WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2023 – 06:24 AM EDT

PDB ID	:	1KEE
Title	:	Inactivation of the Amidotransferase Activity of Carbamoyl Phosphate Synthetase by the Antibiotic Acivicin
Authors	:	Miles, B.W.; Thoden, J.B.; Holden, H.M.; Raushel, F.M.
Deposited on	:	2001-11-15
Resolution	:	2.10 Å(reported)

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

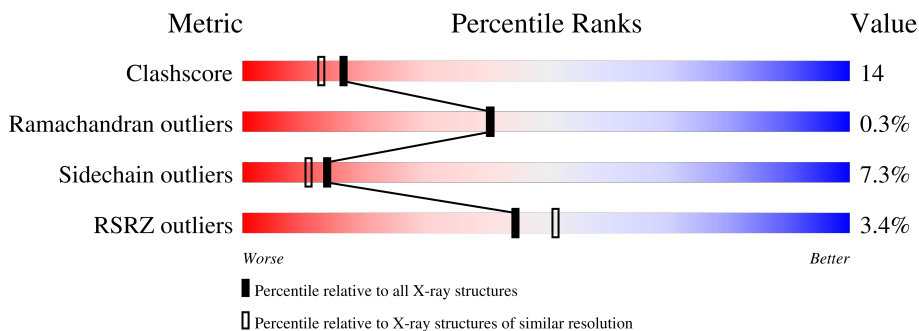|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.3%
Sidechain outliers		7.3%
RSRZ outliers		3.4%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	1073	3% / 63% / 29% / 6% ••
1	C	1073	4% / 63% / 29% / 7% ••
1	E	1073	4% / 64% / 29% / 5% ••
1	G	1073	5% / 60% / 30% / 7% ••
2	B	382	% / 62% / 31% / 5% •
2	D	382	61% / 34% / ••

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Mol	Chain	Length	Quality of chain
2	F	382	3% 61% 33% 6%
2	H	382	3% 55% 36% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	143	B	269	X	-	-	-
2	143	D	269	X	-	-	-
2	143	F	269	X	-	-	-
2	143	H	269	X	-	-	-

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 48896 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 Carbamoyl-phosphate synthetase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total 8181	C 5136	N 1425	O 1575	S 45	0	5	0
1	C	1058	Total 8172	C 5130	N 1425	O 1572	S 45	0	2	0
1	E	1058	Total 8204	C 5150	N 1430	O 1579	S 45	0	8	0
1	G	1058	Total 8160	C 5123	N 1422	O 1570	S 45	0	0	0

- Molecule 2 is a protein called Carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total 2912	C 1834	N 513	O 555	S 10	0	1	0
2	D	379	Total 2907	C 1831	N 510	O 556	S 10	0	1	0
2	F	379	Total 2905	C 1830	N 510	O 555	S 10	0	0	0
2	H	379	Total 2905	C 1830	N 510	O 555	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	143	CYS	modified residue	UNP P00907
D	269	143	CYS	modified residue	UNP P00907
F	269	143	CYS	modified residue	UNP P00907
H	269	143	CYS	modified residue	UNP P00907

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mn 3	0	0
3	C	3	Total 3	Mn 3	0	0
3	E	3	Total 3	Mn 3	0	0
3	G	3	Total 3	Mn 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	K 7	0	0
4	B	1	Total 1	K 1	0	0
4	C	7	Total 7	K 7	0	0
4	D	1	Total 1	K 1	0	0
4	E	7	Total 7	K 7	0	0
4	F	1	Total 1	K 1	0	0
4	G	7	Total 7	K 7	0	0
4	H	1	Total 1	K 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	Cl 5	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	5	Total 5	Cl 5	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	4	Total 4	Cl 4	0	0
5	F	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	4	Total 4	Cl 4	0	0
5	H	1	Total 1	Cl 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
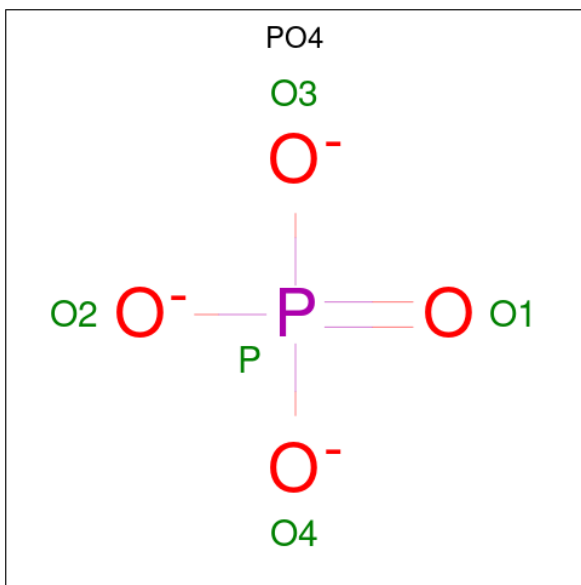
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	P 1	0	0
6	C	1	Total 5	O 4	P 1	0	0
6	E	1	Total 5	O 4	P 1	0	0
6	G	1	Total 5	O 4	P 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

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

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).
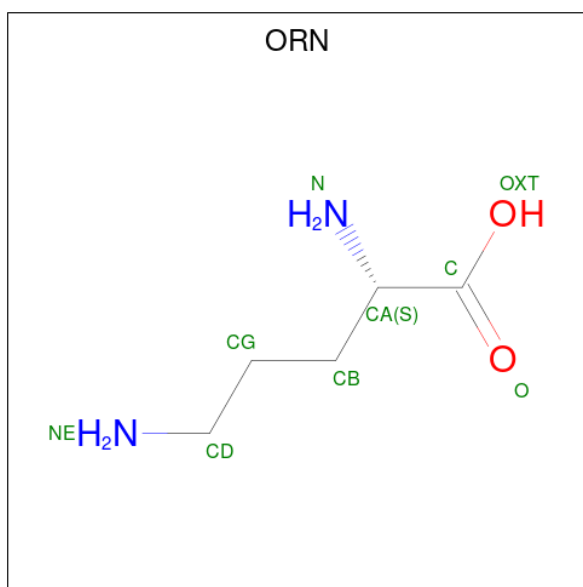
ORN

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).

NET
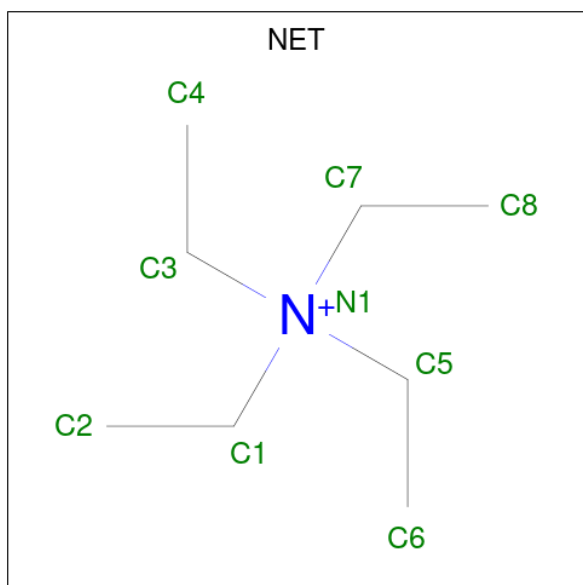
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 9	C 8	N 1	0	0
9	C	1	Total 9	C 8	N 1	0	0
9	E	1	Total 9	C 8	N 1	0	0
9	G	1	Total 9	C 8	N 1	0	0

- Molecule 10 is water.

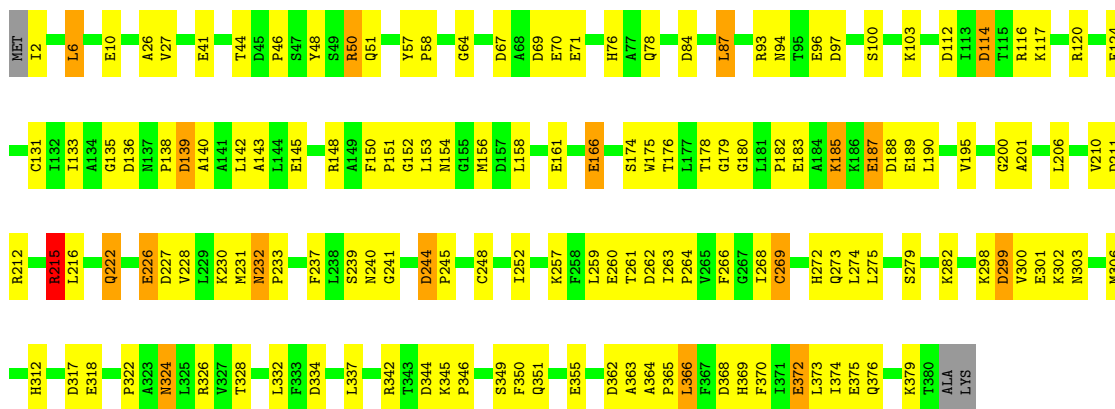| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	841	Total 841	O 841	0	0
10	B	230	Total 230	O 230	0	0
10	C	783	Total 783	O 783	0	0
10	D	304	Total 304	O 304	0	0
10	E	886	Total 886	O 886	0	0
10	F	263	Total 263	O 263	0	0
10	G	678	Total 678	O 678	0	0
10	H	191	Total 191	O 191	0	0

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.

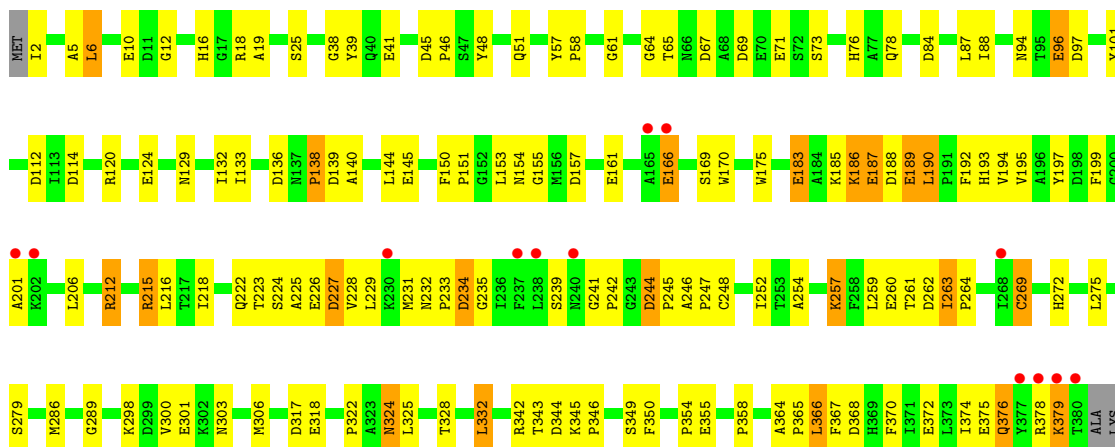• Molecule 1: Carbamoyl-phosphate synthetase large chain

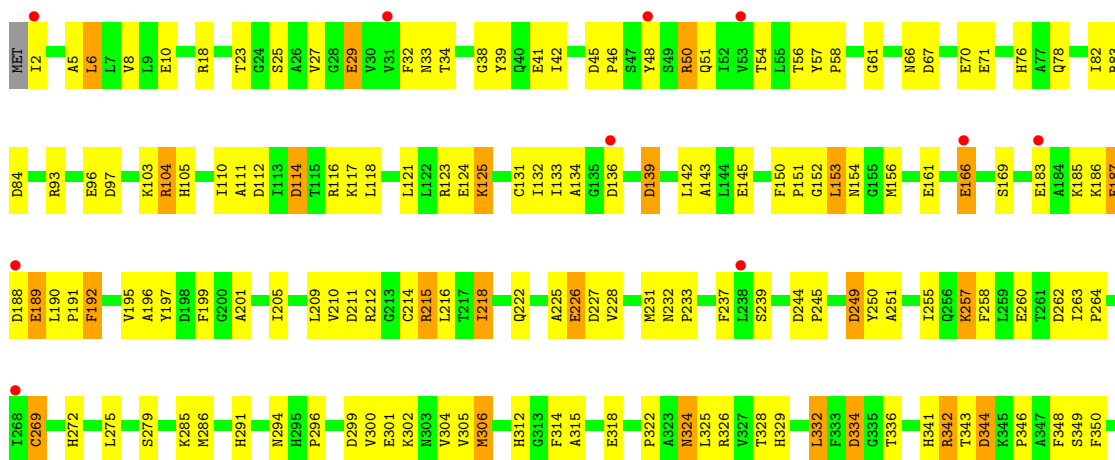S1026 R1031 S1032 Y1036 Y1040 F1048 M1052 T1059 E1060 K1061 E1067 K1073

• Molecule 1: Carbamoyl-phosphate synthetase large chain

Chain C:

4%

63%　　　29%　　　7% ••

M1 P2 K3 R4 T5 D6 I7 I10 L11 I12 P17 C24 D27 R38 E39 E40 G41 Y42 R43 V44 I45 L46 P51 M55 T56 D57 P58 E59 M60 A61 D62 A63 T64 Y65 I66 E67 E72 R75 K76 I77 I78 E79 K80 R82 P83 D84 P88 E101

L102 E103 R104 Q105 G106 V107 L108 E109 E110 D121 D124 E127 D128 R129 R130 R131 F132 D133 E142 R145 S146 G147 I148 A149 H150 T151 M152 E153 E154 A159 A160 D161 C166 I167 F172 T173 M174 G175 G176 G180 R185 E186 E187 F188 E189 E190 L196 D197

P200 T201 K202 E203 L204 L205 I206 D207 W213 K214 E215 Y216 E217 M218 E219 R222 D223 K224 N225 D226 E235 N236 F237 I248 D258 K259 E260 A267 V271 L272 R273 E274 E278 R294 L295 I296 E299 S307 K313 P318 K321 G329 Y330 D333

E334 D338 E349 D353 K358 N363 F364 E365 D372 R373 L374 T375 T376 Q377 E383 V384 M385 E393 R400 E403 D410 P411 K412 V413 S414 L415 D416 D417 P418 E419 T422 K423 I424 R425 R426 E427 L428 D434 D441 L447 D450 D459 R460

E467 V470 R471 L472 E473 E474 K475 V476 A477 E478 T482 D487 F488 L489 R490 A500 A503 K504 R509 E510 A511 E512 I513 R514 R517 D518 Q519 Y520 D521 V525 Y526 K527 D530 A534 E535 D539 Y542 M543 Y544 S545 E548 E549 E550 C551 D558

R559 E660 K561 I562 M563 R571 E577 F578 D579 V583 L587 A588 L589 R590 E591 D592 G593 Y594 E595 N600 P603 E604 T608 D609 D614 F618 V621 T622 L623 E624 D625 E628 I629 V630 E633 K634 P635 T646 P647 R652 A653 L654 E655 V659 P660

D667 D670 R671 A672 E673 D674 R675 E676 R677 F678 Q679 H680 E683 K686 L687 K688 N692 A693 T694 V695 T696 A697 I698 E699 M700 A701 V702 E703 K704 A705 K706 E707 I708 G709 Y710 P711 L712 P716 SER TYR VAL LEU GLY GLY ARG A724 M725 E726 I727 V728 Y729 D730 E731 A732

D733 L734 R735 R736 Y737 F738 Q739 T740 A741 VAL SER VAL ASN ASP ALA PRO V750 L751 L752 D753 H754 D757 E761 V762 D763 V764 D765 D769 G770 E771 M772 V773 L774 I775 E780 H781 I782 E783 Q784 T800 L801 S802 Q803 E804 I805 Q806 V808 M809 R810 Q811 Q812 V813

E819 L820 Q821 V822 R823 G824 L825 M826 N827 K833 E836 V837 E841 T849 K855 G858 K863 V864 A865 A866 R867 V868 M869 K872 S873 E876 Q877 G878 V879 T880 K881 E882 P885 K891 E892 G902 V903 D904 P905 L906 E910 M911 R912 E916 V917 M918

E926 K940 L947 R950 E951 G952 D953 K954 E955 R956 D959 K966 Q967 E970 L971 D972 A973 T974 H975 I979 V980 L981 G982 E983 I986 N987 P988 V991 N992 K993 V994 H995 E996 G997 R998 P999 H1000 I1001 Q1002 D1003 M1007 G1008 E1009 I1013 I1014 T1017 S1018

G1019 R1020 R1021 A1022 I1023 E1024 R1027 K1037 Y1040 D1041 T1042 T1043 L1044 F1048 M1052 A1053 L1054 E1060 K1061 E1067 M1068 H1069 A1070 Q1071 I1072 K1073

• Molecule 1: Carbamoyl-phosphate synthetase large chain

Chain E:

4%

64%　　　29%　　　5% ••

• Molecule 1: Carbamoyl-phosphate synthetase large chain

Chain G:

The protein sequence residue boxes are displayed here as a color-coded validation diagram.

• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain B:

62%   31%   5% •

• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain D:

61%   34%

• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain F:

3%

61%   33%   6%

• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain H:

3%

55%   36%   7%

P354 E355 A356 S357 P358 D362 A363 A364 P365 L366 F367 D368 H369 F370 I371 E372 E375 T380 ALA LYS

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	152.40Å 164.40Å 333.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.00-2.10) 88.9 (29.99-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.186 , 0.211 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 108.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NET, ADP, 143, MN, ORN, CL, K, PO4

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	0.99	76/8327 (0.9%)	1.38	120/11257 (1.1%)
1	C	0.99	79/8306 (1.0%)	1.34	111/11228 (1.0%)
1	E	1.00	77/8362 (0.9%)	1.34	118/11302 (1.0%)
1	G	0.97	74/8286 (0.9%)	1.38	120/11202 (1.1%)
2	B	0.88	20/2961 (0.7%)	1.28	38/4019 (0.9%)
2	D	0.90	19/2956 (0.6%)	1.29	33/4013 (0.8%)
2	F	0.90	18/2950 (0.6%)	1.31	39/4005 (1.0%)
2	H	0.88	20/2950 (0.7%)	1.28	36/4005 (0.9%)
All	All	0.96	383/45098 (0.8%)	1.34	615/61031 (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
2	B	1	0
2	D	1	0
2	F	1	0
2	H	1	0
All	All	4	0

The worst 5 of 383 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	183	GLU	CD-OE2	8.23	1.34	1.25
1	C	110	GLU	CD-OE2	8.18	1.34	1.25
2	D	183	GLU	CD-OE2	8.05	1.34	1.25
1	E	467	GLU	CD-OE2	8.02	1.34	1.25
2	F	355	GLU	CD-OE2	8.01	1.34	1.25

The worst 5 of 615 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	38	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	E	956	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	642	TYR	CB-CG-CD2	-11.19	114.28	121.00
1	E	43	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	1004	ARG	NE-CZ-NH1	10.36	125.48	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8181	0	8215	216	0
1	C	8172	0	8206	231	0
1	E	8204	0	8235	208	0
1	G	8160	0	8196	256	0
2	B	2912	0	2874	84	0
2	D	2907	0	2866	90	0
2	F	2905	0	2864	84	0
2	H	2905	0	2864	109	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	7	0	0	1	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	1	0
5	B	1	0	0	0	0
5	C	5	0	0	1	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	1	0	0	0	0
5	G	4	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	1	0
6	E	5	0	0	0	0
6	G	5	0	0	1	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	4	0
7	G	54	0	24	4	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	4	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	1	0
10	A	841	0	0	23	0
10	B	230	0	0	5	0
10	C	783	0	0	20	0
10	D	304	0	0	8	0
10	E	886	0	0	20	0
10	F	263	0	0	1	0
10	G	678	0	0	13	0
10	H	191	0	0	4	0
All	All	48896	0	44540	1267	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 14.

The worst 5 of 1267 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:E:46:LEU:HD22	1:E:46:LEU:O	1.37	1.20
1:A:46:LEU:O	1:A:46:LEU:HD22	1.42	1.18
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.27	1.14
2:D:228:VAL:HA	2:D:231:MET:HE2	1.26	1.10
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.32	1.09

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	1057/1073 (98%)	998 (94%)	56 (5%)	3 (0%)	41	41
1	C	1054/1073 (98%)	1002 (95%)	48 (5%)	4 (0%)	34	32
1	E	1060/1073 (99%)	1012 (96%)	45 (4%)	3 (0%)	41	41
1	G	1052/1073 (98%)	998 (95%)	49 (5%)	5 (0%)	29	26
2	B	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	376/382 (98%)	364 (97%)	12 (3%)	0	100	100
2	H	376/382 (98%)	362 (96%)	14 (4%)	0	100	100
All	All	5729/5820 (98%)	5462 (95%)	252 (4%)	15 (0%)	41	41

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	996	GLU
1	G	873	SER
1	A	558	ASP
1	A	975	HIS
1	E	675	ARG

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	870/878 (99%)	808 (93%)	62 (7%)	14	11
1	C	867/878 (99%)	797 (92%)	70 (8%)	11	8
1	E	873/878 (99%)	818 (94%)	55 (6%)	18	15
1	G	865/878 (98%)	793 (92%)	72 (8%)	11	7
2	B	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	D	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	F	307/309 (99%)	281 (92%)	26 (8%)	10	7
2	H	307/309 (99%)	286 (93%)	21 (7%)	16	13
All	All	4705/4748 (99%)	4359 (93%)	346 (7%)	14	10

5 of 346 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	87	LEU
1	G	673	GLU
2	F	186	LYS
1	G	103	GLU
1	G	784	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1035	GLN
1	G	784	GLN
1	E	1071	GLN
1	G	150	HIS
1	G	942	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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
2	143	F	269	2	9,16,17	7.68	4 (44%)	3,21,23	1.86	1 (33%)
2	143	D	269	2	9,16,17	6.57	5 (55%)	3,21,23	1.34	0
2	143	B	269	2	9,16,17	5.18	4 (44%)	3,21,23	1.81	1 (33%)
2	143	H	269	2	9,16,17	8.70	5 (55%)	3,21,23	1.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	143	F	269	2	1/1/5/8	4/9/24/26	0/1/1/1
2	143	D	269	2	1/1/5/8	3/9/24/26	0/1/1/1
2	143	B	269	2	1/1/5/8	3/9/24/26	0/1/1/1
2	143	H	269	2	1/1/5/8	4/9/24/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	143	CD-NX	-20.68	1.17	1.45
2	F	269	143	CD-NX	-19.40	1.19	1.45
2	D	269	143	CD-NX	-16.99	1.22	1.45
2	B	269	143	CD-NX	-13.21	1.27	1.45
2	H	269	143	CD-CE	-12.18	1.33	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	143	OJ1-CJ-OJ2	-2.82	117.68	124.09

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PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	269	143	OJ1-CJ-OJ2	-2.43	118.57	124.09

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	143	N-CA-CB-SG
2	B	269	143	OF-CF-CI-CJ
2	D	269	143	N-CA-CB-SG
2	D	269	143	OF-CF-CI-CJ
2	F	269	143	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	269	143	2	0
2	D	269	143	3	0
2	B	269	143	2	0
2	H	269	143	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
7	ADP	E	2045	3	24,29,29	1.01	2 (8%)	29,45,45	1.25	2 (6%)
6	PO4	E	2050	3	4,4,4	1.99	3 (75%)	6,6,6	1.07	0
7	ADP	C	2029	4,3	24,29,29	1.10	2 (8%)	29,45,45	1.29	4 (13%)
7	ADP	A	2001	3	24,29,29	1.21	2 (8%)	29,45,45	1.26	4 (13%)
7	ADP	G	2066	3	24,29,29	1.16	3 (12%)	29,45,45	1.28	4 (13%)
8	ORN	G	5076	-	7,8,8	0.97	1 (14%)	8,9,9	1.11	1 (12%)
6	PO4	A	2006	3	4,4,4	1.85	2 (50%)	6,6,6	1.28	1 (16%)
7	ADP	A	2007	4,3	24,29,29	1.01	1 (4%)	29,45,45	1.27	3 (10%)
7	ADP	G	2072	4,3	24,29,29	1.20	4 (16%)	29,45,45	1.37	4 (13%)
8	ORN	C	5033	-	7,8,8	0.87	0	8,9,9	1.11	1 (12%)
9	NET	G	5077	-	8,8,8	0.83	0	10,10,10	0.35	0
7	ADP	C	2023	3	24,29,29	1.26	4 (16%)	29,45,45	1.22	5 (17%)
6	PO4	C	2028	3	4,4,4	2.28	2 (50%)	6,6,6	0.98	0
9	NET	E	5056	-	8,8,8	0.79	0	10,10,10	0.35	0
7	ADP	E	2051	4,3	24,29,29	1.15	4 (16%)	29,45,45	1.06	3 (10%)
9	NET	C	5034	-	8,8,8	0.60	0	10,10,10	0.45	0
9	NET	A	5012	-	8,8,8	0.64	0	10,10,10	0.52	0
8	ORN	A	5011	-	7,8,8	0.79	0	8,9,9	1.54	2 (25%)
6	PO4	G	2071	3	4,4,4	2.07	1 (25%)	6,6,6	1.05	0
8	ORN	E	5055	-	7,8,8	0.95	0	8,9,9	1.25	1 (12%)

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
8	ORN	E	5055	-	-	6/8/8/8	-
9	NET	E	5056	-	-	3/12/12/12	-
7	ADP	A	2007	4,3	-	3/12/32/32	0/3/3/3
7	ADP	C	2029	4,3	-	3/12/32/32	0/3/3/3
7	ADP	A	2001	3	-	0/12/32/32	0/3/3/3
7	ADP	E	2051	4,3	-	3/12/32/32	0/3/3/3
7	ADP	G	2072	4,3	-	3/12/32/32	0/3/3/3
8	ORN	C	5033	-	-	7/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NET	A	5012	-	-	10/12/12/12	-
8	ORN	A	5011	-	-	5/8/8/8	-
7	ADP	G	2066	3	-	0/12/32/32	0/3/3/3
7	ADP	C	2023	3	-	2/12/32/32	0/3/3/3
9	NET	C	5034	-	-	0/12/12/12	-
8	ORN	G	5076	-	-	6/8/8/8	-
7	ADP	E	2045	3	-	0/12/32/32	0/3/3/3
9	NET	G	5077	-	-	3/12/12/12	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2029	ADP	O3'-C3'	3.44	1.51	1.43
7	G	2066	ADP	O2'-C2'	2.99	1.50	1.43
7	A	2001	ADP	O3'-C3'	2.96	1.49	1.43
7	C	2023	ADP	O3'-C3'	2.95	1.49	1.43
7	C	2023	ADP	O4'-C1'	-2.94	1.37	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2072	ADP	O3B-PB-O3A	3.94	117.86	104.64
7	E	2045	ADP	C5-C6-N6	3.71	125.99	120.35
7	C	2029	ADP	C5-C6-N6	3.35	125.44	120.35
7	G	2066	ADP	O2'-C2'-C3'	3.19	122.15	111.82
7	A	2007	ADP	C5-C6-N6	3.17	125.17	120.35

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2007	ADP	PA-O3A-PB-O3B
7	C	2029	ADP	PA-O3A-PB-O3B
7	E	2051	ADP	PA-O3A-PB-O3B
8	A	5011	ORN	N-CA-CB-CG
8	A	5011	ORN	C-CA-CB-CG

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	2045	ADP	2	0
7	G	2066	ADP	2	0
8	G	5076	ORN	2	0
7	G	2072	ADP	2	0
8	C	5033	ORN	1	0
9	G	5077	NET	1	0
6	C	2028	PO4	1	0
9	E	5056	NET	1	0
7	E	2051	ADP	2	0
9	A	5012	NET	4	0
6	G	2071	PO4	1	0
8	E	5055	ORN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP E 2045

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 2029

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 2066

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 2007

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 2072

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 2023

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 2051

Bond lengths

Bond angles

Torsions

Rings

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	1058/1073 (98%)	-0.33	37 (3%)	44	50	15, 32, 80, 100	0
1	C	1058/1073 (98%)	-0.31	42 (3%)	38	44	15, 33, 81, 100	0
1	E	1058/1073 (98%)	-0.32	40 (3%)	40	46	16, 29, 82, 100	0
1	G	1058/1073 (98%)	-0.20	49 (4%)	32	38	16, 37, 87, 100	0
2	B	378/382 (98%)	-0.29	4 (1%)	80	84	19, 41, 75, 100	0
2	D	378/382 (98%)	-0.39	0	100	100	18, 33, 63, 92	0
2	F	378/382 (98%)	-0.28	13 (3%)	45	51	18, 35, 74, 99	0
2	H	378/382 (98%)	-0.12	10 (2%)	56	61	25, 45, 78, 98	0
All	All	5744/5820 (98%)	-0.29	195 (3%)	45	51	15, 34, 80, 100	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.4
1	A	738	PHE	10.3
1	A	740	THR	9.9
1	A	739	GLN	8.8
1	C	695	VAL	8.3

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

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	143	H	269	16/17	0.90	0.21	29,71,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	143	B	269	16/17	0.91	0.18	34,46,87,90	0
2	143	F	269	16/17	0.93	0.20	25,46,100,100	0
2	143	D	269	16/17	0.94	0.20	21,32,100,100	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
4	K	C	5031	1/1	0.89	0.11	52,52,52,52	0
4	K	A	5013	1/1	0.93	0.10	59,59,59,59	0
5	CL	A	5020	1/1	0.93	0.08	61,61,61,61	0
5	CL	E	5062	1/1	0.94	0.07	59,59,59,59	0
4	K	C	5035	1/1	0.95	0.06	48,48,48,48	0
8	ORN	G	5076	9/9	0.95	0.16	18,27,35,49	0
9	NET	E	5056	9/9	0.95	0.15	19,29,41,43	0
6	PO4	A	2006	5/5	0.96	0.07	22,25,39,50	0
6	PO4	G	2071	5/5	0.96	0.08	20,28,40,56	0
8	ORN	A	5011	9/9	0.96	0.15	21,24,31,40	0
8	ORN	C	5033	9/9	0.96	0.16	12,21,37,46	0
4	K	E	5057	1/1	0.96	0.06	59,59,59,59	0
5	CL	G	5084	1/1	0.96	0.11	65,65,65,65	0
9	NET	G	5077	9/9	0.96	0.15	23,39,55,64	0
5	CL	C	5044	1/1	0.97	0.06	39,39,39,39	0
4	K	C	5036	1/1	0.97	0.07	56,56,56,56	0
5	CL	G	5083	1/1	0.97	0.05	40,40,40,40	0
4	K	C	5037	1/1	0.97	0.08	62,62,62,62	0
5	CL	G	5085	1/1	0.97	0.07	68,68,68,68	0
4	K	A	5009	1/1	0.97	0.13	38,38,38,38	0
4	K	E	5058	1/1	0.97	0.09	53,53,53,53	0
7	ADP	G	2072	27/27	0.97	0.07	24,38,60,83	0
4	K	G	5074	1/1	0.97	0.16	67,67,67,67	0
4	K	G	5079	1/1	0.97	0.09	71,71,71,71	0
4	K	A	5015	1/1	0.97	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NET	A	5012	9/9	0.97	0.12	20,29,37,45	0
5	CL	C	5040	1/1	0.97	0.04	35,35,35,35	0
5	CL	C	5042	1/1	0.97	0.07	55,55,55,55	0
6	PO4	E	2050	5/5	0.98	0.07	22,25,48,48	0
4	K	E	5053	1/1	0.98	0.09	51,51,51,51	0
7	ADP	C	2029	27/27	0.98	0.07	16,35,60,82	0
7	ADP	E	2051	27/27	0.98	0.07	20,32,49,89	0
7	ADP	G	2066	27/27	0.98	0.10	15,21,36,38	0
4	K	G	5080	1/1	0.98	0.07	43,43,43,43	0
4	K	H	5081	1/1	0.98	0.12	57,57,57,57	0
5	CL	A	5019	1/1	0.98	0.06	40,40,40,40	0
8	ORN	E	5055	9/9	0.98	0.11	21,23,35,53	0
4	K	E	5059	1/1	0.98	0.04	43,43,43,43	0
5	CL	A	5022	1/1	0.98	0.17	74,74,74,74	0
5	CL	H	5086	1/1	0.98	0.11	47,47,47,47	0
4	K	C	5027	1/1	0.98	0.10	29,29,29,29	0
5	CL	F	5065	1/1	0.99	0.08	31,31,31,31	0
5	CL	G	5082	1/1	0.99	0.08	39,39,39,39	0
4	K	G	5070	1/1	0.99	0.12	36,36,36,36	0
4	K	A	5010	1/1	0.99	0.08	24,24,24,24	0
4	K	G	5078	1/1	0.99	0.06	54,54,54,54	0
3	MN	C	2024	1/1	0.99	0.09	28,28,28,28	0
4	K	A	5014	1/1	0.99	0.10	52,52,52,52	0
6	PO4	C	2028	5/5	0.99	0.08	13,16,31,35	0
4	K	D	5038	1/1	0.99	0.06	37,37,37,37	0
5	CL	A	5018	1/1	0.99	0.04	34,34,34,34	0
7	ADP	A	2001	27/27	0.99	0.10	16,25,33,41	0
7	ADP	A	2007	27/27	0.99	0.07	17,26,37,45	0
7	ADP	C	2023	27/27	0.99	0.12	13,21,23,26	0
4	K	E	2048	1/1	0.99	0.08	24,24,24,24	0
7	ADP	E	2045	27/27	0.99	0.12	16,27,43,64	0
4	K	E	5049	1/1	0.99	0.13	30,30,30,30	0
3	MN	G	2067	1/1	0.99	0.06	36,36,36,36	0
5	CL	B	5021	1/1	0.99	0.06	33,33,33,33	0
4	K	B	5016	1/1	0.99	0.08	45,45,45,45	0
3	MN	G	2073	1/1	0.99	0.06	42,42,42,42	0
3	MN	A	5008	1/1	0.99	0.06	28,28,28,28	0
5	CL	D	5043	1/1	0.99	0.06	30,30,30,30	0
4	K	F	5060	1/1	0.99	0.09	42,42,42,42	0
9	NET	C	5034	9/9	0.99	0.12	17,19,27,30	0
5	CL	E	5063	1/1	0.99	0.05	45,45,45,45	0
5	CL	E	5064	1/1	0.99	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	2002	1/1	1.00	0.06	31,31,31,31	0
4	K	C	5026	1/1	1.00	0.12	18,18,18,18	0
5	CL	C	5039	1/1	1.00	0.11	27,27,27,27	0
3	MN	G	2068	1/1	1.00	0.07	25,25,25,25	0
5	CL	C	5041	1/1	1.00	0.05	36,36,36,36	0
3	MN	A	2003	1/1	1.00	0.08	25,25,25,25	0
4	K	G	2069	1/1	1.00	0.09	23,23,23,23	0
4	K	C	5032	1/1	1.00	0.07	31,31,31,31	0
5	CL	E	5061	1/1	1.00	0.12	30,30,30,30	0
4	K	A	5004	1/1	1.00	0.10	24,24,24,24	0
4	K	G	5075	1/1	1.00	0.08	29,29,29,29	0
4	K	A	5005	1/1	1.00	0.09	27,27,27,27	0
3	MN	C	2025	1/1	1.00	0.09	22,22,22,22	0
3	MN	C	2030	1/1	1.00	0.06	38,38,38,38	0
3	MN	E	2046	1/1	1.00	0.08	34,34,34,34	0
5	CL	A	5017	1/1	1.00	0.07	29,29,29,29	0
3	MN	E	2047	1/1	1.00	0.08	27,27,27,27	0
3	MN	E	2052	1/1	1.00	0.05	34,34,34,34	0
4	K	E	5054	1/1	1.00	0.07	24,24,24,24	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.
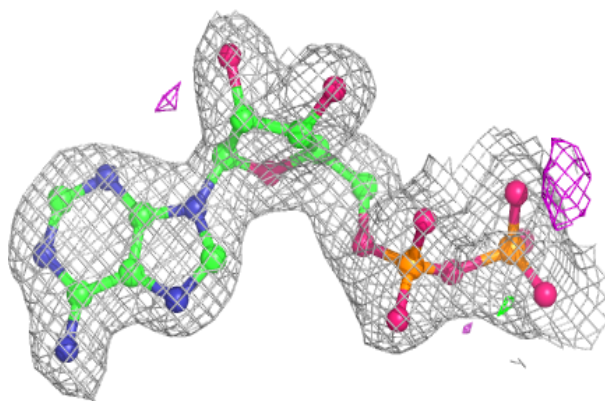
Electron density around ADP G 2072:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
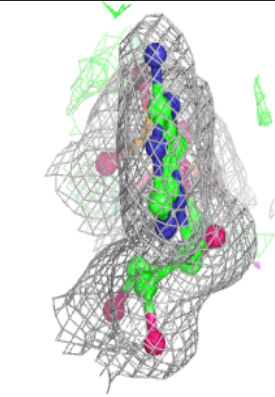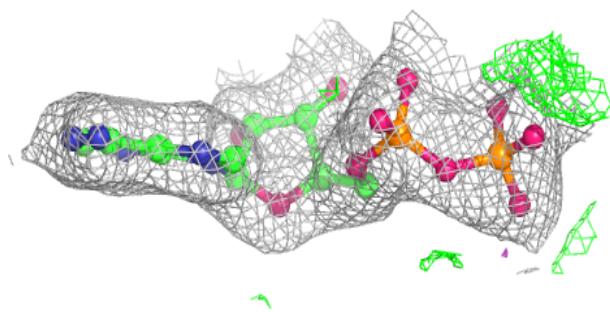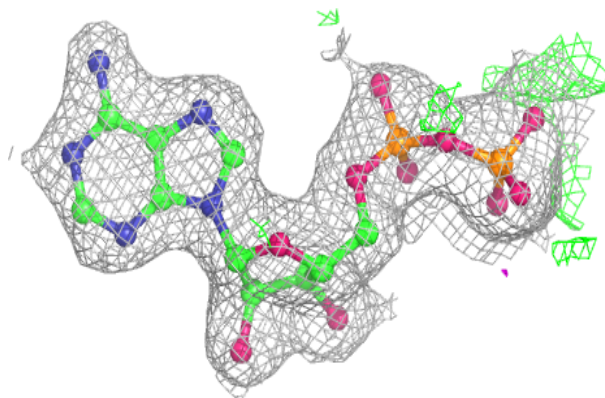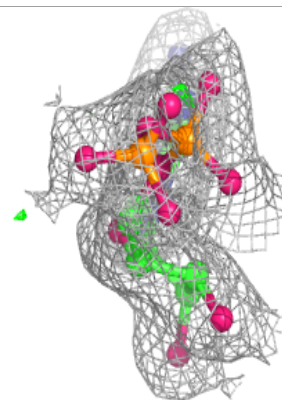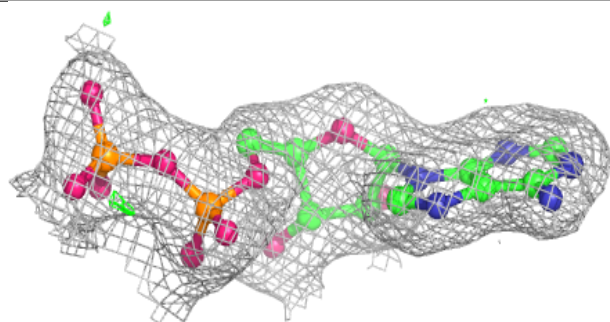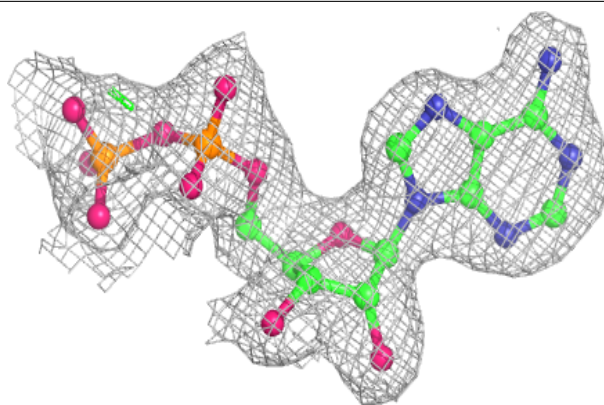mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
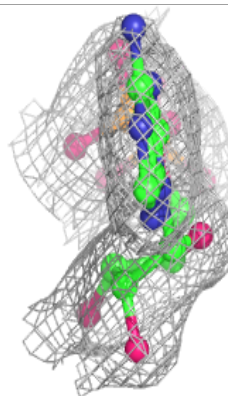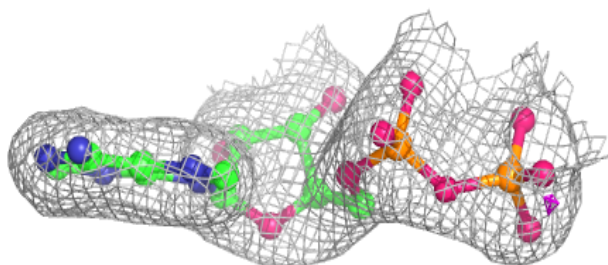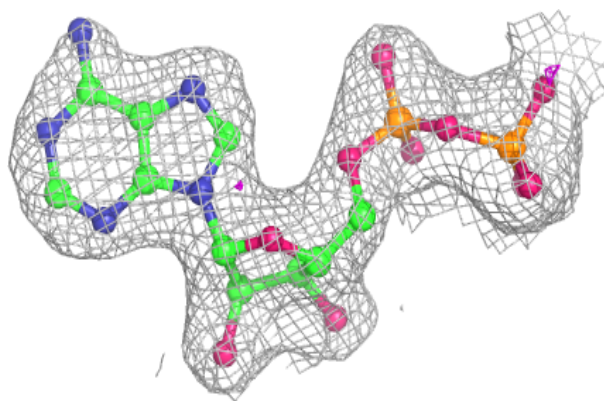
Electron density around ADP C 2029:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
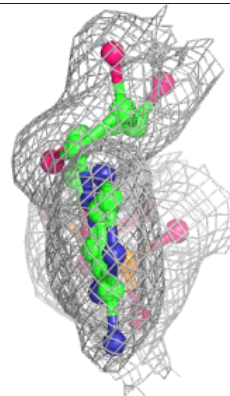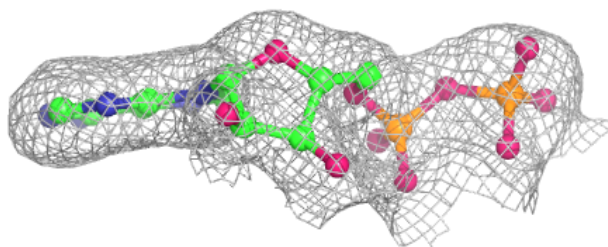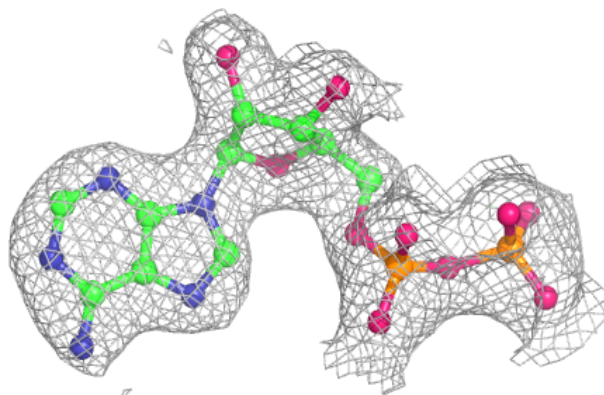
Electron density around ADP E 2051:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
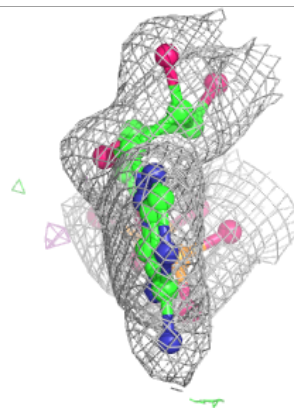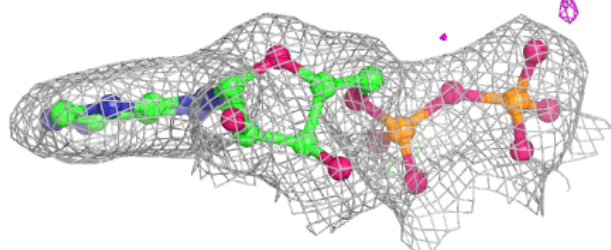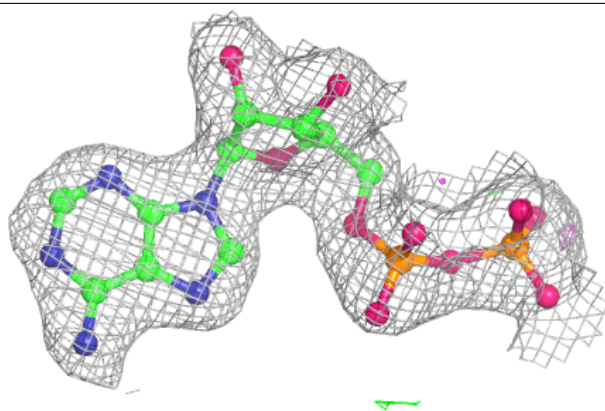
Electron density around ADP G 2066:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
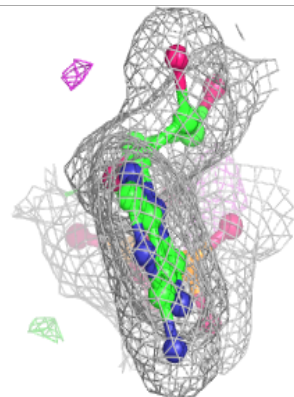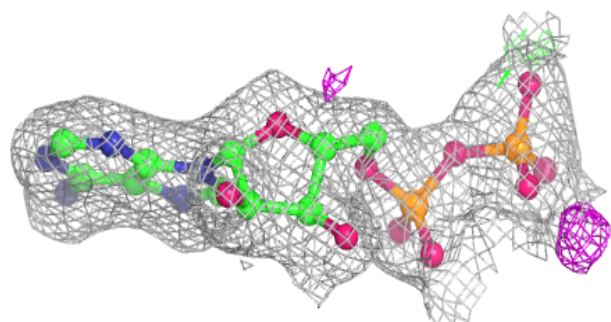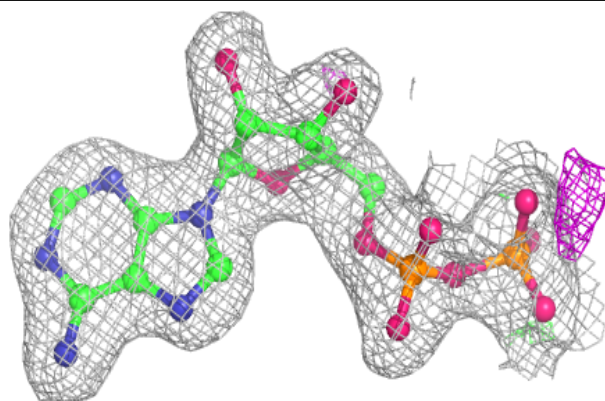
Electron density around ADP A 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
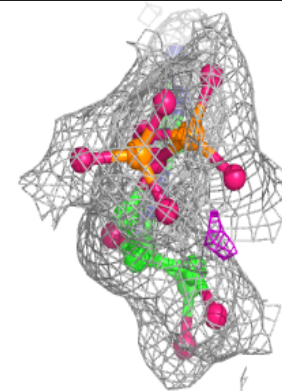mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
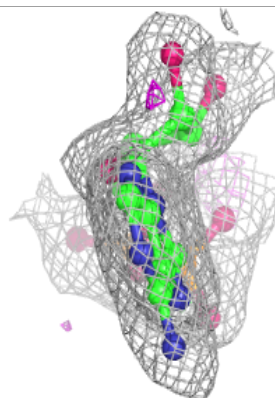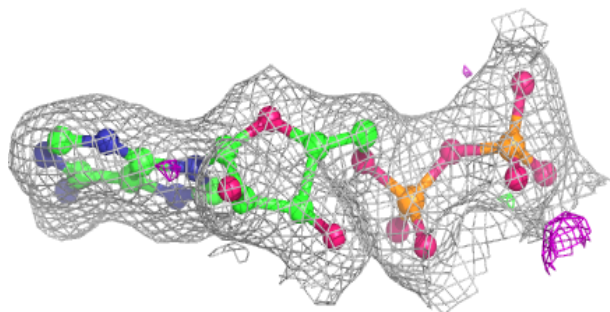
Electron density around ADP A 2007:

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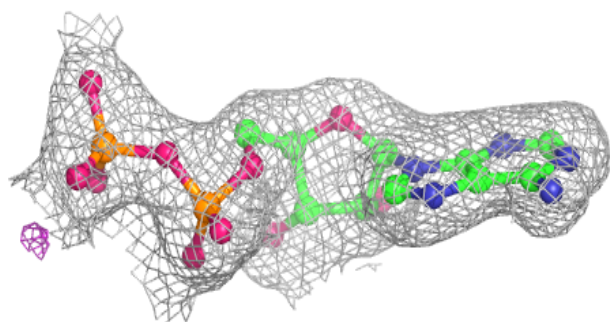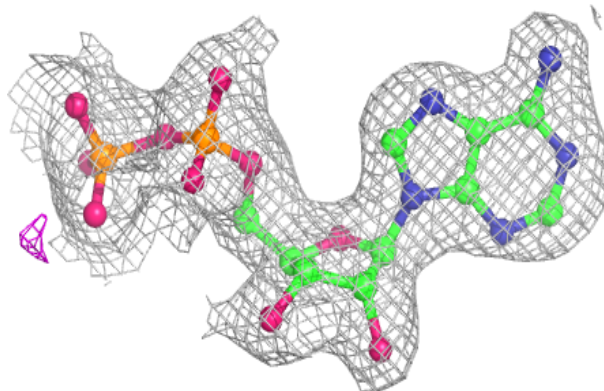mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ADP C 2023:

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

Electron density around ADP E 2045:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.