



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CHQ
Title : REPLICATION FACTOR C ADPNP COMPLEX
Authors : Seybert, A.; Singleton, M.R.; Cook, N.; Hall, D.R.; Wigley, D.B.
Deposited on : 2006-03-16
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

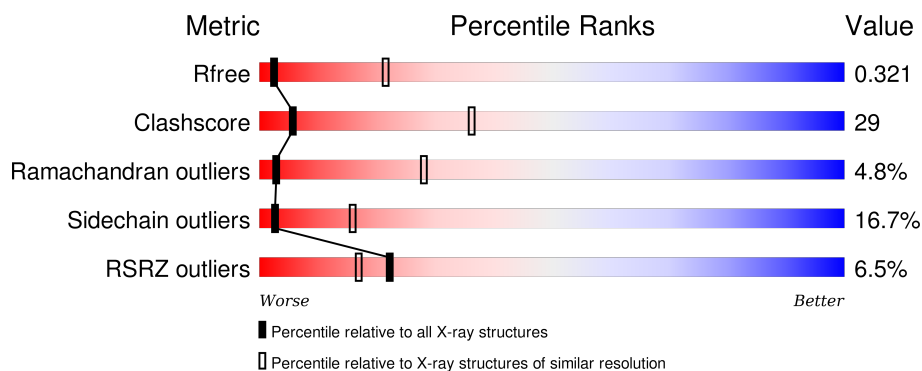
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	319	<div> <div>6%</div> <div>50% 36% 11% ..</div> </div>
1	B	319	<div> <div>6%</div> <div>51% 37% 10% ..</div> </div>
1	C	319	<div> <div>8%</div> <div>50% 37% 10% ..</div> </div>

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

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

2 Entry composition [i](#)

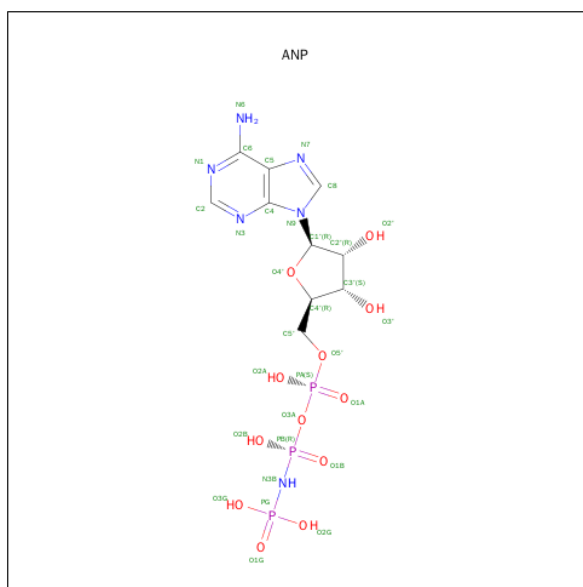
There are 2 unique types of molecules in this entry. The entry contains 7512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 REPLICATION FACTOR C SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	1
			2473	1570	427	463	13			
1	B	314	Total	C	N	O	S	0	0	1
			2473	1570	427	463	13			
1	C	314	Total	C	N	O	S	0	0	1
			2473	1570	427	463	13			

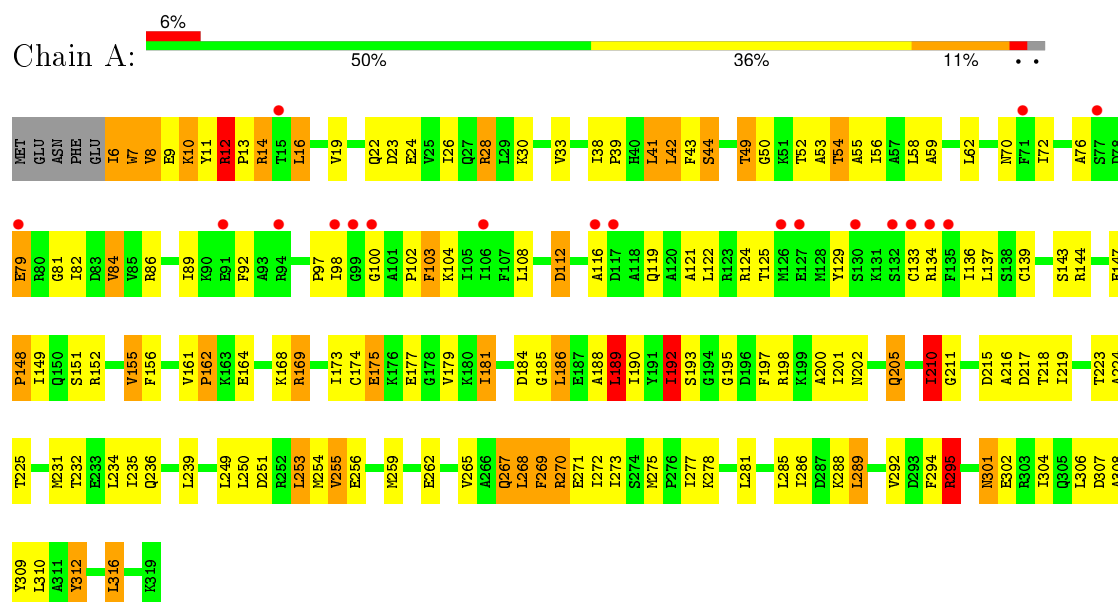
- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



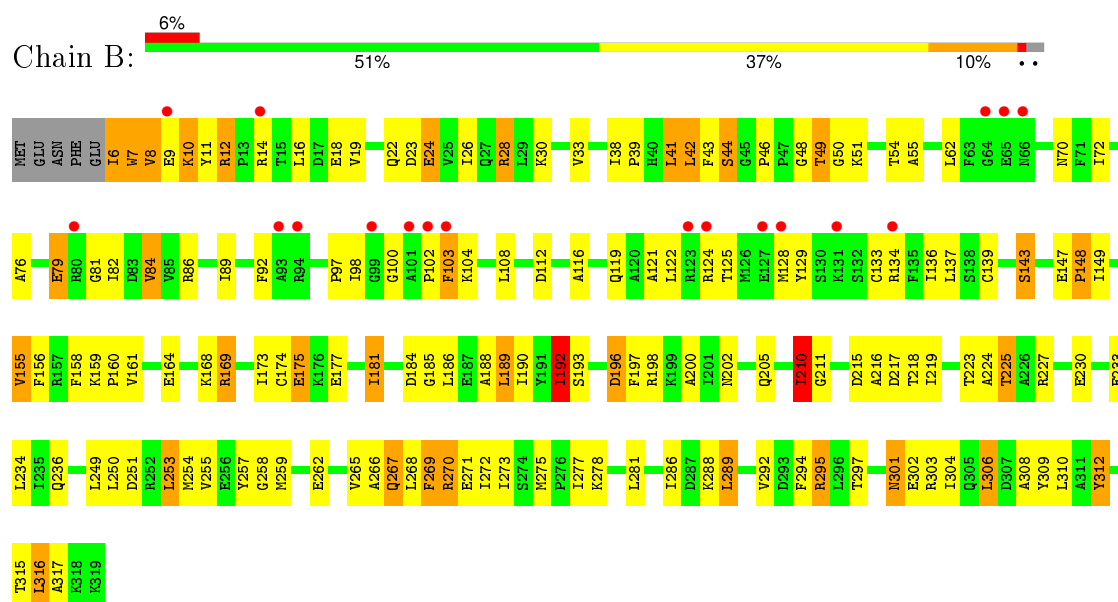
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

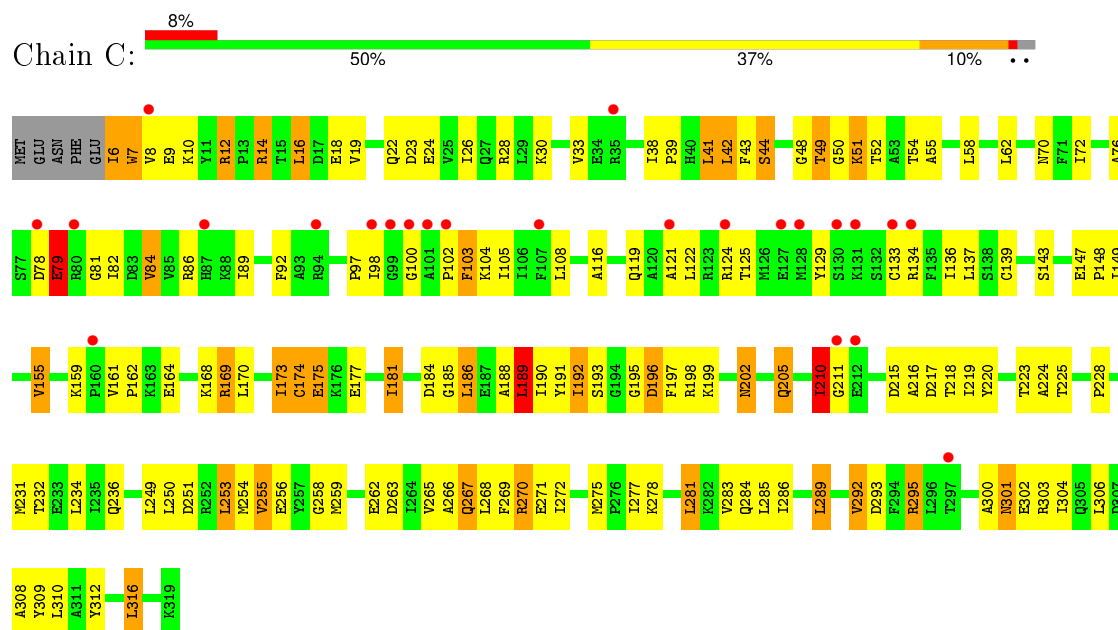
• Molecule 1: REPLICATION FACTOR C SMALL SUBUNIT



• Molecule 1: REPLICATION FACTOR C SMALL SUBUNIT



• Molecule 1: REPLICATION FACTOR C SMALL SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.17Å 109.17Å 257.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 3.50 19.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (95.35-3.50) 99.8 (19.94-3.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.297 , 0.324 0.287 , 0.321	Depositor DCC
R_{free} test set	1175 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	126.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 161.3	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22929 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å ²)	204.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.81	1/2511 (0.0%)	0.85	4/3384 (0.1%)
1	B	0.79	0/2511	0.84	0/3384
1	C	0.79	1/2511 (0.0%)	0.84	2/3384 (0.1%)
All	All	0.79	2/7533 (0.0%)	0.84	6/10152 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	CYS	CB-SG	-5.87	1.72	1.81
1	A	12	ARG	CG-CD	5.22	1.65	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASP	CB-CG-OD1	6.69	124.33	118.30
1	A	268	LEU	CB-CG-CD2	5.92	121.06	111.00
1	A	268	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	C	281	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	295	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	79	GLU	N-CA-C	5.08	124.71	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2473	0	2522	170	1
1	B	2473	0	2522	159	0
1	C	2473	0	2522	133	1
2	A	31	0	13	19	0
2	B	31	0	13	9	0
2	C	31	0	13	7	0
All	All	7512	0	7605	442	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 29.

All (442) 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:152:ARG:HG3	1:B:6:ILE:HD11	1.29	1.11
1:B:147:GLU:HG3	1:C:199:LYS:NZ	1.71	1.05
1:B:268:LEU:O	1:B:272:ILE:HG12	1.55	1.04
1:A:268:LEU:O	1:A:272:ILE:HG12	1.57	1.04
1:A:174:CYS:SG	1:A:181:ILE:HD11	2.04	0.96
1:C:191:TYR:OH	1:C:270:ARG:HD2	1.65	0.96
1:C:268:LEU:O	1:C:272:ILE:HG12	1.65	0.95
1:B:224:ALA:HA	1:B:257:TYR:HB3	1.48	0.95
1:B:50:GLY:O	1:B:54:THR:HG23	1.68	0.93
1:C:7:TRP:H	1:C:7:TRP:HD1	1.04	0.92
1:A:147:GLU:HB3	1:B:198:ARG:NH1	1.84	0.92
1:A:9:GLU:HG3	1:A:12:ARG:NE	1.84	0.92
1:C:92:PHE:CZ	1:C:104:LYS:HB3	2.05	0.91
1:A:92:PHE:CZ	1:A:104:LYS:HB3	2.06	0.91
1:B:147:GLU:HG3	1:C:199:LYS:HZ1	1.30	0.91
1:B:7:TRP:H	1:B:7:TRP:HD1	1.12	0.90
1:B:270:ARG:HH12	1:C:303:ARG:NH1	1.69	0.90
1:A:147:GLU:HB3	1:B:198:ARG:HH11	1.36	0.90
1:A:7:TRP:H	1:A:7:TRP:HD1	1.00	0.90
1:A:50:GLY:O	1:A:54:THR:HG23	1.72	0.89
1:B:92:PHE:CZ	1:B:104:LYS:HB3	2.08	0.89
1:A:301:ASN:HD22	1:A:302:GLU:N	1.71	0.88
1:B:174:CYS:SG	1:B:181:ILE:HD11	2.15	0.86
1:A:10:LYS:NZ	1:A:177:GLU:OE2	2.09	0.86
1:A:9:GLU:HA	1:A:12:ARG:HE	1.41	0.86
1:C:184:ASP:HB3	1:C:216:ALA:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG13	1:A:278:LYS:H	1.41	0.86
1:C:19:VAL:HG11	1:C:54:THR:HG22	1.57	0.85
1:A:148:PRO:HD3	1:B:198:ARG:NH1	1.92	0.85
1:C:7:TRP:CE2	1:C:205:GLN:NE2	2.45	0.84
1:A:147:GLU:OE2	1:B:198:ARG:HG2	1.77	0.84
1:B:9:GLU:HG3	1:B:12:ARG:NE	1.91	0.84
1:B:103:PHE:HD2	1:B:103:PHE:H	1.26	0.84
1:A:19:VAL:HG11	1:A:54:THR:HG22	1.60	0.84
1:B:270:ARG:NH1	1:C:303:ARG:NH1	2.25	0.83
1:A:147:GLU:OE1	1:B:202:ASN:ND2	2.10	0.82
1:B:19:VAL:HG11	1:B:54:THR:HG22	1.63	0.80
1:C:174:CYS:SG	1:C:181:ILE:HD11	2.20	0.80
1:B:184:ASP:HB3	1:B:216:ALA:HB2	1.63	0.80
1:B:301:ASN:HD22	1:B:302:GLU:N	1.79	0.80
1:C:9:GLU:HA	1:C:12:ARG:HE	1.46	0.80
1:B:6:ILE:HG23	1:B:6:ILE:O	1.81	0.80
1:B:9:GLU:HA	1:B:12:ARG:HE	1.47	0.80
1:C:103:PHE:HD2	1:C:103:PHE:H	1.26	0.80
1:A:103:PHE:H	1:A:103:PHE:HD2	1.27	0.80
1:A:184:ASP:HB3	1:A:216:ALA:HB2	1.63	0.80
1:B:277:ILE:HG12	1:B:281:LEU:HD22	1.64	0.80
1:A:152:ARG:CG	1:B:6:ILE:HD11	2.09	0.79
1:C:277:ILE:HG13	1:C:278:LYS:H	1.46	0.78
2:A:700:ANP:H8	2:A:700:ANP:O5'	1.83	0.78
1:B:254:MET:HA	1:B:259:MET:CE	2.14	0.77
1:A:7:TRP:CD1	1:A:7:TRP:N	2.48	0.77
2:A:700:ANP:O5'	2:A:700:ANP:C8	2.34	0.76
1:C:301:ASN:HD22	1:C:302:GLU:N	1.84	0.76
1:A:277:ILE:HG13	1:A:278:LYS:N	1.97	0.76
1:A:9:GLU:HG3	1:A:12:ARG:CZ	2.15	0.75
1:A:86:ARG:HA	1:A:89:ILE:HG12	1.68	0.75
1:C:18:GLU:O	1:C:169:ARG:NH2	2.20	0.75
1:A:53:ALA:HB2	2:A:700:ANP:O2A	1.86	0.75
1:C:271:GLU:O	1:C:275:MET:HG2	1.86	0.75
1:B:277:ILE:HG13	1:B:278:LYS:H	1.51	0.74
1:C:86:ARG:HA	1:C:89:ILE:HG12	1.70	0.74
1:B:86:ARG:HA	1:B:89:ILE:HG12	1.68	0.74
1:A:152:ARG:HG3	1:B:6:ILE:CD1	2.15	0.74
2:B:700:ANP:H8	2:B:700:ANP:C5'	2.18	0.73
1:C:277:ILE:HG12	1:C:281:LEU:HD22	1.71	0.73
1:C:50:GLY:O	1:C:54:THR:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG12	1:A:281:LEU:HD22	1.71	0.73
1:B:271:GLU:O	1:B:275:MET:HG2	1.89	0.72
1:B:169:ARG:O	1:B:173:ILE:HG12	1.89	0.72
1:C:169:ARG:O	1:C:173:ILE:HG12	1.88	0.72
1:B:217:ASP:OD1	1:B:227:ARG:HD2	1.89	0.72
1:A:271:GLU:O	1:A:275:MET:HG2	1.88	0.72
1:A:147:GLU:CD	1:B:202:ASN:HD22	1.93	0.72
2:B:700:ANP:H8	2:B:700:ANP:H5'1	1.71	0.72
1:B:270:ARG:HH12	1:C:303:ARG:HH11	1.34	0.72
1:B:39:PRO:O	1:B:41:LEU:HD13	1.90	0.71
1:C:119:GLN:HB3	1:C:149:ILE:HD11	1.73	0.70
1:C:198:ARG:O	1:C:202:ASN:HB2	1.92	0.70
1:A:39:PRO:O	1:A:41:LEU:HD13	1.92	0.69
1:A:169:ARG:O	1:A:173:ILE:HG12	1.92	0.69
1:A:6:ILE:O	1:A:8:VAL:N	2.24	0.69
1:A:301:ASN:HD22	1:A:301:ASN:C	1.94	0.69
1:A:12:ARG:HA	2:A:700:ANP:O2'	1.93	0.69
1:C:277:ILE:HG13	1:C:278:LYS:N	2.07	0.69
1:C:125:THR:HG22	1:C:129:TYR:CE1	2.28	0.69
1:B:42:LEU:HB3	1:B:155:VAL:HG22	1.75	0.68
1:B:270:ARG:NH1	1:C:303:ARG:HH11	1.90	0.68
1:C:103:PHE:HD2	1:C:103:PHE:N	1.92	0.68
1:B:304:ILE:O	1:B:308:ALA:HB2	1.94	0.68
1:A:103:PHE:N	1:A:103:PHE:HD2	1.93	0.67
1:C:39:PRO:O	1:C:41:LEU:HD13	1.93	0.67
1:C:9:GLU:HG3	1:C:12:ARG:NE	2.10	0.67
1:C:6:ILE:HG23	1:C:6:ILE:O	1.94	0.67
1:C:19:VAL:HB	1:C:26:ILE:HD11	1.75	0.67
1:B:277:ILE:HG13	1:B:278:LYS:N	2.10	0.67
1:A:19:VAL:HB	1:A:26:ILE:HD11	1.76	0.67
1:A:38:ILE:HG22	1:A:134:ARG:HG2	1.77	0.67
1:A:125:THR:HG22	1:A:129:TYR:CE1	2.30	0.66
1:B:48:GLY:HA2	2:B:700:ANP:HNB1	1.61	0.66
1:B:38:ILE:HG22	1:B:134:ARG:HG2	1.76	0.66
1:A:6:ILE:HA	1:A:205:GLN:OE1	1.96	0.66
1:A:231:MET:HE3	1:A:268:LEU:HD23	1.77	0.66
1:B:119:GLN:HB3	1:B:149:ILE:HD11	1.78	0.66
1:B:125:THR:HG22	1:B:129:TYR:CE1	2.29	0.66
1:C:103:PHE:N	1:C:103:PHE:CD2	2.64	0.65
1:B:103:PHE:N	1:B:103:PHE:HD2	1.91	0.65
2:B:700:ANP:O1A	2:B:700:ANP:N3B	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:MET:HA	1:C:259:MET:CE	2.27	0.65
1:B:9:GLU:HG3	1:B:12:ARG:CZ	2.27	0.65
1:C:38:ILE:HG22	1:C:134:ARG:HG2	1.79	0.65
1:B:198:ARG:O	1:B:202:ASN:HB2	1.98	0.64
1:B:223:THR:OG1	1:B:225:THR:OG1	2.15	0.64
1:A:151:SER:HA	1:B:202:ASN:OD1	1.98	0.64
1:C:7:TRP:CD1	1:C:7:TRP:N	2.52	0.64
1:A:231:MET:CE	1:A:268:LEU:HD23	2.28	0.64
1:B:49:THR:HG21	1:B:159:LYS:O	1.97	0.64
1:A:119:GLN:HB3	1:A:149:ILE:HD11	1.80	0.64
1:C:129:TYR:CB	1:C:133:CYS:HB2	2.28	0.63
1:B:129:TYR:CB	1:B:133:CYS:HB2	2.28	0.63
2:C:700:ANP:O2G	2:C:700:ANP:O1A	2.16	0.63
1:B:6:ILE:CG2	1:B:6:ILE:O	2.46	0.63
1:A:198:ARG:O	1:A:202:ASN:HB2	1.99	0.63
1:B:48:GLY:H	2:B:700:ANP:HNB1	1.46	0.63
2:C:700:ANP:N3B	2:C:700:ANP:O1A	2.31	0.63
1:C:48:GLY:HA2	2:C:700:ANP:HNB1	1.63	0.63
1:B:19:VAL:HB	1:B:26:ILE:HD11	1.80	0.62
1:B:297:THR:HG21	1:C:300:ALA:HA	1.80	0.62
1:A:254:MET:HA	1:A:259:MET:CE	2.29	0.62
1:A:8:VAL:HG23	2:A:700:ANP:H4'	1.82	0.62
1:B:103:PHE:N	1:B:103:PHE:CD2	2.64	0.62
1:A:129:TYR:CB	1:A:133:CYS:HB2	2.30	0.61
1:A:81:GLY:HA2	1:A:84:VAL:HG12	1.82	0.61
1:B:48:GLY:CA	2:B:700:ANP:HNB1	2.13	0.61
1:C:97:PRO:HG3	1:C:104:LYS:HG3	1.81	0.61
1:A:301:ASN:ND2	1:A:301:ASN:C	2.53	0.61
1:A:190:ILE:HA	1:A:193:SER:OG	2.00	0.61
1:B:210:ILE:HG22	1:B:211:GLY:H	1.65	0.61
1:C:250:LEU:HD12	1:C:254:MET:HG3	1.82	0.60
1:A:174:CYS:O	1:A:177:GLU:N	2.32	0.60
1:A:198:ARG:NE	2:A:700:ANP:O1B	2.33	0.60
1:A:42:LEU:HB3	1:A:155:VAL:HG22	1.82	0.60
2:A:700:ANP:H8	2:A:700:ANP:C5'	2.31	0.60
1:A:198:ARG:HE	2:A:700:ANP:PB	2.25	0.59
1:C:42:LEU:HB3	1:C:155:VAL:HG22	1.83	0.59
1:B:224:ALA:CA	1:B:257:TYR:HB3	2.29	0.59
1:C:19:VAL:HB	1:C:26:ILE:CD1	2.33	0.59
1:A:103:PHE:CD2	1:A:103:PHE:N	2.65	0.59
1:B:215:ASP:HB3	1:B:218:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:700:ANP:O5'	2:C:700:ANP:H8	2.03	0.59
1:B:174:CYS:O	1:B:175:GLU:C	2.41	0.59
1:A:9:GLU:CB	1:A:12:ARG:HH21	2.16	0.58
1:A:9:GLU:HG3	1:A:12:ARG:HE	1.65	0.58
1:B:169:ARG:HH11	1:B:169:ARG:HB2	1.68	0.58
1:A:7:TRP:HH2	1:A:179:VAL:HG21	1.68	0.58
1:B:190:ILE:HA	1:B:193:SER:OG	2.03	0.58
1:B:8:VAL:HG23	2:B:700:ANP:H4'	1.83	0.58
1:C:190:ILE:HA	1:C:193:SER:OG	2.02	0.58
1:C:210:ILE:HG22	1:C:211:GLY:H	1.68	0.58
1:B:254:MET:HA	1:B:259:MET:HE1	1.85	0.58
1:C:125:THR:HG22	1:C:129:TYR:HE1	1.67	0.58
1:B:125:THR:HG22	1:B:129:TYR:HE1	1.67	0.58
1:C:51:LYS:HE3	2:C:700:ANP:O3G	2.02	0.58
1:B:48:GLY:N	2:B:700:ANP:HNB1	2.01	0.58
1:A:97:PRO:HG3	1:A:104:LYS:HG3	1.86	0.58
1:B:41:LEU:HB2	1:B:136:ILE:HG12	1.86	0.58
1:A:292:VAL:HG21	1:A:309:TYR:HB2	1.86	0.58
1:B:97:PRO:HG3	1:B:104:LYS:HG3	1.85	0.57
1:C:301:ASN:ND2	1:C:301:ASN:C	2.58	0.57
1:A:49:THR:O	2:A:700:ANP:N6	2.35	0.57
1:A:188:ALA:C	1:A:190:ILE:H	2.08	0.57
1:A:41:LEU:HB2	1:A:136:ILE:HG12	1.85	0.57
1:A:250:LEU:HD23	1:A:310:LEU:HD11	1.85	0.57
1:B:292:VAL:HG21	1:B:309:TYR:HB2	1.85	0.57
1:B:301:ASN:HD22	1:B:301:ASN:C	2.04	0.57
1:C:42:LEU:HD23	1:C:137:LEU:O	2.04	0.57
1:A:6:ILE:O	1:A:6:ILE:HG23	2.05	0.57
1:B:301:ASN:ND2	1:B:301:ASN:C	2.56	0.57
1:A:53:ALA:CB	2:A:700:ANP:O2A	2.51	0.56
1:C:174:CYS:O	1:C:177:GLU:N	2.30	0.56
1:C:30:LYS:O	1:C:33:VAL:HG22	2.05	0.56
1:A:30:LYS:O	1:A:33:VAL:HG22	2.05	0.56
1:A:125:THR:HG22	1:A:129:TYR:HE1	1.68	0.56
1:B:81:GLY:HA2	1:B:84:VAL:HG12	1.86	0.56
1:B:224:ALA:CB	1:B:257:TYR:O	2.53	0.56
1:B:86:ARG:HA	1:B:89:ILE:CG1	2.34	0.56
1:B:304:ILE:O	1:B:308:ALA:CB	2.54	0.56
1:C:86:ARG:HA	1:C:89:ILE:CG1	2.35	0.56
1:B:249:LEU:O	1:B:253:LEU:HB2	2.06	0.56
1:C:7:TRP:CZ2	1:C:205:GLN:NE2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:VAL:HG11	1:C:54:THR:CG2	2.33	0.55
1:A:174:CYS:O	1:A:175:GLU:C	2.44	0.55
1:C:301:ASN:HD22	1:C:301:ASN:C	2.03	0.55
1:B:30:LYS:O	1:B:33:VAL:HG22	2.06	0.55
1:C:129:TYR:HB2	1:C:133:CYS:HB2	1.88	0.55
1:C:81:GLY:HA2	1:C:84:VAL:HG12	1.88	0.55
1:A:19:VAL:HB	1:A:26:ILE:CD1	2.35	0.55
1:B:9:GLU:HG3	1:B:12:ARG:HE	1.71	0.55
1:A:42:LEU:HD23	1:A:137:LEU:O	2.05	0.55
1:C:174:CYS:O	1:C:175:GLU:C	2.44	0.55
1:A:210:ILE:HG22	1:A:211:GLY:H	1.71	0.55
1:B:19:VAL:HB	1:B:26:ILE:CD1	2.36	0.55
1:B:42:LEU:HD23	1:B:137:LEU:O	2.07	0.55
1:A:294:PHE:O	1:A:295:ARG:C	2.44	0.55
1:C:215:ASP:HB3	1:C:218:THR:HG23	1.89	0.55
1:A:86:ARG:HA	1:A:89:ILE:CG1	2.35	0.54
1:C:129:TYR:HB3	1:C:133:CYS:HB2	1.89	0.54
1:C:255:VAL:O	1:C:256:GLU:C	2.45	0.54
1:B:129:TYR:HB3	1:B:133:CYS:HB2	1.89	0.54
1:C:192:ILE:HG13	1:C:223:THR:HG21	1.89	0.54
1:A:76:ALA:HB2	1:A:108:LEU:HG	1.89	0.54
1:A:9:GLU:CA	1:A:12:ARG:HH21	2.20	0.54
1:B:147:GLU:CG	1:C:199:LYS:NZ	2.59	0.54
1:C:231:MET:HE3	1:C:268:LEU:HD23	1.89	0.54
1:A:285:LEU:N	1:A:285:LEU:HD12	2.23	0.54
1:C:292:VAL:HG21	1:C:309:TYR:HB2	1.90	0.54
1:A:8:VAL:HA	1:A:201:ILE:HG21	1.90	0.53
1:B:147:GLU:HG3	1:C:199:LYS:CE	2.37	0.53
1:A:13:PRO:HD3	2:A:700:ANP:O2'	2.08	0.53
1:A:197:PHE:O	1:A:200:ALA:N	2.41	0.53
1:B:9:GLU:CA	1:B:12:ARG:HH21	2.21	0.53
1:A:129:TYR:HB3	1:A:133:CYS:HB2	1.90	0.53
1:A:147:GLU:O	1:A:149:ILE:N	2.42	0.53
1:A:215:ASP:HB3	1:A:218:THR:HG23	1.89	0.53
1:C:249:LEU:O	1:C:253:LEU:HB2	2.09	0.53
1:B:164:GLU:H	1:B:164:GLU:CD	2.12	0.53
1:B:250:LEU:HD12	1:B:254:MET:HG3	1.90	0.53
1:B:192:ILE:HG13	1:B:223:THR:HG21	1.90	0.53
1:C:41:LEU:HB2	1:C:136:ILE:HG12	1.89	0.53
1:B:129:TYR:HB2	1:B:133:CYS:HB2	1.89	0.53
1:B:262:GLU:O	1:B:265:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:H	1:C:164:GLU:CD	2.12	0.53
1:C:231:MET:CE	1:C:268:LEU:HD23	2.39	0.53
1:B:147:GLU:HG3	1:C:199:LYS:HZ3	1.66	0.53
1:C:304:ILE:O	1:C:308:ALA:HB2	2.08	0.53
1:C:6:ILE:O	1:C:6:ILE:CG2	2.57	0.52
1:B:188:ALA:C	1:B:190:ILE:H	2.12	0.52
1:B:301:ASN:ND2	1:B:302:GLU:N	2.54	0.52
1:A:192:ILE:HG13	1:A:223:THR:HG21	1.89	0.52
1:C:285:LEU:N	1:C:285:LEU:HD12	2.24	0.52
1:A:50:GLY:HA2	2:A:700:ANP:O2A	2.09	0.52
1:C:43:PHE:HB3	1:C:51:LYS:HG2	1.90	0.52
1:A:185:GLY:O	1:A:189:LEU:HB2	2.09	0.52
1:C:147:GLU:O	1:C:149:ILE:N	2.43	0.52
1:C:48:GLY:CA	2:C:700:ANP:HNB1	2.22	0.52
1:C:9:GLU:HG3	1:C:12:ARG:CZ	2.39	0.52
1:C:98:ILE:HD12	1:C:98:ILE:H	1.75	0.52
1:A:9:GLU:O	1:A:12:ARG:HB2	2.10	0.52
1:A:98:ILE:H	1:A:98:ILE:HD12	1.75	0.52
1:A:270:ARG:HH12	1:B:303:ARG:NH1	2.07	0.52
1:A:9:GLU:HA	1:A:12:ARG:NE	2.17	0.51
1:B:9:GLU:O	1:B:12:ARG:HB2	2.09	0.51
1:A:217:ASP:O	1:A:218:THR:C	2.49	0.51
1:B:98:ILE:H	1:B:98:ILE:HD12	1.75	0.51
1:A:164:GLU:H	1:A:164:GLU:CD	2.14	0.51
1:A:269:PHE:CZ	1:A:273:ILE:HD11	2.46	0.51
1:B:197:PHE:O	1:B:198:ARG:C	2.47	0.51
1:A:129:TYR:HB2	1:A:133:CYS:HB2	1.92	0.51
1:B:147:GLU:O	1:B:149:ILE:N	2.44	0.51
1:C:250:LEU:HD12	1:C:250:LEU:O	2.11	0.50
1:C:220:TYR:CE1	1:C:228:PRO:HD2	2.46	0.50
1:C:191:TYR:OH	1:C:270:ARG:CD	2.51	0.50
1:B:217:ASP:O	1:B:218:THR:C	2.50	0.50
1:A:28:ARG:HE	1:A:156:PHE:HE2	1.60	0.50
2:A:700:ANP:H5'2	2:A:700:ANP:O1B	2.12	0.49
1:B:224:ALA:HB2	1:B:257:TYR:O	2.12	0.49
1:B:10:LYS:HG2	1:B:11:TYR:CE1	2.47	0.49
1:C:49:THR:HG21	1:C:159:LYS:O	2.11	0.49
1:A:169:ARG:O	1:A:173:ILE:CG1	2.60	0.49
1:A:19:VAL:HG11	1:A:54:THR:CG2	2.39	0.49
1:B:9:GLU:CB	1:B:12:ARG:HH21	2.25	0.49
1:A:44:SER:HB2	1:A:139:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:CB	1:B:202:ASN:HD21	2.26	0.49
1:B:224:ALA:HB1	1:B:257:TYR:O	2.13	0.49
1:A:232:THR:HG22	1:A:271:GLU:HB3	1.93	0.49
1:B:250:LEU:HD23	1:B:310:LEU:HD11	1.95	0.49
1:A:11:TYR:CG	1:A:173:ILE:HD13	2.48	0.48
1:A:250:LEU:HD12	1:A:254:MET:HG3	1.94	0.48
1:A:151:SER:HA	1:B:202:ASN:CG	2.33	0.48
1:A:147:GLU:CD	1:B:202:ASN:ND2	2.64	0.48
1:A:301:ASN:ND2	1:A:302:GLU:N	2.53	0.48
1:A:188:ALA:O	1:A:190:ILE:N	2.45	0.48
1:B:9:GLU:HA	1:B:12:ARG:NE	2.23	0.48
1:B:143:SER:CB	1:C:263:ASP:OD2	2.61	0.48
1:B:185:GLY:O	1:B:189:LEU:HB2	2.14	0.48
1:A:259:MET:HE3	1:A:259:MET:HB2	1.75	0.47
1:B:46:PRO:HG3	1:B:160:PRO:HD3	1.95	0.47
1:C:217:ASP:O	1:C:218:THR:C	2.52	0.47
1:A:7:TRP:CH2	1:A:179:VAL:HG21	2.49	0.47
1:A:255:VAL:O	1:A:256:GLU:C	2.53	0.47
1:C:262:GLU:O	1:C:265:VAL:HG12	2.14	0.47
1:A:262:GLU:O	1:A:265:VAL:HG12	2.14	0.47
1:B:22:GLN:O	1:B:23:ASP:C	2.52	0.47
1:C:185:GLY:O	1:C:189:LEU:HB2	2.15	0.47
1:C:267:GLN:HB3	1:C:267:GLN:HE21	1.55	0.47
1:B:18:GLU:O	1:B:169:ARG:NH2	2.48	0.47
1:C:22:GLN:O	1:C:23:ASP:C	2.52	0.47
1:A:197:PHE:O	1:A:198:ARG:C	2.53	0.47
2:B:700:ANP:O2G	2:B:700:ANP:O2A	2.33	0.47
1:B:217:ASP:O	1:B:219:ILE:N	2.48	0.47
1:C:188:ALA:C	1:C:190:ILE:H	2.19	0.47
1:B:294:PHE:O	1:B:295:ARG:C	2.53	0.47
1:B:44:SER:HA	1:B:139:CYS:O	2.15	0.47
1:B:28:ARG:HE	1:B:156:PHE:HE2	1.62	0.46
1:B:7:TRP:CD1	1:B:7:TRP:N	2.57	0.46
1:B:174:CYS:O	1:B:177:GLU:N	2.38	0.46
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.81	0.46
1:C:102:PRO:HD2	1:C:103:PHE:CD2	2.51	0.46
1:A:151:SER:HA	1:B:202:ASN:ND2	2.30	0.46
1:A:9:GLU:CG	1:A:12:ARG:NH2	2.78	0.46
1:A:304:ILE:O	1:A:308:ALA:HB2	2.16	0.46
1:A:215:ASP:OD1	1:A:216:ALA:N	2.49	0.46
1:A:161:VAL:O	1:A:162:PRO:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PRO:HD2	1:B:103:PHE:CD2	2.51	0.46
1:A:197:PHE:CD1	2:A:700:ANP:C5	2.98	0.46
1:A:56:ILE:O	1:A:59:ALA:N	2.49	0.46
1:B:267:GLN:HE21	1:B:267:GLN:HB3	1.50	0.46
1:B:121:ALA:HA	1:B:124:ARG:HH21	1.81	0.46
1:C:121:ALA:HA	1:C:124:ARG:HH21	1.82	0.45
1:B:7:TRP:N	1:B:7:TRP:HD1	1.93	0.45
1:B:76:ALA:HB2	1:B:108:LEU:HG	1.97	0.45
1:C:254:MET:O	1:C:258:GLY:HA2	2.17	0.45
1:A:149:ILE:C	1:A:151:SER:N	2.70	0.45
1:A:102:PRO:HD2	1:A:103:PHE:CD2	2.51	0.45
1:A:270:ARG:NH1	1:B:303:ARG:NH1	2.64	0.45
1:B:230:GLU:O	1:B:233:GLU:HB3	2.17	0.45
1:A:152:ARG:NE	1:B:6:ILE:HG13	2.31	0.45
1:C:33:VAL:HA	1:C:62:LEU:HD21	1.99	0.45
1:B:294:PHE:CD1	1:C:295:ARG:HD2	2.52	0.45
1:C:44:SER:HB2	1:C:139:CYS:SG	2.56	0.45
1:A:249:LEU:O	1:A:253:LEU:HB2	2.17	0.45
1:C:9:GLU:HA	1:C:12:ARG:NE	2.24	0.45
1:C:43:PHE:HE1	1:C:55:ALA:HB2	1.81	0.45
1:C:219:ILE:O	1:C:223:THR:HG23	2.16	0.45
1:A:269:PHE:O	1:A:270:ARG:C	2.55	0.45
1:B:43:PHE:HE1	1:B:55:ALA:HB2	1.82	0.45
1:A:267:GLN:HE21	1:A:267:GLN:HB3	1.51	0.45
1:A:169:ARG:HD2	1:A:173:ILE:HD11	1.99	0.45
1:A:151:SER:OG	1:B:8:VAL:HG11	2.16	0.45
1:B:288:LYS:HD3	1:B:312:TYR:CG	2.51	0.45
1:A:181:ILE:HG21	1:A:186:LEU:HD13	1.99	0.44
1:C:281:LEU:O	1:C:284:GLN:N	2.50	0.44
1:C:169:ARG:HH11	1:C:169:ARG:HB2	1.83	0.44
1:A:33:VAL:HA	1:A:62:LEU:HD21	1.98	0.44
1:A:147:GLU:CD	1:B:198:ARG:HG2	2.37	0.44
1:B:33:VAL:HA	1:B:62:LEU:HD21	1.98	0.44
1:A:43:PHE:HE1	1:A:55:ALA:HB2	1.82	0.44
1:A:41:LEU:HG	1:A:156:PHE:CE1	2.53	0.44
1:C:186:LEU:HD12	1:C:186:LEU:HA	1.45	0.44
1:A:121:ALA:HA	1:A:124:ARG:HH21	1.83	0.44
1:A:70:ASN:HB3	1:A:92:PHE:HE1	1.82	0.44
1:B:44:SER:HB2	1:B:139:CYS:SG	2.57	0.44
1:C:70:ASN:HB3	1:C:92:PHE:HE1	1.82	0.44
1:C:304:ILE:O	1:C:308:ALA:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:CG	1:A:12:ARG:CZ	2.91	0.44
2:A:700:ANP:C5'	2:A:700:ANP:O1B	2.66	0.44
1:B:70:ASN:HB3	1:B:92:PHE:HE1	1.83	0.44
1:B:254:MET:O	1:B:258:GLY:HA2	2.18	0.44
1:B:269:PHE:CZ	1:B:273:ILE:HD11	2.52	0.44
1:B:219:ILE:O	1:B:223:THR:HG23	2.18	0.43
1:C:265:VAL:CG2	1:C:289:LEU:HD22	2.48	0.43
1:C:295:ARG:H	1:C:295:ARG:HG2	1.66	0.43
1:B:128:MET:CE	1:C:78:ASP:OD1	2.66	0.43
1:C:193:SER:C	1:C:195:GLY:H	2.22	0.43
1:B:19:VAL:HG11	1:B:54:THR:CG2	2.43	0.43
1:A:108:LEU:HD23	1:A:137:LEU:HD21	1.99	0.43
1:A:41:LEU:HG	1:A:156:PHE:HE1	1.83	0.43
1:A:43:PHE:CE1	1:A:55:ALA:HB2	2.54	0.43
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.84	0.43
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.68	0.43
1:B:250:LEU:CD2	1:B:310:LEU:HD11	2.49	0.43
1:C:14:ARG:HH11	1:C:14:ARG:HG2	1.83	0.43
1:C:14:ARG:HG2	1:C:14:ARG:NH1	2.32	0.43
1:A:8:VAL:CA	1:A:201:ILE:HG21	2.47	0.43
1:A:81:GLY:CA	1:A:84:VAL:HG12	2.48	0.43
1:C:169:ARG:O	1:C:173:ILE:CG1	2.62	0.43
1:C:43:PHE:CE1	1:C:55:ALA:HB2	2.53	0.43
1:B:193:SER:HB3	1:B:200:ALA:HB2	2.00	0.43
1:A:147:GLU:OE2	1:B:202:ASN:ND2	2.52	0.43
1:C:250:LEU:HD23	1:C:310:LEU:HD11	1.99	0.43
2:C:700:ANP:C8	2:C:700:ANP:O5'	2.66	0.42
1:A:14:ARG:NH1	1:A:14:ARG:HG2	2.33	0.42
1:C:161:VAL:HA	1:C:162:PRO:HD3	1.89	0.42
1:C:301:ASN:OD1	1:C:304:ILE:HG13	2.19	0.42
1:A:193:SER:C	1:A:195:GLY:H	2.21	0.42
1:B:266:ALA:O	1:B:269:PHE:HB3	2.18	0.42
1:A:197:PHE:HB2	2:A:700:ANP:C8	2.50	0.42
1:A:301:ASN:HB3	1:A:304:ILE:HD12	2.01	0.42
1:B:217:ASP:C	1:B:219:ILE:N	2.71	0.42
1:B:41:LEU:HG	1:B:156:PHE:CE1	2.55	0.42
1:A:217:ASP:C	1:A:219:ILE:N	2.72	0.42
1:C:197:PHE:O	1:C:198:ARG:C	2.58	0.42
1:C:289:LEU:HA	1:C:289:LEU:HD23	1.63	0.42
1:A:52:THR:N	2:A:700:ANP:O2G	2.50	0.42
1:C:232:THR:HG22	1:C:271:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:CE1	1:B:55:ALA:HB2	2.55	0.42
1:B:169:ARG:HD2	1:B:173:ILE:HD11	2.01	0.41
1:B:108:LEU:HD23	1:B:137:LEU:HD21	2.02	0.41
1:B:295:ARG:H	1:B:295:ARG:HG2	1.68	0.41
1:B:315:THR:C	1:B:317:ALA:H	2.23	0.41
1:B:147:GLU:HB3	1:B:148:PRO:HD3	2.02	0.41
1:A:219:ILE:O	1:A:223:THR:HG23	2.20	0.41
1:A:9:GLU:C	1:A:11:TYR:H	2.23	0.41
1:B:23:ASP:O	1:B:24:GLU:C	2.59	0.41
1:A:197:PHE:HD1	2:A:700:ANP:N7	2.19	0.41
1:B:259:MET:HB2	1:B:259:MET:HE3	1.76	0.41
1:B:158:PHE:N	1:B:158:PHE:CD1	2.88	0.41
1:A:198:ARG:HH21	2:A:700:ANP:HNB1	1.66	0.41
1:C:283:VAL:O	1:C:284:GLN:C	2.58	0.41
1:A:250:LEU:CD2	1:A:310:LEU:HD11	2.50	0.41
1:A:10:LYS:O	1:A:10:LYS:CG	2.68	0.41
1:C:259:MET:HE3	1:C:259:MET:HB2	1.72	0.41
1:A:44:SER:HB2	1:A:139:CYS:HG	1.86	0.41
1:C:267:GLN:H	1:C:267:GLN:HG2	1.41	0.41
1:C:192:ILE:HA	1:C:192:ILE:HD13	1.74	0.41
1:A:10:LYS:HE2	1:A:11:TYR:OH	2.21	0.41
1:C:92:PHE:HZ	1:C:105:ILE:N	2.19	0.41
1:A:304:ILE:O	1:A:308:ALA:CB	2.69	0.41
1:A:217:ASP:O	1:A:219:ILE:N	2.54	0.41
1:C:129:TYR:HB3	1:C:133:CYS:H	1.86	0.41
1:A:285:LEU:CD1	1:A:285:LEU:N	2.84	0.41
1:B:265:VAL:CG2	1:B:289:LEU:HD22	2.51	0.41
1:C:285:LEU:N	1:C:285:LEU:CD1	2.84	0.41
1:A:14:ARG:CG	1:A:14:ARG:HH11	2.34	0.41
1:A:235:ILE:O	1:A:239:LEU:HD12	2.21	0.41
1:A:22:GLN:O	1:A:23:ASP:C	2.59	0.41
1:A:16:LEU:HD21	1:A:58:LEU:HA	2.02	0.41
1:C:196:ASP:C	1:C:196:ASP:OD1	2.59	0.41
1:A:288:LYS:NZ	1:A:312:TYR:CD1	2.78	0.41
1:B:129:TYR:HB3	1:B:133:CYS:H	1.86	0.40
1:A:188:ALA:C	1:A:190:ILE:N	2.73	0.40
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.84	0.40
1:A:112:ASP:HB2	1:A:144:ARG:HB3	2.03	0.40
1:C:76:ALA:HB2	1:C:108:LEU:HG	2.03	0.40
1:C:51:LYS:O	1:C:52:THR:C	2.60	0.40
1:A:22:GLN:HA	1:A:22:GLN:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.67	0.40
1:C:169:ARG:HD2	1:C:173:ILE:HD11	2.04	0.40
1:B:193:SER:O	1:B:196:ASP:HB3	2.21	0.40
1:C:16:LEU:HD21	1:C:58:LEU:HA	2.03	0.40
1:B:302:GLU:O	1:B:306:LEU:HB2	2.21	0.40
1:C:121:ALA:HA	1:C:124:ARG:NH2	2.36	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:304:ILE:CD1	1:C:293:ASP:OD2[6_765]	2.16	0.04

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	312/319 (98%)	238 (76%)	58 (19%)	16 (5%)	2	26
1	B	312/319 (98%)	239 (77%)	60 (19%)	13 (4%)	3	32
1	C	312/319 (98%)	246 (79%)	50 (16%)	16 (5%)	2	26
All	All	936/957 (98%)	723 (77%)	168 (18%)	45 (5%)	3	28

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	TRP
1	A	24	GLU
1	A	189	LEU
1	B	7	TRP
1	B	24	GLU
1	C	7	TRP

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Mol	Chain	Res	Type
1	C	24	GLU
1	A	10	LYS
1	A	79	GLU
1	B	10	LYS
1	B	79	GLU
1	C	79	GLU
1	C	189	LEU
1	A	100	GLY
1	A	116	ALA
1	A	210	ILE
1	A	269	PHE
1	A	295	ARG
1	B	51	LYS
1	B	100	GLY
1	B	148	PRO
1	C	10	LYS
1	C	100	GLY
1	C	116	ALA
1	A	148	PRO
1	A	224	ALA
1	B	112	ASP
1	B	210	ILE
1	C	51	LYS
1	C	148	PRO
1	C	266	ALA
1	C	269	PHE
1	C	316	LEU
1	A	112	ASP
1	A	316	LEU
1	B	116	ALA
1	B	269	PHE
1	B	316	LEU
1	C	202	ASN
1	C	210	ILE
1	A	162	PRO
1	C	224	ALA
1	C	292	VAL
1	A	192	ILE
1	B	192	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	261/267 (98%)	218 (84%)	43 (16%)	3	16
1	B	261/267 (98%)	217 (83%)	44 (17%)	2	15
1	C	261/267 (98%)	217 (83%)	44 (17%)	2	15
All	All	783/801 (98%)	652 (83%)	131 (17%)	3	16

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	8	VAL
1	A	12	ARG
1	A	14	ARG
1	A	16	LEU
1	A	28	ARG
1	A	41	LEU
1	A	42	LEU
1	A	44	SER
1	A	49	THR
1	A	54	THR
1	A	72	ILE
1	A	79	GLU
1	A	82	ILE
1	A	84	VAL
1	A	103	PHE
1	A	122	LEU
1	A	143	SER
1	A	155	VAL
1	A	168	LYS
1	A	169	ARG
1	A	175	GLU
1	A	181	ILE
1	A	186	LEU
1	A	189	LEU
1	A	192	ILE

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	210	ILE
1	A	225	THR
1	A	234	LEU
1	A	236	GLN
1	A	251	ASP
1	A	253	LEU
1	A	255	VAL
1	A	267	GLN
1	A	270	ARG
1	A	286	ILE
1	A	289	LEU
1	A	295	ARG
1	A	301	ASN
1	A	306	LEU
1	A	312	TYR
1	A	316	LEU
1	B	6	ILE
1	B	8	VAL
1	B	12	ARG
1	B	14	ARG
1	B	16	LEU
1	B	28	ARG
1	B	41	LEU
1	B	42	LEU
1	B	44	SER
1	B	49	THR
1	B	72	ILE
1	B	79	GLU
1	B	82	ILE
1	B	84	VAL
1	B	103	PHE
1	B	122	LEU
1	B	143	SER
1	B	155	VAL
1	B	161	VAL
1	B	168	LYS
1	B	169	ARG
1	B	175	GLU
1	B	181	ILE
1	B	186	LEU
1	B	189	LEU

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Mol	Chain	Res	Type
1	B	192	ILE
1	B	196	ASP
1	B	205	GLN
1	B	210	ILE
1	B	225	THR
1	B	234	LEU
1	B	236	GLN
1	B	251	ASP
1	B	253	LEU
1	B	255	VAL
1	B	267	GLN
1	B	270	ARG
1	B	286	ILE
1	B	289	LEU
1	B	295	ARG
1	B	301	ASN
1	B	306	LEU
1	B	312	TYR
1	B	316	LEU
1	C	6	ILE
1	C	8	VAL
1	C	12	ARG
1	C	14	ARG
1	C	16	LEU
1	C	28	ARG
1	C	41	LEU
1	C	42	LEU
1	C	44	SER
1	C	49	THR
1	C	72	ILE
1	C	79	GLU
1	C	82	ILE
1	C	84	VAL
1	C	103	PHE
1	C	122	LEU
1	C	143	SER
1	C	155	VAL
1	C	168	LYS
1	C	169	ARG
1	C	173	ILE
1	C	175	GLU
1	C	181	ILE

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Mol	Chain	Res	Type
1	C	186	LEU
1	C	189	LEU
1	C	192	ILE
1	C	196	ASP
1	C	205	GLN
1	C	210	ILE
1	C	225	THR
1	C	234	LEU
1	C	236	GLN
1	C	251	ASP
1	C	253	LEU
1	C	255	VAL
1	C	267	GLN
1	C	270	ARG
1	C	286	ILE
1	C	289	LEU
1	C	295	ARG
1	C	301	ASN
1	C	306	LEU
1	C	312	TYR
1	C	316	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	66	ASN
1	A	267	GLN
1	A	301	ASN
1	B	27	GLN
1	B	66	ASN
1	B	202	ASN
1	B	205	GLN
1	B	301	ASN
1	C	27	GLN
1	C	66	ASN
1	C	205	GLN
1	C	267	GLN
1	C	301	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	A	700	-	27,33,33	3.93	8 (29%)	30,52,52	2.88	11 (36%)
2	ANP	B	700	-	27,33,33	3.57	7 (25%)	30,52,52	2.73	10 (33%)
2	ANP	C	700	-	27,33,33	3.83	8 (29%)	30,52,52	2.74	11 (36%)

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	700	-	-	0/12/38/38	0/3/3/3
2	ANP	B	700	-	-	0/12/38/38	0/3/3/3
2	ANP	C	700	-	-	0/12/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	700	ANP	C5-N7	-2.38	1.31	1.39
2	B	700	ANP	C5-N7	-2.26	1.31	1.39
2	C	700	ANP	PA-O1A	2.03	1.58	1.51
2	C	700	ANP	C5-C4	2.07	1.45	1.40
2	B	700	ANP	PA-O1A	2.08	1.58	1.51
2	A	700	ANP	PB-O3A	2.14	1.61	1.59
2	A	700	ANP	C5-C4	2.25	1.45	1.40
2	A	700	ANP	PA-O1A	2.38	1.59	1.51
2	C	700	ANP	PB-N3B	3.21	1.71	1.63
2	C	700	ANP	PG-N3B	3.50	1.72	1.63
2	B	700	ANP	PG-N3B	3.54	1.72	1.63
2	B	700	ANP	PB-N3B	3.68	1.73	1.63
2	B	700	ANP	C4-N3	4.50	1.42	1.35
2	A	700	ANP	PG-N3B	4.50	1.75	1.63
2	C	700	ANP	C4-N3	5.57	1.43	1.35
2	A	700	ANP	PB-N3B	5.58	1.78	1.63
2	A	700	ANP	C4-N3	5.86	1.44	1.35
2	B	700	ANP	PG-O1G	11.64	1.59	1.46
2	B	700	ANP	PB-O1B	11.81	1.59	1.46
2	A	700	ANP	PB-O1B	12.14	1.60	1.46
2	C	700	ANP	PG-O1G	12.28	1.60	1.46
2	A	700	ANP	PG-O1G	12.39	1.60	1.46
2	C	700	ANP	PB-O1B	12.89	1.61	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ANP	C2'-C1'-N9	-8.97	100.58	114.29
2	B	700	ANP	C2'-C1'-N9	-8.39	101.48	114.29
2	A	700	ANP	N3-C2-N1	-7.61	123.06	128.89
2	C	700	ANP	C2'-C1'-N9	-7.57	102.73	114.29
2	C	700	ANP	N3-C2-N1	-7.07	123.48	128.89
2	C	700	ANP	PA-O3A-PB	-5.70	113.56	132.67
2	B	700	ANP	N3-C2-N1	-5.38	124.78	128.89
2	B	700	ANP	PA-O3A-PB	-4.79	116.61	132.67
2	B	700	ANP	C4-C5-N7	-4.56	105.29	109.48
2	A	700	ANP	O1B-PB-N3B	-4.36	105.21	111.90
2	A	700	ANP	PA-O3A-PB	-4.06	119.07	132.67
2	A	700	ANP	C4-C5-N7	-3.79	106.00	109.48
2	C	700	ANP	C4-C5-N7	-3.45	106.31	109.48
2	C	700	ANP	O3A-PA-O5'	-3.11	94.70	102.94
2	B	700	ANP	O1G-PG-N3B	-3.07	107.19	111.90
2	A	700	ANP	O1G-PG-N3B	-2.94	107.39	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ANP	C5'-C4'-C3'	-2.79	104.13	115.21
2	B	700	ANP	O4'-C1'-N9	-2.54	102.77	108.10
2	A	700	ANP	C1'-N9-C4	2.08	130.08	126.94
2	A	700	ANP	O3'-C3'-C2'	2.10	118.66	111.83
2	C	700	ANP	O2B-PB-O1B	2.23	114.65	110.00
2	C	700	ANP	C2-N1-C6	2.24	122.77	118.77
2	B	700	ANP	O3'-C3'-C4'	2.25	117.79	111.05
2	C	700	ANP	C1'-N9-C4	2.27	130.36	126.94
2	B	700	ANP	O3'-C3'-C2'	2.32	119.37	111.83
2	C	700	ANP	O3A-PB-N3B	2.33	112.86	106.44
2	A	700	ANP	C2-N1-C6	2.74	123.67	118.77
2	A	700	ANP	O3A-PB-N3B	2.94	114.51	106.44
2	B	700	ANP	C4'-O4'-C1'	3.34	113.39	109.72
2	C	700	ANP	O3'-C3'-C2'	3.36	122.75	111.83
2	C	700	ANP	C4'-O4'-C1'	3.43	113.49	109.72
2	B	700	ANP	C1'-N9-C4	4.30	133.43	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	ANP	19	0
2	B	700	ANP	9	0
2	C	700	ANP	7	0

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, 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	314/319 (98%)	0.24	19 (6%)	25 19	121, 188, 291, 295	0
1	B	314/319 (98%)	0.12	18 (5%)	27 21	121, 189, 291, 295	0
1	C	314/319 (98%)	0.18	24 (7%)	17 14	121, 188, 291, 295	0
All	All	942/957 (98%)	0.18	61 (6%)	22 17	121, 189, 291, 295	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	9.6
1	A	127	GLU	9.4
1	A	79	GLU	8.9
1	C	127	GLU	8.5
1	A	133	CYS	7.5
1	B	127	GLU	6.3
1	B	94	ARG	6.3
1	C	100	GLY	6.0
1	B	93	ALA	5.9
1	B	99	GLY	5.9
1	A	100	GLY	5.1
1	C	131	LYS	4.7
1	A	126	MET	4.6
1	A	98	ILE	4.4
1	B	102	PRO	4.1
1	C	212	GLU	4.1
1	B	65	GLU	3.9
1	B	124	ARG	3.6
1	A	130	SER	3.4
1	C	98	ILE	3.4
1	B	123	ARG	3.3
1	B	128	MET	3.3
1	C	80	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	124	ARG	3.2
1	C	94	ARG	3.1
1	C	101	ALA	3.0
1	B	131	LYS	3.0
1	C	35	ARG	3.0
1	A	132	SER	2.9
1	C	130	SER	2.9
1	A	134	ARG	2.8
1	C	78	ASP	2.8
1	A	106	ILE	2.7
1	C	99	GLY	2.7
1	A	117	ASP	2.7
1	C	8	VAL	2.7
1	C	133	CYS	2.6
1	B	64	GLY	2.6
1	B	101	ALA	2.4
1	C	128	MET	2.4
1	C	87	HIS	2.4
1	B	9	GLU	2.4
1	A	91	GLU	2.3
1	B	14	ARG	2.3
1	C	107	PHE	2.3
1	C	297	THR	2.3
1	A	135	PHE	2.2
1	B	80	ARG	2.2
1	B	134	ARG	2.2
1	A	77	SER	2.2
1	C	211	GLY	2.2
1	A	15	THR	2.2
1	C	121	ALA	2.1
1	C	160	PRO	2.1
1	A	71	PHE	2.1
1	A	94	ARG	2.1
1	A	116	ALA	2.1
1	B	103	PHE	2.1
1	C	102	PRO	2.0
1	C	134	ARG	2.0
1	B	66	ASN	2.0

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ANP	A	700	31/31	0.80	0.43	1.07	142,146,163,164	0
2	ANP	C	700	31/31	0.88	0.36	0.18	141,146,160,162	0
2	ANP	B	700	31/31	0.89	0.30	-0.17	141,144,161,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.