



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:13 PM EDT

PDB ID : 6QV3 / pdb_00006qv3
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 types of validation reports are described at

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

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

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

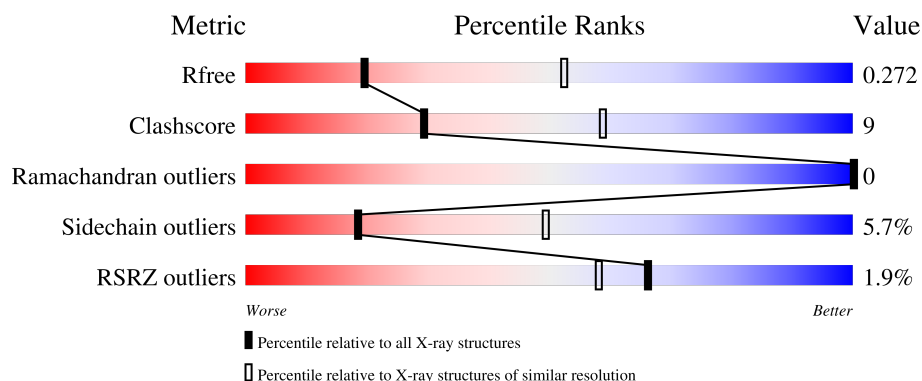
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

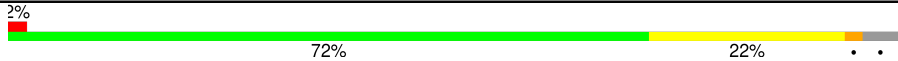
The reported resolution of this entry is 2.90 Å.

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1725	

2 Entry composition [i](#)

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.

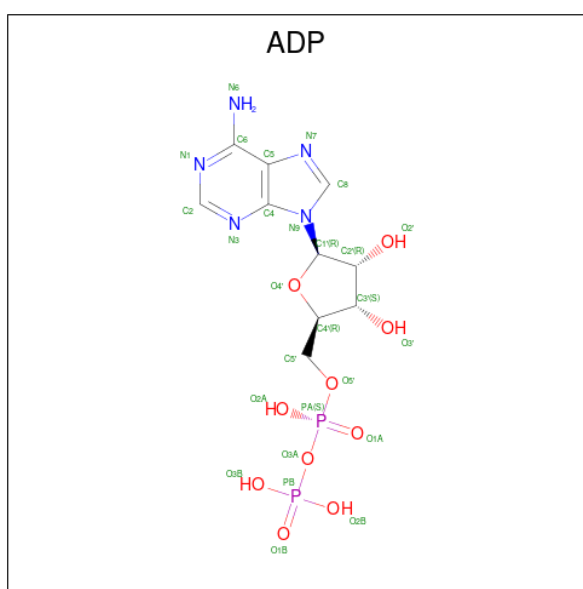
- Molecule 1 is a protein called Pre-mRNA splicing helicase-like protein.

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

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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

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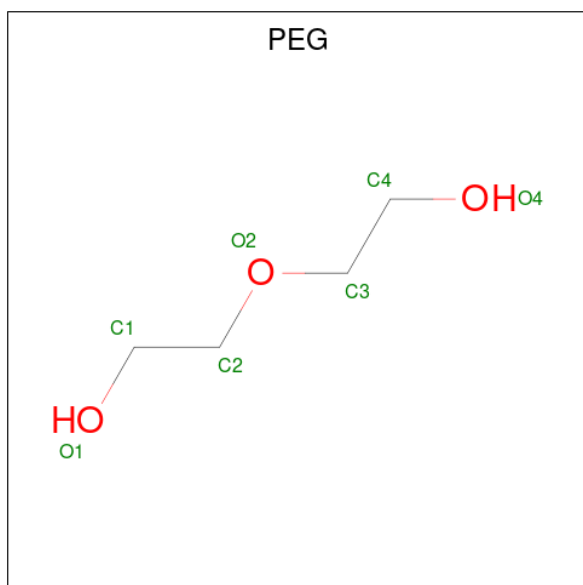
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

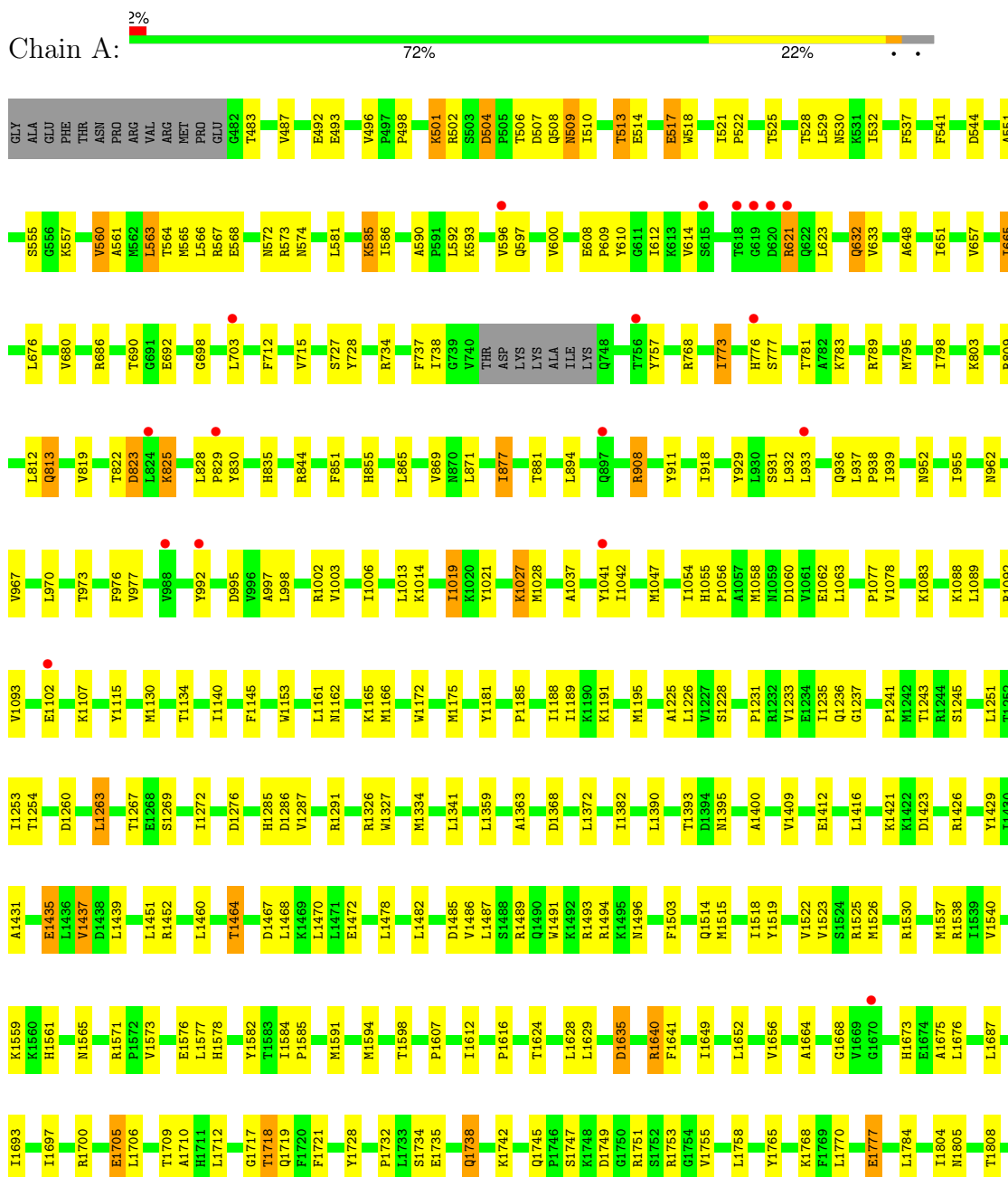
- Molecule 5 is water.

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

3 Residue-property plots

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: Pre-mRNA splicing helicase-like protein





4 Data and refinement statistics

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 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.65-2.90) 99.6 (44.65-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14 _ 3260: ???)	Depositor
R, R_{free}	0.220 , 0.271 0.224 , 0.272	Depositor DCC
R_{free} test set	2720 reflections (4.92%)	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 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, PEG, ADP

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	0.13	0/13576	0.34	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 [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	13284	0	13360	230	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	1	0
All	All	13417	0	13406	230	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 9.

All (230) 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:590:ALA:HB3	1:A:596:VAL:HG12	1.78	0.66
1:A:1243:THR:HG23	1:A:1245:SER:H	1.60	0.66
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:1431:ALA:HB3	1:A:1437:VAL:HG12	1.80	0.64
1:A:1530:ARG:HD3	1:A:1537:MET:HE2	1.80	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:N	1:A:504:ASP:OD1	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:OD1	1:A:823:ASP:N	2.34	0.61
1:A:530:ASN:ND2	1:A:555:SER:O	2.35	0.60
1:A:1578:HIS:HB2	1:A:1755:VAL:HG12	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:ALA:HB3	1:A:1565:ASN:HA	1.89	0.55
1:A:789:ARG:HD2	1:A:830:TYR:HD1	1.71	0.55
1:A:2033:ASP:OD1	1:A:2034:ILE:N	2.40	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:932:LEU:HD13	1:A:937:LEU:HD23	1.89	0.54
1:A:1709:THR:HG22	1:A:1745:GLN:HG3	1.89	0.54
1:A:1950:ALA:HA	1:A:1955:MET:HE3	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:H	1:A:632:GLN:HE21	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:1899:LEU:HA	1:A:1997:MET:HE1	1.91	0.52
1:A:1161:LEU:HG	1:A:1165:LYS:HE3	1.90	0.52
1:A:2000:MET:HE3	1:A:2006:TRP:HA	1.91	0.52
1:A:1988:HIS:CD2	1:A:1988:HIS:H	2.28	0.52
1:A:851:PHE:HB3	1:A:871:LEU:HD11	1.92	0.52
1:A:2144:LYS:HB2	1:A:2156:LEU:HD12	1.91	0.52
1:A:1594:MET:O	1:A:1598:THR:HG23	2.10	0.52
1:A:686:ARG:O	1:A:690:THR:HG22	2.09	0.52
1:A:1853:ILE:HG23	1:A:1854:ILE:HG23	1.92	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:998:LEU:O	1:A:1002:ARG:HG3	2.10	0.51
1:A:2075:PRO:HG2	1:A:2180:VAL:HG21	1.91	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:1225:ALA:O	1:A:1228:SER:OG	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	1:A:2007:ASP:N	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:1088:LYS:NZ	5:A:2304:HOH:O	2.46	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:1055:HIS:CD2	1:A:1058:MET:HE3	2.49	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:1491:TRP:C	1:A:1493:ARG:H	2.21	0.48
1:A:621:ARG:HD2	1:A:621:ARG:HA	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:1928:VAL:HG11	1:A:1949:GLN:CD	2.40	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:537:PHE:HA	1:A:563:LEU:HD23	1.97	0.47
1:A:551:ALA:HB3	1:A:557:LYS:HE2	1.96	0.47
1:A:1732:PRO:HG2	1:A:1735:GLU:HG2	1.96	0.47
1:A:1996:GLU:O	1:A:1999:GLN:HG2	2.14	0.46
1:A:703:LEU:HB3	1:A:939:ILE:HD11	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1987:GLY:C	1:A:2139:THR:HA	2.41	0.46
1:A:593:LYS:O	1:A:596:VAL:HG22	2.15	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: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
1:A:835:HIS:NE2	1:A:844:ARG:HG3	2.31	0.45
1:A:1902:VAL:HG22	1:A:1979:ILE:HD12	1.99	0.45
1:A:1526:MET:HB3	1:A:1537:MET:HE1	1.98	0.45
1:A:937:LEU:HD12	1:A:938:PRO:HD2	1.97	0.45
1:A:665:ILE:HD11	1:A:698:GLY:HA3	1.98	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:783:LYS:HE3	1:A:783:LYS:HB3	1.86	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: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:648:ALA:HA	1:A:651:ILE:HD11	1.99	0.45
1:A:1260:ASP:HB3	1:A:1263:LEU:HD11	1.98	0.45
1:A:1577:LEU:HD11	1:A:1770:LEU:HD13	1.99	0.44
1:A:1628:LEU:HD21	1:A:1641:PHE:CE2	2.51	0.44
1:A:483:THR:HG22	1:A:496:VAL:HG22	1.98	0.44
1:A:623:LEU:HD11	1:A:1269:SER:HB2	1.99	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:812:LEU:HD13	1:A:855:HIS:HB3	1.99	0.44
1:A:1041:TYR:O	1:A:1041:TYR:CG	2.70	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:1932:MET:HE1	1:A:1942:PHE:HA	1.99	0.44
1:A:501:LYS:O	1:A:727:SER:HB2	2.18	0.44
1:A:813:GLN:H	1:A:813:GLN:HG3	1.48	0.44
1:A:1181:TYR:CD1	1:A:1226:LEU:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:541:PHE:O	1:A:567:ARG:HD3	2.19	0.43
1:A:1914:ARG:NH2	1:A:1964:ASP:OD2	2.51	0.43
1:A:1482:LEU:O	1:A:1486:VAL:HG23	2.18	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
1:A:1875:TYR:OH	1:A:1981:ASP:OD2	2.32	0.43
1:A:1077:PRO:O	1:A:1107:LYS:NZ	2.49	0.43
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:608:GLU:N	1:A:609:PRO:HD2	2.34	0.42
1:A:1089:LEU:O	1:A:1093:VAL:HG13	2.19	0.42
1:A:2123:LYS:HG3	1:A:2124:LYS:O	2.19	0.42
1:A:768:ARG:HG3	1:A:803:LYS:HZ2	1.84	0.42
1:A:1991:ALA:O	1:A:1995:MET:HG3	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:1712:LEU:HA	1:A:1753:ARG:O	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:HD23	1:A:1784:LEU:HA	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:1237:GLY:N	1:A:1334:MET:HE1	2.35	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:585:LYS:HB2	1:A:657:VAL:HG12	2.01	0.41
1:A:1514:GLN:OE1	1:A:1514:GLN:N	2.51	0.41
1:A:2097:LEU:HB2	1:A:2158:PHE:CE2	2.54	0.41
1:A:1060:ASP:N	1:A:1060:ASP:OD1	2.53	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:1412:GLU:O	1:A:1416:LEU:HG	2.20	0.41
1:A:2148:VAL:HG22	1:A:2152:LEU:HD12	2.01	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:737:PHE:CE2	1:A:933:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:ASN:C	1:A:1028:MET:HE2	2.45	0.41
1:A:1584:ILE:HA	1:A:1585:PRO:HD3	1.87	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
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:517:GLU:OE1	1:A:518:TRP:N	2.54	0.40
1:A:1706:LEU:O	1:A:1742:LYS:HE3	2.21	0.40
1:A:2103:ARG:HH22	1:A:2126:GLU:CD	2.27	0.40
1:A:1172:TRP:H	1:A:1175:MET:HE2	1.85	0.40
1:A:1582:TYR:CZ	1:A:1594:MET:HG2	2.56	0.40
1:A:573:ARG:HG2	1:A:574:ASN:O	2.22	0.40
1:A:1923:ARG:O	1:A:1927:HIS:ND1	2.55	0.40
1:A:795:MET:HE3	1:A:795:MET:HB2	1.98	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 ⓘ

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%)	1381 (94%)	83 (6%)	18 49

All (83) 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	560	VAL
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	665	ILE
1	A	715	VAL
1	A	757	TYR
1	A	773	ILE
1	A	798	ILE

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Mol	Chain	Res	Type
1	A	809	ARG
1	A	813	GLN
1	A	819	VAL
1	A	823	ASP
1	A	825	LYS
1	A	877	ILE
1	A	908	ARG
1	A	1006	ILE
1	A	1019	ILE
1	A	1027	LYS
1	A	1063	LEU
1	A	1078	VAL
1	A	1189	ILE
1	A	1233	VAL
1	A	1254	THR
1	A	1263	LEU
1	A	1276	ASP
1	A	1382	ILE
1	A	1409	VAL
1	A	1435	GLU
1	A	1437	VAL
1	A	1439	LEU
1	A	1464	THR
1	A	1540	VAL
1	A	1571	ARG
1	A	1573	VAL
1	A	1591	MET
1	A	1635	ASP
1	A	1640	ARG
1	A	1676	LEU
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	1895	LEU

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Mol	Chain	Res	Type
1	A	1914	ARG
1	A	1930	VAL
1	A	1979	ILE
1	A	1984	SER
1	A	1992	LEU
1	A	2008	ARG
1	A	2123	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	559	ASN
1	A	622	GLN
1	A	799	ASN
1	A	1017	ASN
1	A	1442	GLN
1	A	1689	ASN
1	A	1826	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 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
4	PEG	A	2206	-	6,6,6	0.51	0	5,5,5	0.25	0
2	ADP	A	2203	-	28,29,29	1.46	5 (17%)	43,45,45	1.81	8 (18%)
2	ADP	A	2202	3	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
2	ADP	A	2201	-	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)

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	PEG	A	2206	-	-	0/4/4/4	-
2	ADP	A	2203	-	-	3/16/32/32	0/3/3/3
2	ADP	A	2202	3	-	3/16/32/32	0/3/3/3
2	ADP	A	2201	-	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2203	ADP	C5-C4	4.81	1.47	1.39
2	A	2201	ADP	C5-C4	4.71	1.47	1.39
2	A	2202	ADP	C5-C4	4.67	1.47	1.39
2	A	2202	ADP	C5-C6	2.73	1.48	1.41
2	A	2203	ADP	C5-C6	2.69	1.48	1.41
2	A	2201	ADP	C5-C6	2.68	1.48	1.41
2	A	2203	ADP	PA-O3A	2.49	1.62	1.59
2	A	2202	ADP	C8-N7	2.40	1.36	1.31
2	A	2201	ADP	C8-N7	2.36	1.36	1.31
2	A	2203	ADP	C8-N7	2.32	1.36	1.31
2	A	2201	ADP	C5-N7	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2202	ADP	C5-N7	-2.26	1.35	1.39
2	A	2203	ADP	C5-N7	-2.22	1.35	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2202	ADP	C5-C4-N3	-5.78	118.76	126.72
2	A	2201	ADP	C5-C4-N3	-5.74	118.81	126.72
2	A	2203	ADP	C5-C4-N3	-5.74	118.82	126.72
2	A	2203	ADP	N3-C4-N9	4.66	135.10	127.17
2	A	2201	ADP	N3-C4-N9	4.55	134.91	127.17
2	A	2202	ADP	N3-C4-N9	4.51	134.84	127.17
2	A	2202	ADP	C2-N3-C4	3.70	120.86	111.83
2	A	2201	ADP	C2-N3-C4	3.69	120.84	111.83
2	A	2203	ADP	C2-N3-C4	3.61	120.65	111.83
2	A	2202	ADP	C4-C5-N7	-3.58	106.48	110.58
2	A	2201	ADP	C4-C5-N7	-3.44	106.65	110.58
2	A	2202	ADP	N3-C2-N1	-3.30	123.59	128.58
2	A	2201	ADP	N3-C2-N1	-3.29	123.60	128.58
2	A	2203	ADP	C4-C5-N7	-3.29	106.82	110.58
2	A	2203	ADP	N3-C2-N1	-3.11	123.87	128.58
2	A	2202	ADP	C4-N9-C8	2.71	108.59	105.74
2	A	2203	ADP	C4-N9-C8	2.70	108.58	105.74
2	A	2201	ADP	C4-N9-C8	2.70	108.57	105.74
2	A	2202	ADP	C5-N7-C8	2.64	107.60	103.45
2	A	2203	ADP	C3'-C2'-C1'	2.59	106.36	101.46
2	A	2201	ADP	C5-N7-C8	2.53	107.42	103.45
2	A	2203	ADP	C5-N7-C8	2.43	107.27	103.45
2	A	2202	ADP	C6-C5-N7	2.19	136.31	132.09
2	A	2201	ADP	C6-C5-N7	2.13	136.19	132.09
2	A	2202	ADP	N9-C8-N7	-2.12	110.94	113.94
2	A	2201	ADP	N9-C8-N7	-2.01	111.09	113.94

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'

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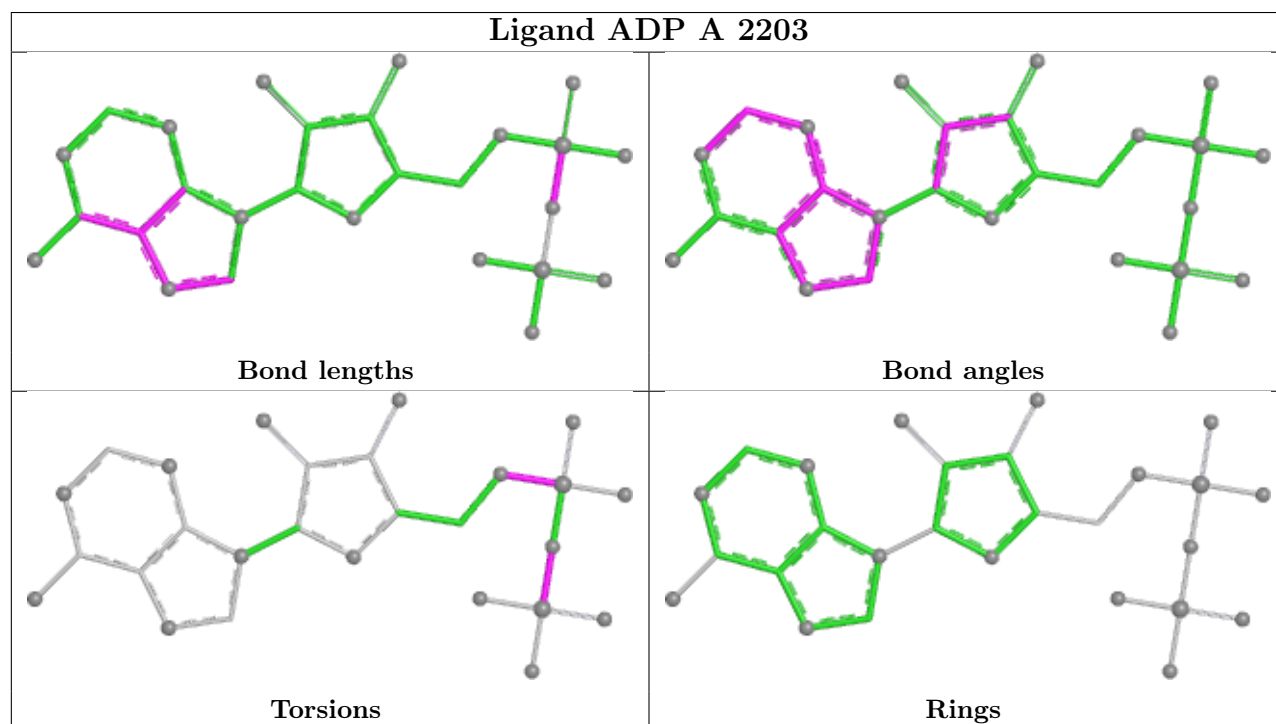
Mol	Chain	Res	Type	Atoms
2	A	2202	ADP	C5'-O5'-PA-O1A
2	A	2203	ADP	C5'-O5'-PA-O1A
2	A	2203	ADP	PA-O3A-PB-O2B
2	A	2201	ADP	PB-O3A-PA-O2A
2	A	2201	ADP	PB-O3A-PA-O1A

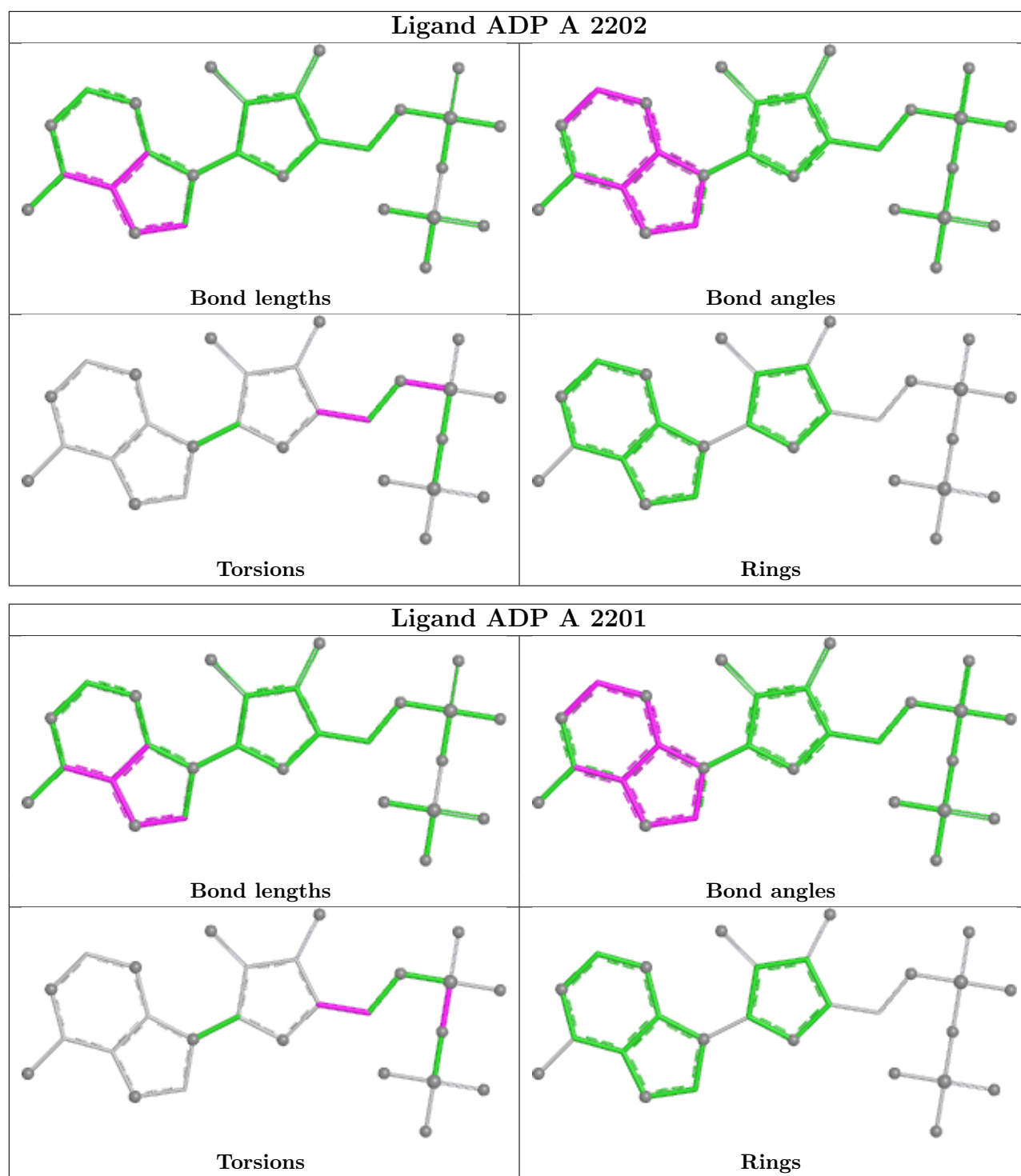
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

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, 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	1657/1725 (96%)	0.13	31 (1%) 66 58	35, 83, 155, 229	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2041	MET	4.0
1	A	829	PRO	3.8
1	A	1887	LEU	3.3
1	A	596	VAL	3.1
1	A	1041	TYR	3.1
1	A	1893	SER	3.1
1	A	1866	LEU	2.8
1	A	619	GLY	2.6
1	A	988	VAL	2.6
1	A	2131	VAL	2.6
1	A	1886	LEU	2.5
1	A	824	LEU	2.5
1	A	933	LEU	2.5
1	A	2148	VAL	2.4
1	A	2141	LEU	2.3
1	A	756	THR	2.3
1	A	1670	GLY	2.3
1	A	2123	LYS	2.2
1	A	2077	ILE	2.2
1	A	776	HIS	2.2
1	A	2018	PHE	2.2
1	A	621	ARG	2.2
1	A	615	SER	2.1
1	A	618	THR	2.1
1	A	1102	GLU	2.1
1	A	897	GLN	2.1
1	A	703	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	620	ASP	2.1
1	A	992	TYR	2.1
1	A	2049	TYR	2.1
1	A	2171	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

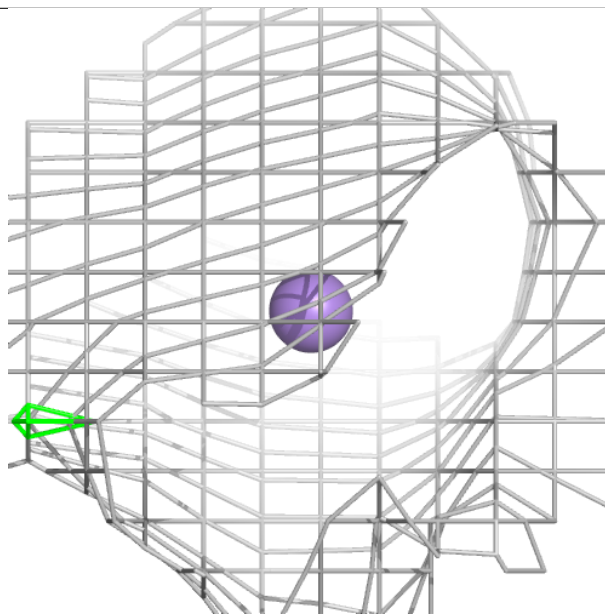
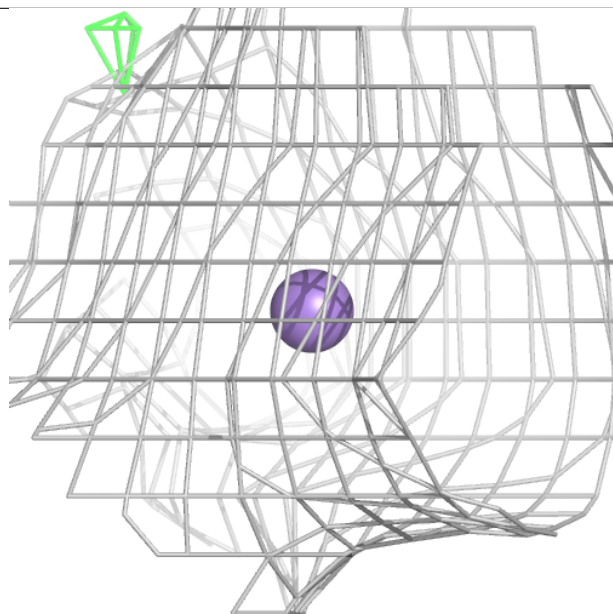
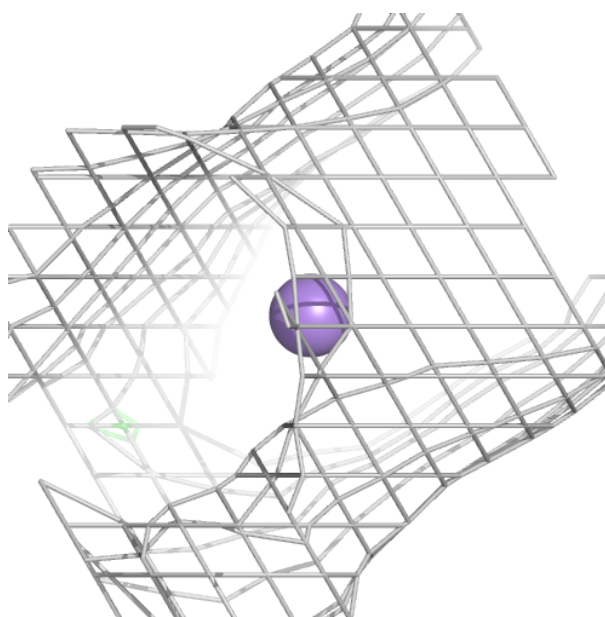
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	A	2206	7/7	0.86	0.14	41,44,57,63	0
3	MN	A	2205	1/1	0.88	0.11	133,133,133,133	0
2	ADP	A	2203	27/27	0.89	0.10	50,71,101,103	0
2	ADP	A	2201	27/27	0.93	0.07	86,105,119,121	0
2	ADP	A	2202	27/27	0.95	0.08	46,61,74,85	0
3	MN	A	2204	1/1	0.95	0.19	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.

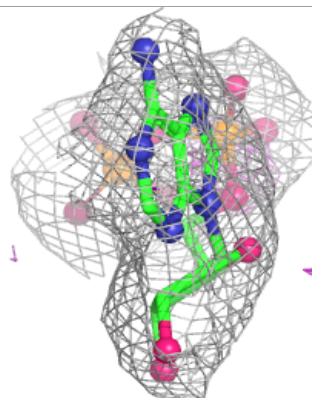
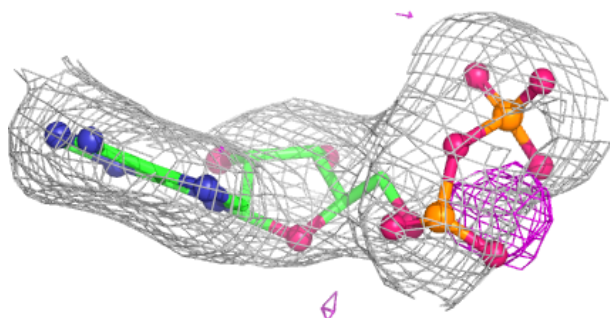
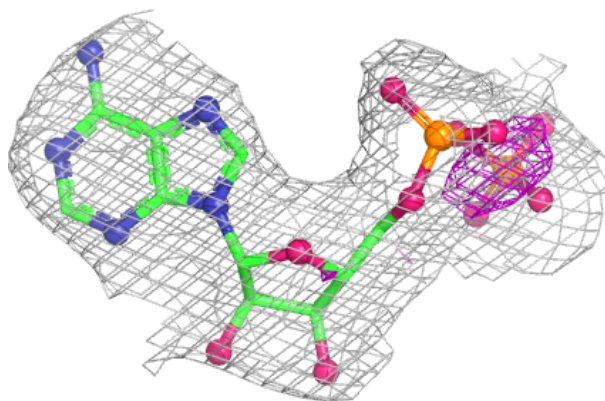
Electron density around MN A 2205:

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

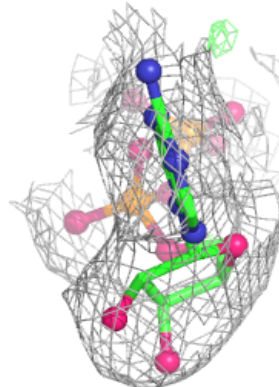
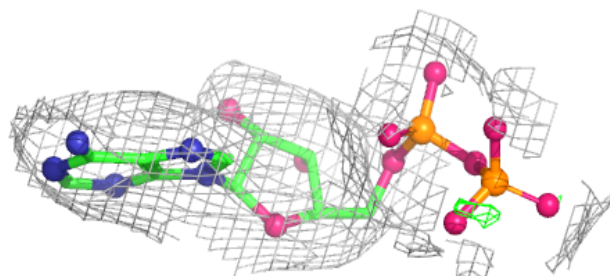
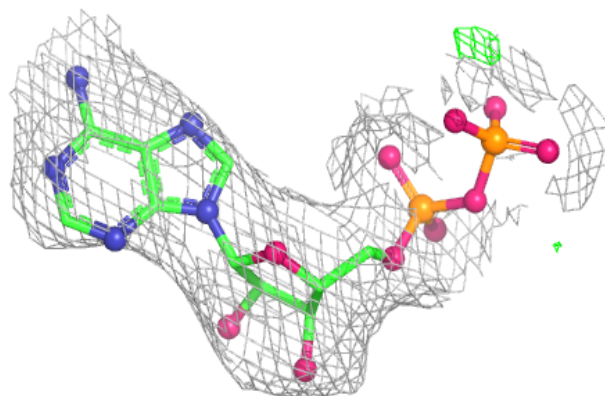


Electron density around ADP A 2203:

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

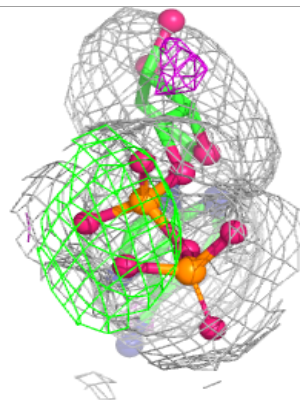
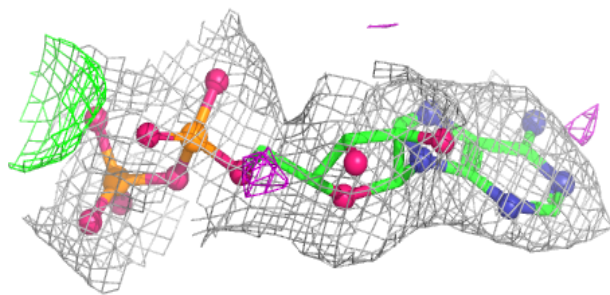
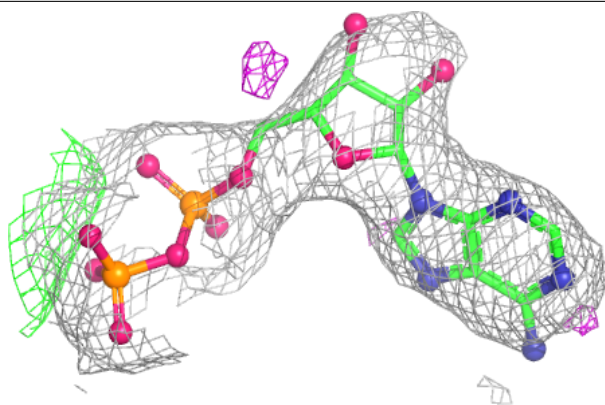
**Electron density around ADP A 2201:**

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



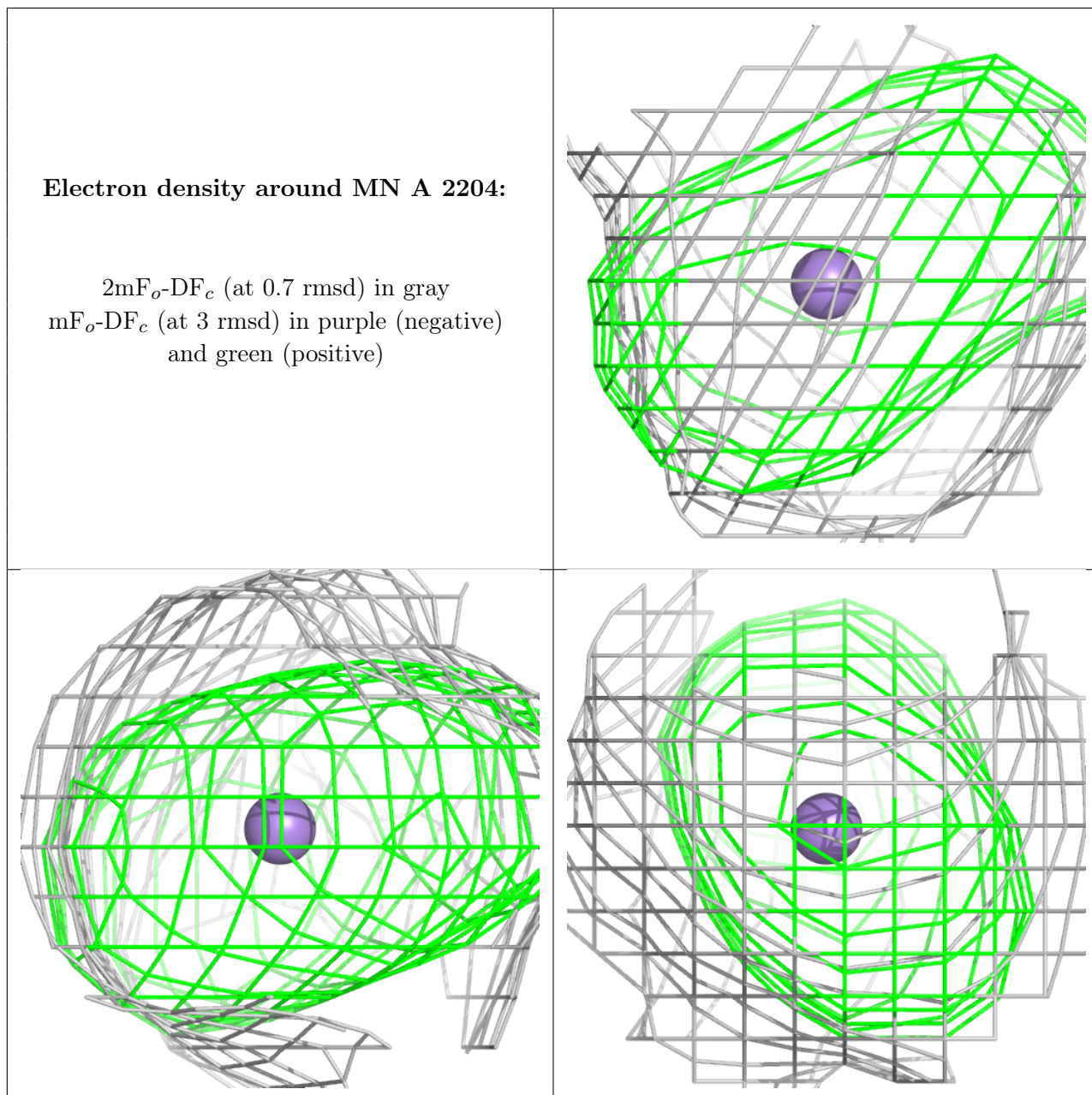
Electron density around ADP A 2202:

$2mF_o - DF_c$ (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 ⓘ

There are no such residues in this entry.