Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 06:03 am BST

PDB ID	:	4CEJ / pdb_00004cej
Title	:	Crystal structure of AddAB-DNA-ADPNP complex at 3 Angstrom resolution
Authors	:	Krajewski, W.W.; Wilkinson, M.; Fu, X.; Cronin, N.B.; Wigley, D.
Deposited on	:	2013-11-11
Resolution	:	3.00 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:

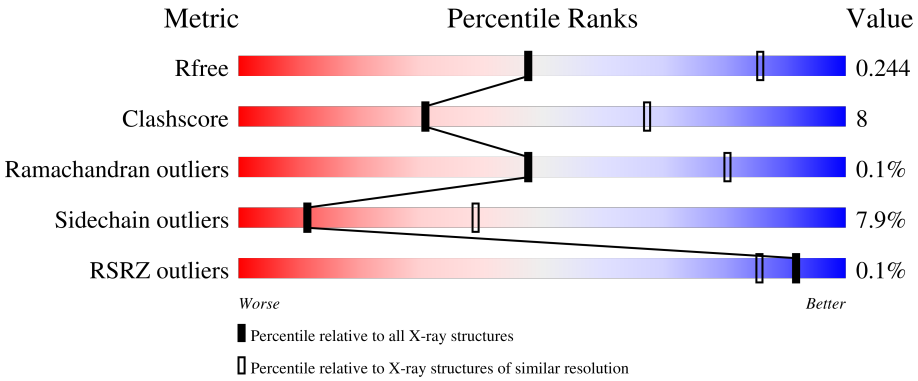
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1232	69% 23%
2	B	1166	75% 22%
3	X	70	44% 21% 34%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19953 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 ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0	0
			9539	6084	1627	1800	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	variant	UNP P23478
A	1172	ALA	ASP	engineered mutation	UNP P23478

- Molecule 2 is a protein called ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1156	Total	C	N	O	S	0	1	0
			9410	5979	1613	1774	44			

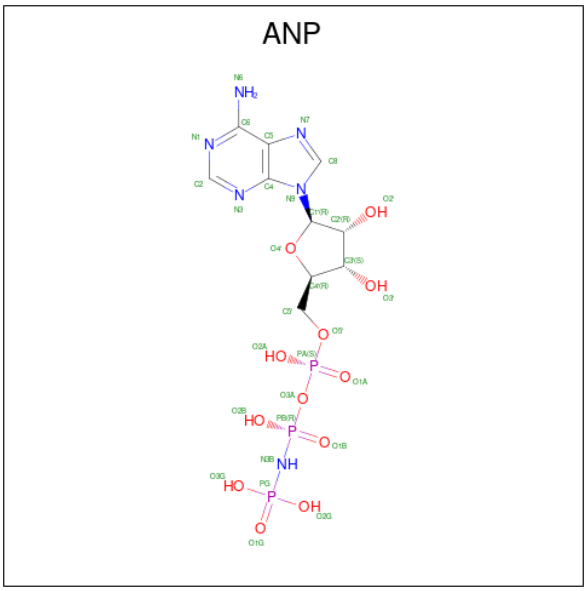
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	variant	UNP P23477
B	844	GLU	GLN	variant	UNP P23477
B	961	ALA	ASP	engineered mutation	UNP P23477

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	46	Total	C	N	O	P	0	0	0
			925	443	151	285	46			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

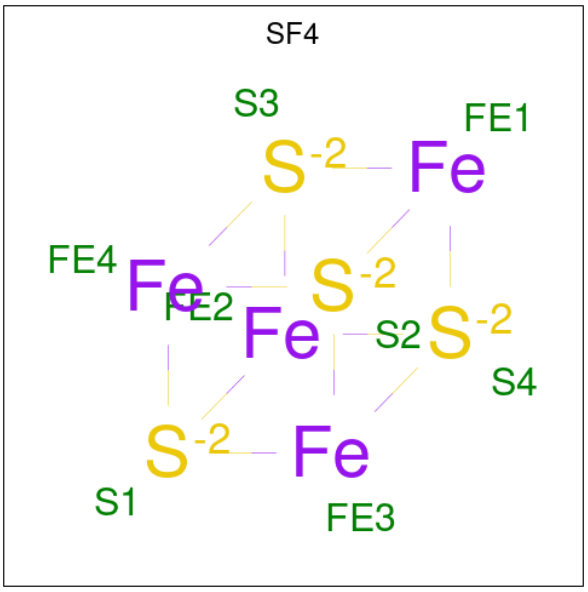


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Fe S 8 4 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total O 4 4	0	0
7	B	3	Total O 3 3	0	0

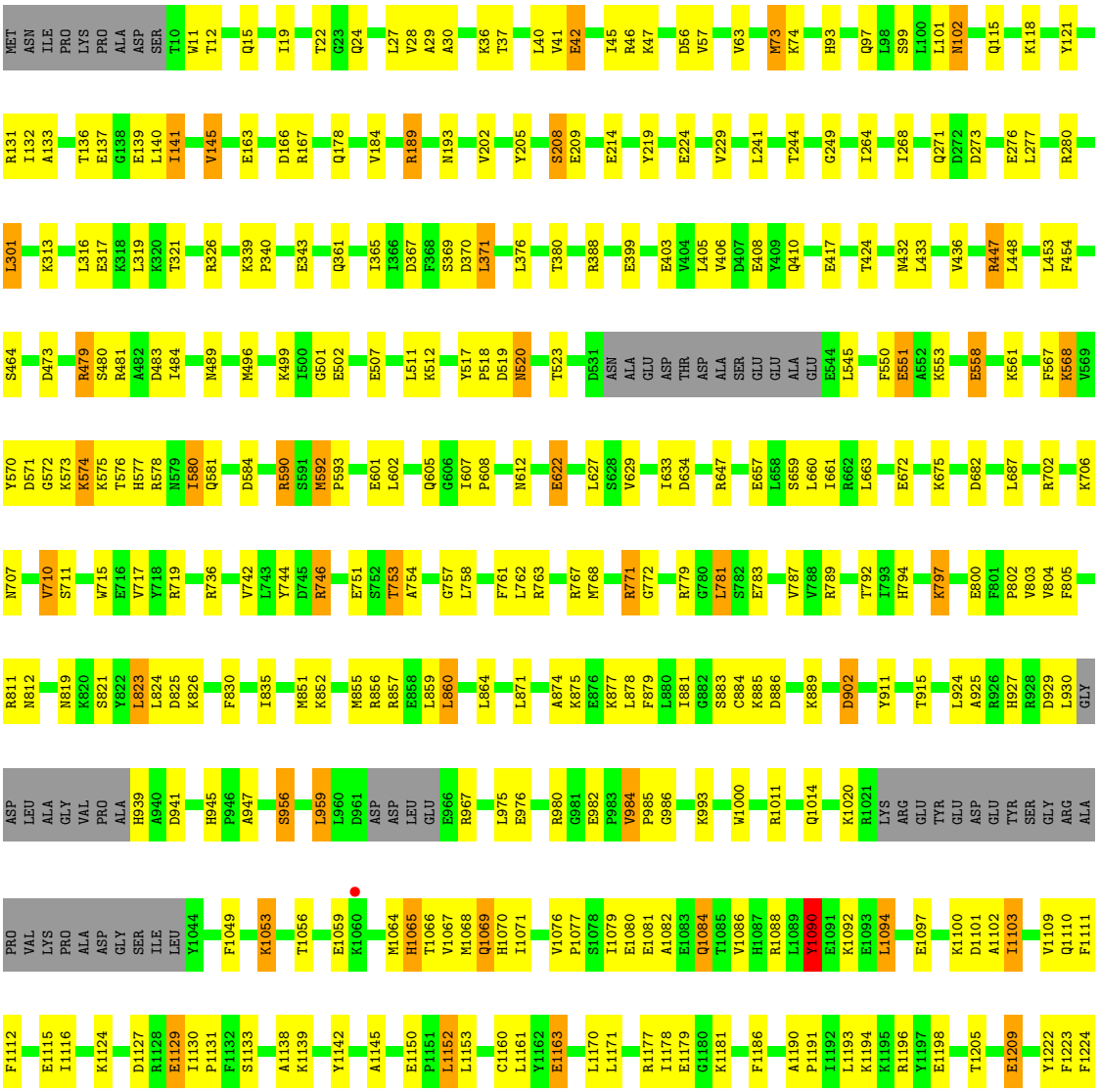
3 Residue-property plots (i)

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: ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A

Chain A:



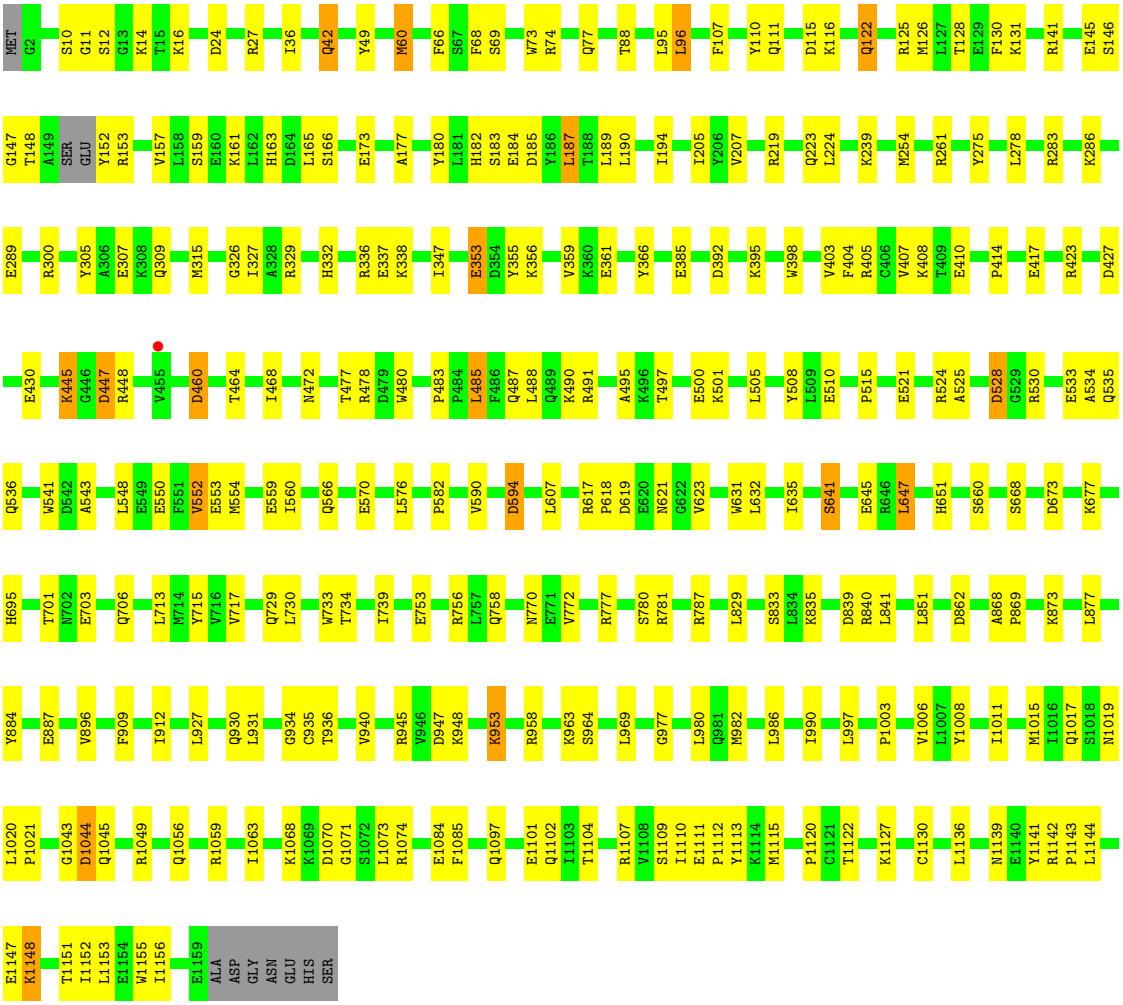




• Molecule 2: ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B

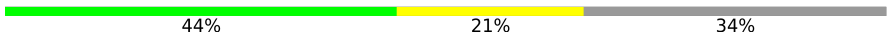
Chain B:

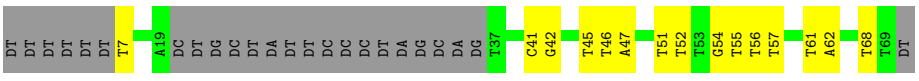




• Molecule 3: DNA

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.44Å 152.94Å 125.24Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	29.73 – 3.00 29.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.73-3.00) 99.5 (29.73-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.243 0.205 , 0.244	Depositor DCC
R_{free} test set	2924 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19953	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0.31	0/9731	0.78	12/13128 (0.1%)
2	B	0.29	0/9601	0.75	4/12936 (0.0%)
3	X	0.29	0/1031	0.60	0/1589
All	All	0.30	0/20363	0.76	16/27653 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1142	TYR	CA-C-N	-7.29	112.82	120.03
1	A	1142	TYR	C-N-CA	-7.29	112.82	120.03
1	A	193	ASN	CA-C-N	6.36	125.59	118.97
1	A	193	ASN	C-N-CA	6.36	125.59	118.97
2	B	660	SER	CA-C-N	-6.17	114.42	120.52
2	B	660	SER	C-N-CA	-6.17	114.42	120.52
2	B	483	PRO	N-CA-C	5.86	117.85	110.70
1	A	1178	ILE	CB-CA-C	-5.70	106.87	111.71
1	A	984	VAL	CA-C-N	5.35	126.53	119.84
1	A	984	VAL	C-N-CA	5.35	126.53	119.84
1	A	986	GLY	N-CA-C	5.27	125.67	113.18
1	A	1076	VAL	CA-C-N	5.17	125.38	120.31
1	A	1076	VAL	C-N-CA	5.17	125.38	120.31
1	A	1090	TYR	CA-CB-CG	5.16	123.18	113.90
1	A	772	GLY	N-CA-C	-5.13	107.98	115.63
2	B	934	GLY	N-CA-C	-5.08	108.61	115.21

There are no chirality outliers.

There are no planarity outliers.

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	9539	0	9505	193	0
2	B	9410	0	9357	145	0
3	X	925	0	516	16	0
4	A	31	0	13	2	0
4	B	31	0	13	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	8	0	0	1	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
All	All	19953	0	19404	327	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 8.

All (327) 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)
2:B:912:ILE:HD11	2:B:948:LYS:HB3	1.64	0.79
2:B:165:LEU:HD11	2:B:623:VAL:HG11	1.65	0.77
1:A:30:ALA:HB3	1:A:36:LYS:HD2	1.68	0.75
2:B:414:PRO:HB2	2:B:417:GLU:HG3	1.68	0.74
1:A:28:VAL:HB	1:A:436:VAL:HG12	1.69	0.74
1:A:276:GLU:HG3	1:A:280:ARG:HE	1.52	0.72
1:A:167:ARG:NH1	1:A:835:ILE:O	2.22	0.72
1:A:590:ARG:HH21	1:A:794:HIS:HE1	1.37	0.70
1:A:856:ARG:NH1	1:A:911:TYR:O	2.25	0.69
1:A:417:GLU:HB2	1:A:453:LEU:HD21	1.74	0.69
1:A:578:ARG:NH2	1:A:584:ASP:OD1	2.26	0.69
1:A:479:ARG:HD3	1:A:800:GLU:HB3	1.75	0.69
1:A:480:SER:OG	1:A:874:ALA:O	2.10	0.68
2:B:180:TYR:OH	2:B:553:GLU:OE1	2.13	0.67
1:A:166:ASP:OD1	2:B:884:TYR:OH	2.11	0.67
2:B:11:GLY:H	4:B:2161:ANP:HNB1	1.42	0.67
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:GLU:OE1	2:B:706:GLN:NE2	2.27	0.67
2:B:14:LYS:NZ	4:B:2161:ANP:O2B	2.27	0.66
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.79	0.65
2:B:930:GLN:O	2:B:1097:GLN:NE2	2.30	0.65
2:B:772:VAL:HG21	2:B:1109:SER:HA	1.79	0.65
2:B:835:LYS:NZ	2:B:839:ASP:OD2	2.30	0.65
2:B:787:ARG:HG3	2:B:787:ARG:HH11	1.63	0.64
1:A:578:ARG:NH1	1:A:581:GLN:OE1	2.31	0.64
1:A:1077:PRO:HD2	1:A:1112:PHE:HD2	1.63	0.64
2:B:448:ARG:HH22	2:B:472:ASN:HA	1.63	0.64
1:A:825:ASP:HB2	1:A:851:MET:HE3	1.80	0.64
2:B:1111:GLU:HB3	2:B:1142:ARG:HD3	1.80	0.64
2:B:521:GLU:OE2	2:B:524:ARG:NH1	2.32	0.63
1:A:647:ARG:HH21	2:B:772:VAL:HG12	1.62	0.62
2:B:283:ARG:HD3	4:B:2161:ANP:H4'	1.80	0.62
1:A:715:TRP:CD1	1:A:719:ARG:HH21	2.16	0.62
1:A:1138:ALA:HA	1:A:1152:LEU:HD11	1.81	0.62
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.82	0.62
2:B:385:GLU:OE2	2:B:405:ARG:NH1	2.33	0.62
1:A:1079:ILE:HA	1:A:1109:VAL:HG21	1.80	0.61
2:B:931:LEU:HD12	2:B:935:CYS:HB2	1.81	0.61
1:A:40:LEU:HD22	1:A:73:MET:HE3	1.81	0.61
2:B:460:ASP:OD1	2:B:460:ASP:N	2.33	0.61
1:A:380:THR:HG21	1:A:388:ARG:HE	1.65	0.61
2:B:1113:TYR:CE2	2:B:1120:PRO:HG3	2.36	0.61
1:A:819:ASN:HB3	3:X:7:DT:H4'	1.81	0.61
1:A:131:ARG:NH2	1:A:137:GLU:OE2	2.33	0.60
1:A:871:LEU:HD22	1:A:878:LEU:HD21	1.83	0.60
1:A:812:ASN:HB2	3:X:51:DT:H5"	1.83	0.60
2:B:528:ASP:HB3	2:B:530:ARG:HD3	1.84	0.60
2:B:447:ASP:OD1	2:B:447:ASP:N	2.32	0.59
2:B:10:SER:OG	2:B:283:ARG:NH2	2.35	0.59
1:A:313:LYS:NZ	3:X:42:DG:OP2	2.36	0.59
1:A:571:ASP:O	1:A:575:LYS:N	2.34	0.59
2:B:305:TYR:CZ	2:B:307:GLU:HB2	2.37	0.59
2:B:947:ASP:HB2	2:B:958:ARG:HG2	1.85	0.58
1:A:1082:ALA:O	1:A:1086:VAL:HG23	2.03	0.58
1:A:1011:ARG:HD3	2:B:582:PRO:HB2	1.85	0.58
1:A:481:ARG:NH2	1:A:518:PRO:O	2.36	0.58
1:A:823:LEU:HB3	1:A:851:MET:HE2	1.86	0.58
1:A:612:ASN:HD22	1:A:779:ARG:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ARG:NH2	3:X:52:DT:OP1	2.37	0.57
2:B:594:ASP:OD1	2:B:594:ASP:N	2.37	0.57
1:A:1111:PHE:HB2	1:A:1222:TYR:CZ	2.40	0.57
1:A:802:PRO:HA	1:A:875:LYS:HB2	1.87	0.57
1:A:121:TYR:OH	2:B:122:GLN:NE2	2.38	0.56
1:A:321:THR:O	2:B:1019:ASN:ND2	2.38	0.56
1:A:711:SER:N	1:A:751:GLU:OE2	2.36	0.56
1:A:1133:SER:HB3	1:A:1153:LEU:HD11	1.86	0.56
2:B:909:PHE:HB3	2:B:947:ASP:HB3	1.88	0.56
2:B:982:MET:HE3	2:B:1006:VAL:HB	1.87	0.56
1:A:1124:LYS:NZ	1:A:1163:GLU:OE1	2.35	0.56
2:B:1059:ARG:HD3	3:X:45:DT:H5"	1.88	0.56
1:A:805:PHE:HD2	1:A:881:ILE:HD11	1.71	0.56
1:A:1090:TYR:CD1	1:A:1090:TYR:C	2.83	0.56
3:X:68:DT:H5'	3:X:68:DT:C6	2.40	0.55
1:A:141:ILE:HD12	1:A:365:ILE:HD11	1.87	0.55
1:A:408:GLU:OE1	1:A:410:GLN:NE2	2.31	0.55
2:B:205:ILE:HD13	2:B:224:LEU:HD13	1.88	0.55
2:B:787:ARG:NH1	2:B:936:THR:OG1	2.40	0.55
1:A:984:VAL:HG13	1:A:985:PRO:HD2	1.88	0.55
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.89	0.54
3:X:55:DT:H2"	3:X:56:DT:O5'	2.08	0.54
2:B:501:LYS:NZ	2:B:560:ILE:O	2.36	0.54
2:B:963:LYS:HG3	2:B:1008:TYR:HD2	1.72	0.54
2:B:42:GLN:H	2:B:42:GLN:CD	2.16	0.53
2:B:131:LYS:NZ	2:B:173:GLU:OE2	2.35	0.53
2:B:953:LYS:NZ	2:B:1044:ASP:OD1	2.39	0.53
2:B:990:ILE:HG13	2:B:1003:PRO:HG3	1.90	0.53
2:B:329:ARG:HD3	2:B:715:TYR:HA	1.90	0.53
2:B:16:LYS:HD3	4:B:2161:ANP:C8	2.39	0.53
2:B:157:VAL:HG12	2:B:161:LYS:HE3	1.91	0.53
2:B:1112:PRO:HG3	6:B:2160:SF4:S4	2.49	0.53
2:B:12:SER:HB3	2:B:278:LEU:HB2	1.90	0.52
2:B:125:ARG:HG2	3:X:61:DT:H72	1.91	0.52
2:B:770:ASN:H	2:B:1136:LEU:HD21	1.72	0.52
1:A:141:ILE:O	1:A:145:VAL:HG13	2.10	0.52
1:A:11:TRP:HZ2	1:A:42:GLU:HG3	1.74	0.52
1:A:133:ALA:HB2	1:A:365:ILE:HD12	1.92	0.52
1:A:567:PHE:HB3	1:A:580:ILE:HG13	1.92	0.52
1:A:241:LEU:O	1:A:244:THR:OG1	2.25	0.51
1:A:1194:LYS:NZ	1:A:1198:GLU:OE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ARG:O	2:B:145:GLU:HG2	2.10	0.51
1:A:264:ILE:O	1:A:268:ILE:HG13	2.11	0.51
1:A:622:GLU:HG2	1:A:736:ARG:HB3	1.92	0.51
1:A:975:LEU:HG	2:B:733:TRP:CZ3	2.45	0.51
1:A:975:LEU:HG	2:B:733:TRP:HZ3	1.75	0.51
2:B:16:LYS:HD3	4:B:2161:ANP:N7	2.26	0.51
1:A:229:VAL:HG21	1:A:319:LEU:HD13	1.92	0.51
1:A:835:ILE:HG23	2:B:1015:MET:HE2	1.93	0.51
1:A:1097:GLU:HG2	1:A:1100:LYS:HD2	1.92	0.51
2:B:392:ASP:OD2	2:B:405:ARG:NH2	2.43	0.51
1:A:1116:ILE:HD12	1:A:1229:ILE:HG21	1.93	0.51
1:A:574:LYS:HD2	1:A:574:LYS:O	2.11	0.51
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.93	0.51
2:B:289:GLU:OE1	2:B:695:HIS:NE2	2.34	0.51
2:B:410:GLU:OE2	2:B:423:ARG:NH1	2.37	0.51
1:A:1127:ASP:HB3	1:A:1130:ILE:HD11	1.94	0.50
2:B:969:LEU:HB2	2:B:1008:TYR:HE1	1.76	0.50
1:A:479:ARG:NH2	4:A:2233:ANP:HNB1	2.09	0.50
1:A:612:ASN:HD22	1:A:779:ARG:HH11	1.59	0.50
1:A:753:THR:HG22	1:A:754:ALA:N	2.25	0.50
1:A:902:ASP:N	1:A:902:ASP:OD1	2.42	0.50
1:A:1069:GLN:HE21	1:A:1069:GLN:HA	1.76	0.50
1:A:273:ASP:OD2	1:A:276:GLU:HB2	2.12	0.50
1:A:1090:TYR:C	1:A:1090:TYR:HD1	2.19	0.50
1:A:605:GLN:HB2	1:A:607:ILE:HD12	1.94	0.49
2:B:347:ILE:HG23	2:B:607:LEU:HD13	1.94	0.49
1:A:884:CYS:SG	1:A:885:LYS:N	2.85	0.49
2:B:1102:GLN:OE1	2:B:1107:ARG:NH1	2.42	0.49
1:A:925:ALA:HA	1:A:930:LEU:HD23	1.94	0.49
1:A:823:LEU:HD21	1:A:855:MET:SD	2.53	0.49
1:A:1205:THR:O	1:A:1209:GLU:HB2	2.13	0.49
2:B:1147:GLU:HG3	2:B:1155:TRP:CH2	2.48	0.49
1:A:403:GLU:HA	1:A:432:ASN:HB2	1.94	0.49
1:A:479:ARG:HH22	4:A:2233:ANP:HNB1	1.60	0.49
2:B:326:GLY:HA2	2:B:329:ARG:NH1	2.27	0.49
1:A:11:TRP:CZ2	1:A:42:GLU:HG3	2.48	0.49
2:B:366:TYR:CD2	2:B:717:VAL:HG21	2.47	0.48
1:A:205:TYR:OH	1:A:830:PHE:O	2.29	0.48
2:B:641:SER:OG	2:B:645:GLU:OE1	2.28	0.48
2:B:543:ALA:HB1	2:B:576:LEU:HD22	1.95	0.48
2:B:36:ILE:HG23	2:B:66:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:THR:OG1	3:X:54:DG:OP1	2.18	0.48
1:A:742:VAL:O	1:A:746:ARG:HD3	2.13	0.48
1:A:27:LEU:HD11	1:A:454:PHE:CE2	2.48	0.48
2:B:1068:LYS:HB2	2:B:1070:ASP:OD1	2.14	0.48
2:B:1153:LEU:HA	2:B:1156:ILE:HD12	1.94	0.48
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.49	0.48
2:B:1148:LYS:O	2:B:1151:THR:OG1	2.19	0.48
1:A:980:ARG:NH1	1:A:982:GLU:OE2	2.46	0.48
2:B:730:LEU:O	2:B:734:THR:HG23	2.14	0.48
1:A:132:ILE:N	3:X:57:DT:O4	2.25	0.47
2:B:110:TYR:OH	2:B:623:VAL:HG13	2.14	0.47
1:A:367:ASP:HB2	1:A:370:ASP:CG	2.39	0.47
2:B:355:TYR:O	2:B:359:VAL:HG23	2.15	0.47
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.97	0.47
1:A:507:GLU:O	1:A:512:LYS:NZ	2.38	0.47
1:A:1102:ALA:O	1:A:1103:ILE:HG12	2.15	0.47
2:B:261[B]:ARG:HG2	2:B:261[B]:ARG:HH11	1.80	0.47
1:A:523:THR:HA	1:A:877:LYS:HD3	1.96	0.47
2:B:477:THR:HA	2:B:480:TRP:NE1	2.30	0.47
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.49	0.47
1:A:570:TYR:HD1	1:A:577:HIS:CE1	2.32	0.47
1:A:1064:MET:SD	1:A:1103:ILE:HD13	2.55	0.47
2:B:115:ASP:HB3	2:B:116:LYS:HZ2	1.80	0.47
2:B:182:HIS:HB3	2:B:185:ASP:OD2	2.15	0.47
2:B:395:LYS:HD3	2:B:566:GLN:OE1	2.14	0.47
2:B:403:VAL:O	2:B:407:VAL:HG23	2.14	0.47
1:A:657:GLU:HB3	1:A:687:LEU:HD13	1.97	0.47
2:B:147:GLY:HA3	2:B:159:SER:HB3	1.96	0.47
1:A:993:LYS:HD2	2:B:713:LEU:HD21	1.96	0.47
2:B:42:GLN:OE1	3:X:62:DA:H1'	2.13	0.46
2:B:353:GLU:OE1	2:B:356:LYS:NZ	2.37	0.46
1:A:781:LEU:HD22	1:A:787:VAL:HG11	1.96	0.46
1:A:1071:ILE:HG21	1:A:1112:PHE:HZ	1.79	0.46
2:B:1141:TYR:O	2:B:1143:PRO:HD3	2.16	0.46
1:A:484:ILE:HD12	1:A:878:LEU:HB2	1.98	0.46
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.81	0.46
1:A:1161:LEU:HD23	1:A:1170:LEU:HA	1.96	0.46
2:B:96:LEU:HD12	2:B:96:LEU:HA	1.79	0.46
1:A:367:ASP:HB3	1:A:369:SER:H	1.80	0.46
1:A:629:VAL:O	1:A:633:ILE:HG13	2.16	0.46
1:A:719:ARG:NH2	2:B:361:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:GLU:OE1	1:A:883:SER:OG	2.25	0.46
1:A:1020:LYS:NZ	1:A:1196:ARG:O	2.39	0.46
1:A:1139:LYS:HD3	1:A:1145:ALA:O	2.16	0.46
1:A:224:GLU:OE1	1:A:857:ARG:NH1	2.49	0.45
1:A:976:GLU:O	1:A:980:ARG:HG3	2.16	0.45
2:B:107:PHE:HB2	2:B:111:GLN:HG2	1.97	0.45
2:B:152:TYR:HB2	2:B:631:TRP:CD1	2.51	0.45
1:A:489:ASN:HD21	1:A:511:LEU:N	2.15	0.45
1:A:592:MET:N	1:A:593:PRO:HD2	2.31	0.45
2:B:88:THR:OG1	2:B:550:GLU:OE2	2.26	0.45
1:A:553:LYS:NZ	1:A:601:GLU:OE2	2.43	0.45
2:B:36:ILE:HB	2:B:205:ILE:HG12	1.99	0.45
2:B:1070:ASP:OD1	2:B:1071:GLY:N	2.49	0.45
1:A:163:GLU:OE1	1:A:167:ARG:NH2	2.44	0.45
1:A:1150:GLU:HB3	2:B:49:TYR:OH	2.16	0.45
1:A:249:GLY:HA2	1:A:301:LEU:HD22	1.99	0.45
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	1.97	0.45
1:A:424:THR:HG21	1:A:433:LEU:HD13	1.99	0.45
1:A:1092:LYS:HB3	1:A:1094:LEU:HD12	1.99	0.45
2:B:673:ASP:HB2	2:B:677:LYS:HB3	1.99	0.45
2:B:128:THR:HG23	2:B:184:GLU:HG3	1.99	0.45
1:A:939:HIS:HD2	1:A:941:ASP:H	1.66	0.44
1:A:945:HIS:C	1:A:947:ALA:H	2.24	0.44
1:A:1129:GLU:O	1:A:1131:PRO:HD3	2.16	0.44
1:A:1194:LYS:O	1:A:1198:GLU:HB2	2.17	0.44
2:B:190:LEU:O	2:B:194:ILE:HG13	2.17	0.44
2:B:632:LEU:HD23	2:B:632:LEU:HA	1.86	0.44
2:B:1045:GLN:HG3	2:B:1049:ARG:HD2	2.00	0.44
2:B:868:ALA:HB3	2:B:869:PRO:HD3	1.99	0.44
1:A:447:ARG:HH21	3:X:54:DG:H1'	1.82	0.44
1:A:804:VAL:HB	1:A:874:ALA:HB2	1.99	0.44
1:A:1112:PHE:CD1	1:A:1112:PHE:N	2.84	0.44
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.99	0.44
1:A:93:HIS:O	1:A:97:GLN:HG2	2.18	0.44
1:A:376:LEU:O	1:A:380:THR:HG23	2.18	0.44
1:A:481:ARG:HD3	1:A:523:THR:HG21	2.00	0.44
1:A:558:GLU:HG2	1:A:879:PHE:CE1	2.52	0.44
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.99	0.44
2:B:505:LEU:O	2:B:508:TYR:HB3	2.17	0.44
1:A:553:LYS:HD2	1:A:959:LEU:HB3	1.99	0.44
1:A:574:LYS:HB3	1:A:576:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:GLN:HB2	2:B:695:HIS:CE1	2.53	0.44
1:A:1186:PHE:O	1:A:1190:ALA:N	2.45	0.44
1:A:496:MET:HG3	1:A:501:GLY:HA3	1.99	0.44
1:A:682:ASP:OD1	1:A:682:ASP:N	2.51	0.44
2:B:254:MET:HE2	2:B:254:MET:HB3	1.85	0.44
1:A:271:GLN:HA	1:A:277:LEU:HD11	2.00	0.43
2:B:485:LEU:HD12	2:B:485:LEU:HA	1.88	0.43
2:B:525:ALA:HB3	2:B:534:ALA:HB2	1.99	0.43
1:A:99:SER:O	1:A:102:ASN:ND2	2.51	0.43
1:A:1081:GLU:HA	1:A:1084:GLN:NE2	2.33	0.43
1:A:706:LYS:HA	1:A:706:LYS:HD3	1.77	0.43
2:B:515:PRO:HG3	2:B:541:TRP:CH2	2.54	0.43
3:X:41:DC:H2"	3:X:42:DG:C8	2.53	0.43
1:A:189:ARG:NH1	1:A:370:ASP:OD1	2.42	0.43
1:A:202:VAL:HG12	1:A:343:GLU:HG2	2.00	0.43
1:A:857:ARG:HG3	1:A:911:TYR:HE1	1.83	0.43
1:A:15:GLN:O	1:A:19:ILE:HG13	2.19	0.43
1:A:56:ASP:HA	1:A:97:GLN:OE1	2.19	0.43
2:B:261[B]:ARG:HG2	2:B:261[B]:ARG:NH1	2.33	0.43
1:A:1190:ALA:HB3	1:A:1191:PRO:HD3	2.01	0.43
2:B:398:TRP:CH2	2:B:485:LEU:HB3	2.53	0.43
2:B:445:LYS:O	2:B:478:ARG:NH2	2.52	0.43
2:B:1107:ARG:NH2	2:B:1111:GLU:OE2	2.51	0.43
1:A:710:VAL:HG22	1:A:757:GLY:C	2.43	0.42
3:X:61:DT:H6	3:X:61:DT:H2'	1.63	0.42
1:A:118:LYS:HB3	2:B:621:ASN:ND2	2.34	0.42
2:B:126:MET:HE2	2:B:130:PHE:CE1	2.54	0.42
1:A:136:THR:HG21	1:A:768:MET:HG3	2.01	0.42
1:A:339:LYS:HB3	1:A:340:PRO:HD3	2.01	0.42
1:A:1193:LEU:HD13	1:A:1223:PHE:CZ	2.54	0.42
2:B:24:ASP:HA	2:B:27:ARG:HD2	2.01	0.42
1:A:1077:PRO:CD	1:A:1112:PHE:HD2	2.32	0.42
2:B:841:LEU:HD21	2:B:851:LEU:HD21	2.01	0.42
1:A:567:PHE:HB3	1:A:580:ILE:CG1	2.49	0.42
1:A:1053:LYS:H	1:A:1053:LYS:HG2	1.70	0.42
2:B:729:GLN:O	2:B:739:ILE:HG21	2.20	0.42
1:A:326:ARG:HG2	2:B:1021:PRO:HG3	2.00	0.42
1:A:634:ASP:OD1	2:B:408:LYS:HE2	2.20	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.92	0.42
2:B:68:PHE:HB3	2:B:187:LEU:HD11	2.01	0.42
1:A:864:LEU:HA	1:A:864:LEU:HD12	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HD13	2:B:1130:CYS:HB2	2.01	0.42
1:A:29:ALA:O	1:A:473:ASP:HA	2.19	0.42
1:A:479:ARG:HB2	1:A:800:GLU:OE1	2.20	0.42
1:A:707:ASN:OD1	1:A:707:ASN:N	2.51	0.42
1:A:753:THR:CG2	1:A:754:ALA:N	2.82	0.42
2:B:533:GLU:O	2:B:536:GLN:HG2	2.20	0.42
2:B:787:ARG:HG3	2:B:787:ARG:NH1	2.29	0.42
2:B:548:LEU:O	2:B:552:VAL:HG13	2.20	0.42
1:A:63:VAL:HG22	1:A:406:VAL:HG22	2.01	0.42
1:A:276:GLU:CG	1:A:280:ARG:HE	2.27	0.42
1:A:886:ASP:OD2	1:A:889:LYS:HB2	2.19	0.42
3:X:68:DT:H5'	3:X:68:DT:H6	1.83	0.42
1:A:42:GLU:HA	1:A:45:ILE:HD12	2.02	0.41
1:A:570:TYR:CE2	1:A:572:GLY:HA2	2.54	0.41
2:B:829:LEU:O	2:B:833:SER:OG	2.37	0.41
1:A:339:LYS:O	1:A:343:GLU:HG3	2.20	0.41
1:A:517:TYR:HA	1:A:518:PRO:HD2	1.91	0.41
1:A:550:PHE:CZ	1:A:956:SER:HB3	2.55	0.41
1:A:1194:LYS:HB2	1:A:1230:LEU:HD21	2.02	0.41
2:B:95:LEU:HB2	2:B:554:MET:HE2	2.01	0.41
2:B:327:ILE:HD13	2:B:607:LEU:HD11	2.01	0.41
1:A:40:LEU:HG	1:A:405:LEU:HD23	2.02	0.41
1:A:711:SER:HB2	1:A:744:TYR:CE1	2.55	0.41
1:A:927:HIS:HD2	1:A:929:ASP:H	1.67	0.41
1:A:208:SER:OG	1:A:209:GLU:N	2.54	0.41
1:A:710:VAL:HG13	1:A:758:LEU:HA	2.02	0.41
2:B:338:LYS:N	2:B:338:LYS:HD2	2.35	0.41
1:A:37:THR:O	1:A:41:VAL:HG23	2.20	0.41
1:A:702:ARG:HH22	2:B:427:ASP:CG	2.28	0.41
1:A:1000:TRP:HB2	2:B:336:ARG:HH11	1.86	0.41
1:A:408:GLU:CD	1:A:797:LYS:HD2	2.45	0.41
1:A:607:ILE:HA	1:A:608:PRO:HD3	1.90	0.41
1:A:803:VAL:HG22	1:A:877:LYS:HB2	2.02	0.41
2:B:163:HIS:O	2:B:166:SER:OG	2.33	0.41
1:A:568:LYS:HD2	1:A:568:LYS:HA	1.72	0.41
1:A:608:PRO:HB2	1:A:787:VAL:HG12	2.02	0.41
1:A:622:GLU:CD	1:A:622:GLU:H	2.29	0.41
1:A:675:LYS:HE2	1:A:675:LYS:HB3	1.93	0.41
1:A:710:VAL:HG11	1:A:761:PHE:CD2	2.56	0.41
1:A:781:LEU:HD12	1:A:781:LEU:H	1.85	0.41
1:A:1049:PHE:CD1	2:B:552:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:HIS:O	1:A:1069:GLN:HG2	2.21	0.41
2:B:60:MET:HE2	2:B:60:MET:HB2	1.85	0.41
2:B:953:LYS:H	2:B:953:LYS:HG2	1.54	0.41
1:A:12:THR:HB	1:A:15:GLN:HG3	2.03	0.41
3:X:46:DT:H2"	3:X:47:DA:H8	1.85	0.41
1:A:629:VAL:HG11	1:A:717:VAL:HG11	2.03	0.40
2:B:219:ARG:NH1	2:B:223:GLN:OE1	2.53	0.40
2:B:497:THR:HA	2:B:559:GLU:HA	2.03	0.40
2:B:618:PRO:HD3	2:B:647:LEU:HG	2.03	0.40
1:A:519:ASP:O	1:A:520:ASN:ND2	2.54	0.40
1:A:561:LYS:HE2	1:A:561:LYS:HB3	1.90	0.40
1:A:1068:MET:HE3	1:A:1224:PHE:HE1	1.86	0.40
2:B:487:GLN:HG2	2:B:491:ARG:HD2	2.03	0.40
2:B:1068:LYS:HG2	2:B:1074:ARG:HB3	2.04	0.40
1:A:139:GLU:HB3	1:A:771:ARG:NH2	2.36	0.40
1:A:657:GLU:O	1:A:661:ILE:HG13	2.22	0.40
2:B:189:LEU:HD12	2:B:189:LEU:HA	1.94	0.40
2:B:315:MET:O	2:B:668:SER:HA	2.20	0.40
1:A:860:LEU:HD12	1:A:860:LEU:HA	1.80	0.40
2:B:1152:ILE:O	2:B:1156:ILE:HG13	2.21	0.40
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.94	0.40
2:B:73:TRP:O	2:B:77:GLN:HG2	2.20	0.40
2:B:464:THR:O	2:B:468:ILE:HG13	2.22	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	1167/1232 (95%)	1137 (97%)	29 (2%)	1 (0%)	48 80
2	B	1153/1166 (99%)	1120 (97%)	31 (3%)	2 (0%)	43 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2320/2398 (97%)	2257 (97%)	60 (3%)	3 (0%)	48 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	177	ALA
1	A	592	MET
2	B	1043	GLY

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	1019/1062 (96%)	927 (91%)	92 (9%)	9 34
2	B	1022/1029 (99%)	953 (93%)	69 (7%)	14 45
All	All	2041/2091 (98%)	1880 (92%)	161 (8%)	11 39

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	24	GLN
1	A	42	GLU
1	A	46	ARG
1	A	47	LYS
1	A	57	VAL
1	A	73	MET
1	A	74	LYS
1	A	101	LEU
1	A	102	ASN
1	A	115	GLN
1	A	141	ILE
1	A	145	VAL
1	A	178	GLN
1	A	189	ARG

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Mol	Chain	Res	Type
1	A	208	SER
1	A	301	LEU
1	A	316	LEU
1	A	317	GLU
1	A	361	GLN
1	A	371	LEU
1	A	399	GLU
1	A	447	ARG
1	A	448	LEU
1	A	464	SER
1	A	479	ARG
1	A	483	ASP
1	A	499	LYS
1	A	502	GLU
1	A	520	ASN
1	A	545	LEU
1	A	551	GLU
1	A	558	GLU
1	A	568	LYS
1	A	573	LYS
1	A	574	LYS
1	A	580	ILE
1	A	590	ARG
1	A	602	LEU
1	A	622	GLU
1	A	627	LEU
1	A	659	SER
1	A	660	LEU
1	A	672	GLU
1	A	710	VAL
1	A	746	ARG
1	A	753	THR
1	A	762	LEU
1	A	763	ARG
1	A	767	ARG
1	A	771	ARG
1	A	781	LEU
1	A	783	GLU
1	A	789	ARG
1	A	797	LYS
1	A	821	SER
1	A	823	LEU

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Mol	Chain	Res	Type
1	A	826	LYS
1	A	852	LYS
1	A	859	LEU
1	A	860	LEU
1	A	902	ASP
1	A	915	THR
1	A	924	LEU
1	A	956	SER
1	A	959	LEU
1	A	967	ARG
1	A	1014	GLN
1	A	1053	LYS
1	A	1056	THR
1	A	1059	GLU
1	A	1065	HIS
1	A	1066	THR
1	A	1067	VAL
1	A	1069	GLN
1	A	1070	HIS
1	A	1080	GLU
1	A	1084	GLN
1	A	1088	ARG
1	A	1090	TYR
1	A	1094	LEU
1	A	1101	ASP
1	A	1103	ILE
1	A	1110	GLN
1	A	1115	GLU
1	A	1129	GLU
1	A	1152	LEU
1	A	1163	GLU
1	A	1177	ARG
1	A	1179	GLU
1	A	1181	LYS
1	A	1209	GLU
2	B	42	GLN
2	B	60	MET
2	B	69	SER
2	B	74	ARG
2	B	96	LEU
2	B	122	GLN
2	B	146	SER

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Mol	Chain	Res	Type
2	B	148	THR
2	B	153	ARG
2	B	183	SER
2	B	187	LEU
2	B	207	VAL
2	B	239	LYS
2	B	275	TYR
2	B	286	LYS
2	B	300	ARG
2	B	332	HIS
2	B	337	GLU
2	B	353	GLU
2	B	445	LYS
2	B	447	ASP
2	B	460	ASP
2	B	485	LEU
2	B	490	LYS
2	B	510	GLU
2	B	528	ASP
2	B	535	GLN
2	B	552	VAL
2	B	570	GLU
2	B	590	VAL
2	B	594	ASP
2	B	617	ARG
2	B	619	ASP
2	B	635	ILE
2	B	641	SER
2	B	647	LEU
2	B	651	HIS
2	B	701	THR
2	B	753	GLU
2	B	756	ARG
2	B	758	GLN
2	B	777	ARG
2	B	780	SER
2	B	781	ARG
2	B	840	ARG
2	B	862	ASP
2	B	873	LYS
2	B	877	LEU
2	B	887	GLU

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Mol	Chain	Res	Type
2	B	927	LEU
2	B	940	VAL
2	B	945	ARG
2	B	953	LYS
2	B	964	SER
2	B	997	LEU
2	B	1017	GLN
2	B	1020	LEU
2	B	1044	ASP
2	B	1056	GLN
2	B	1063	ILE
2	B	1073	LEU
2	B	1084	GLU
2	B	1085	PHE
2	B	1101	GLU
2	B	1104	THR
2	B	1122	THR
2	B	1127	LYS
2	B	1139	ASN
2	B	1148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	75	HIS
1	A	102	ASN
1	A	110	HIS
1	A	183	GLN
1	A	383	ASN
1	A	402	HIS
1	A	520	ASN
1	A	577	HIS
1	A	579	ASN
1	A	612	ASN
1	A	638	GLN
1	A	749	GLN
1	A	769	GLN
1	A	794	HIS
1	A	819	ASN
1	A	887	HIS
1	A	890	GLN

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Mol	Chain	Res	Type
1	A	912	GLN
1	A	939	HIS
1	A	955	HIS
1	A	1069	GLN
1	A	1084	GLN
1	A	1110	GLN
1	A	1146	HIS
1	A	1202	GLN
2	B	20	ASN
2	B	122	GLN
2	B	163	HIS
2	B	171	GLN
2	B	428	GLN
2	B	487	GLN
2	B	567	GLN
2	B	621	ASN
2	B	809	HIS
2	B	812	HIS
2	B	1017	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ANP	A	2233	5	32,33,33	0.87	3 (9%)	44,52,52	0.80	2 (4%)
4	ANP	B	2161	5	32,33,33	0.94	3 (9%)	44,52,52	1.02	3 (6%)
6	SF4	B	2160	2	0,12,12	-	-	-		

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	ANP	A	2233	5	-	3/18/38/38	0/3/3/3
4	ANP	B	2161	5	-	0/18/38/38	0/3/3/3
6	SF4	B	2160	2	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2161	ANP	PB-O3A	-2.65	1.55	1.59
4	A	2233	ANP	PB-O3A	-2.62	1.55	1.59
4	A	2233	ANP	PG-N3B	2.37	1.69	1.63
4	B	2161	ANP	PG-N3B	2.30	1.69	1.63
4	B	2161	ANP	PG-O1G	2.29	1.49	1.46
4	A	2233	ANP	PG-O1G	2.15	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2161	ANP	PB-O3A-PA	-2.99	122.07	132.62
4	B	2161	ANP	O1G-PG-N3B	-2.76	107.71	111.77
4	A	2233	ANP	PB-O3A-PA	-2.67	123.22	132.62
4	B	2161	ANP	C5-C4-N9	2.37	108.54	105.78
4	A	2233	ANP	O3G-PG-O1G	-2.14	108.07	113.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2233	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
4	A	2233	ANP	PG-N3B-PB-O1B
4	A	2233	ANP	PG-N3B-PB-O3A

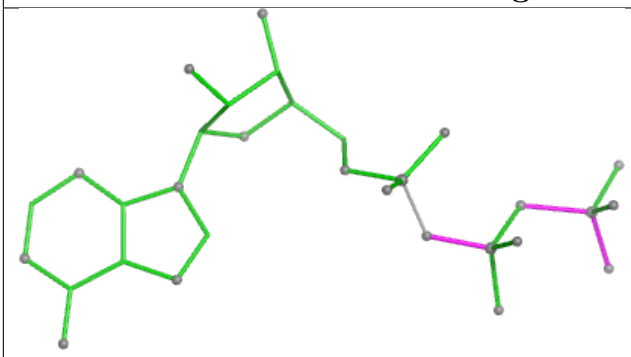
There are no ring outliers.

3 monomers are involved in 8 short contacts:

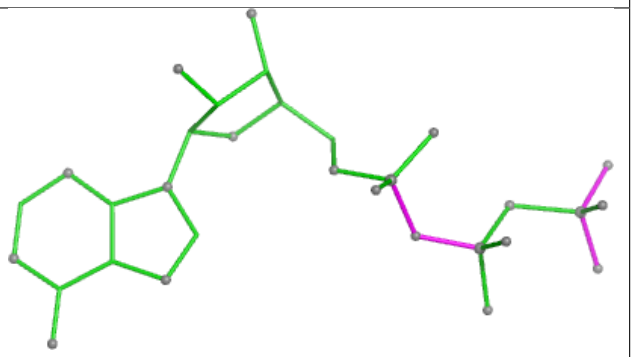
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2233	ANP	2	0
4	B	2161	ANP	5	0
6	B	2160	SF4	1	0

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.

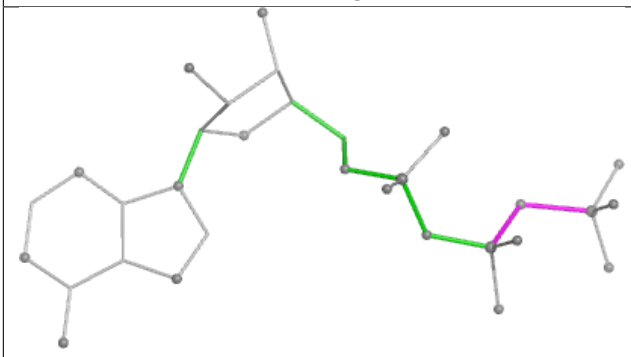
Ligand ANP A 2233



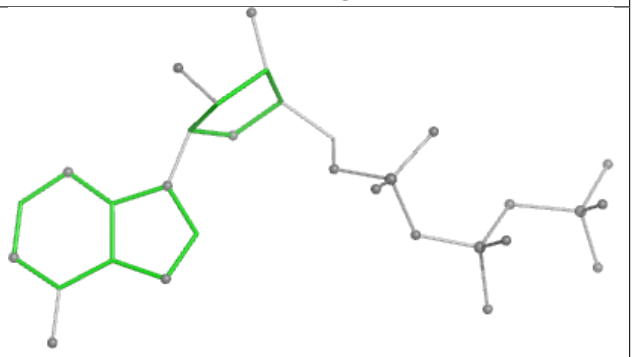
Bond lengths



Bond angles

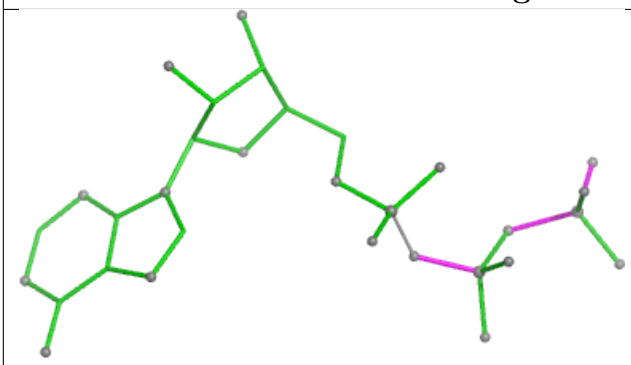


Torsions

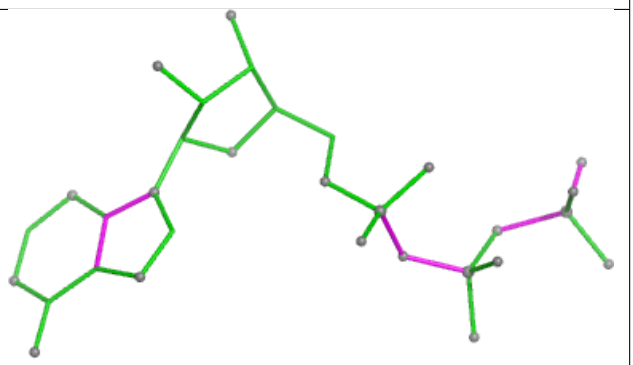


Rings

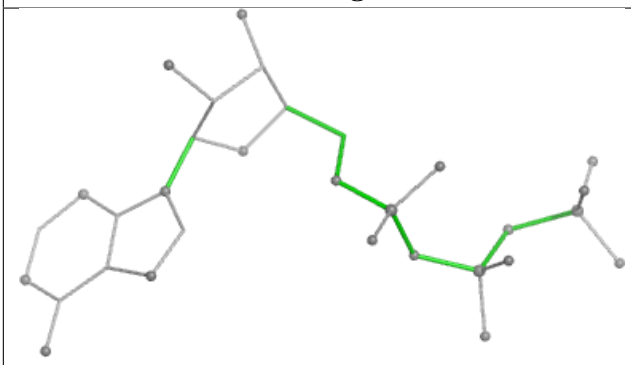
Ligand ANP B 2161



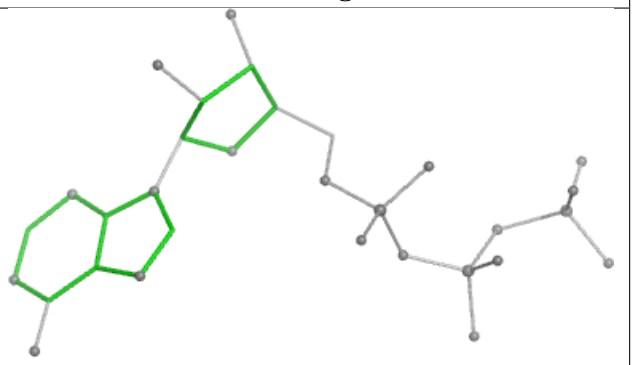
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1177/1232 (95%)	-0.37	1 (0%)	92	86	35, 79, 137, 163	0
2	B	1156/1166 (99%)	-0.40	1 (0%)	92	86	33, 76, 120, 142	1 (0%)
3	X	46/70 (65%)	0.16	0	100	100	67, 143, 166, 176	0
All	All	2379/2468 (96%)	-0.37	2 (0%)	92	86	33, 78, 132, 176	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	455	VAL	2.2
1	A	1060	LYS	2.2

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ANP	A	2233	31/31	0.91	0.07	64,84,94,97	0

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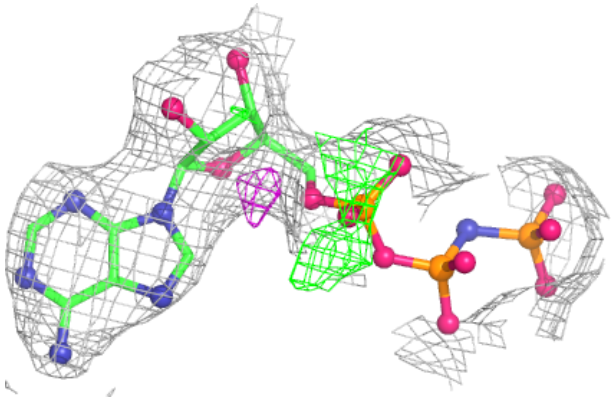
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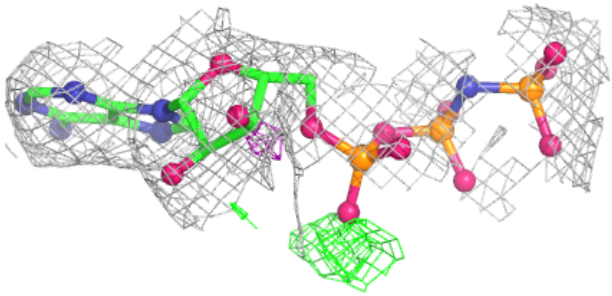
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ANP	B	2161	31/31	0.93	0.08	60,89,109,111	0
6	SF4	B	2160	8/8	0.94	0.05	86,113,125,125	0
5	MG	B	2162	1/1	0.98	0.05	78,78,78,78	0
5	MG	A	2234	1/1	0.99	0.06	85,85,85,85	0

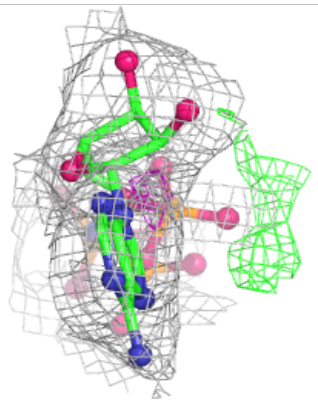
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 2233:

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

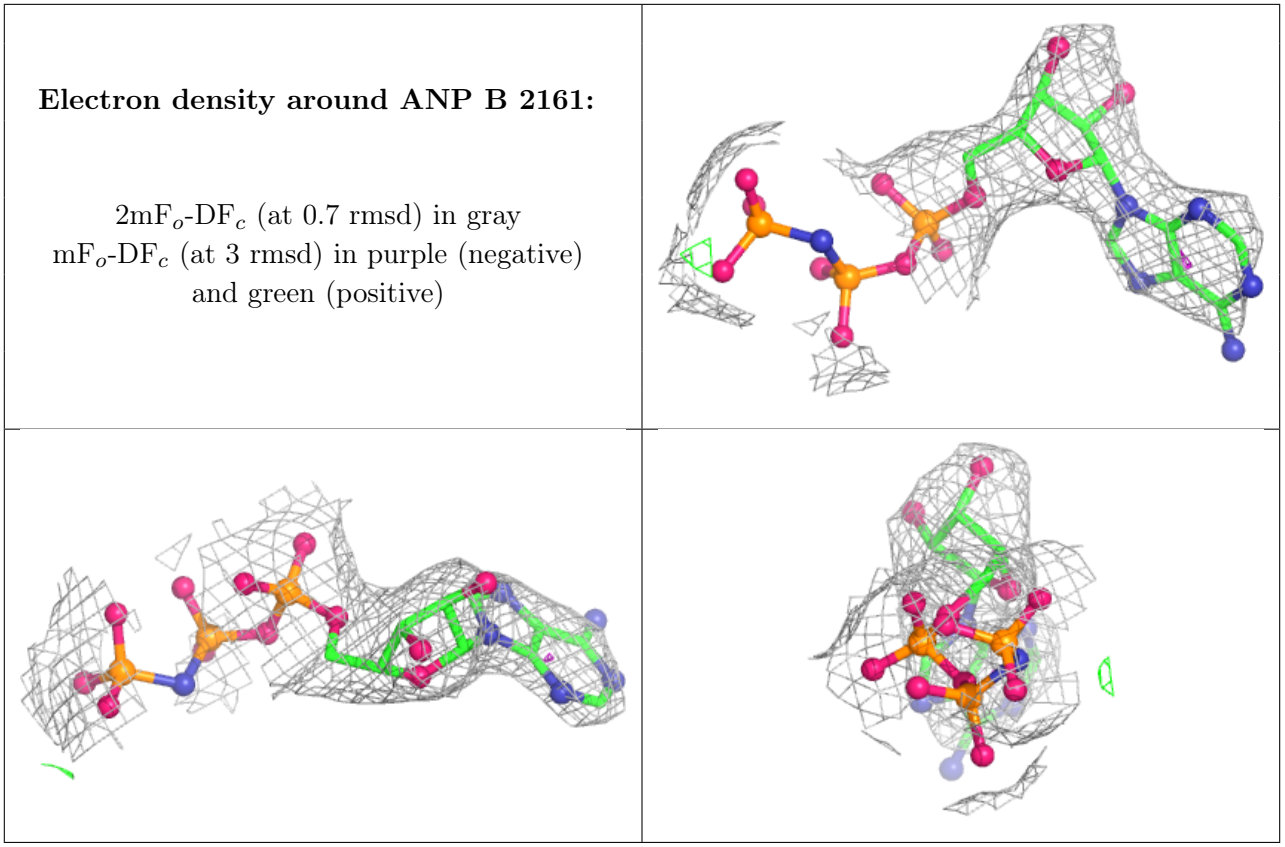






Electron density around ANP B 2161:

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



6.5 Other polymers

There are no such residues in this entry.