Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:35 am BST

PDB ID	:	6QV3
Title	:	Crystal structure of the Ski2 RNA-helicase Brr2 from Chaetomium thermophilum bound to ADP
Authors	:	Absmeier, E.; Santos, K.F.; Wahl, M.C.
Deposited on	:	2019-03-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

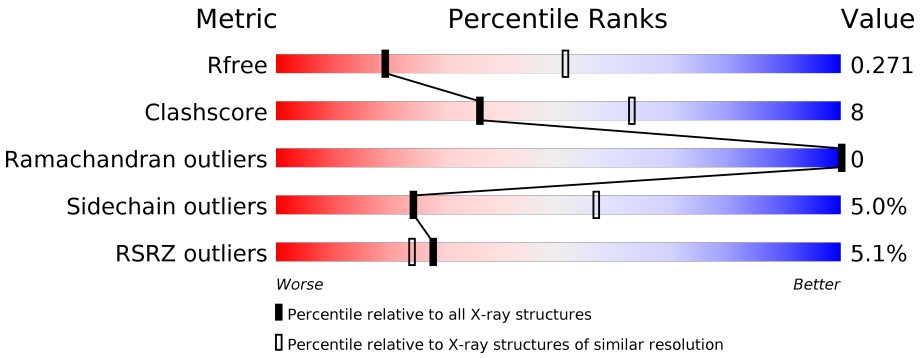
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	1725	5% 73% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13417 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.

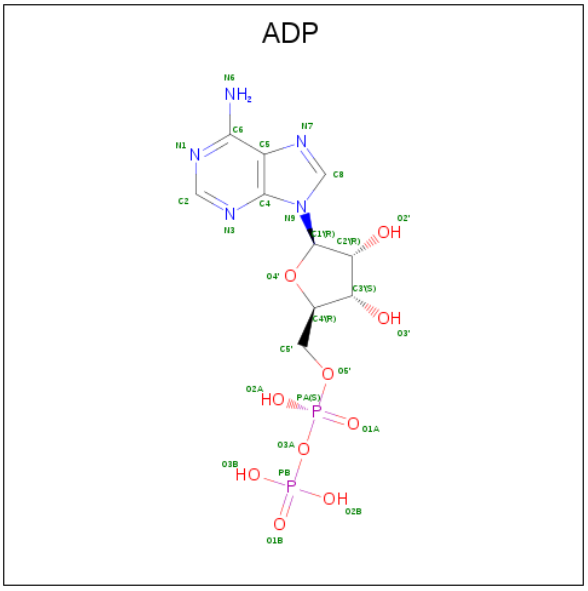
- Molecule 1 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1657	Total	C	N	O	S	0	0	0
			13284	8499	2260	2462	63			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLY	-	expression tag	UNP G0S0B9
A	470	ALA	-	expression tag	UNP G0S0B9
A	471	GLU	-	expression tag	UNP G0S0B9
A	472	PHE	-	expression tag	UNP G0S0B9

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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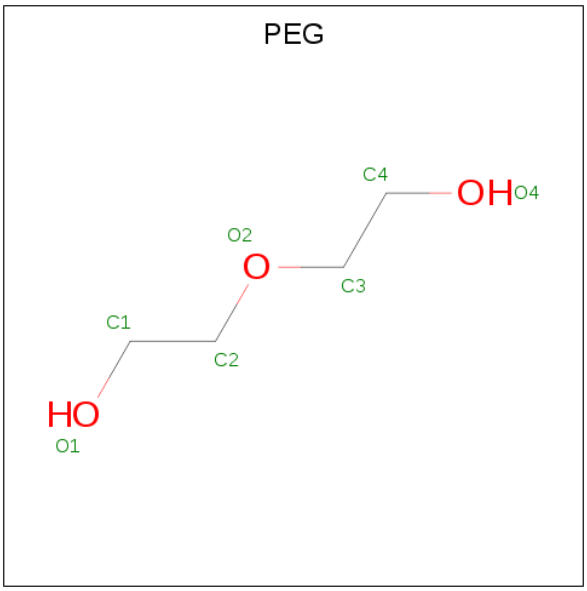
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			7	4	3			

- Molecule 5 is water.

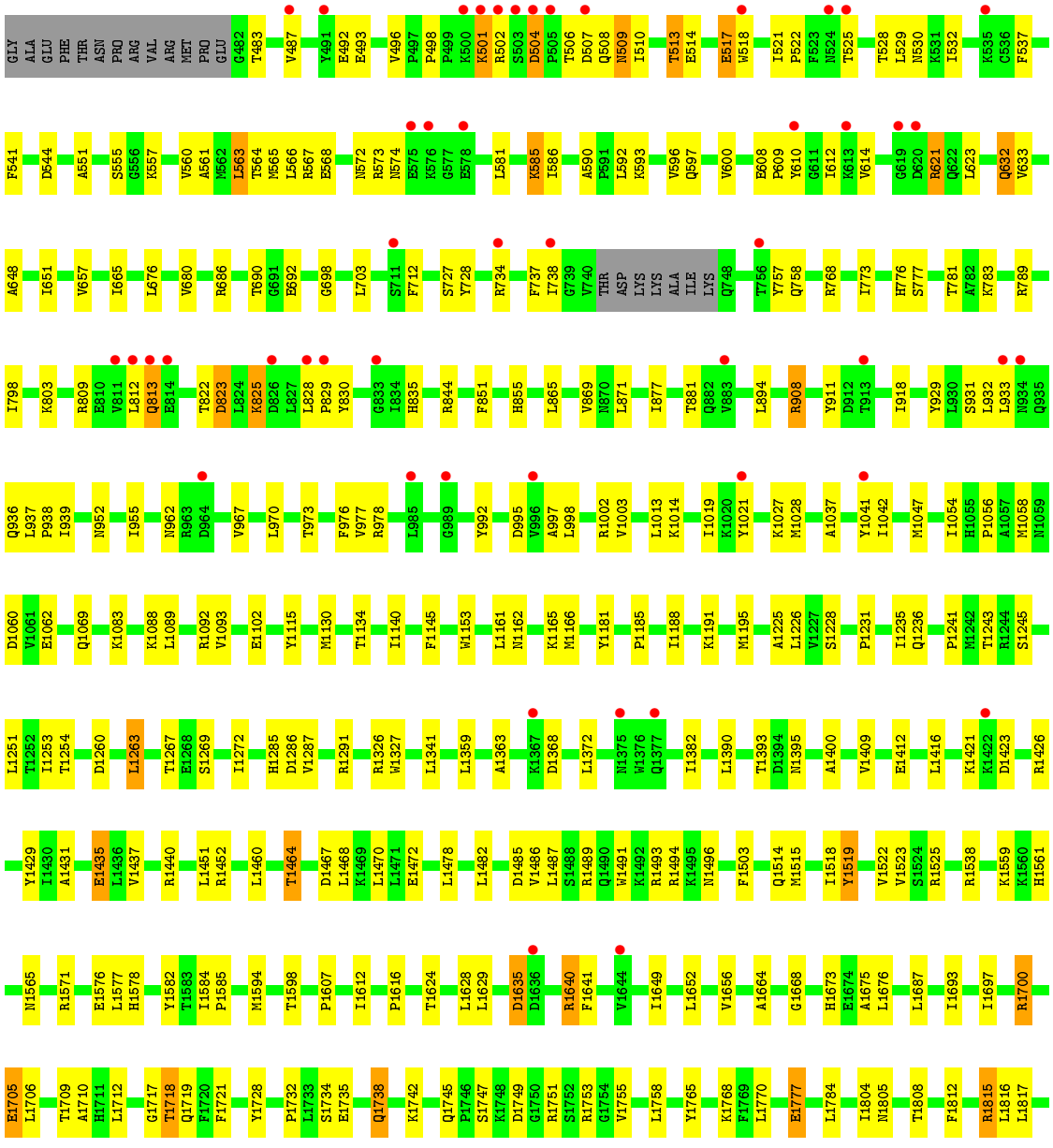
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		

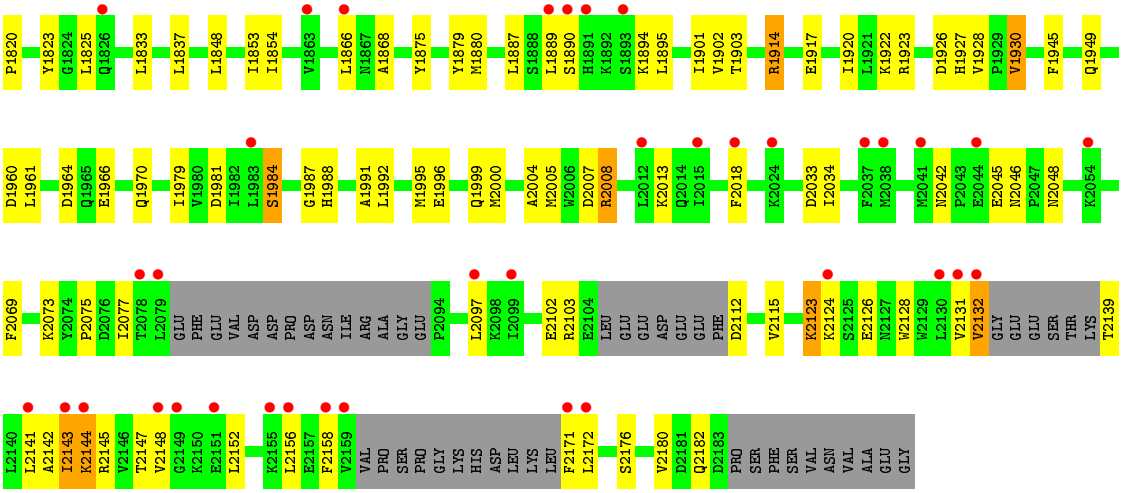
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Pre-mRNA splicing helicase-like protein

Chain A:




P1820 Y1823 G1824 L1825 Q1826 L1833 L1837 L1848 I1853 I1854 V1863 L1866 N1867 A1868 Y1875 Y1879 M1880 L1887 S1888 L1889 S1890 H1891 K1892 S1893 K1894 L1895 I1901 V1902 T1903 R1914 E1917 I1920 L1921 K1922 R1923 D1926 H1927 V1928 P1929 V1930 F1945 Q1949
D1960 L1961 D1964 Q1965 E1966 Q1970 I1979 V1980 D1981 I1982 L1983 S1984 G1987 H1988 A1991 L1992 M1995 E1996 Q1999 M2000 A2004 M2005 W2006 D2007 R2008 L2012 K2013 Q2014 I2015 F2018 K2024 D2033 I2034 F2037 M2038 M2041 N2042 P2043 E2044 E2045 N2046 P2047 N2048 K2054
F2069 K2073 Y2074 P2075 D2076 I2077 T2078 L2079 GLU PHE GLU VAL ASP ASP PRO ASP ASN ILE ARG ALA GLY GLU P2094 L2097 K2098 I2099 E2102 R2103 E2104 LEU GLU GLU ASP GLU GLU PHE D2112 V2115 K2123 K2124 S2125 E2126 W2127 W2128 W2129 L2130 V2131 V2132 GLY GLU GLU SER THR LYS T2139
L2140 L2141 A2142 I2143 K2144 R2145 V2146 T2147 V2148 G2149 K2150 E2151 L2152 K2155 L2156 E2157 F2158 V2159 VAL PRO SER PRO GLY LYS HIS ASP LEU LYS LEU F2171 L2172 S2176 V2180 D2181 Q2182 D2183 PRO SER PHE SER VAL ASN VAL ALA GLU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	125.17Å 125.17Å 127.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 2.90 44.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.65-2.90) 99.5 (44.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.220 , 0.271 0.220 , 0.271	Depositor DCC
R_{free} test set	2720 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.031 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13417	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: PEG, ADP, MN

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	0.25	0/13576	0.43	0/18414

There are no bond length outliers.

There are no bond angle outliers.

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	13284	0	13360	215	0
2	A	81	0	36	1	0
3	A	2	0	0	0	0
4	A	7	0	10	0	0
5	A	43	0	0	0	0
All	All	13417	0	13406	215	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 (215) 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:1460:LEU:HD22	1:A:1467:ASP:HB2	1.60	0.83
1:A:1777:GLU:OE2	1:A:1815:ARG:NH1	2.24	0.71
1:A:1390:LEU:HA	1:A:1538:ARG:HH22	1.54	0.70
1:A:1635:ASP:OD1	1:A:1635:ASP:N	2.24	0.69
1:A:865:LEU:HD12	1:A:869:VAL:HG11	1.75	0.68
1:A:1037:ALA:HB2	1:A:1047:MET:HG3	1.76	0.68
1:A:1393:THR:HG22	1:A:1395:ASN:H	1.59	0.67
1:A:1503:PHE:HE2	1:A:1523:VAL:HG12	1.60	0.66
1:A:1243:THR:HG23	1:A:1245:SER:H	1.60	0.66
1:A:590:ALA:HB3	1:A:596:VAL:HG12	1.78	0.66
1:A:1431:ALA:HB3	1:A:1437:VAL:HG12	1.80	0.64
1:A:513:THR:HG22	1:A:529:LEU:HG	1.78	0.64
1:A:955:ILE:HD13	1:A:1019:ILE:HD12	1.79	0.64
1:A:532:ILE:HD11	1:A:728:TYR:HB3	1.80	0.64
1:A:568:GLU:OE2	1:A:572:ASN:ND2	2.30	0.64
1:A:690:THR:HG23	1:A:692:GLU:H	1.62	0.64
1:A:962:ASN:HB3	1:A:1027:LYS:HE3	1.80	0.63
1:A:504:ASP:OD1	1:A:504:ASP:N	2.30	0.61
1:A:908:ARG:HG3	1:A:911:TYR:HB2	1.82	0.61
1:A:563:LEU:HD12	1:A:566:LEU:HD12	1.83	0.61
1:A:823:ASP:N	1:A:823:ASP:OD1	2.34	0.61
1:A:1578:HIS:HB2	1:A:1755:VAL:HG12	1.83	0.60
1:A:530:ASN:ND2	1:A:555:SER:O	2.35	0.60
1:A:1241:PRO:HG3	1:A:1341:LEU:HD11	1.82	0.60
1:A:822:THR:HB	1:A:825:LYS:HG2	1.84	0.60
1:A:973:THR:HG23	1:A:976:PHE:H	1.67	0.59
1:A:1519:TYR:O	1:A:1523:VAL:HG22	2.02	0.59
1:A:1019:ILE:HD11	1:A:1028:MET:HB2	1.83	0.59
1:A:621:ARG:HD3	1:A:1326:ARG:HE	1.66	0.58
1:A:1014:LYS:HD2	1:A:1021:TYR:HB3	1.85	0.58
1:A:1966:GLU:O	1:A:1970:GLN:HG2	2.04	0.58
1:A:1185:PRO:HG2	1:A:1188:ILE:HG12	1.86	0.57
1:A:1668:GLY:HA2	1:A:1693:ILE:HG22	1.86	0.57
1:A:1042:ILE:HD12	1:A:1140:ILE:HD13	1.86	0.57
1:A:1088:LYS:O	1:A:1092:ARG:HG2	2.03	0.57
1:A:1576:GLU:HG3	1:A:1751:ARG:HD3	1.85	0.57
1:A:1928:VAL:HG11	1:A:1949:GLN:HB3	1.88	0.56
1:A:931:SER:HB2	1:A:936:GLN:HB3	1.88	0.56
1:A:2097:LEU:HB2	1:A:2158:PHE:HE2	1.71	0.56
1:A:1467:ASP:HA	1:A:1470:LEU:HB2	1.87	0.55
1:A:1083:LYS:HE2	1:A:1102:GLU:HG3	1.89	0.55
1:A:1400:ALA:HB3	1:A:1565:ASN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2033:ASP:OD1	1:A:2034:ILE:N	2.40	0.55
1:A:789:ARG:HD2	1:A:830:TYR:HD1	1.71	0.55
1:A:877:ILE:HD13	1:A:918:ILE:HB	1.87	0.55
1:A:1468:LEU:HD13	1:A:1487:LEU:HD22	1.88	0.55
1:A:828:LEU:N	1:A:829:PRO:HD3	2.22	0.55
1:A:1429:TYR:HB3	1:A:1478:LEU:HD22	1.87	0.55
1:A:2115:VAL:HG11	1:A:2176:SER:HB2	1.88	0.55
1:A:1914:ARG:NH1	1:A:1960:ASP:HB3	2.22	0.55
1:A:1709:THR:HG22	1:A:1745:GLN:HG3	1.89	0.54
1:A:932:LEU:HD13	1:A:937:LEU:HD23	1.89	0.54
1:A:952:ASN:HB2	1:A:1013:LEU:HD11	1.90	0.54
1:A:1058:MET:HG3	1:A:1062:GLU:HB2	1.88	0.54
1:A:560:VAL:O	1:A:564:THR:HG23	2.07	0.54
1:A:789:ARG:HD2	1:A:830:TYR:CD1	2.42	0.54
1:A:992:TYR:HB3	1:A:995:ASP:HB2	1.90	0.53
1:A:676:LEU:O	1:A:680:VAL:HG22	2.09	0.53
1:A:632:GLN:HE21	1:A:632:GLN:H	1.57	0.53
1:A:2046:ASN:O	1:A:2048:ASN:N	2.40	0.53
1:A:1368:ASP:OD2	1:A:1452:ARG:NH1	2.42	0.52
1:A:1700:ARG:NH2	1:A:1735:GLU:OE2	2.42	0.52
1:A:1777:GLU:HG3	1:A:1823:TYR:OH	2.10	0.52
1:A:1161:LEU:HG	1:A:1165:LYS:HE3	1.90	0.52
1:A:1988:HIS:H	1:A:1988:HIS:CD2	2.28	0.52
1:A:2144:LYS:HB2	1:A:2156:LEU:HD12	1.91	0.52
1:A:851:PHE:HB3	1:A:871:LEU:HD11	1.92	0.52
1:A:1594:MET:O	1:A:1598:THR:HG23	2.10	0.52
1:A:1853:ILE:HG23	1:A:1854:ILE:HG23	1.92	0.52
1:A:686:ARG:O	1:A:690:THR:HG22	2.09	0.52
1:A:493:GLU:HG2	1:A:738:ILE:HG12	1.91	0.52
1:A:1421:LYS:HE3	1:A:1423:ASP:HB3	1.91	0.51
1:A:1624:THR:HG22	1:A:1697:ILE:HD13	1.91	0.51
1:A:1747:SER:OG	1:A:1749:ASP:OD1	2.25	0.51
1:A:2075:PRO:HG2	1:A:2180:VAL:HG21	1.91	0.51
1:A:998:LEU:O	1:A:1002:ARG:HG3	2.10	0.51
1:A:1485:ASP:OD1	1:A:1525:ARG:NH1	2.36	0.51
1:A:1820:PRO:HB3	1:A:1825:LEU:HD23	1.91	0.50
1:A:1272:ILE:O	1:A:1285:HIS:HA	2.11	0.50
1:A:1286:ASP:OD1	1:A:1287:VAL:N	2.44	0.50
1:A:1804:ILE:HG23	1:A:1837:LEU:HD23	1.94	0.50
1:A:1130:MET:O	1:A:1134:THR:HG23	2.11	0.50
1:A:1903:THR:HG21	1:A:1945:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:SER:N	2:A:2201:ADP:O2B	2.45	0.50
1:A:1917:GLU:HG2	1:A:1920:ILE:HD11	1.94	0.49
1:A:2042:ASN:HB3	1:A:2045:GLU:HB2	1.93	0.49
1:A:1805:ASN:O	1:A:1808:THR:OG1	2.29	0.49
1:A:2000:MET:O	1:A:2004:ALA:N	2.44	0.49
1:A:2007:ASP:N	1:A:2007:ASP:OD1	2.45	0.49
1:A:1191:LYS:O	1:A:1195:MET:HG3	2.11	0.49
1:A:2103:ARG:NH2	1:A:2126:GLU:OE2	2.39	0.49
1:A:1056:PRO:HG3	1:A:1153:TRP:CE2	2.48	0.49
1:A:507:ASP:OD1	1:A:509:ASN:ND2	2.46	0.48
1:A:703:LEU:HD13	1:A:939:ILE:HD11	1.93	0.48
1:A:1426:ARG:NH1	1:A:1496:ASN:OD1	2.46	0.48
1:A:1652:LEU:O	1:A:1656:VAL:HG23	2.13	0.48
1:A:1231:PRO:HG2	1:A:1327:TRP:CD1	2.48	0.48
1:A:1464:THR:O	1:A:1468:LEU:HB2	2.14	0.48
1:A:1612:ILE:HG13	1:A:1710:ALA:HB2	1.95	0.48
1:A:1235:ILE:HG22	1:A:1253:ILE:HG12	1.96	0.48
1:A:2172:LEU:HB2	1:A:2182:GLN:HB3	1.94	0.48
1:A:621:ARG:HA	1:A:621:ARG:HD2	1.59	0.47
1:A:773:ILE:HG23	1:A:877:ILE:HB	1.95	0.47
1:A:1649:ILE:HG23	1:A:1687:LEU:HD21	1.96	0.47
1:A:621:ARG:HD3	1:A:1326:ARG:NE	2.30	0.47
1:A:2069:PHE:HA	1:A:2073:LYS:HG3	1.95	0.47
1:A:612:ILE:HG23	1:A:632:GLN:HB2	1.95	0.47
1:A:1145:PHE:CE1	1:A:1161:LEU:HB2	2.50	0.47
1:A:1732:PRO:HG2	1:A:1735:GLU:HG2	1.96	0.47
1:A:551:ALA:HB3	1:A:557:LYS:HE2	1.96	0.47
1:A:537:PHE:HA	1:A:563:LEU:HD23	1.97	0.47
1:A:1996:GLU:O	1:A:1999:GLN:HG2	2.14	0.46
1:A:967:VAL:HG21	1:A:1003:VAL:HG22	1.97	0.46
1:A:1472:GLU:HB2	1:A:1494:ARG:HH22	1.81	0.46
1:A:703:LEU:HB3	1:A:939:ILE:HD11	1.98	0.46
1:A:712:PHE:HB2	1:A:977:VAL:HG21	1.96	0.46
1:A:1984:SER:HB2	1:A:2143:ILE:HG12	1.96	0.46
1:A:2132:VAL:HG22	1:A:2142:ALA:HB3	1.97	0.46
1:A:1435:GLU:HB3	1:A:1705:GLU:HB2	1.97	0.46
1:A:1765:TYR:O	1:A:1768:LYS:HB3	2.16	0.46
1:A:1848:LEU:HD22	1:A:1853:ILE:HG21	1.97	0.46
1:A:593:LYS:O	1:A:596:VAL:HG22	2.15	0.46
1:A:597:GLN:O	1:A:600:VAL:HG12	2.15	0.46
1:A:997:ALA:O	1:A:1002:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1902:VAL:HG22	1:A:1979:ILE:HD12	1.99	0.45
1:A:835:HIS:NE2	1:A:844:ARG:HG3	2.31	0.45
1:A:937:LEU:HD12	1:A:938:PRO:HD2	1.97	0.45
1:A:1515:MET:O	1:A:1518:ILE:HG12	2.17	0.45
1:A:2077:ILE:HD13	1:A:2103:ARG:HG2	1.97	0.45
1:A:2147:THR:O	1:A:2152:LEU:HD11	2.16	0.45
1:A:665:ILE:HD11	1:A:698:GLY:HA3	1.98	0.45
1:A:1629:LEU:HD11	1:A:1664:ALA:HA	1.98	0.45
1:A:1721:PHE:HB2	1:A:1728:TYR:CE2	2.52	0.45
1:A:783:LYS:HB3	1:A:783:LYS:HE3	1.86	0.45
1:A:1559:LYS:HE3	1:A:1561:HIS:NE2	2.31	0.45
1:A:1930:VAL:HG13	1:A:1949:GLN:NE2	2.31	0.45
1:A:2008:ARG:O	1:A:2008:ARG:HG2	2.16	0.45
1:A:592:LEU:O	1:A:596:VAL:HG13	2.17	0.45
1:A:1260:ASP:HB3	1:A:1263:LEU:HD11	1.98	0.45
1:A:648:ALA:HA	1:A:651:ILE:HD11	1.99	0.45
1:A:1628:LEU:HD21	1:A:1641:PHE:CE2	2.51	0.44
1:A:1577:LEU:HD11	1:A:1770:LEU:HD13	1.99	0.44
1:A:623:LEU:HD11	1:A:1269:SER:HB2	1.99	0.44
1:A:483:THR:HG22	1:A:496:VAL:HG22	1.98	0.44
1:A:776:HIS:CE1	1:A:894:LEU:HD22	2.52	0.44
1:A:881:THR:HB	1:A:929:TYR:OH	2.17	0.44
1:A:1041:TYR:CG	1:A:1041:TYR:O	2.70	0.44
1:A:812:LEU:HD13	1:A:855:HIS:HB3	1.99	0.44
1:A:522:PRO:HG3	1:A:610:TYR:HE2	1.81	0.44
1:A:768:ARG:HG3	1:A:803:LYS:NZ	2.33	0.44
1:A:501:LYS:O	1:A:727:SER:HB2	2.18	0.44
1:A:813:GLN:HG3	1:A:813:GLN:H	1.48	0.44
1:A:1181:TYR:CD1	1:A:1226:LEU:HD12	2.53	0.44
1:A:1225:ALA:O	1:A:1228:SER:OG	2.25	0.43
1:A:1817:LEU:HD11	1:A:1833:LEU:HD22	2.00	0.43
1:A:1848:LEU:O	1:A:1853:ILE:HG22	2.18	0.43
1:A:1115:TYR:CG	1:A:1134:THR:HG21	2.52	0.43
1:A:1887:LEU:HD11	1:A:1901:ILE:HG12	1.99	0.43
1:A:1491:TRP:C	1:A:1493:ARG:H	2.21	0.43
1:A:1914:ARG:NH2	1:A:1964:ASP:OD2	2.51	0.43
1:A:541:PHE:O	1:A:567:ARG:HD3	2.19	0.43
1:A:1482:LEU:O	1:A:1486:VAL:HG23	2.18	0.43
1:A:1875:TYR:OH	1:A:1981:ASP:OD2	2.32	0.43
1:A:487:VAL:HG22	1:A:492:GLU:HG3	2.01	0.43
1:A:557:LYS:O	1:A:560:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:ASN:O	1:A:1166:MET:HG3	2.19	0.43
1:A:600:VAL:HG23	1:A:614:VAL:HG12	2.00	0.43
1:A:1089:LEU:O	1:A:1093:VAL:HG13	2.19	0.42
1:A:1928:VAL:HG11	1:A:1949:GLN:CD	2.40	0.42
1:A:2123:LYS:HG3	1:A:2124:LYS:O	2.19	0.42
1:A:608:GLU:N	1:A:609:PRO:HD2	2.34	0.42
1:A:1991:ALA:O	1:A:1995:MET:HG3	2.19	0.42
1:A:1712:LEU:HA	1:A:1753:ARG:O	2.19	0.42
1:A:561:ALA:O	1:A:565:MET:HG3	2.20	0.42
1:A:777:SER:O	1:A:781:THR:HG23	2.19	0.42
1:A:537:PHE:HD1	1:A:563:LEU:HD21	1.84	0.42
1:A:1267:THR:HG22	1:A:1291:ARG:HD3	2.01	0.42
1:A:1784:LEU:HA	1:A:1784:LEU:HD23	1.89	0.42
1:A:1616:PRO:HG3	1:A:1717:GLY:HA3	2.02	0.42
1:A:1037:ALA:CB	1:A:1047:MET:HG3	2.48	0.42
1:A:1738:GLN:OE1	1:A:1742:LYS:NZ	2.52	0.42
1:A:1922:LYS:NZ	1:A:1926:ASP:OD1	2.52	0.42
1:A:1607:PRO:O	1:A:1640:ARG:NH1	2.51	0.42
1:A:1514:GLN:N	1:A:1514:GLN:OE1	2.51	0.41
1:A:2097:LEU:HB2	1:A:2158:PHE:CE2	2.54	0.41
1:A:585:LYS:HB2	1:A:657:VAL:HG12	2.01	0.41
1:A:1060:ASP:N	1:A:1060:ASP:OD1	2.53	0.41
1:A:1412:GLU:O	1:A:1416:LEU:HG	2.20	0.41
1:A:1987:GLY:C	1:A:2139:THR:HA	2.41	0.41
1:A:2148:VAL:HG22	1:A:2152:LEU:HD12	2.01	0.41
1:A:532:ILE:HG13	1:A:555:SER:OG	2.20	0.41
1:A:970:LEU:O	1:A:973:THR:HG22	2.21	0.41
1:A:1812:PHE:CZ	1:A:1816:LEU:HD11	2.55	0.41
1:A:2005:MET:HG2	1:A:2013:LYS:HE3	2.01	0.41
1:A:1584:ILE:HA	1:A:1585:PRO:HD3	1.87	0.41
1:A:737:PHE:CE2	1:A:933:LEU:HD12	2.55	0.41
1:A:1236:GLN:O	1:A:1251:LEU:HD12	2.21	0.41
1:A:1372:LEU:HD11	1:A:1451:LEU:HD11	2.02	0.41
1:A:1718:THR:HG22	1:A:1719:GLN:HG3	2.03	0.41
1:A:1928:VAL:HG11	1:A:1949:GLN:CB	2.51	0.41
1:A:1961:LEU:HD12	1:A:1961:LEU:HA	1.97	0.41
1:A:1673:HIS:CE1	1:A:1675:ALA:HB3	2.56	0.41
1:A:498:PRO:HG3	1:A:734:ARG:HG2	2.03	0.41
1:A:1054:ILE:HG22	1:A:1153:TRP:HZ3	1.85	0.41
1:A:1494:ARG:NH1	1:A:1496:ASN:HB2	2.36	0.41
1:A:2102:GLU:HG2	1:A:2103:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:LEU:HD13	1:A:1363:ALA:HB3	2.03	0.40
1:A:1485:ASP:O	1:A:1489:ARG:HG3	2.21	0.40
1:A:1706:LEU:O	1:A:1742:LYS:HE3	2.21	0.40
1:A:517:GLU:OE1	1:A:518:TRP:N	2.54	0.40
1:A:1582:TYR:CZ	1:A:1594:MET:HG2	2.56	0.40
1:A:1923:ARG:O	1:A:1927:HIS:ND1	2.55	0.40
1:A:573:ARG:HG2	1:A:574:ASN:O	2.22	0.40
1:A:1518:ILE:O	1:A:1522:VAL:HG13	2.22	0.40
1:A:1866:LEU:O	1:A:1868:ALA:N	2.55	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	1645/1725 (95%)	1585 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1464/1523 (96%)	1391 (95%)	73 (5%)	24	57

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	501	LYS
1	A	502	ARG
1	A	504	ASP
1	A	506	THR
1	A	508	GLN
1	A	509	ASN
1	A	510	ILE
1	A	513	THR
1	A	514	GLU
1	A	517	GLU
1	A	521	ILE
1	A	525	THR
1	A	528	THR
1	A	544	ASP
1	A	563	LEU
1	A	581	LEU
1	A	585	LYS
1	A	586	ILE
1	A	621	ARG
1	A	632	GLN
1	A	633	VAL
1	A	757	TYR
1	A	758	GLN
1	A	798	ILE
1	A	809	ARG
1	A	813	GLN
1	A	823	ASP
1	A	825	LYS
1	A	908	ARG
1	A	978	ARG
1	A	1069	GLN
1	A	1254	THR
1	A	1263	LEU
1	A	1382	ILE
1	A	1409	VAL
1	A	1435	GLU
1	A	1440	ARG
1	A	1464	THR
1	A	1519	TYR
1	A	1571	ARG
1	A	1635	ASP
1	A	1640	ARG

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Mol	Chain	Res	Type
1	A	1676	LEU
1	A	1700	ARG
1	A	1705	GLU
1	A	1718	THR
1	A	1734	SER
1	A	1738	GLN
1	A	1758	LEU
1	A	1777	GLU
1	A	1815	ARG
1	A	1879	TYR
1	A	1880	MET
1	A	1889	LEU
1	A	1890	SER
1	A	1894	LYS
1	A	1895	LEU
1	A	1914	ARG
1	A	1930	VAL
1	A	1984	SER
1	A	1992	LEU
1	A	2008	ARG
1	A	2018	PHE
1	A	2112	ASP
1	A	2123	LYS
1	A	2128	TRP
1	A	2131	VAL
1	A	2132	VAL
1	A	2141	LEU
1	A	2143	ILE
1	A	2144	LYS
1	A	2145	ARG
1	A	2171	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	2202	3	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	A	2201	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
2	ADP	A	2203	-	24,29,29	0.97	1 (4%)	29,45,45	1.38	4 (13%)
4	PEG	A	2206	-	6,6,6	0.50	0	5,5,5	0.25	0

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	ADP	A	2202	3	-	3/12/32/32	0/3/3/3
2	ADP	A	2201	-	-	3/12/32/32	0/3/3/3
2	ADP	A	2203	-	-	4/12/32/32	0/3/3/3
4	PEG	A	2206	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2203	ADP	C5-C4	2.54	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2201	ADP	C5-C4	2.48	1.47	1.40
2	A	2202	ADP	C5-C4	2.45	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2203	ADP	C3'-C2'-C1'	3.57	106.36	100.98
2	A	2202	ADP	PA-O3A-PB	-3.55	120.64	132.83
2	A	2201	ADP	PA-O3A-PB	-3.33	121.41	132.83
2	A	2202	ADP	N3-C2-N1	-3.26	123.59	128.68
2	A	2201	ADP	N3-C2-N1	-3.25	123.60	128.68
2	A	2203	ADP	N3-C2-N1	-3.08	123.87	128.68
2	A	2202	ADP	C4-C5-N7	-2.80	106.48	109.40
2	A	2201	ADP	C4-C5-N7	-2.63	106.65	109.40
2	A	2202	ADP	C3'-C2'-C1'	2.59	104.88	100.98
2	A	2203	ADP	C4-C5-N7	-2.47	106.82	109.40
2	A	2203	ADP	PA-O3A-PB	-2.32	124.88	132.83
2	A	2201	ADP	C3'-C2'-C1'	2.25	104.37	100.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	ADP	O4'-C4'-C5'-O5'
2	A	2203	ADP	C5'-O5'-PA-O3A
2	A	2202	ADP	C3'-C4'-C5'-O5'
2	A	2201	ADP	C3'-C4'-C5'-O5'
2	A	2202	ADP	O4'-C4'-C5'-O5'
2	A	2203	ADP	C5'-O5'-PA-O1A
2	A	2203	ADP	PA-O3A-PB-O2B
2	A	2201	ADP	PB-O3A-PA-O2A
2	A	2202	ADP	C5'-O5'-PA-O1A
2	A	2203	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

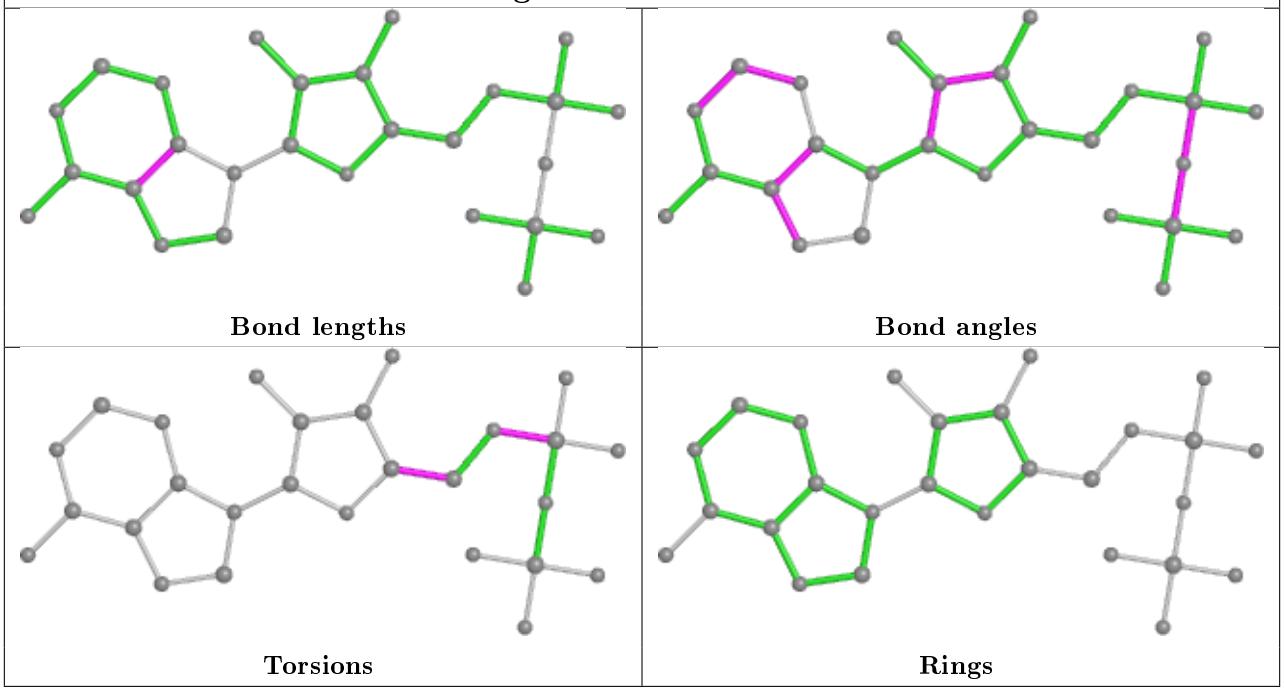
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2201	ADP	1	0

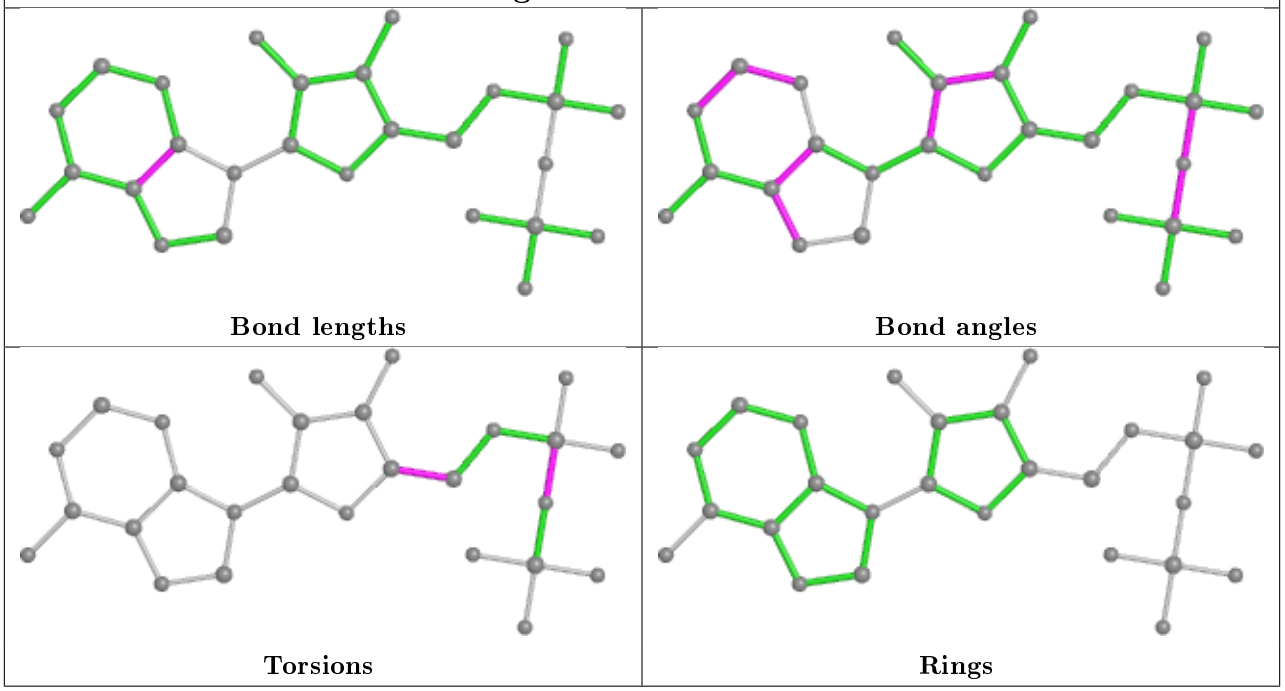
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

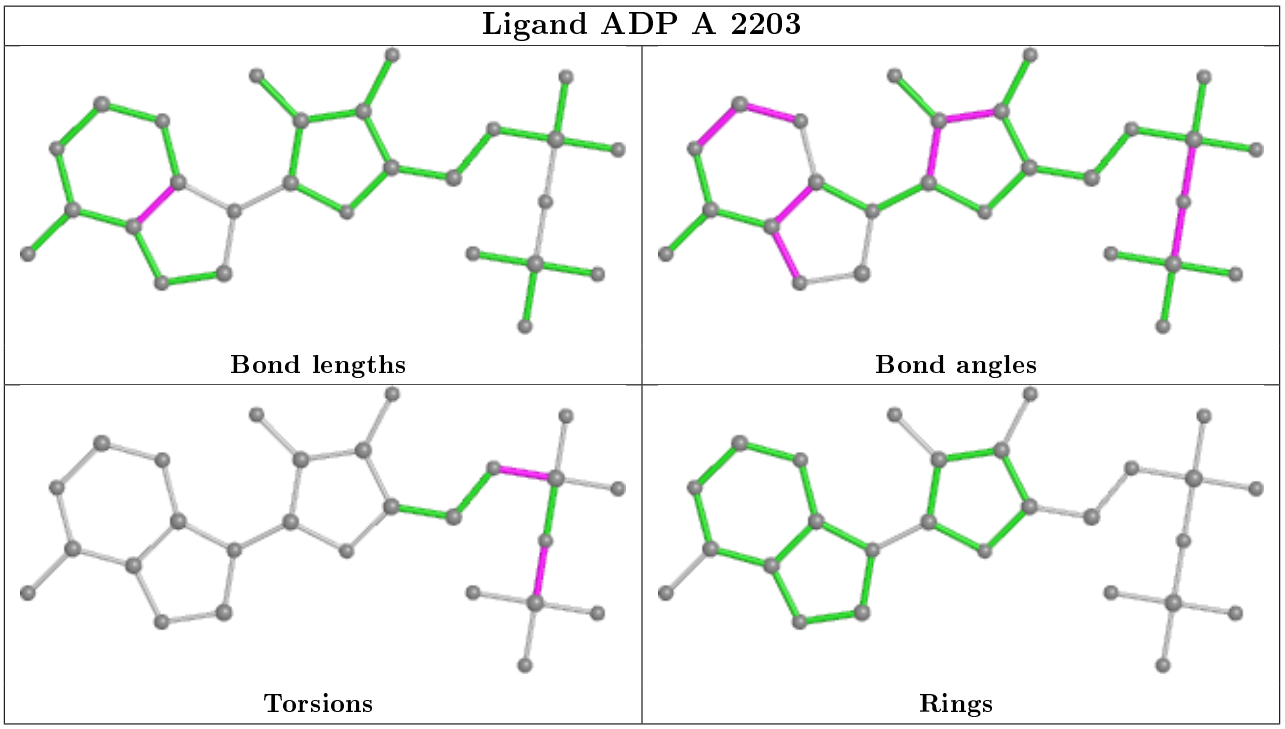
Ligand ADP A 2202



Ligand ADP A 2201



Ligand ADP A 2203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1657/1725 (96%)	0.24	85 (5%) 28 24	35, 83, 155, 229	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2158	PHE	5.3
1	A	620	ASP	5.1
1	A	2141	LEU	4.9
1	A	505	PRO	4.7
1	A	575	GLU	4.6
1	A	576	LYS	4.0
1	A	2038	MET	3.9
1	A	502	ARG	3.8
1	A	2131	VAL	3.6
1	A	811	VAL	3.5
1	A	525	THR	3.4
1	A	1636	ASP	3.3
1	A	1375	ASN	3.3
1	A	828	LEU	3.3
1	A	829	PRO	3.3
1	A	619	GLY	3.2
1	A	500	LYS	3.2
1	A	2097	LEU	3.1
1	A	2018	PHE	3.1
1	A	2156	LEU	3.1
1	A	518	TRP	3.1
1	A	1983	LEU	3.1
1	A	2041	MET	3.1
1	A	2124	LYS	3.1
1	A	2130	LEU	3.1
1	A	503	SER	3.0
1	A	2037	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	501	LYS	3.0
1	A	613	LYS	3.0
1	A	734	ARG	3.0
1	A	989	GLY	2.9
1	A	814	GLU	2.9
1	A	2148	VAL	2.9
1	A	1891	HIS	2.8
1	A	2099	ILE	2.8
1	A	2012	LEU	2.8
1	A	2132	VAL	2.7
1	A	578	GLU	2.7
1	A	1367	LYS	2.7
1	A	1893	SER	2.6
1	A	2155	LYS	2.6
1	A	1866	LEU	2.6
1	A	1041	TYR	2.6
1	A	2078	THR	2.6
1	A	2171	PHE	2.6
1	A	2079	LEU	2.5
1	A	933	LEU	2.5
1	A	1644	VAL	2.5
1	A	2151	GLU	2.5
1	A	491	TYR	2.5
1	A	738	ILE	2.5
1	A	2143	ILE	2.4
1	A	2172	LEU	2.4
1	A	1889	LEU	2.4
1	A	826	ASP	2.4
1	A	964	ASP	2.4
1	A	487	VAL	2.4
1	A	524	ASN	2.3
1	A	813	GLN	2.3
1	A	504	ASP	2.3
1	A	1890	SER	2.3
1	A	2149	GLY	2.3
1	A	812	LEU	2.3
1	A	1422	LYS	2.3
1	A	2044	GLU	2.3
1	A	535	LYS	2.3
1	A	2144	LYS	2.3
1	A	1377	GLN	2.3
1	A	507	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	996	VAL	2.2
1	A	833	GLY	2.2
1	A	985	LEU	2.2
1	A	1021	TYR	2.2
1	A	610	TYR	2.1
1	A	2024	LYS	2.1
1	A	1826	GLN	2.1
1	A	711	SER	2.1
1	A	913	THR	2.0
1	A	883	VAL	2.0
1	A	1863	VAL	2.0
1	A	2054	LYS	2.0
1	A	2015	ILE	2.0
1	A	756	THR	2.0
1	A	2159	VAL	2.0
1	A	934	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

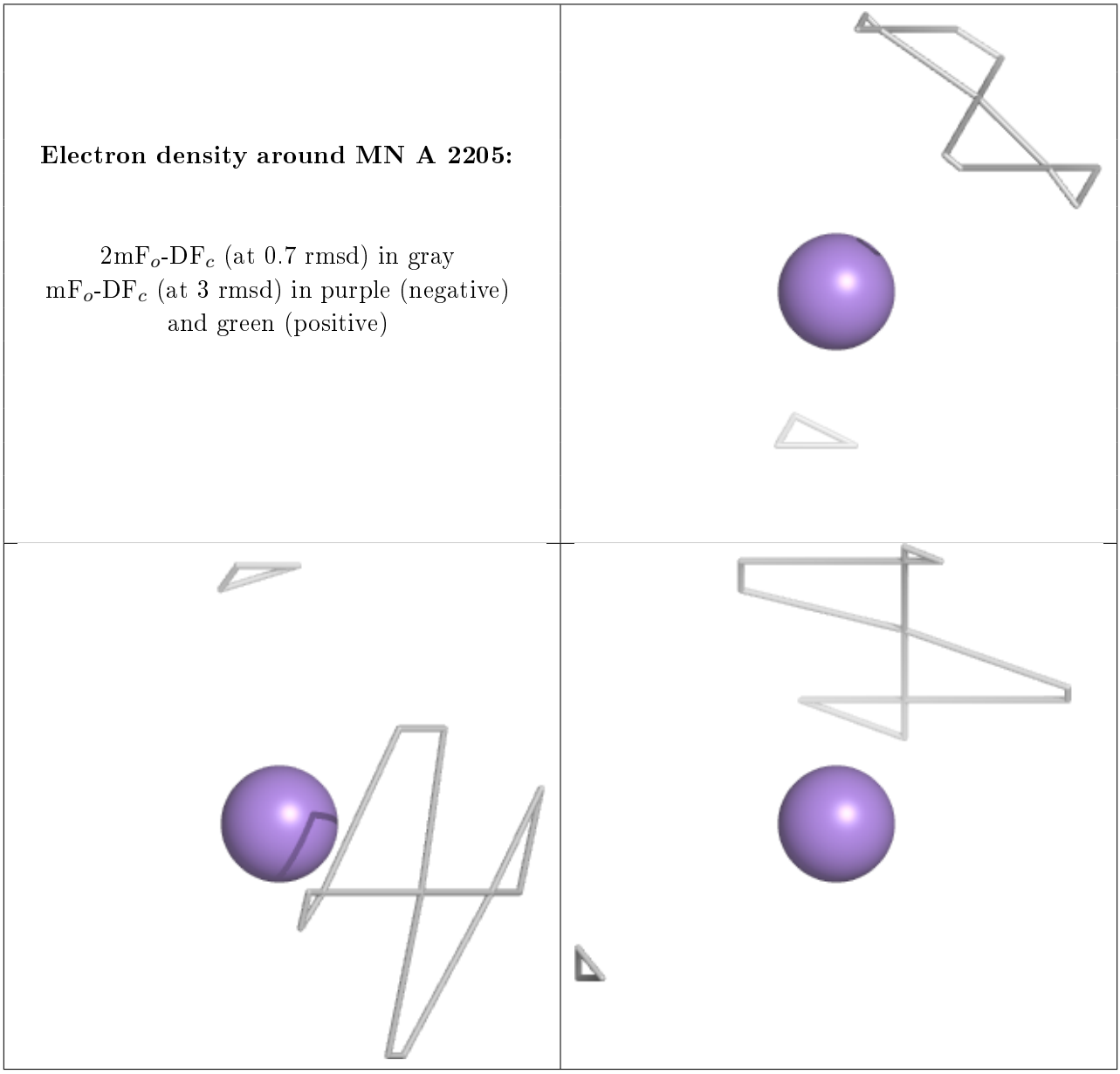
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MN	A	2205	1/1	0.66	0.30	133,133,133,133	0
4	PEG	A	2206	7/7	0.89	0.18	41,44,57,63	0
2	ADP	A	2203	27/27	0.92	0.17	50,71,101,103	0
2	ADP	A	2201	27/27	0.92	0.18	86,105,119,121	0
2	ADP	A	2202	27/27	0.93	0.20	46,61,74,85	0
3	MN	A	2204	1/1	0.94	0.39	69,69,69,69	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.

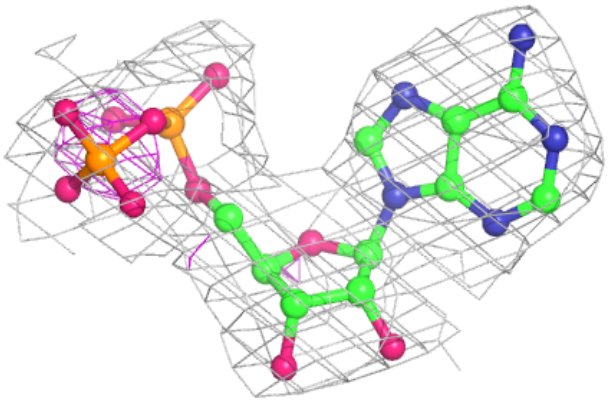
Electron density around MN A 2205:

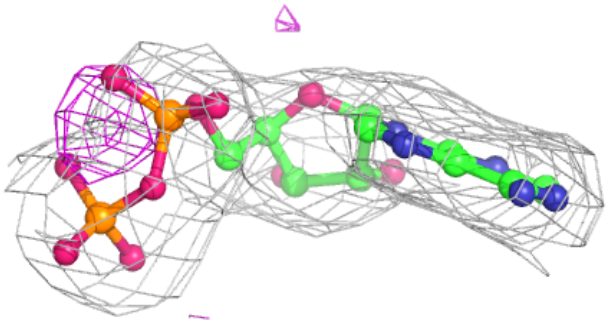
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

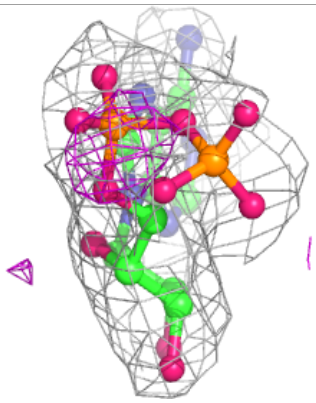


Electron density around ADP A 2203:

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

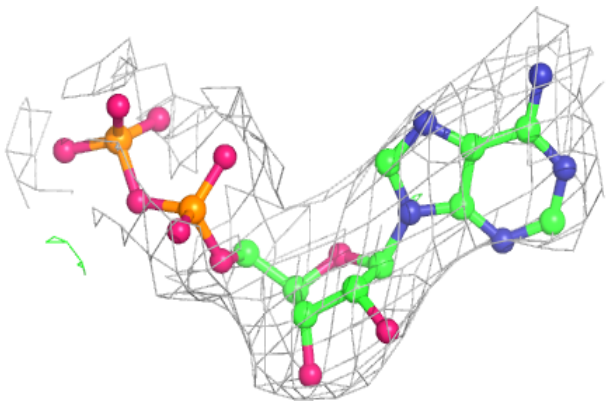


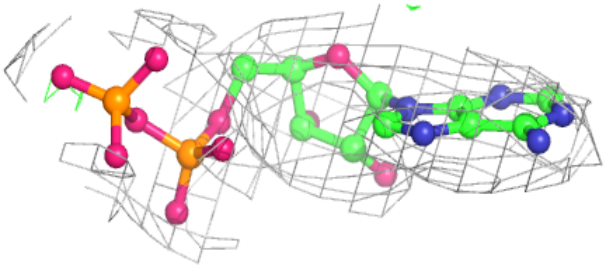


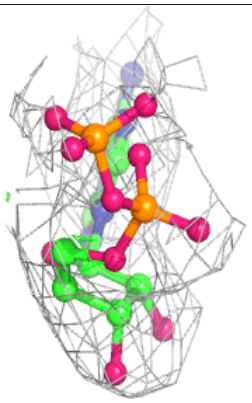


Electron density around ADP A 2201:

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

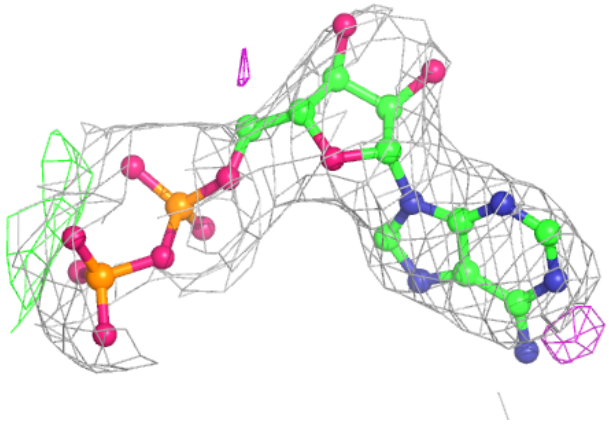


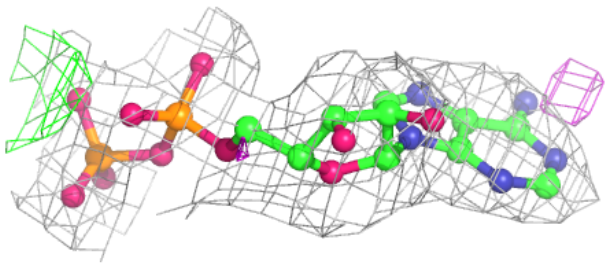


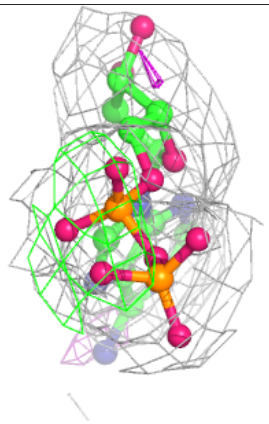


Electron density around ADP A 2202:

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

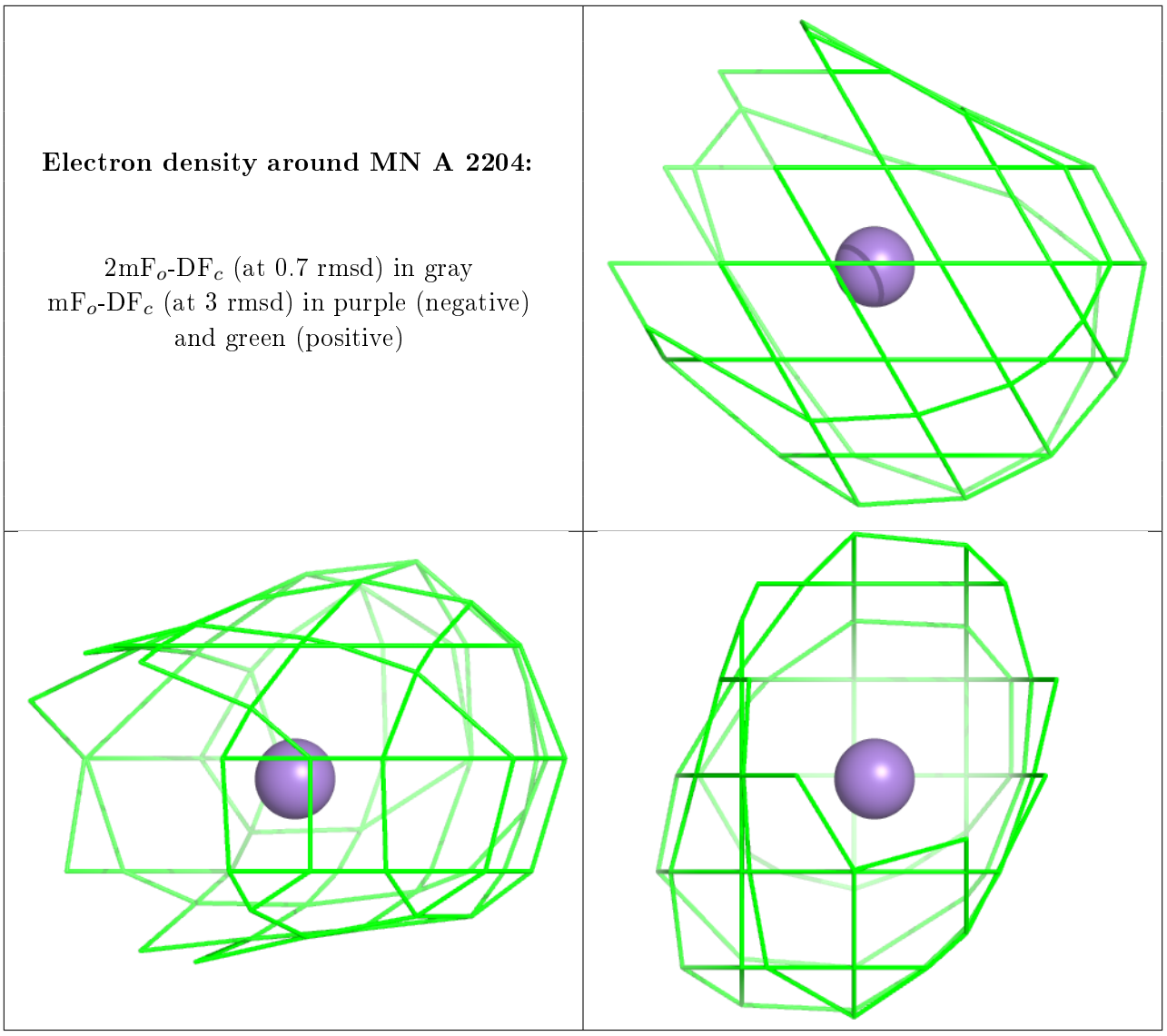






Electron density around MN A 2204:

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



6.5 Other polymers (i)

There are no such residues in this entry.