



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 12:35 AM EDT

PDB ID : 4DB1
Title : Cardiac human myosin S1dC, beta isoform complexed with Mn-AMPPNP
Authors : Klenchin, V.A.; Deacon, J.C.; Combs, A.C.; Leinwand, L.A.; Rayment, I.
Deposited on : 2012-01-13
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

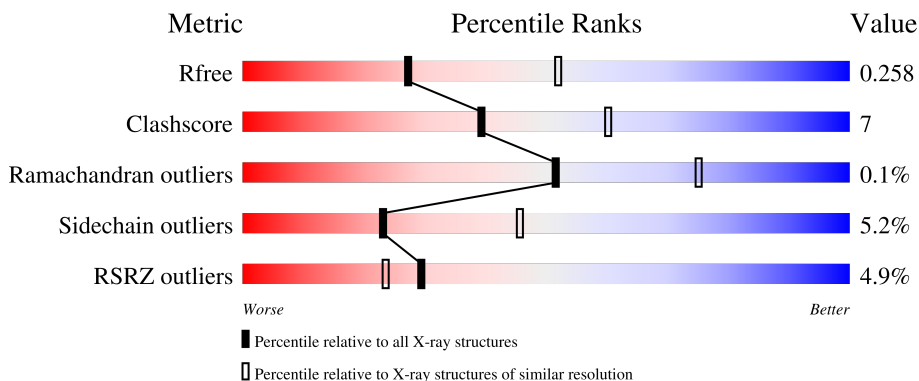
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	783	 4% 74% 16% • 9%
1	B	783	 5% 76% 14% • 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11340 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.

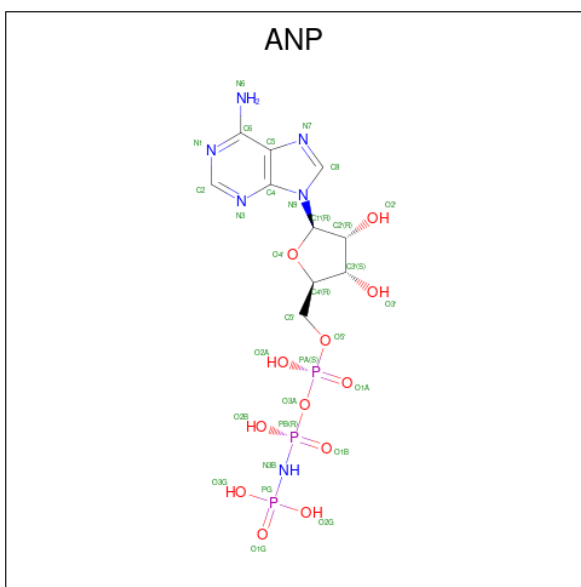
- Molecule 1 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	716	Total 5572	C 3576	N 934	O 1030	S 32	0	1	0
1	B	718	Total 5502	C 3530	N 921	O 1022	S 29	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P12883
B	1	GLY	-	expression tag	UNP P12883

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

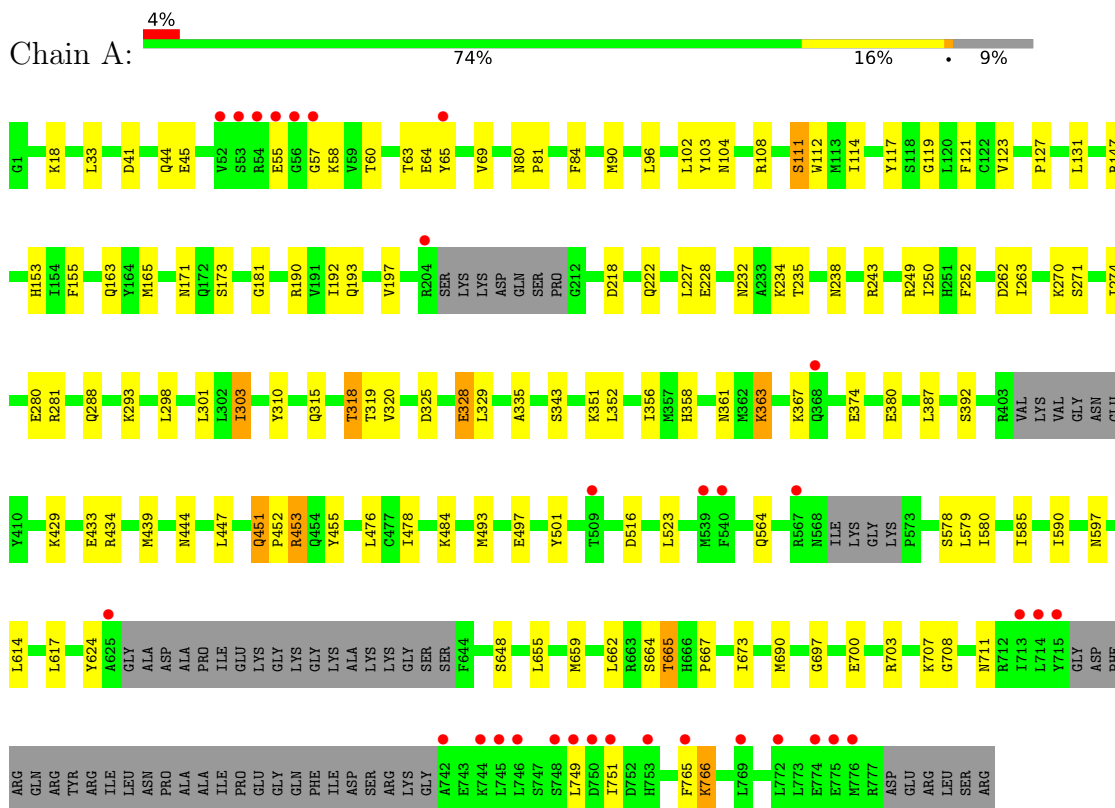
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	85	85	85	0	0
4	B	117	117	117	0	0

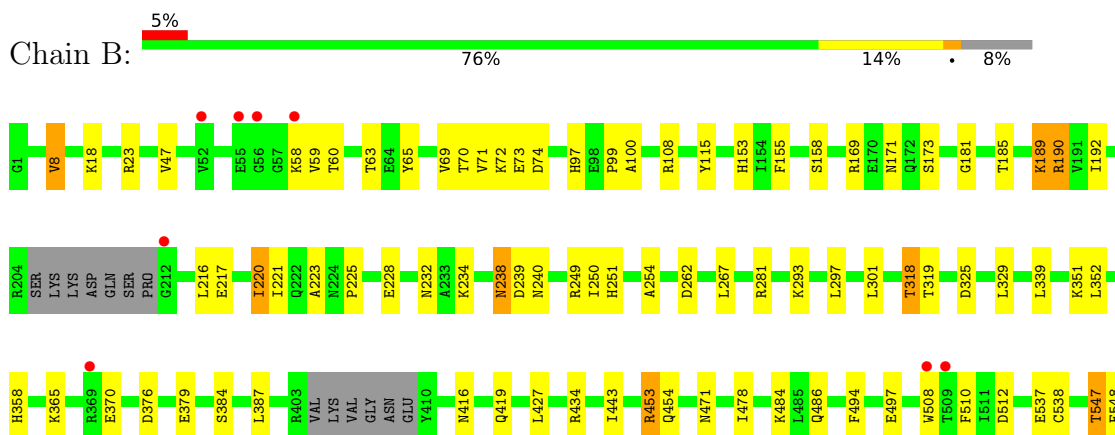
3 Residue-property plots [i](#)

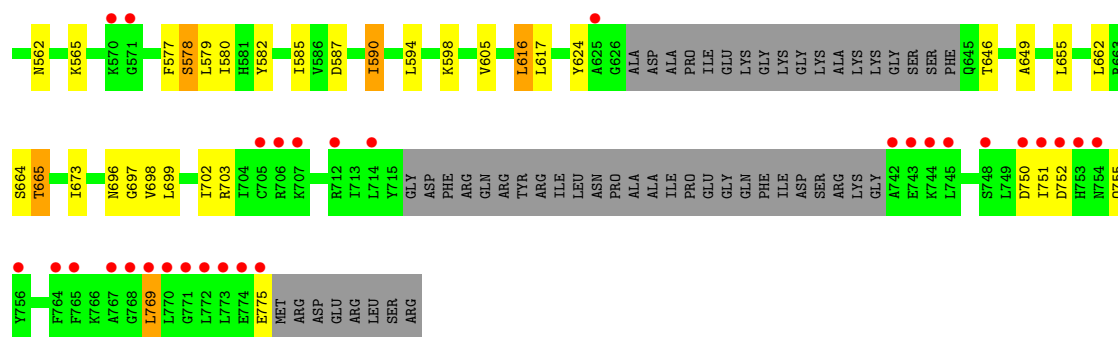
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Myosin-7



- Molecule 1: Myosin-7





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.21Å 94.31Å 110.89Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.60) 99.4 (24.97-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.60Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.257 0.211 , 0.258	Depositor DCC
R_{free} test set	2961 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11340	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4695e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ANP, 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	0.44	0/5697	0.57	0/7705
1	B	0.46	0/5622	0.58	0/7613
All	All	0.45	0/11319	0.57	0/15318

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	751	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5572	0	5333	90	0
1	B	5502	0	5215	71	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	85	0	0	4	0
4	B	117	0	0	2	0
All	All	11340	0	10574	160	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 7.

All (160) 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:173:SER:HB2	1:A:665:THR:CG2	1.79	1.11
1:A:173:SER:HB2	1:A:665:THR:HG21	1.18	1.08
1:A:181:GLY:H	2:A:801:ANP:HNB1	1.08	0.92
1:A:173:SER:CB	1:A:665:THR:HG21	2.00	0.92
1:A:153:HIS:HD2	1:A:155:PHE:H	1.14	0.91
1:B:153:HIS:HD2	1:B:155:PHE:H	1.18	0.89
1:A:263:ILE:H	1:A:444:ASN:HD21	1.22	0.86
1:B:755:GLN:CB	1:B:769:LEU:HD13	2.07	0.83
1:A:434:ARG:HH21	1:A:624:TYR:HD2	1.25	0.82
1:B:698:VAL:O	1:B:702:ILE:HG12	1.81	0.79
1:B:63:THR:HG22	1:B:65:TYR:H	1.47	0.79
1:B:234:LYS:HE2	4:B:987:HOH:O	1.84	0.77
1:B:646:THR:HG22	1:B:649:ALA:H	1.50	0.77
1:B:752:ASP:CB	1:B:769:LEU:HD11	2.16	0.74
1:B:434:ARG:HH22	1:B:624:TYR:HD1	1.36	0.74
1:A:434:ARG:NH2	1:A:624:TYR:HD2	1.85	0.73
1:B:108:ARG:NH1	1:B:115:TYR:O	2.22	0.72
1:A:41:ASP:HB3	1:A:44:GLN:O	1.89	0.72
1:B:173:SER:OG	1:B:665:THR:HG21	1.89	0.72
1:B:108:ARG:NH2	4:B:904:HOH:O	2.22	0.71
1:B:752:ASP:HB2	1:B:769:LEU:HD11	1.72	0.71
1:A:153:HIS:CD2	1:A:155:PHE:H	2.03	0.70
1:B:153:HIS:CD2	1:B:155:PHE:H	2.06	0.70
1:B:216:LEU:O	1:B:220:ILE:HG12	1.90	0.70
1:B:254:ALA:HB2	1:B:454:GLN:HE21	1.55	0.70
1:B:537:GLU:OE1	1:B:547:THR:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HB3	1:B:74:ASP:HB2	1.75	0.67
1:A:173:SER:HB2	1:A:665:THR:HG23	1.74	0.67
1:A:749:LEU:HB3	1:A:751:ILE:HG12	1.77	0.66
1:B:181:GLY:H	2:B:801:ANP:HNB1	1.41	0.66
1:A:192:ILE:HD12	1:A:250:ILE:HD11	1.77	0.66
1:B:339:LEU:HD13	1:B:443:ILE:HD12	1.76	0.66
1:A:281:ARG:HD3	4:A:968:HOH:O	1.96	0.66
1:B:416:ASN:H	1:B:419:GLN:HE21	1.43	0.65
1:A:303:ILE:HG13	1:A:310:TYR:OH	1.96	0.65
1:A:173:SER:HB3	1:A:667:PRO:HA	1.80	0.63
1:A:597:ASN:HD21	1:A:648:SER:H	1.48	0.62
1:B:238:ASN:ND2	1:B:240:ASN:H	1.98	0.61
1:B:434:ARG:NH2	1:B:624:TYR:HD1	1.97	0.60
1:A:63:THR:CG2	1:A:64:GLU:O	2.50	0.59
1:A:190:ARG:HH21	1:A:193:GLN:HE22	1.50	0.59
1:A:114:ILE:HD13	1:A:131:LEU:HD11	1.84	0.58
1:B:238:ASN:HD22	1:B:239:ASP:N	2.00	0.58
1:A:597:ASN:HD21	1:A:648:SER:HB2	1.67	0.58
1:B:752:ASP:HB3	1:B:769:LEU:HD11	1.85	0.58
1:A:301:LEU:O	1:A:358:HIS:HE1	1.87	0.58
1:A:708:GLY:O	1:A:766:LYS:HE2	2.05	0.57
1:A:173:SER:CB	1:A:665:THR:CG2	2.68	0.57
1:A:165:MET:HE3	1:A:252:PHE:CD1	2.39	0.57
1:B:301:LEU:O	1:B:358:HIS:HE1	1.88	0.56
1:A:63:THR:HG22	1:A:64:GLU:O	2.06	0.56
1:A:249:ARG:HD3	1:A:262:ASP:OD2	2.06	0.56
1:A:104:ASN:O	1:A:108:ARG:HG2	2.05	0.55
1:B:185:THR:O	1:B:189:LYS:HG3	2.06	0.55
1:B:434:ARG:NH2	1:B:624:TYR:CD1	2.75	0.55
1:A:453:ARG:NH2	4:A:959:HOH:O	2.38	0.55
1:A:303:ILE:HG13	1:A:310:TYR:CZ	2.43	0.53
1:B:484:LYS:HG3	1:B:655:LEU:HD21	1.89	0.52
1:A:165:MET:HE2	1:A:455:TYR:HB2	1.92	0.52
1:B:352:LEU:HD12	1:B:616:LEU:CD1	2.41	0.51
1:B:537:GLU:OE1	1:B:547:THR:CG2	2.58	0.51
1:A:218:ASP:OD1	1:B:8:VAL:HG11	2.11	0.50
1:A:523:LEU:HD21	1:A:579:LEU:HD22	1.94	0.50
1:A:165:MET:CE	1:A:455:TYR:HB2	2.41	0.50
1:A:102:LEU:HD22	1:A:690:MET:HE2	1.93	0.49
1:A:516:ASP:OD1	1:A:707:LYS:NZ	2.43	0.49
1:A:18:LYS:HE3	1:A:111:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:O	1:A:197:VAL:HG23	2.11	0.49
1:B:301:LEU:HD22	1:B:351:LYS:HA	1.94	0.49
1:A:263:ILE:H	1:A:444:ASN:ND2	2.01	0.49
1:A:119:GLY:O	1:A:147:ARG:NH2	2.45	0.49
1:B:173:SER:CB	1:B:665:THR:HG21	2.43	0.49
1:B:190:ARG:HH11	1:B:190:ARG:HG3	1.78	0.49
1:A:484:LYS:HB2	1:A:659:MET:CE	2.44	0.48
1:A:147:ARG:HG2	4:A:962:HOH:O	2.14	0.48
1:A:222:GLN:HE21	1:A:335:ALA:HA	1.78	0.48
1:B:699:LEU:O	1:B:702:ILE:HB	2.14	0.48
1:B:190:ARG:HH11	1:B:190:ARG:CG	2.27	0.47
1:B:365:LYS:HG3	1:B:376:ASP:HB2	1.95	0.47
1:A:318:THR:HG22	1:A:319:THR:HG23	1.96	0.47
1:A:484:LYS:HG3	1:A:655:LEU:HD21	1.97	0.47
1:B:318:THR:HG22	1:B:319:THR:HG23	1.95	0.47
1:B:192:ILE:HD12	1:B:250:ILE:HD11	1.96	0.47
1:B:673:ILE:HD11	1:B:696:ASN:HD21	1.80	0.47
1:A:497:GLU:HG3	1:A:501:TYR:CE2	2.49	0.47
1:B:249:ARG:HD3	1:B:262:ASP:OD2	2.14	0.47
1:A:64:GLU:O	1:A:65:TYR:CB	2.63	0.47
1:A:352:LEU:O	1:A:356:ILE:HG12	2.15	0.46
1:B:59:VAL:HG23	1:B:73:GLU:CG	2.46	0.46
1:A:274:ILE:O	1:A:315:GLN:NE2	2.45	0.46
1:A:63:THR:HG23	1:A:64:GLU:O	2.15	0.46
1:A:60:THR:HA	1:A:69:VAL:O	2.15	0.46
1:B:97:HIS:ND1	1:B:99:PRO:HG2	2.30	0.46
1:B:232:ASN:HD22	1:B:240:ASN:ND2	2.14	0.46
1:A:281:ARG:HH22	1:A:325:ASP:CG	2.19	0.46
1:B:673:ILE:CD1	1:B:696:ASN:HD21	2.29	0.46
1:A:64:GLU:OE2	1:A:103:TYR:OH	2.27	0.46
1:B:297:LEU:O	1:B:301:LEU:HG	2.15	0.46
1:B:562:ASN:ND2	1:B:580:ILE:O	2.45	0.45
1:A:165:MET:CE	1:A:252:PHE:CD1	2.99	0.45
1:B:494:PHE:CD1	1:B:512:ASP:HA	2.51	0.45
1:B:548:PHE:CE2	1:B:590:ILE:HD11	2.52	0.45
1:A:523:LEU:CD2	1:A:579:LEU:HD22	2.47	0.45
1:A:114:ILE:HD11	1:A:127:PRO:HB3	1.99	0.45
1:A:81:PRO:HD2	1:A:84:PHE:CD2	2.52	0.45
1:A:358:HIS:HD2	1:A:380:GLU:OE2	1.99	0.45
1:B:582:TYR:OH	1:B:697:GLY:HA2	2.17	0.45
1:A:45:GLU:HG2	1:A:690:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HA	1:A:303:ILE:HG22	1.99	0.44
1:B:72:LYS:HB3	1:B:74:ASP:CB	2.45	0.44
1:A:235:THR:HA	1:A:280:GLU:HG2	1.99	0.44
1:B:97:HIS:CE1	1:B:100:ALA:HB2	2.53	0.44
1:B:223:ALA:HA	1:B:339:LEU:HD11	1.99	0.44
1:B:351:LYS:HG2	1:B:387:LEU:HD22	2.00	0.43
1:A:227:LEU:HD23	1:A:439:MET:HE3	2.00	0.43
1:B:471:ASN:HB2	1:B:587:ASP:O	2.18	0.43
1:A:117:TYR:HA	1:A:121:PHE:O	2.18	0.43
1:A:190:ARG:NH2	1:A:193:GLN:HE22	2.15	0.43
1:A:523:LEU:HD21	1:A:579:LEU:CD2	2.49	0.43
1:B:58:LYS:HB3	1:B:71:VAL:O	2.19	0.43
1:A:564:GLN:HB2	1:A:578:SER:HB2	2.01	0.43
1:B:281:ARG:NH2	1:B:325:ASP:OD2	2.52	0.43
1:B:171:ASN:HB2	1:B:664:SER:O	2.19	0.42
1:B:427:LEU:HD13	1:B:605:VAL:HG11	2.01	0.42
1:B:60:THR:HA	1:B:70:THR:HA	2.01	0.42
1:A:288:GLN:NE2	1:A:328:GLU:HB3	2.34	0.42
1:A:484:LYS:HB2	1:A:659:MET:HE2	2.01	0.42
1:B:251:HIS:HB3	1:B:453:ARG:HG3	2.02	0.42
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.89	0.42
1:A:580:ILE:HG12	1:A:585:ILE:HD12	2.02	0.42
1:B:577:PHE:HE1	1:B:579:LEU:HG	1.83	0.42
1:A:90:MET:O	1:A:96:LEU:HD21	2.20	0.42
1:A:711:ASN:HB2	1:A:765:PHE:HB2	2.02	0.42
1:B:217:GLU:O	1:B:221:ILE:HG12	2.20	0.42
1:B:565:LYS:O	1:B:578:SER:HB2	2.19	0.42
1:B:18:LYS:O	1:B:23:ARG:NH1	2.53	0.42
1:A:293:LYS:HB3	1:A:329:LEU:HD23	2.02	0.41
1:A:55:GLU:HB3	1:A:58:LYS:H	1.84	0.41
1:A:64:GLU:O	1:A:65:TYR:HB2	2.20	0.41
1:A:361:ASN:HB3	1:A:380:GLU:HG3	2.01	0.41
1:A:697:GLY:HA2	1:A:700:GLU:HB3	2.02	0.41
1:B:293:LYS:HB3	1:B:329:LEU:HD23	2.02	0.41
1:A:165:MET:HE1	1:A:252:PHE:HB2	2.02	0.41
1:A:111:SER:O	1:A:112:TRP:HB2	2.21	0.41
1:B:228:GLU:O	1:B:232:ASN:HB2	2.21	0.41
1:B:662:LEU:O	1:B:665:THR:HB	2.21	0.41
1:B:538:CYS:O	1:B:598:LYS:HE3	2.20	0.41
1:A:171:ASN:HB2	1:A:664:SER:O	2.21	0.41
1:A:228:GLU:O	1:A:232:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:GLU:HB3	1:B:594:LEU:HD21	2.03	0.41
1:A:351:LYS:HD3	1:A:387:LEU:HD22	2.03	0.41
1:A:303:ILE:HD12	1:A:358:HIS:CE1	2.56	0.40
1:A:363:LYS:HG3	4:A:952:HOH:O	2.21	0.40
1:A:451:GLN:HA	1:A:452:PRO:HD3	1.91	0.40
1:A:270:LYS:O	1:A:429:LYS:HG2	2.21	0.40
1:A:367:LYS:HD3	1:A:374:GLU:OE1	2.20	0.40
1:A:123:VAL:HG13	1:A:673:ILE:HD13	2.02	0.40
1:A:80:ASN:HA	1:A:81:PRO:HD3	1.97	0.40
1:B:47:VAL:HG21	1:B:63:THR:HG23	2.03	0.40
1:A:662:LEU:O	1:A:665:THR:HB	2.21	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	705/783 (90%)	684 (97%)	20 (3%)	1 (0%)	51 75
1	B	709/783 (90%)	688 (97%)	20 (3%)	1 (0%)	51 75
All	All	1414/1566 (90%)	1372 (97%)	40 (3%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	750	ASP
1	A	57	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/673 (84%)	538 (95%)	27 (5%)	25	49
1	B	543/673 (81%)	513 (94%)	30 (6%)	21	43
All	All	1108/1346 (82%)	1051 (95%)	57 (5%)	23	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	111	SER
1	A	163	GLN
1	A	234	LYS
1	A	238	ASN
1	A	243	ARG
1	A	271	SER
1	A	303	ILE
1	A	318	THR
1	A	320	VAL
1	A	328	GLU
1	A	343	SER
1	A	363	LYS
1	A	392	SER
1	A	433	GLU
1	A	447	LEU
1	A	451	GLN
1	A	453	ARG
1	A	476	LEU
1	A	478	ILE
1	A	493	MET
1	A	590	ILE
1	A	614	LEU
1	A	617	LEU
1	A	665	THR
1	A	703	ARG
1	A	766	LYS

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Mol	Chain	Res	Type
1	B	8	VAL
1	B	69	VAL
1	B	158	SER
1	B	169	ARG
1	B	189	LYS
1	B	190	ARG
1	B	220	ILE
1	B	225	PRO
1	B	238	ASN
1	B	267	LEU
1	B	318	THR
1	B	370	GLU
1	B	379	GLU
1	B	384	SER
1	B	453	ARG
1	B	478	ILE
1	B	486	GLN
1	B	497	GLU
1	B	508	TRP
1	B	510	PHE
1	B	547	THR
1	B	578	SER
1	B	585	ILE
1	B	590	ILE
1	B	616	LEU
1	B	617	LEU
1	B	665	THR
1	B	703	ARG
1	B	769	LEU
1	B	775	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	79	GLN
1	A	153	HIS
1	A	187	ASN
1	A	193	GLN
1	A	222	GLN
1	A	238	ASN
1	A	292	ASN

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Mol	Chain	Res	Type
1	A	334	ASN
1	A	358	HIS
1	A	372	GLN
1	A	444	ASN
1	A	482	ASN
1	A	518	GLN
1	A	568	ASN
1	A	589	ASN
1	A	597	ASN
1	A	666	HIS
1	B	153	HIS
1	B	160	ASN
1	B	224	ASN
1	B	238	ASN
1	B	240	ASN
1	B	358	HIS
1	B	419	GLN
1	B	437	ASN
1	B	454	GLN
1	B	696	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	A	801	3	29,33,33	1.43	5 (17%)	31,52,52	1.98	8 (25%)
2	ANP	B	801	3	29,33,33	1.41	4 (13%)	31,52,52	2.26	10 (32%)

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	801	3	-	4/14/38/38	0/3/3/3
2	ANP	B	801	3	-	4/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-N3B	3.56	1.72	1.63
2	B	801	ANP	PB-N3B	3.49	1.72	1.63
2	A	801	ANP	PB-N3B	3.48	1.72	1.63
2	B	801	ANP	PG-N3B	3.23	1.71	1.63
2	B	801	ANP	PB-O1B	2.49	1.50	1.46
2	A	801	ANP	PG-O2G	-2.34	1.50	1.56
2	A	801	ANP	C5-C4	2.28	1.47	1.40
2	B	801	ANP	C5-C4	2.23	1.46	1.40
2	A	801	ANP	PG-O1G	2.13	1.49	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	O1B-PB-N3B	-6.78	101.78	111.77
2	B	801	ANP	O1G-PG-N3B	-5.95	103.01	111.77
2	B	801	ANP	O1B-PB-N3B	-5.10	104.26	111.77
2	B	801	ANP	O2B-PB-O1B	5.06	120.53	109.92
2	A	801	ANP	O1G-PG-N3B	-4.09	105.75	111.77
2	B	801	ANP	O2B-PB-O3A	3.61	116.70	104.64
2	B	801	ANP	N3-C2-N1	-3.58	123.08	128.68
2	A	801	ANP	O2B-PB-O1B	3.33	116.90	109.92
2	A	801	ANP	N3-C2-N1	-3.15	123.76	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ANP	O2G-PG-O3G	3.14	116.00	107.64
2	A	801	ANP	PB-O3A-PA	-2.66	123.26	132.62
2	B	801	ANP	O3A-PB-N3B	-2.62	99.32	106.59
2	B	801	ANP	PB-O3A-PA	-2.57	123.56	132.62
2	A	801	ANP	C4-C5-N7	-2.46	106.83	109.40
2	A	801	ANP	O2B-PB-O3A	2.45	112.82	104.64
2	A	801	ANP	O2G-PG-O3G	2.40	114.03	107.64
2	B	801	ANP	C2-N1-C6	2.08	122.30	118.75
2	B	801	ANP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

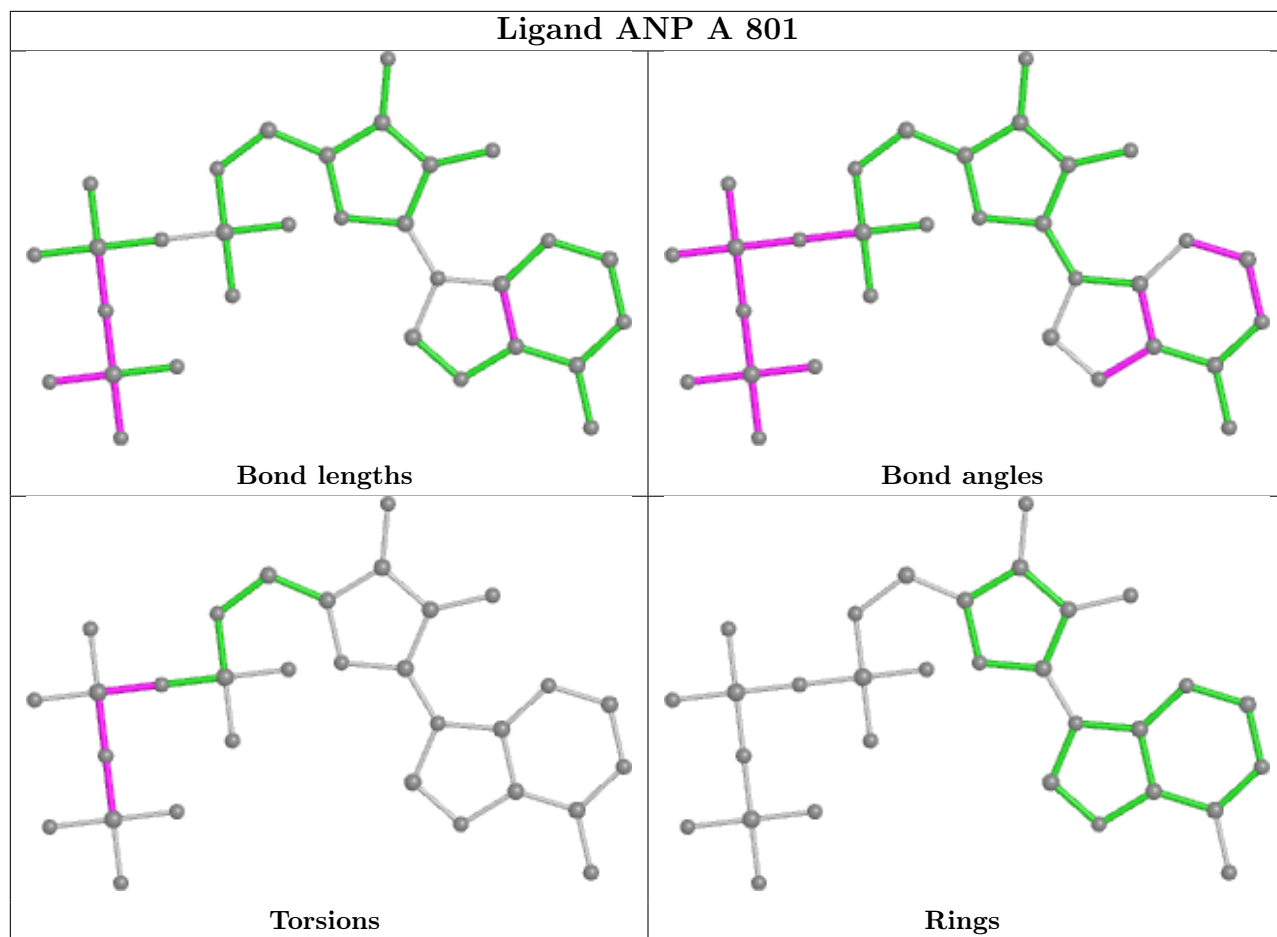
Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	PA-O3A-PB-O1B
2	A	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PB-N3B-PG-O1G
2	B	801	ANP	PG-N3B-PB-O1B
2	B	801	ANP	PA-O3A-PB-O1B
2	B	801	ANP	PA-O3A-PB-O2B

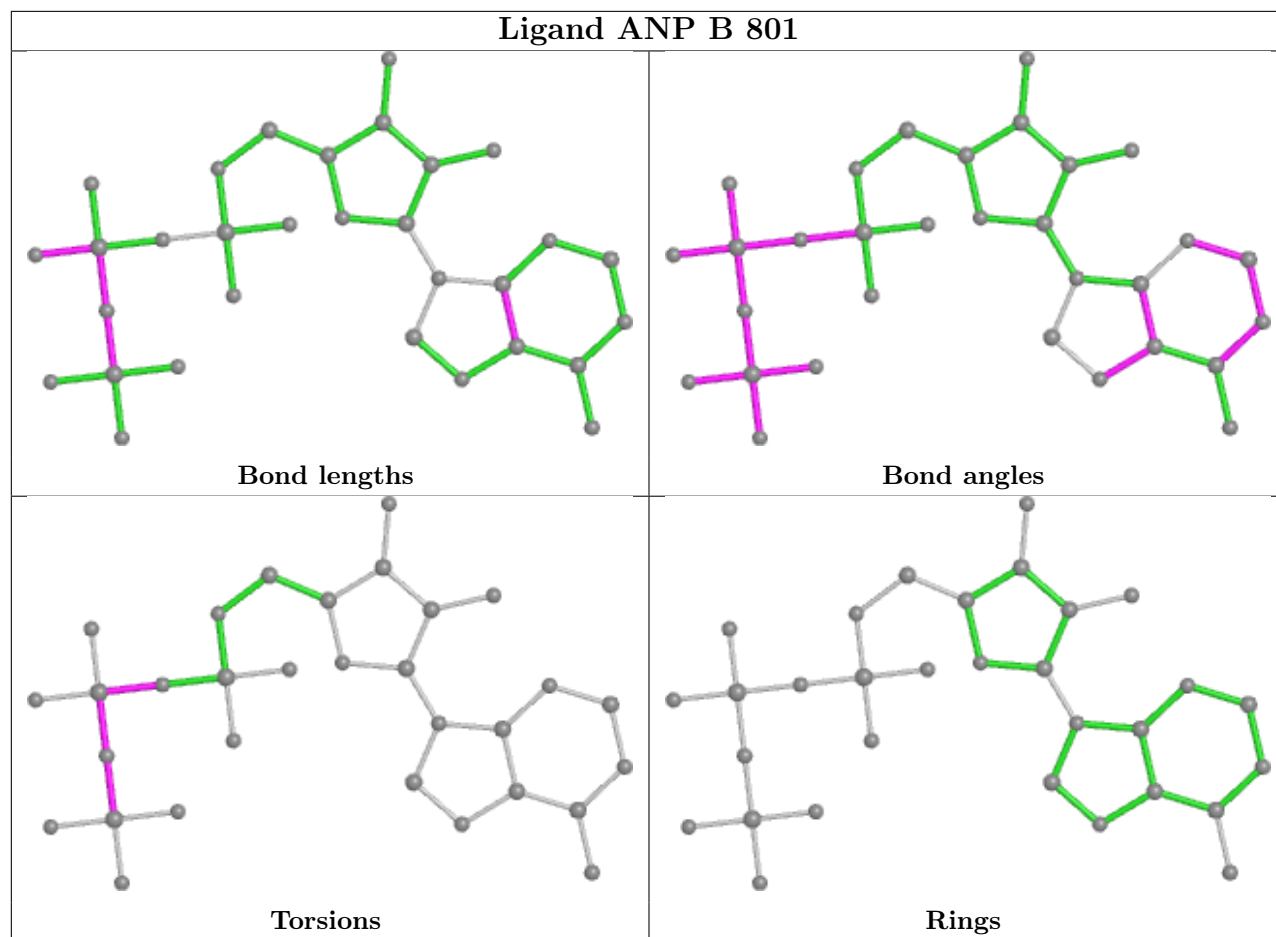
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	1	0
2	B	801	ANP	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 [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	716/783 (91%)	-0.23	32 (4%) 33 26	19, 35, 84, 114	0
1	B	718/783 (91%)	-0.12	38 (5%) 26 20	17, 34, 106, 145	0
All	All	1434/1566 (91%)	-0.18	70 (4%) 29 23	17, 34, 93, 145	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	772	LEU	10.7
1	B	771	GLY	7.2
1	B	756	TYR	5.0
1	B	769	LEU	5.0
1	B	706	ARG	4.6
1	B	770	LEU	4.6
1	A	714	LEU	4.6
1	B	748	SER	4.4
1	B	775	GLU	4.3
1	A	52	VAL	4.2
1	B	773	LEU	4.2
1	B	508	TRP	4.2
1	B	764	PHE	4.0
1	B	753	HIS	4.0
1	B	765	PHE	4.0
1	A	775	GLU	3.8
1	B	712	ARG	3.7
1	A	713	ILE	3.7
1	B	742	ALA	3.6
1	B	750	ASP	3.6
1	A	55	GLU	3.5
1	B	56	GLY	3.5
1	A	56	GLY	3.4
1	A	715	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	3.2
1	B	754	ASN	3.2
1	A	746	LEU	3.2
1	A	57	GLY	3.2
1	A	509	THR	3.1
1	A	53	SER	3.1
1	B	571	GLY	3.0
1	B	751	ILE	3.0
1	A	749	LEU	3.0
1	A	751	ILE	3.0
1	B	714	LEU	2.9
1	A	368	GLN	2.9
1	A	539	MET	2.9
1	B	774	GLU	2.8
1	B	52	VAL	2.7
1	B	744	LYS	2.7
1	A	772	LEU	2.7
1	B	707	LYS	2.7
1	B	768	GLY	2.7
1	A	204	ARG	2.7
1	A	742	ALA	2.6
1	A	744	LYS	2.6
1	B	625	ALA	2.6
1	A	769	LEU	2.6
1	B	743	GLU	2.5
1	A	625	ALA	2.5
1	B	58	LYS	2.5
1	A	540	PHE	2.5
1	A	748	SER	2.4
1	B	752	ASP	2.4
1	B	55	GLU	2.4
1	B	705	CYS	2.4
1	A	776	MET	2.4
1	B	369	ARG	2.4
1	A	774	GLU	2.3
1	B	767	ALA	2.3
1	A	753	HIS	2.3
1	B	570	LYS	2.3
1	A	750	ASP	2.2
1	A	54	ARG	2.2
1	B	745	LEU	2.2
1	B	509	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	765	PHE	2.1
1	A	745	LEU	2.0
1	B	212	GLY	2.0
1	A	567	ARG	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](#)

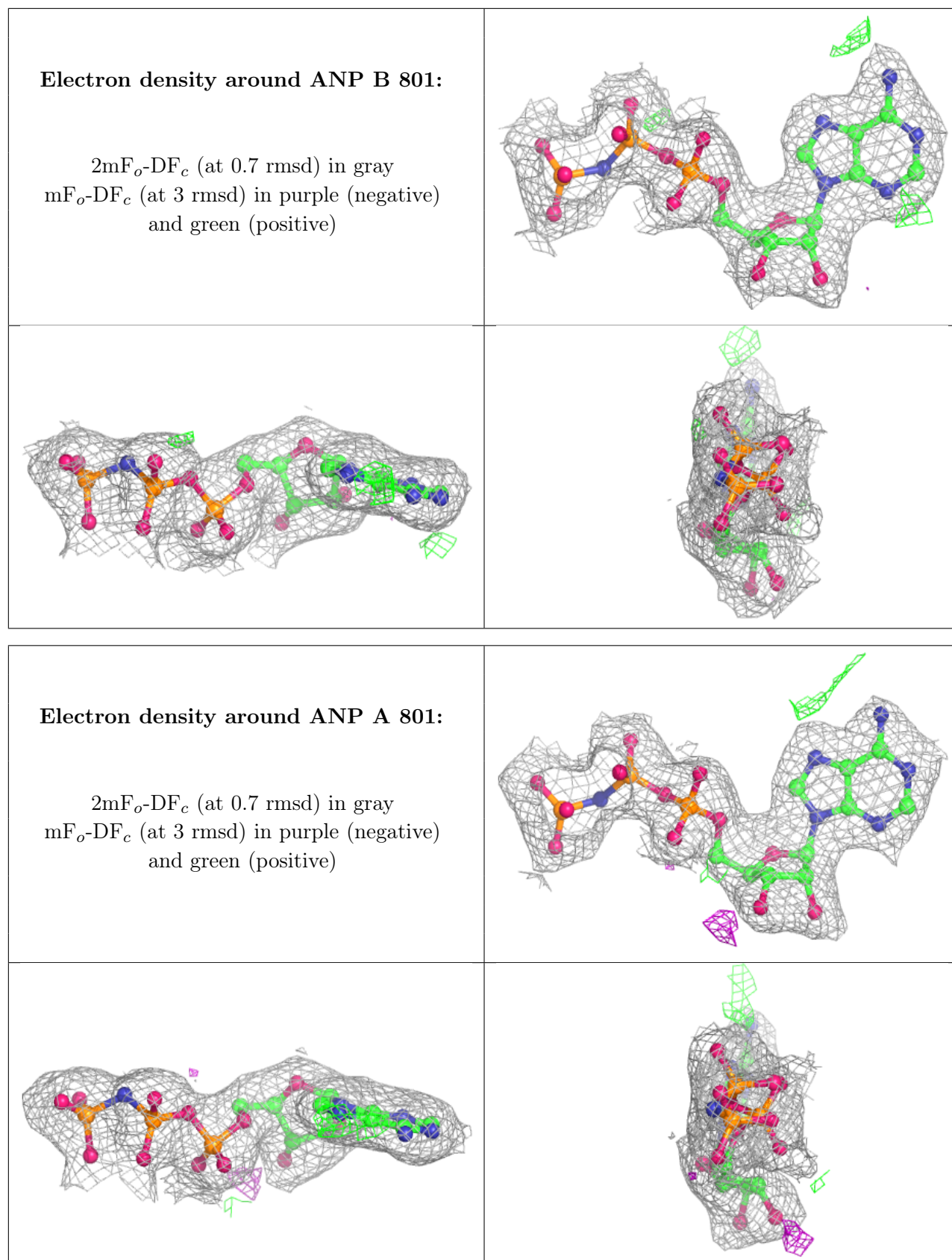
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q < 0.9
2	ANP	B	801	31/31	0.98	0.09	10,19,25,31	0
2	ANP	A	801	31/31	0.99	0.09	12,19,27,30	0
3	MN	A	802	1/1	1.00	0.04	21,21,21,21	0
3	MN	B	802	1/1	1.00	0.07	17,17,17,17	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.