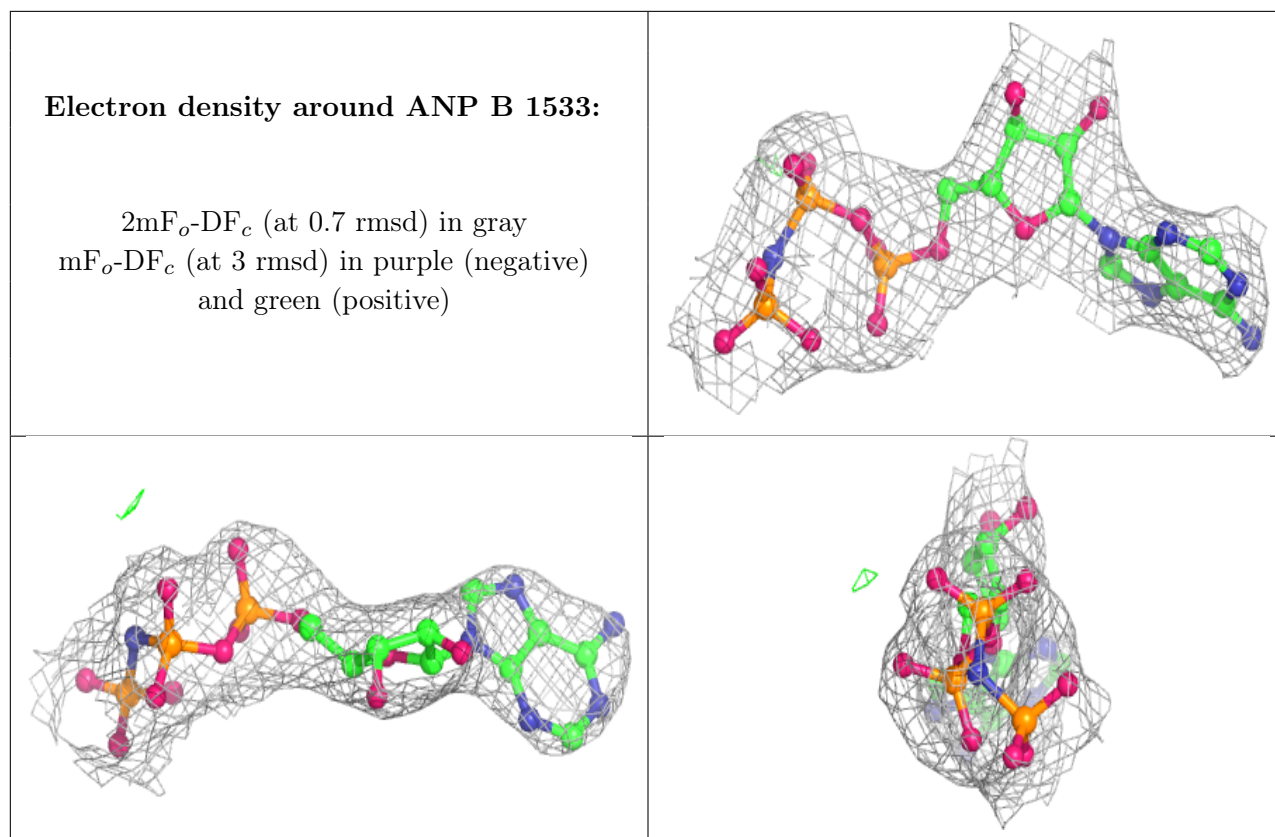
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	B	1533	31/31	0.96	0.14	66,70,87,87	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.