



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:17 PM UTC

PDB ID : 4DB1 / pdb_00004db1
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 : 4-5-2 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

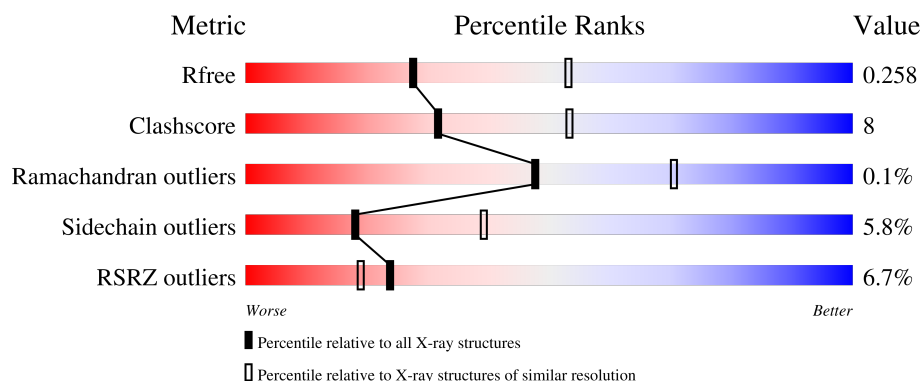
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	5% 73% 17% • 9%
1	B	783	7% 75% 15% • 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.

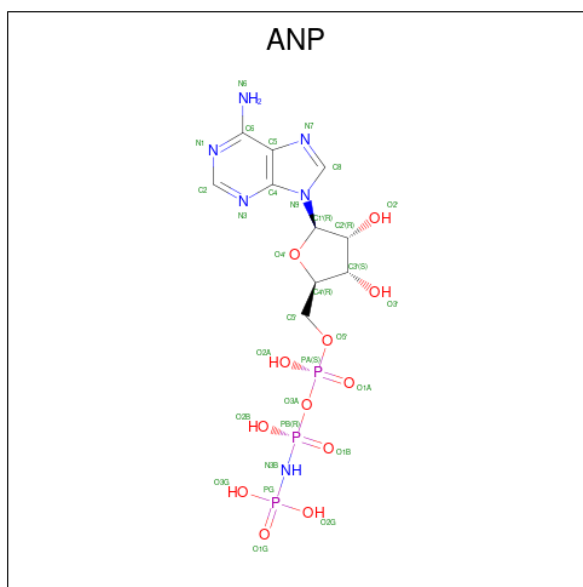
- Molecule 1 is a protein called Myosin-7.

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

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 (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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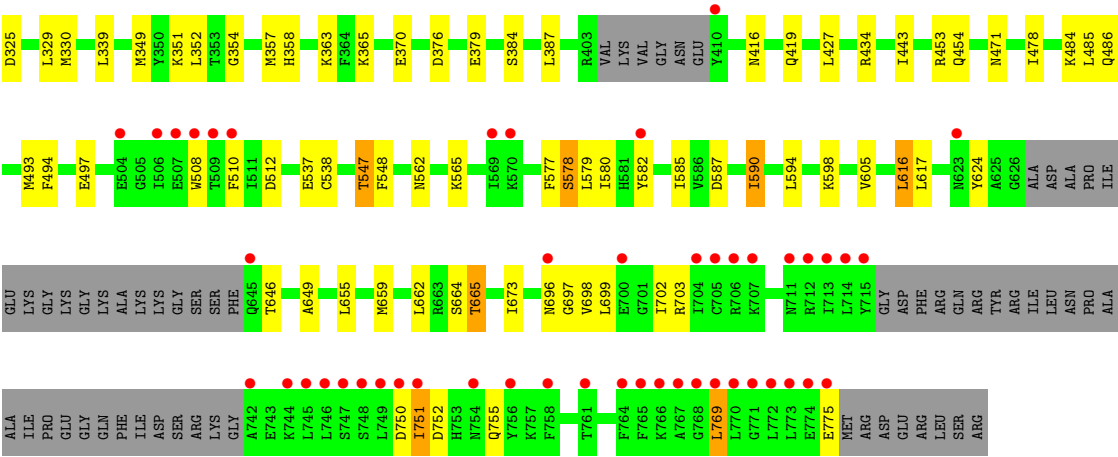
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

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



4 Data and refinement statistics

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 25.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.60) 99.3 (25.00-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.60Å)	Xtriage
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	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.55	0/5697	0.84	2/7705 (0.0%)
1	B	0.57	1/5622 (0.0%)	0.86	3/7613 (0.0%)
All	All	0.56	1/11319 (0.0%)	0.85	5/15318 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	751	ILE	C-O	6.08	1.31	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	751	ILE	N-CA-C	7.03	123.96	109.34
1	A	559	LYS	N-CA-C	5.70	119.41	112.23
1	A	56	GLY	N-CA-C	-5.13	108.59	114.69
1	B	751	ILE	CA-C-N	-5.04	114.75	122.62
1	B	751	ILE	C-N-CA	-5.04	114.75	122.62

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 ⓘ

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	97	0
1	B	5502	0	5215	79	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	5	0
4	B	117	0	0	3	0
All	All	11340	0	10574	175	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 (175) 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:165:MET:HE2	1:A:455:TYR:HB2	1.49	0.93
1:A:165:MET:HE1	1:A:252:PHE:CD1	2.04	0.92
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:A:484:LYS:CB	1:A:659:MET:HE3	2.13	0.78
1:B:493:MET:HE1	4:B:964:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:484:LYS:HB2	1:A:659:MET:HE3	1.70	0.72
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
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:A:484:LYS:HB3	1:A:659:MET:HE3	1.78	0.65
1:A:165:MET:HE1	1:A:252:PHE:HD1	1.61	0.65
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:227:LEU:HD23	1:A:439:MET:HE3	1.78	0.64
1:A:173:SER:HB3	1:A:667:PRO:HA	1.80	0.63
1:A:354:GLY:HA2	1:A:357:MET:HE3	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:A:485:LEU:HD23	1:A:659:MET:HE1	1.84	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:485:LEU:HD23	1:B:659:MET:HE1	1.90	0.53
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:102:LEU:HD22	1:A:690:MET:HE2	1.92	0.51
1:B:352:LEU:HD12	1:B:616:LEU:CD1	2.41	0.51
4:A:904:HOH:O	1:B:330:MET:HE1	2.11	0.51
1:A:281:ARG:HH22	1:A:325:ASP:CG	2.19	0.51
1:B:354:GLY:HA2	1:B:357:MET:HE3	1.93	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: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
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:6:MET:HE1	1:B:151:PRO:HD3	1.94	0.49
1:A:64:GLU:OE2	1:A:103:TYR:OH	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:673:ILE:CD1	1:B:696:ASN:HD21	2.29	0.46
1:B:297:LEU:O	1:B:301:LEU:HG	2.15	0.46
1:B:485:LEU:CD2	1:B:659:MET:HE1	2.46	0.45
1:B:562:ASN:ND2	1:B:580:ILE:O	2.45	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:B:655:LEU:HD11	1:B:659:MET:HE3	1.99	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
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:6:MET:HE1	1:A:151:PRO:HD3	1.97	0.44
1:A:277:LEU:O	1:A:278:LYS:C	2.60	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: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:A:484:LYS:HB2	1:A:659:MET:CE	2.44	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLN:NE2	1:A:328:GLU:HB3	2.34	0.42
1:A:749:LEU:C	1:A:751:ILE:H	2.27	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:A:655:LEU:HD11	1:A:659:MET:HE2	2.01	0.42
1:B:577:PHE:HE1	1:B:579:LEU:HG	1.83	0.42
1:A:6:MET:HE3	1:A:17:ARG:NH1	2.35	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:B:349:MET:HE3	1:B:349:MET:HB2	1.86	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: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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	48	70
1	B	709/783 (90%)	688 (97%)	20 (3%)	1 (0%)	48	70
All	All	1414/1566 (90%)	1372 (97%)	40 (3%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

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

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	565/673 (84%)	530 (94%)	35 (6%)	16	36
1	B	543/673 (81%)	514 (95%)	29 (5%)	20	43
All	All	1108/1346 (82%)	1044 (94%)	64 (6%)	18	39

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	63	THR
1	A	111	SER
1	A	114	ILE

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Mol	Chain	Res	Type
1	A	163	GLN
1	A	166	LEU
1	A	224	ASN
1	A	234	LYS
1	A	246	LYS
1	A	248	ILE
1	A	271	SER
1	A	298	LEU
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	370	GLU
1	A	392	SER
1	A	433	GLU
1	A	447	LEU
1	A	451	GLN
1	A	453	ARG
1	A	462	ILE
1	A	476	LEU
1	A	478	ILE
1	A	585	ILE
1	A	590	ILE
1	A	614	LEU
1	A	617	LEU
1	A	665	THR
1	A	673	ILE
1	A	703	ARG
1	A	766	LYS
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	248	ILE
1	B	267	LEU
1	B	318	THR
1	B	363	LYS

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Mol	Chain	Res	Type
1	B	370	GLU
1	B	379	GLU
1	B	384	SER
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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	153	HIS
1	A	187	ASN
1	A	193	GLN
1	A	222	GLN
1	A	224	ASN
1	A	238	ASN
1	A	292	ASN
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	555	ASN
1	A	564	GLN
1	A	568	ASN
1	A	589	ASN
1	A	597	ASN
1	A	666	HIS

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Mol	Chain	Res	Type
1	B	153	HIS
1	B	187	ASN
1	B	238	ASN
1	B	240	ASN
1	B	315	GLN
1	B	358	HIS
1	B	419	GLN
1	B	437	ASN
1	B	454	GLN
1	B	487	GLN
1	B	492	HIS
1	B	518	GLN
1	B	555	ASN
1	B	696	ASN

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 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	B	801	3	33,33,33	1.64	8 (24%)	45,52,52	2.32	16 (35%)
2	ANP	A	801	3	33,33,33	1.65	8 (24%)	45,52,52	2.19	14 (31%)

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	B	801	3	-	4/18/38/38	0/3/3/3
2	ANP	A	801	3	-	3/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	C5-C4	4.42	1.47	1.39
2	B	801	ANP	C5-C4	4.34	1.46	1.39
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	A	801	ANP	C5-C6	2.69	1.48	1.41
2	B	801	ANP	PB-O1B	2.58	1.50	1.46
2	B	801	ANP	C4-N9	-2.54	1.32	1.37
2	A	801	ANP	C8-N7	2.53	1.36	1.31
2	B	801	ANP	C5-C6	2.51	1.48	1.41
2	A	801	ANP	C5-N7	-2.48	1.34	1.39
2	B	801	ANP	C5-N7	-2.47	1.34	1.39
2	A	801	ANP	PG-O2G	-2.39	1.50	1.56
2	A	801	ANP	PG-O1G	2.20	1.49	1.46
2	B	801	ANP	C8-N7	2.05	1.35	1.31

All (30) 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	A	801	ANP	C5-C4-N3	-5.81	118.72	126.72
2	B	801	ANP	C5-C4-N3	-5.14	119.64	126.72
2	B	801	ANP	O1B-PB-N3B	-5.10	104.26	111.77
2	B	801	ANP	O2B-PB-O1B	4.97	120.53	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	N3-C4-N9	4.53	134.88	127.17
2	B	801	ANP	N3-C4-N9	4.37	134.60	127.17
2	A	801	ANP	O1G-PG-N3B	-4.09	105.75	111.77
2	A	801	ANP	C2-N3-C4	3.80	121.11	111.83
2	B	801	ANP	N3-C2-N1	-3.63	123.08	128.58
2	B	801	ANP	O2B-PB-O3A	3.61	116.70	104.64
2	B	801	ANP	C2-N3-C4	3.53	120.45	111.83
2	A	801	ANP	O2B-PB-O1B	3.28	116.90	109.87
2	A	801	ANP	C4-C5-N7	-3.28	106.83	110.58
2	B	801	ANP	C4-N9-C8	3.21	109.11	105.74
2	A	801	ANP	N3-C2-N1	-3.19	123.76	128.58
2	B	801	ANP	O2G-PG-O3G	3.13	116.00	107.59
2	B	801	ANP	C4-C5-N7	-2.86	107.31	110.58
2	B	801	ANP	O3A-PB-N3B	-2.62	99.32	106.59
2	A	801	ANP	C5-N7-C8	2.55	107.46	103.45
2	A	801	ANP	C4-N9-C8	2.52	108.38	105.74
2	A	801	ANP	O2B-PB-O3A	2.45	112.82	104.64
2	A	801	ANP	O2G-PG-O3G	2.39	114.03	107.59
2	A	801	ANP	C6-C5-N7	2.31	136.54	132.09
2	B	801	ANP	C2-N1-C6	2.18	122.30	118.73
2	A	801	ANP	N9-C8-N7	-2.13	110.92	113.94
2	B	801	ANP	C5-N7-C8	2.09	106.74	103.45
2	B	801	ANP	C6-C5-N7	2.06	136.06	132.09
2	B	801	ANP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

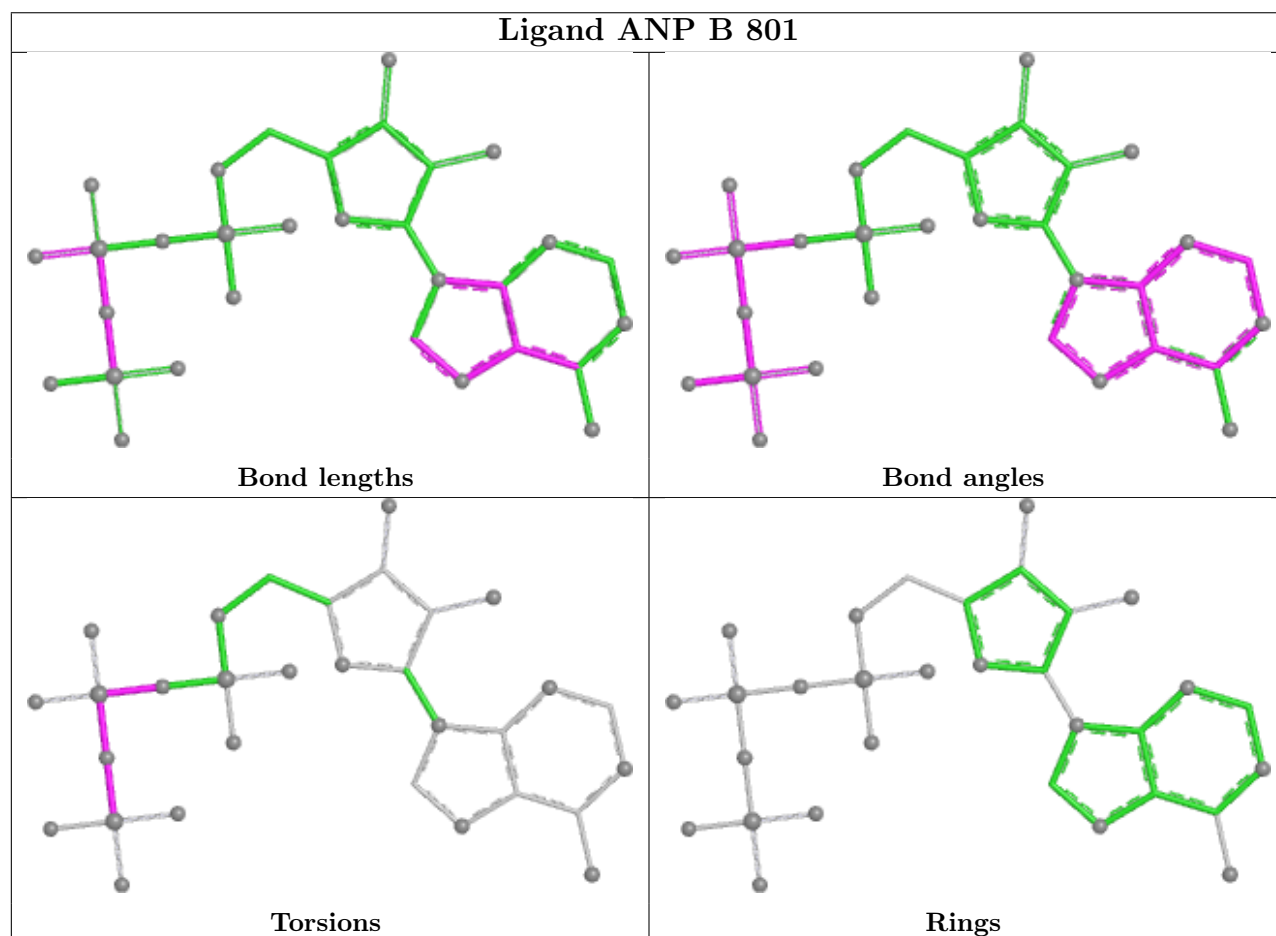
Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PB-N3B-PG-O1G
2	B	801	ANP	PG-N3B-PB-O1B
2	B	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PA-O3A-PB-O1B

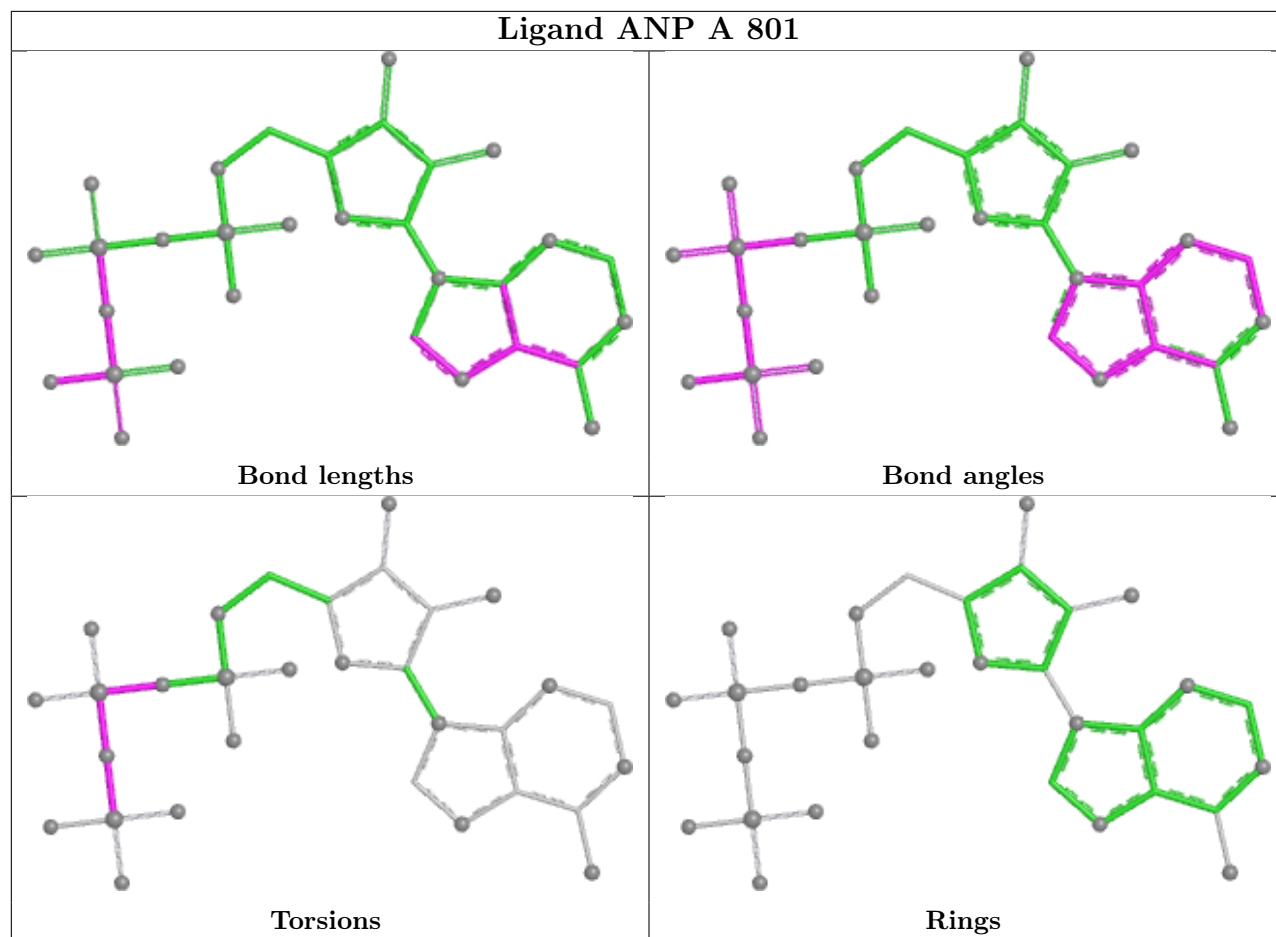
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ANP	1	0
2	A	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%)	-0.03	39 (5%)	31 26	16, 35, 84, 114	1 (0%)
1	B	718/783 (91%)	0.04	57 (7%)	18 14	17, 34, 106, 145	1 (0%)
All	All	1434/1566 (91%)	0.01	96 (6%)	24 19	16, 34, 93, 145	2 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	ALA	6.2
1	B	756	TYR	5.6
1	B	715	TYR	5.3
1	B	772	LEU	5.2
1	B	771	GLY	5.0
1	A	774	GLU	4.7
1	B	746	LEU	4.7
1	A	714	LEU	4.5
1	B	774	GLU	4.3
1	A	509	THR	4.3
1	B	706	ARG	4.1
1	B	712	ARG	4.1
1	B	764	PHE	4.1
1	B	770	LEU	4.0
1	B	767	ALA	3.9
1	B	750	ASP	3.9
1	B	742	ALA	3.7
1	A	715	TYR	3.7
1	B	748	SER	3.6
1	B	705	CYS	3.6
1	A	508	TRP	3.5
1	B	769	LEU	3.5
1	B	508	TRP	3.5
1	B	751	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	761	THR	3.4
1	B	707	LYS	3.3
1	B	507	GLU	3.3
1	A	750	ASP	3.2
1	B	761	THR	3.2
1	A	769	LEU	3.2
1	B	714	LEU	3.2
1	B	65	TYR	3.2
1	B	504	GLU	3.1
1	B	711	ASN	3.1
1	B	700	GLU	3.0
1	B	758	PHE	2.9
1	B	744	LYS	2.9
1	A	623	ASN	2.9
1	B	754	ASN	2.9
1	B	747	SER	2.9
1	B	775	GLU	2.8
1	A	713	ILE	2.8
1	B	66	GLY	2.8
1	B	68	THR	2.8
1	A	558	GLY	2.7
1	A	71	VAL	2.7
1	B	749	LEU	2.7
1	A	410	TYR	2.6
1	A	56	GLY	2.6
1	A	510	PHE	2.6
1	B	773	LEU	2.6
1	B	569	ILE	2.6
1	B	212	GLY	2.6
1	B	52	VAL	2.5
1	B	410	TYR	2.5
1	B	509	THR	2.4
1	A	538	CYS	2.4
1	A	574	GLU	2.4
1	A	57	GLY	2.4
1	A	65	TYR	2.4
1	A	507	GLU	2.4
1	B	27	GLN	2.4
1	B	645	GLN	2.4
1	A	58	LYS	2.4
1	A	625	ALA	2.4
1	B	713	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	53	SER	2.3
1	A	204	ARG	2.3
1	A	74	ASP	2.3
1	B	510	PHE	2.3
1	A	765	PHE	2.3
1	B	696	ASN	2.2
1	A	66	GLY	2.2
1	A	51	ILE	2.2
1	B	765	PHE	2.2
1	A	539	MET	2.2
1	B	506	ILE	2.2
1	A	644	PHE	2.2
1	B	704	ILE	2.1
1	A	61	ALA	2.1
1	A	70	THR	2.1
1	B	768	GLY	2.1
1	A	42	ASP	2.1
1	A	763	VAL	2.1
1	B	42	ASP	2.1
1	B	570	LYS	2.1
1	A	760	HIS	2.1
1	A	775	GLU	2.1
1	B	766	LYS	2.1
1	A	60	THR	2.1
1	A	53	SER	2.0
1	B	745	LEU	2.0
1	B	623	ASN	2.0
1	A	73	GLU	2.0
1	B	44	GLN	2.0
1	B	582	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

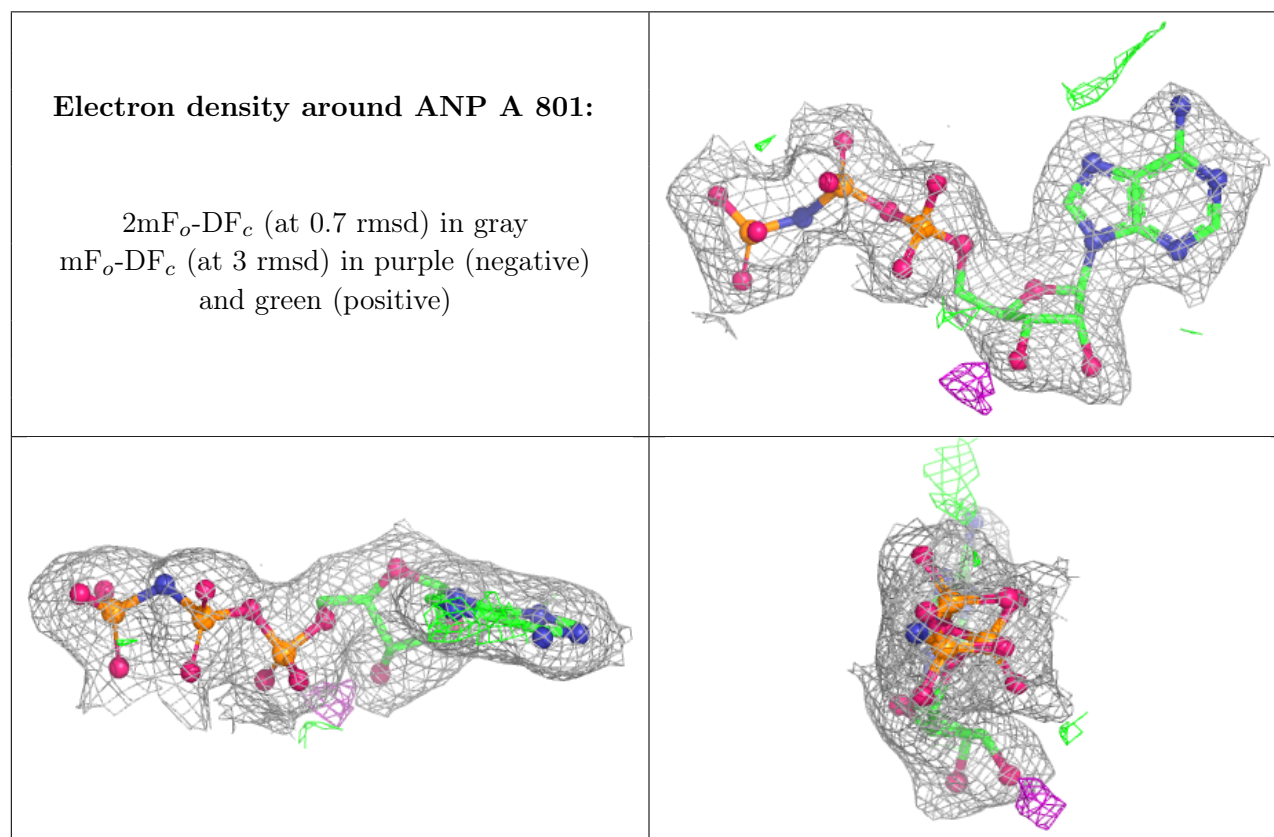
There are no oligosaccharides in this entry.

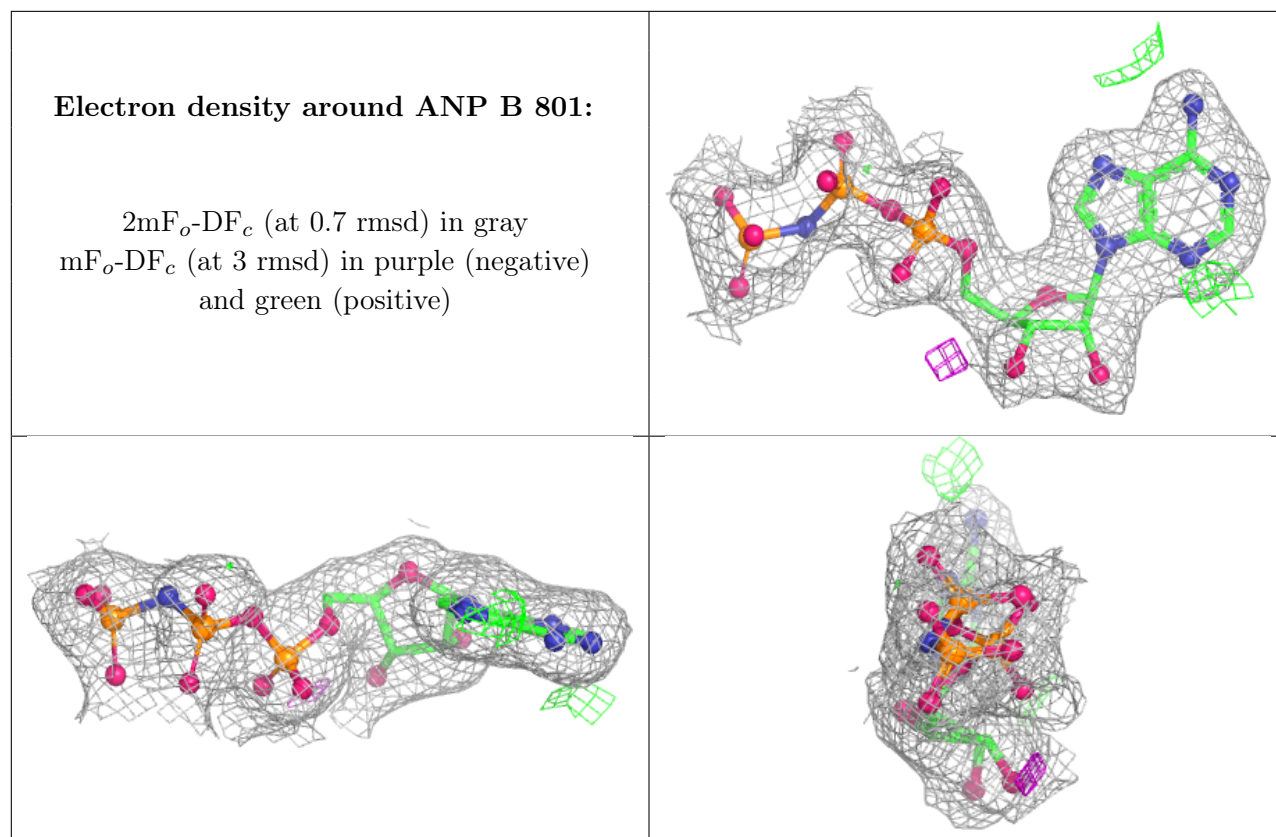
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	ANP	A	801	31/31	0.98	0.05	12,19,27,30	0
2	ANP	B	801	31/31	0.98	0.05	10,19,25,31	0
3	MN	A	802	1/1	1.00	0.03	21,21,21,21	0
3	MN	B	802	1/1	1.00	0.01	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.