



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:57 PM UTC

PDB ID : 4LQP / pdb_00004lqp
Title : Crystal structure of the Cbk1(T743E)-Mob2 kinase-coactivator complex, in crystal form A
Authors : Gogl, G.; Remenyi, A.
Deposited on : 2013-07-19
Resolution : 4.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

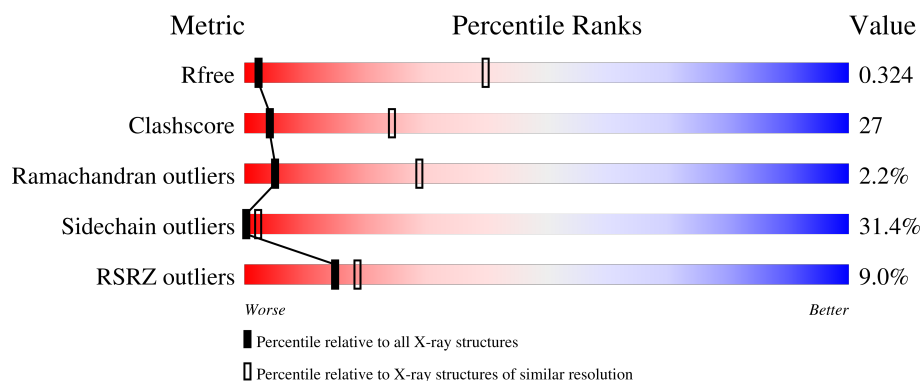
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	508	7% 28% 33% 14% • 25%
2	B	244	5% 35% 22% 8% • 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4131 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 Serine/threonine-protein kinase CBK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2954	1888	513	541	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	expression tag	UNP P53894
A	250	SER	-	expression tag	UNP P53894
A	475	ALA	ASP	engineered mutation	UNP P53894
A	743	GLU	THR	engineered mutation	UNP P53894

- Molecule 2 is a protein called CBK1 kinase activator protein MOB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	163	Total	C	N	O	S	0	0	0
			1146	749	191	205	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	GLY	-	expression tag	UNP P43563
B	45	SER	-	expression tag	UNP P43563

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

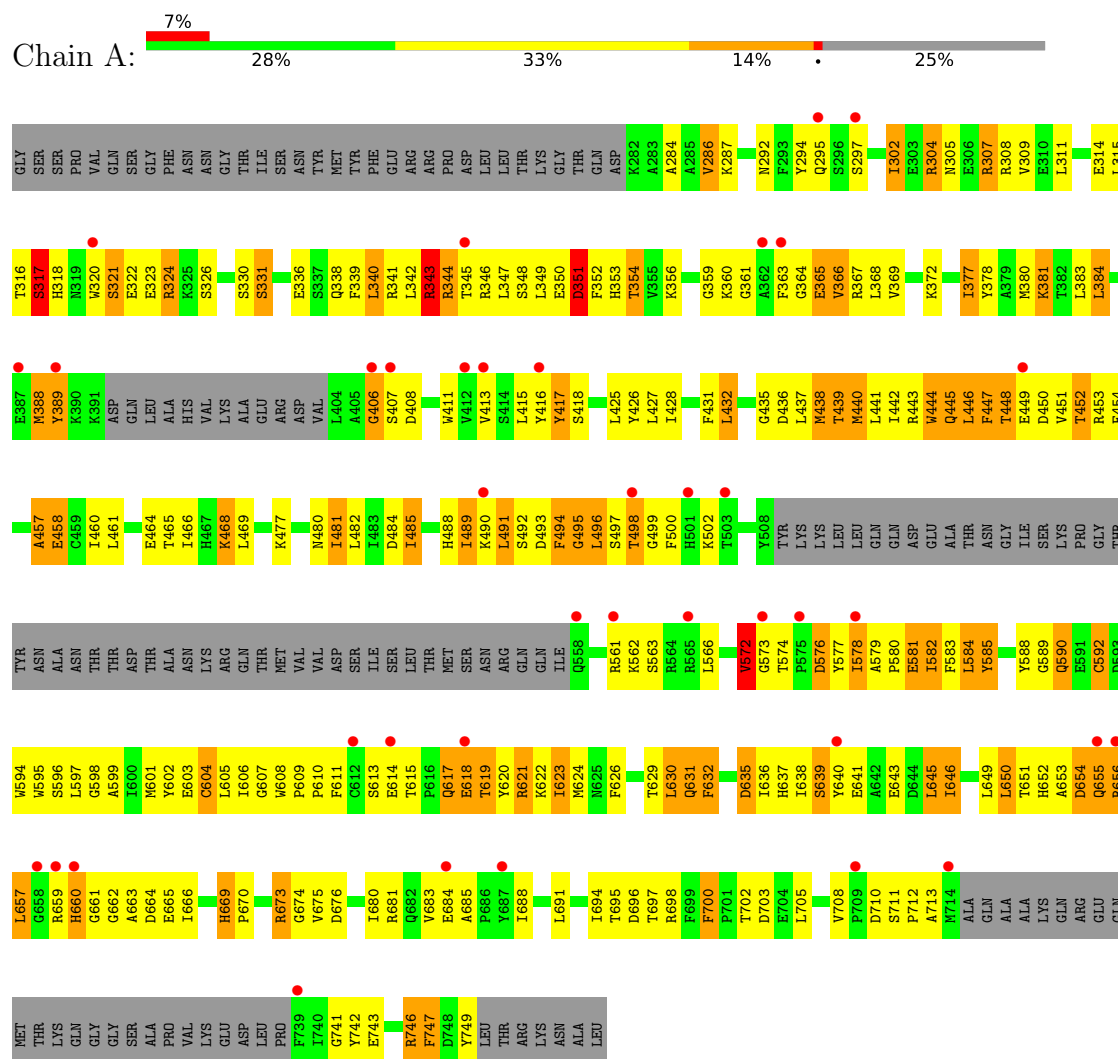


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

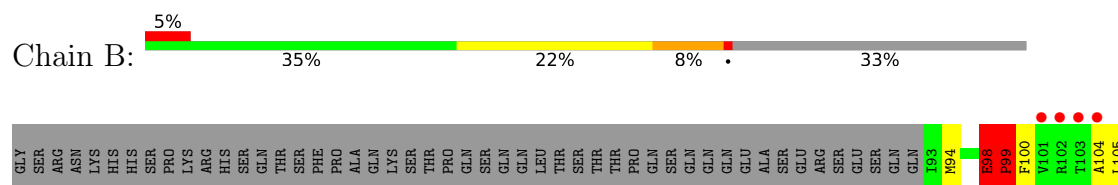
3 Residue-property plots

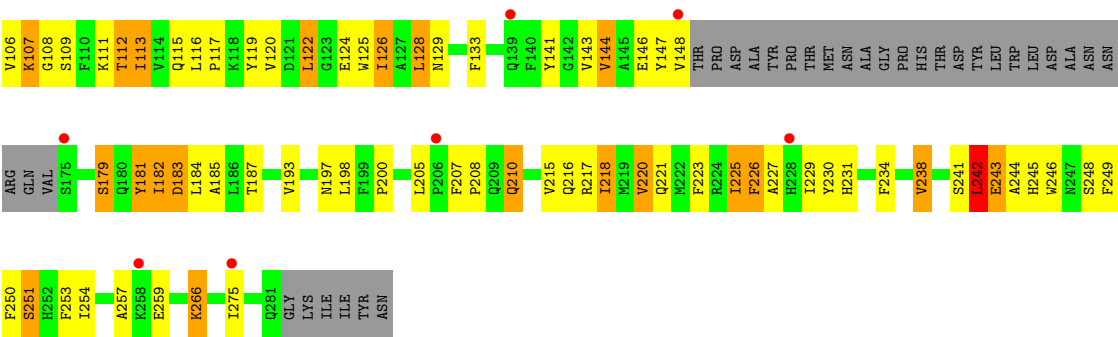
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein kinase CBK1



• Molecule 2: CBK1 kinase activator protein MOB2





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.38Å 129.38Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 4.50 49.59 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.59-4.50) 94.9 (49.59-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.288 , 0.310 0.291 , 0.324	Depositor DCC
R_{free} test set	588 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	242.2	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 739.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4131	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/3024	1.19	37/4100 (0.9%)
2	B	0.51	1/1180 (0.1%)	1.28	20/1629 (1.2%)
All	All	0.47	1/4204 (0.0%)	1.22	57/5729 (1.0%)

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	A	0	7
2	B	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	PRO	CA-CB	-5.59	1.45	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	TYR	N-CA-C	11.95	128.29	112.88
1	A	495	GLY	N-CA-C	11.46	128.33	114.69
2	B	106	VAL	N-CA-C	10.35	123.22	108.42
1	A	583	PHE	N-CA-C	-8.39	96.42	109.76
2	B	183	ASP	N-CA-C	-8.31	101.46	111.69
2	B	107	LYS	N-CA-C	8.20	120.77	108.31
2	B	108	GLY	N-CA-C	8.11	126.31	110.83
1	A	284	ALA	N-CA-C	8.01	118.82	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	THR	CB-CA-C	-7.95	106.42	117.23
2	B	105	LEU	N-CA-C	7.65	120.58	111.02
1	A	351	ASP	N-CA-C	-7.59	104.01	113.20
1	A	635	ASP	N-CA-C	-7.47	95.39	108.23
1	A	653	ALA	N-CA-C	-7.30	104.46	113.15
1	A	287	LYS	N-CA-C	6.92	119.67	111.02
2	B	104	ALA	N-CA-C	6.88	121.98	109.32
1	A	498	THR	N-CA-C	6.85	120.47	109.79
2	B	210	GLN	N-CA-C	-6.76	105.02	113.20
1	A	491	LEU	N-CA-C	6.71	121.17	112.92
1	A	607	GLY	N-CA-C	6.58	125.86	115.08
2	B	98	GLU	N-CA-C	6.30	123.74	109.81
1	A	317	SER	N-CA-C	-6.27	105.59	113.18
1	A	407	SER	N-CA-C	6.25	124.11	110.80
1	A	448	THR	N-CA-C	6.25	119.10	108.67
1	A	741	GLY	N-CA-C	6.18	121.37	110.80
2	B	242	LEU	N-CA-C	-6.17	105.51	113.16
1	A	700	PHE	CA-C-N	6.17	127.55	119.84
1	A	700	PHE	C-N-CA	6.17	127.55	119.84
1	A	326	SER	N-CA-C	-6.15	105.43	113.17
1	A	347	LEU	N-CA-C	6.01	116.50	108.38
2	B	216	GLN	N-CA-C	-5.92	105.32	112.54
1	A	618	GLU	N-CA-C	-5.90	105.93	113.01
1	A	651	THR	N-CA-C	-5.89	102.88	110.19
2	B	207	PHE	CA-C-N	5.83	125.53	119.05
2	B	207	PHE	C-N-CA	5.83	125.53	119.05
1	A	406	GLY	N-CA-C	5.75	126.81	113.18
1	A	489	ILE	N-CA-C	5.71	116.10	108.11
1	A	389	TYR	N-CA-C	5.66	118.63	109.86
1	A	669	HIS	CA-C-N	5.66	126.91	119.84
1	A	669	HIS	C-N-CA	5.66	126.91	119.84
1	A	685	ALA	N-CA-C	-5.63	102.55	109.65
2	B	104	ALA	CB-CA-C	-5.58	109.15	115.79
2	B	94	MET	N-CA-C	5.54	117.40	110.91
1	A	295	GLN	N-CA-C	-5.51	104.68	111.40
2	B	109	SER	CB-CA-C	-5.50	109.24	115.79
1	A	417	TYR	N-CA-C	5.49	115.08	107.73
2	B	205	LEU	CA-C-N	5.45	126.65	119.84
2	B	205	LEU	C-N-CA	5.45	126.65	119.84
1	A	447	PHE	N-CA-C	-5.41	106.36	113.17
2	B	218	ILE	N-CA-C	5.34	118.60	111.44
1	A	609	PRO	CA-C-N	5.28	125.59	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	PRO	C-N-CA	5.28	125.59	119.47
1	A	343	ARG	N-CA-C	5.15	117.08	108.99
1	A	563	SER	N-CA-C	-5.15	107.02	113.15
1	A	432	LEU	CA-C-N	5.11	124.72	119.56
1	A	432	LEU	C-N-CA	5.11	124.72	119.56
2	B	126	ILE	CB-CA-C	-5.06	105.34	111.87
2	B	179	SER	CB-CA-C	-5.06	109.21	115.89

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	VAL	Peptide
1	A	292	ASN	Peptide
1	A	331	SER	Peptide
1	A	406	GLY	Peptide
1	A	572	VAL	Peptide
1	A	582	ILE	Peptide
1	A	619	THR	Peptide
2	B	181	TYR	Peptide
2	B	98	GLU	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	2954	0	2727	177	0
2	B	1146	0	921	41	0
3	A	31	0	13	3	0
All	All	4131	0	3661	213	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 27.

All (213) 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:339:PHE:HB3	1:A:341:ARG:HE	1.47	0.80
1:A:356:LYS:HD2	1:A:697:THR:HG21	1.65	0.79
1:A:308:ARG:HH22	2:B:249:PHE:HA	1.47	0.79
1:A:381:LYS:NZ	3:A:801:ANP:O1A	2.16	0.78
2:B:218:ILE:HA	2:B:221:GLN:HG2	1.65	0.78
2:B:183:ASP:O	2:B:187:THR:OG1	2.02	0.77
1:A:477:LYS:HB2	1:A:480:ASN:HB2	1.69	0.74
1:A:343:ARG:HB3	1:A:345:THR:HG23	1.70	0.72
1:A:673:ARG:HD3	1:A:674:GLY:H	1.55	0.71
2:B:181:TYR:O	2:B:183:ASP:N	2.19	0.70
1:A:448:THR:HB	1:A:452:THR:HB	1.74	0.70
1:A:632:PHE:HE1	1:A:643:GLU:HG3	1.56	0.70
1:A:588:TYR:HD2	1:A:589:GLY:H	1.39	0.69
1:A:453:ARG:HD3	1:A:673:ARG:HD2	1.74	0.68
2:B:182:ILE:HA	2:B:185:ALA:HB3	1.74	0.68
1:A:664:ASP:C	1:A:666:ILE:H	1.99	0.68
1:A:613:SER:HB2	1:A:618:GLU:HB3	1.77	0.67
2:B:227:ALA:HA	2:B:230:TYR:HB2	1.76	0.67
1:A:663:ALA:H	1:A:666:ILE:HD12	1.60	0.66
1:A:314:GLU:HA	1:A:317:SER:HB2	1.79	0.65
1:A:610:PRO:HB3	1:A:630:LEU:HD21	1.79	0.64
1:A:708:VAL:O	1:A:710:ASP:N	2.31	0.64
1:A:346:ARG:NH1	2:B:193:VAL:O	2.31	0.63
2:B:125:TRP:O	2:B:129:ASN:ND2	2.31	0.63
1:A:598:GLY:HA2	1:A:649:LEU:HD13	1.80	0.63
1:A:618:GLU:O	1:A:621:ARG:HB3	1.99	0.63
1:A:330:SER:OG	1:A:331:SER:N	2.32	0.62
1:A:311:LEU:HD21	2:B:113:ILE:HG21	1.81	0.62
2:B:238:VAL:HA	2:B:243:GLU:HB3	1.82	0.61
1:A:652:HIS:C	1:A:654:ASP:H	2.09	0.61
1:A:461:LEU:HA	1:A:464:GLU:HB2	1.82	0.60
1:A:613:SER:C	1:A:615:THR:H	2.10	0.60
1:A:494:PHE:C	1:A:496:LEU:HA	2.27	0.59
1:A:348:SER:OG	1:A:349:LEU:O	2.16	0.59
1:A:495:GLY:N	1:A:496:LEU:HA	2.16	0.59
1:A:652:HIS:HB2	1:A:654:ASP:HB3	1.85	0.59
1:A:413:VAL:HG21	1:A:482:LEU:HD12	1.85	0.59
1:A:635:ASP:HB3	1:A:637:HIS:HE1	1.68	0.59
2:B:116:LEU:HD13	2:B:122:LEU:HD13	1.83	0.59
1:A:349:LEU:HD23	1:A:350:GLU:H	1.67	0.59
2:B:179:SER:HA	2:B:181:TYR:CD1	2.38	0.58
1:A:432:LEU:HD21	1:A:490:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ILE:HA	1:A:649:LEU:HD12	1.85	0.58
2:B:116:LEU:HD12	2:B:117:PRO:HD2	1.85	0.58
1:A:604:CYS:SG	1:A:605:LEU:N	2.77	0.58
2:B:215:VAL:HA	2:B:218:ILE:H	1.67	0.58
1:A:366:VAL:HG23	1:A:381:LYS:HG2	1.85	0.58
1:A:603:GLU:HA	1:A:608:TRP:H	1.67	0.57
1:A:353:HIS:HB2	1:A:372:LYS:HG3	1.86	0.57
1:A:377:ILE:H	1:A:377:ILE:HD13	1.68	0.57
1:A:366:VAL:HG21	3:A:801:ANP:H8	1.88	0.56
1:A:645:LEU:HG	1:A:669:HIS:CD2	2.42	0.55
1:A:364:GLY:HA3	1:A:383:LEU:HA	1.88	0.55
1:A:662:GLY:C	1:A:664:ASP:H	2.14	0.55
1:A:500:PHE:HE1	1:A:582:ILE:HG22	1.71	0.55
1:A:638:ILE:HG22	1:A:639:SER:O	2.07	0.55
1:A:435:GLY:HA2	1:A:700:PHE:CE1	2.42	0.54
1:A:584:LEU:HD23	1:A:585:TYR:HD2	1.72	0.54
1:A:457:ALA:O	1:A:460:ILE:N	2.40	0.54
1:A:349:LEU:C	1:A:351:ASP:H	2.15	0.54
1:A:343:ARG:HA	1:A:343:ARG:NE	2.23	0.54
1:A:602:TYR:CG	1:A:610:PRO:HG3	2.43	0.54
1:A:712:PRO:N	1:A:713:ALA:HA	2.23	0.53
1:A:340:LEU:N	1:A:341:ARG:HA	2.24	0.53
2:B:141:TYR:HA	2:B:144:VAL:HG23	1.89	0.53
1:A:361:GLY:N	1:A:364:GLY:O	2.42	0.53
1:A:577:TYR:HD1	1:A:596:SER:HB3	1.72	0.53
1:A:448:THR:HA	1:A:451:VAL:HB	1.90	0.53
1:A:621:ARG:HD3	1:A:622:LYS:H	1.73	0.53
1:A:339:PHE:HB3	1:A:341:ARG:NE	2.22	0.52
1:A:577:TYR:HB2	1:A:596:SER:HB3	1.92	0.52
2:B:98:GLU:CB	2:B:99:PRO:HD3	2.39	0.52
1:A:438:MET:O	1:A:442:ILE:HG13	2.09	0.52
1:A:417:TYR:CE1	1:A:428:ILE:HD13	2.45	0.52
1:A:637:HIS:O	1:A:638:ILE:HG12	2.10	0.52
1:A:383:LEU:HB2	1:A:425:LEU:HB3	1.92	0.51
1:A:702:THR:HG23	1:A:703:ASP:H	1.75	0.51
1:A:383:LEU:HD12	1:A:425:LEU:HD12	1.92	0.51
1:A:498:THR:OG1	1:A:499:GLY:N	2.34	0.51
1:A:440:MET:HE2	1:A:443:ARG:HH12	1.74	0.51
1:A:315:LEU:HG	1:A:318:HIS:NE2	2.26	0.51
2:B:223:PHE:HA	2:B:226:PHE:HB2	1.93	0.51
1:A:342:LEU:HB2	1:A:747:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HD3	1:A:577:TYR:CE2	2.46	0.51
1:A:620:TYR:HA	1:A:623:ILE:HG22	1.92	0.50
1:A:354:THR:HA	1:A:369:VAL:HG12	1.93	0.50
2:B:229:ILE:O	2:B:234:PHE:N	2.44	0.50
1:A:438:MET:HE2	1:A:442:ILE:HD11	1.94	0.50
1:A:605:LEU:HD22	1:A:638:ILE:HD12	1.93	0.50
1:A:485:ILE:HD12	1:A:485:ILE:H	1.77	0.50
1:A:582:ILE:HD11	1:A:592:CYS:HB2	1.92	0.50
1:A:660:HIS:N	1:A:661:GLY:HA3	2.27	0.50
1:A:304:ARG:HH11	1:A:304:ARG:HB3	1.77	0.49
1:A:305:ASN:O	1:A:309:VAL:HG23	2.11	0.49
1:A:411:TRP:O	1:A:490:LYS:HA	2.12	0.49
1:A:413:VAL:HB	1:A:492:SER:HA	1.94	0.49
1:A:314:GLU:OE2	1:A:344:ARG:NH1	2.45	0.49
1:A:584:LEU:HD23	1:A:585:TYR:CD2	2.47	0.49
1:A:620:TYR:O	1:A:623:ILE:N	2.46	0.49
1:A:363:PHE:HB3	1:A:383:LEU:HD22	1.95	0.49
1:A:448:THR:OG1	1:A:449:GLU:N	2.45	0.49
1:A:619:THR:HG22	1:A:623:ILE:HB	1.95	0.49
1:A:646:ILE:HG22	1:A:650:LEU:HD22	1.95	0.49
2:B:107:LYS:H	2:B:244:ALA:HB1	1.78	0.48
1:A:367:ARG:HB2	1:A:380:MET:HB3	1.95	0.48
2:B:122:LEU:O	2:B:126:ILE:HG12	2.13	0.48
2:B:179:SER:HA	2:B:181:TYR:HD1	1.74	0.48
3:A:801:ANP:O2A	3:A:801:ANP:N3B	2.46	0.48
1:A:360:LYS:HA	1:A:365:GLU:HA	1.94	0.48
1:A:444:TRP:N	1:A:444:TRP:CD1	2.81	0.48
2:B:226:PHE:CD1	2:B:250:PHE:HD1	2.32	0.48
1:A:669:HIS:HA	1:A:670:PRO:HD2	1.72	0.47
1:A:457:ALA:H	1:A:460:ILE:HD12	1.79	0.47
1:A:595:TRP:CD1	1:A:595:TRP:C	2.92	0.47
2:B:98:GLU:CB	2:B:99:PRO:CD	2.91	0.47
1:A:580:PRO:HG3	1:A:626:PHE:HE1	1.78	0.47
2:B:266:LYS:H	2:B:266:LYS:HD3	1.78	0.47
2:B:181:TYR:CG	2:B:182:ILE:N	2.82	0.47
1:A:441:LEU:HD13	1:A:603:GLU:HG2	1.96	0.47
1:A:619:THR:HA	1:A:620:TYR:C	2.40	0.47
1:A:572:VAL:CB	1:A:573:GLY:HA2	2.45	0.46
1:A:613:SER:CB	1:A:618:GLU:HB3	2.44	0.46
1:A:359:GLY:O	1:A:366:VAL:N	2.42	0.46
1:A:302:ILE:H	1:A:302:ILE:HG12	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:CZ	1:A:388:MET:HG3	2.50	0.46
1:A:500:PHE:CE2	1:A:502:LYS:HB3	2.51	0.46
1:A:577:TYR:CG	1:A:578:ILE:N	2.73	0.46
1:A:601:MET:HE1	1:A:645:LEU:HD13	1.97	0.46
1:A:318:HIS:CD2	2:B:117:PRO:HG3	2.51	0.46
1:A:494:PHE:CE2	1:A:496:LEU:HD22	2.50	0.46
1:A:617:GLN:CD	1:A:617:GLN:H	2.23	0.46
1:A:297:SER:HB3	2:B:143:VAL:HG22	1.98	0.46
1:A:458:GLU:OE2	1:A:489:ILE:N	2.46	0.46
2:B:248:SER:HA	2:B:251:SER:HB3	1.98	0.46
1:A:342:LEU:O	1:A:343:ARG:NH2	2.49	0.46
1:A:577:TYR:CD1	1:A:596:SER:HB3	2.51	0.46
1:A:603:GLU:HA	1:A:608:TRP:N	2.30	0.46
1:A:641:GLU:H	1:A:641:GLU:CD	2.17	0.46
1:A:746:ARG:H	1:A:746:ARG:HG3	1.37	0.46
1:A:595:TRP:CD2	1:A:650:LEU:HD12	2.51	0.45
2:B:217:ARG:O	2:B:220:VAL:HG22	2.16	0.45
1:A:321:SER:OG	1:A:322:GLU:N	2.50	0.45
1:A:673:ARG:CD	1:A:674:GLY:H	2.24	0.45
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.87	0.45
2:B:181:TYR:C	2:B:183:ASP:H	2.17	0.45
1:A:574:THR:HG23	1:A:576:ASP:H	1.81	0.45
1:A:576:ASP:O	1:A:599:ALA:HB1	2.17	0.45
1:A:577:TYR:H	1:A:577:TYR:HD2	1.64	0.45
1:A:584:LEU:H	1:A:584:LEU:HD22	1.81	0.44
2:B:225:ILE:O	2:B:229:ILE:HG13	2.18	0.44
2:B:254:ILE:O	2:B:257:ALA:N	2.50	0.44
1:A:352:PHE:CE2	1:A:428:ILE:HD11	2.52	0.44
1:A:440:MET:HE3	1:A:440:MET:HB2	1.88	0.44
1:A:446:LEU:HB2	1:A:448:THR:HG22	2.00	0.44
1:A:324:ARG:HE	1:A:324:ARG:HA	1.82	0.44
1:A:363:PHE:O	1:A:384:LEU:N	2.50	0.44
1:A:574:THR:HG23	1:A:576:ASP:N	2.31	0.44
1:A:464:GLU:O	1:A:468:LYS:HB2	2.18	0.44
2:B:122:LEU:HD13	2:B:122:LEU:HA	1.89	0.44
1:A:448:THR:OG1	1:A:605:LEU:HD23	2.17	0.43
1:A:659:ARG:C	1:A:661:GLY:HA3	2.43	0.43
1:A:465:THR:O	1:A:469:LEU:HG	2.18	0.43
1:A:481:ILE:HG23	1:A:489:ILE:HG23	2.00	0.43
1:A:611:PHE:CE1	1:A:626:PHE:HB3	2.54	0.43
1:A:494:PHE:CZ	1:A:496:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LYS:HB2	1:A:427:LEU:HB2	1.99	0.43
1:A:341:ARG:HG3	1:A:342:LEU:HB3	2.00	0.43
1:A:656:ARG:HB2	1:A:657:LEU:H	1.70	0.43
1:A:674:GLY:HA3	1:A:675:VAL:HA	1.72	0.43
1:A:747:PHE:HD1	1:A:747:PHE:HA	1.59	0.43
1:A:447:PHE:CD1	1:A:447:PHE:N	2.85	0.42
1:A:377:ILE:HG12	1:A:377:ILE:O	2.19	0.42
1:A:451:VAL:O	1:A:454:PHE:HB3	2.20	0.42
1:A:611:PHE:HE1	1:A:626:PHE:HB3	1.84	0.42
2:B:146:GLU:HB3	2:B:147:TYR:H	1.63	0.42
2:B:254:ILE:HD13	2:B:254:ILE:HA	1.91	0.42
1:A:294:TYR:CB	1:A:297:SER:HB2	2.49	0.42
1:A:580:PRO:HG3	1:A:626:PHE:CE1	2.53	0.42
1:A:655:GLN:O	1:A:656:ARG:HG2	2.20	0.42
1:A:675:VAL:HG22	1:A:676:ASP:H	1.85	0.42
2:B:266:LYS:NZ	2:B:266:LYS:HB2	2.35	0.42
1:A:307:ARG:HH12	1:A:311:LEU:HD22	1.83	0.42
1:A:345:THR:HB	1:A:346:ARG:H	1.51	0.42
1:A:611:PHE:CD2	1:A:623:ILE:HG12	2.54	0.42
1:A:359:GLY:N	1:A:366:VAL:HG12	2.34	0.42
1:A:632:PHE:HD2	1:A:632:PHE:HA	1.71	0.42
1:A:584:LEU:HD12	1:A:624:MET:HE1	2.02	0.42
1:A:602:TYR:OH	1:A:631:GLN:O	2.32	0.42
1:A:590:GLN:CD	1:A:594:TRP:HE1	2.28	0.42
1:A:620:TYR:O	1:A:621:ARG:C	2.62	0.42
1:A:621:ARG:HD3	1:A:622:LYS:N	2.33	0.42
1:A:378:TYR:HE1	1:A:416:TYR:HE2	1.68	0.41
2:B:133:PHE:CZ	2:B:253:PHE:HA	2.55	0.41
1:A:663:ALA:N	1:A:666:ILE:HD12	2.32	0.41
1:A:436:ASP:OD2	1:A:439:THR:HB	2.21	0.41
1:A:484:ASP:OD1	1:A:488:HIS:N	2.52	0.41
1:A:601:MET:HE3	1:A:645:LEU:HB3	2.03	0.41
1:A:620:TYR:CB	1:A:624:MET:HG2	2.50	0.41
1:A:343:ARG:HA	1:A:343:ARG:CZ	2.51	0.41
1:A:579:ALA:C	1:A:581:GLU:H	2.29	0.41
1:A:746:ARG:HH21	1:A:747:PHE:HA	1.85	0.41
2:B:208:PRO:C	2:B:210:GLN:H	2.29	0.41
1:A:359:GLY:H	1:A:366:VAL:HG12	1.86	0.41
1:A:694:ILE:HD12	1:A:694:ILE:HA	1.89	0.41
1:A:343:ARG:NH1	2:B:128:LEU:HD21	2.36	0.41
1:A:425:LEU:HD22	1:A:426:TYR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:431:PHE:CD1	2.56	0.40
1:A:342:LEU:HB2	1:A:747:PHE:HZ	1.86	0.40
1:A:630:LEU:HD23	1:A:630:LEU:HA	1.92	0.40
1:A:439:THR:HA	1:A:442:ILE:HD12	2.02	0.40
2:B:218:ILE:HA	2:B:221:GLN:CG	2.44	0.40
1:A:445:GLN:OE1	1:A:445:GLN:N	2.53	0.40
2:B:242:LEU:HD22	2:B:245:HIS:HB2	2.02	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	375/508 (74%)	291 (78%)	80 (21%)	4 (1%)	11	45
2	B	159/244 (65%)	127 (80%)	24 (15%)	8 (5%)	1	16
All	All	534/752 (71%)	418 (78%)	104 (20%)	12 (2%)	5	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLU
2	B	182	ILE
1	A	286	VAL
1	A	572	VAL
2	B	99	PRO
2	B	100	PHE
2	B	111	LYS
2	B	112	THR
1	A	457	ALA
2	B	231	HIS
2	B	200	PRO

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Mol	Chain	Res	Type
1	A	578	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/449 (64%)	192 (67%)	93 (33%)	0	2
2	B	91/223 (41%)	66 (72%)	25 (28%)	0	3
All	All	376/672 (56%)	258 (69%)	118 (31%)	0	2

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ILE
1	A	304	ARG
1	A	307	ARG
1	A	316	THR
1	A	317	SER
1	A	320	TRP
1	A	321	SER
1	A	323	GLU
1	A	324	ARG
1	A	336	GLU
1	A	338	GLN
1	A	340	LEU
1	A	343	ARG
1	A	344	ARG
1	A	351	ASP
1	A	354	THR
1	A	365	GLU
1	A	366	VAL
1	A	377	ILE
1	A	381	LYS
1	A	384	LEU
1	A	388	MET

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Mol	Chain	Res	Type
1	A	389	TYR
1	A	408	ASP
1	A	415	LEU
1	A	418	SER
1	A	437	LEU
1	A	438	MET
1	A	439	THR
1	A	440	MET
1	A	444	TRP
1	A	445	GLN
1	A	446	LEU
1	A	450	ASP
1	A	452	THR
1	A	458	GLU
1	A	466	ILE
1	A	468	LYS
1	A	481	ILE
1	A	485	ILE
1	A	491	LEU
1	A	493	ASP
1	A	494	PHE
1	A	496	LEU
1	A	497	SER
1	A	561	ARG
1	A	562	LYS
1	A	566	LEU
1	A	576	ASP
1	A	581	GLU
1	A	584	LEU
1	A	585	TYR
1	A	590	GLN
1	A	592	CYS
1	A	597	LEU
1	A	604	CYS
1	A	606	ILE
1	A	614	GLU
1	A	617	GLN
1	A	621	ARG
1	A	623	ILE
1	A	629	THR
1	A	630	LEU
1	A	631	GLN

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Mol	Chain	Res	Type
1	A	632	PHE
1	A	636	ILE
1	A	639	SER
1	A	640	TYR
1	A	645	LEU
1	A	646	ILE
1	A	650	LEU
1	A	654	ASP
1	A	655	GLN
1	A	656	ARG
1	A	657	LEU
1	A	660	HIS
1	A	665	GLU
1	A	673	ARG
1	A	680	ILE
1	A	681	ARG
1	A	683	VAL
1	A	684	GLU
1	A	688	ILE
1	A	691	LEU
1	A	695	THR
1	A	696	ASP
1	A	698	ARG
1	A	705	LEU
1	A	711	SER
1	A	743	GLU
1	A	746	ARG
1	A	747	PHE
1	A	749	TYR
2	B	112	THR
2	B	113	ILE
2	B	115	GLN
2	B	119	TYR
2	B	120	VAL
2	B	122	LEU
2	B	124	GLU
2	B	128	LEU
2	B	144	VAL
2	B	148	VAL
2	B	184	LEU
2	B	197	ASN
2	B	198	LEU

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Mol	Chain	Res	Type
2	B	220	VAL
2	B	225	ILE
2	B	226	PHE
2	B	238	VAL
2	B	241	SER
2	B	242	LEU
2	B	243	GLU
2	B	246	TRP
2	B	251	SER
2	B	259	GLU
2	B	266	LYS
2	B	275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	655	GLN
1	A	678	ASN
2	B	194	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	801	-	33,33,33	2.49	8 (24%)	45,52,52	2.65	12 (26%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	PB-O1B	9.26	1.60	1.46
3	A	801	ANP	PB-N3B	4.66	1.75	1.63
3	A	801	ANP	C2'-C3'	-4.34	1.41	1.53
3	A	801	ANP	C6-N6	4.00	1.44	1.34
3	A	801	ANP	PG-O1G	3.65	1.51	1.46
3	A	801	ANP	O4'-C4'	-3.06	1.38	1.45
3	A	801	ANP	C3'-C4'	-2.13	1.47	1.53
3	A	801	ANP	C2'-C1'	-2.01	1.47	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	O1B-PB-N3B	-10.91	95.70	111.77
3	A	801	ANP	C5-C4-N3	-5.13	119.65	126.72
3	A	801	ANP	O2B-PB-O1B	4.78	120.11	109.87
3	A	801	ANP	N3-C2-N1	-4.74	121.41	128.58
3	A	801	ANP	O2B-PB-O3A	4.35	119.16	104.64
3	A	801	ANP	N3-C4-N9	3.94	133.87	127.17
3	A	801	ANP	N9-C8-N7	-3.76	108.61	113.94
3	A	801	ANP	C2-N3-C4	3.58	120.57	111.83
3	A	801	ANP	C5-N7-C8	3.22	108.51	103.45
3	A	801	ANP	C4-N9-C8	3.03	108.92	105.74
3	A	801	ANP	O5'-C5'-C4'	2.94	119.00	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	C4-C5-N7	-2.72	107.48	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

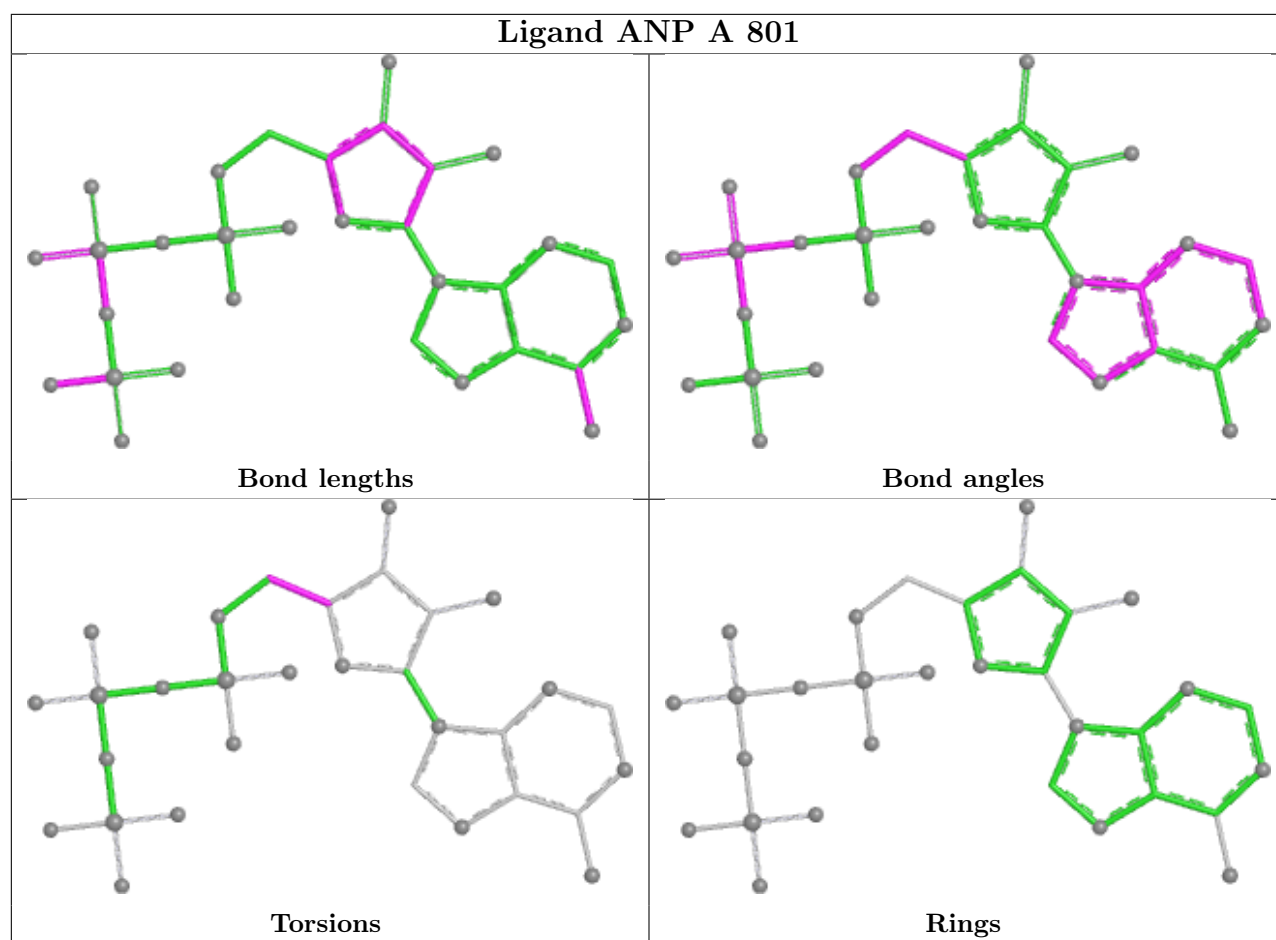
Mol	Chain	Res	Type	Atoms
3	A	801	ANP	O4'-C4'-C5'-O5'
3	A	801	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ANP	3	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	383/508 (75%)	0.64	38 (9%) 13 17	79, 147, 221, 293	0
2	B	163/244 (66%)	0.46	11 (6%) 24 25	84, 136, 200, 240	0
All	All	546/752 (72%)	0.59	49 (8%) 15 19	79, 145, 216, 293	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	GLU	5.0
1	A	501	HIS	4.5
1	A	656	ARG	4.4
1	A	498	THR	4.4
1	A	389	TYR	4.3
1	A	655	GLN	4.2
1	A	503	THR	4.1
1	A	565	ARG	4.1
1	A	387	GLU	4.0
1	A	490	LYS	3.8
1	A	362	ALA	3.6
1	A	684	GLU	3.6
1	A	558	GLN	3.5
1	A	658	GLY	3.4
1	A	640	TYR	3.4
2	B	148	VAL	3.4
2	B	101	VAL	3.3
2	B	175	SER	3.2
1	A	739	PHE	3.2
1	A	561	ARG	3.0
1	A	660	HIS	3.0
2	B	103	THR	3.0
1	A	612	CYS	3.0
1	A	320	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	363	PHE	2.9
2	B	275	ILE	2.8
1	A	659	ARG	2.8
1	A	687	TYR	2.7
1	A	407	SER	2.7
1	A	406	GLY	2.7
1	A	573	GLY	2.6
1	A	575	PRO	2.6
1	A	412	VAL	2.6
2	B	139	GLN	2.5
1	A	416	TYR	2.5
1	A	297	SER	2.4
2	B	102	ARG	2.4
2	B	104	ALA	2.4
2	B	206	PRO	2.3
1	A	295	GLN	2.3
1	A	449	GLU	2.2
1	A	618	GLU	2.2
2	B	228	HIS	2.2
1	A	578	ILE	2.1
1	A	714	MET	2.1
1	A	709	PRO	2.1
1	A	345	THR	2.0
1	A	413	VAL	2.0
2	B	258	LYS	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 ⓘ

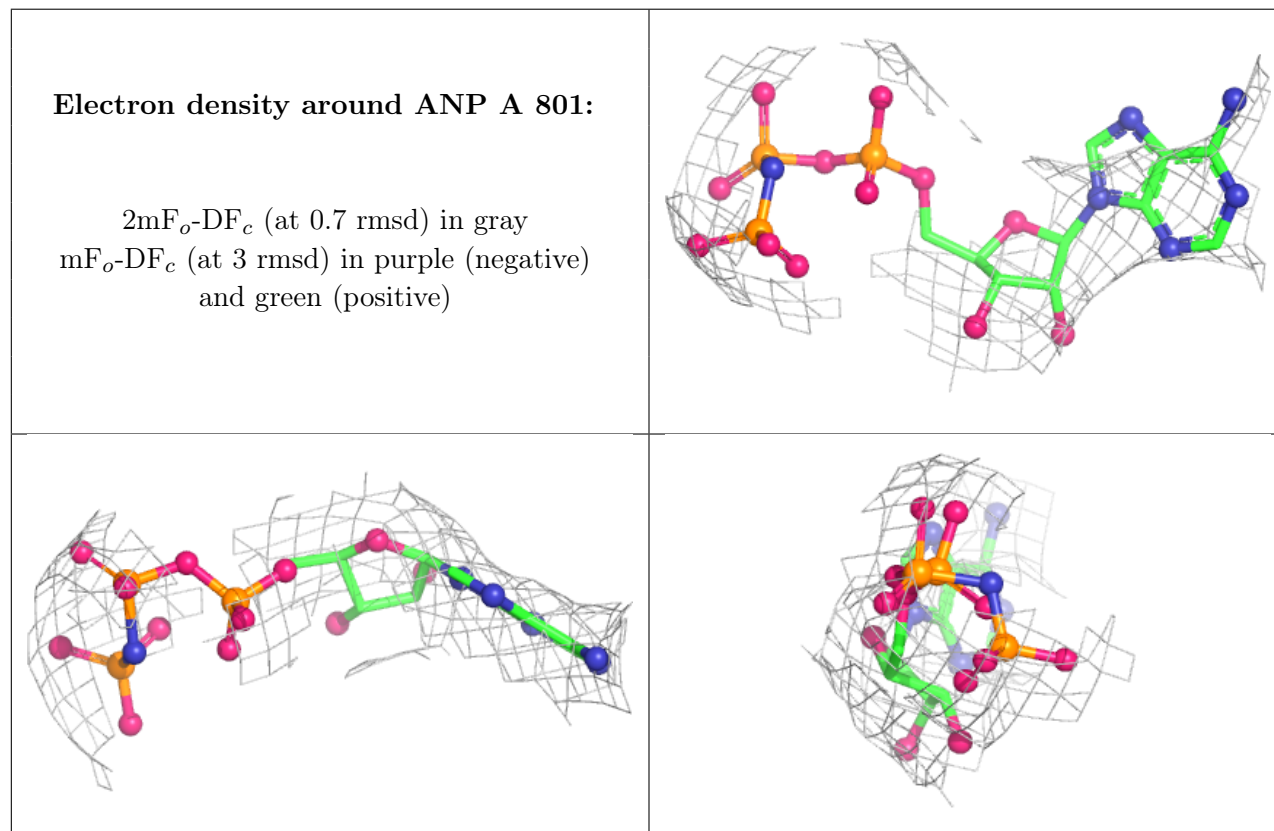
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	ANP	A	801	31/31	0.95	0.09	134,163,204,223	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.