WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 01:41 AM EST

PDB ID	:	3UK6
Title	:	Crystal Structure of the Tip48 (Tip49b) hexamer
Authors	:	Petukhov, M.; Dagkessamanskaja, A.; Bommer, M.; Barrett, T.; Tsaneva, I.; Yakimov, A.; Queval, R.; Shvetsov, A.; Khodorkovskiy, M.; Kas, E.; Grigoriev, M.
Deposited on	:	2011-11-09
Resolution	:	2.95 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 (i) 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 (i)) 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	:	2.36
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)	:	2.36

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 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
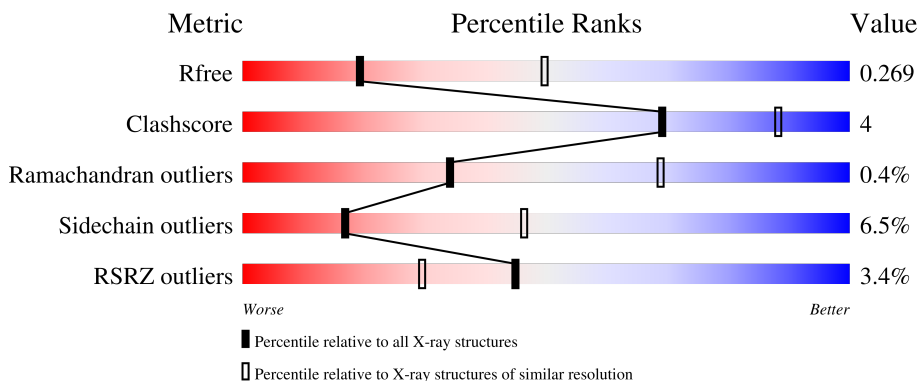
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	368	73% 7% · 19%
1	B	368	.% 72% 8% · 18%
1	C	368	78% 8% · 13%
1	D	368	.% 72% 8% · 19%

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Mol	Chain	Length	Quality of chain
1	E	368	% 70% 9% 21%
1	F	368	% 73% 7% 18%
1	G	368	2% 80% 10% 10%
1	H	368	4% 70% 5% 25%
1	I	368	3% 73% 6% 20%
1	J	368	2% 75% 7% 18%
1	K	368	12% 71% 5% 23%
1	L	368	5% 59% 37%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 22870 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 RuvB-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			1944	1211	345	379	9			
1	B	300	Total	C	N	O	S	0	0	0
			1962	1228	350	377	7			
1	C	321	Total	C	N	O	S	0	0	0
			2117	1324	372	412	9			
1	D	299	Total	C	N	O	S	0	0	0
			1932	1211	341	371	9			
1	E	290	Total	C	N	O	S	0	0	0
			1886	1178	331	368	9			
1	F	301	Total	C	N	O	S	0	0	0
			1964	1232	346	377	9			
1	G	330	Total	C	N	O	S	0	0	0
			2182	1368	387	417	10			
1	H	277	Total	C	N	O	S	0	0	0
			1731	1083	304	339	5			
1	I	294	Total	C	N	O	S	0	0	0
			1829	1140	323	359	7			
1	J	300	Total	C	N	O	S	0	0	0
			1857	1155	337	360	5			
1	K	283	Total	C	N	O	S	0	0	0
			1752	1089	310	351	2			
1	L	233	Total	C	N	O	S	0	0	0
			1392	868	246	274	4			

There are 131 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	-	expression tag	UNP Q9Y230
A	237	GLY	-	expression tag	UNP Q9Y230
A	238	ALA	-	expression tag	UNP Q9Y230
A	464	LEU	-	expression tag	UNP Q9Y230
A	465	GLU	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
A	466	HIS	-	expression tag	UNP Q9Y230
A	467	HIS	-	expression tag	UNP Q9Y230
A	468	HIS	-	expression tag	UNP Q9Y230
A	469	HIS	-	expression tag	UNP Q9Y230
A	470	HIS	-	expression tag	UNP Q9Y230
A	471	HIS	-	expression tag	UNP Q9Y230
B	236	ALA	-	expression tag	UNP Q9Y230
B	237	GLY	-	expression tag	UNP Q9Y230
B	238	ALA	-	expression tag	UNP Q9Y230
B	464	LEU	-	expression tag	UNP Q9Y230
B	465	GLU	-	expression tag	UNP Q9Y230
B	466	HIS	-	expression tag	UNP Q9Y230
B	467	HIS	-	expression tag	UNP Q9Y230
B	468	HIS	-	expression tag	UNP Q9Y230
B	469	HIS	-	expression tag	UNP Q9Y230
B	470	HIS	-	expression tag	UNP Q9Y230
B	471	HIS	-	expression tag	UNP Q9Y230
C	236	ALA	-	expression tag	UNP Q9Y230
C	237	GLY	-	expression tag	UNP Q9Y230
C	238	ALA	-	expression tag	UNP Q9Y230
C	465	GLU	-	expression tag	UNP Q9Y230
C	466	HIS	-	expression tag	UNP Q9Y230
C	467	HIS	-	expression tag	UNP Q9Y230
C	468	HIS	-	expression tag	UNP Q9Y230
C	469	HIS	-	expression tag	UNP Q9Y230
C	470	HIS	-	expression tag	UNP Q9Y230
C	471	HIS	-	expression tag	UNP Q9Y230
D	236	ALA	-	expression tag	UNP Q9Y230
D	237	GLY	-	expression tag	UNP Q9Y230
D	238	ALA	-	expression tag	UNP Q9Y230
D	464	LEU	-	expression tag	UNP Q9Y230
D	465	GLU	-	expression tag	UNP Q9Y230
D	466	HIS	-	expression tag	UNP Q9Y230
D	467	HIS	-	expression tag	UNP Q9Y230
D	468	HIS	-	expression tag	UNP Q9Y230
D	469	HIS	-	expression tag	UNP Q9Y230
D	470	HIS	-	expression tag	UNP Q9Y230
D	471	HIS	-	expression tag	UNP Q9Y230
E	236	ALA	-	expression tag	UNP Q9Y230
E	237	GLY	-	expression tag	UNP Q9Y230
E	238	ALA	-	expression tag	UNP Q9Y230
E	464	LEU	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
E	465	GLU	-	expression tag	UNP Q9Y230
E	466	HIS	-	expression tag	UNP Q9Y230
E	467	HIS	-	expression tag	UNP Q9Y230
E	468	HIS	-	expression tag	UNP Q9Y230
E	469	HIS	-	expression tag	UNP Q9Y230
E	470	HIS	-	expression tag	UNP Q9Y230
E	471	HIS	-	expression tag	UNP Q9Y230
F	236	ALA	-	expression tag	UNP Q9Y230
F	237	GLY	-	expression tag	UNP Q9Y230
F	238	ALA	-	expression tag	UNP Q9Y230
F	464	LEU	-	expression tag	UNP Q9Y230
F	465	GLU	-	expression tag	UNP Q9Y230
F	466	HIS	-	expression tag	UNP Q9Y230
F	467	HIS	-	expression tag	UNP Q9Y230
F	468	HIS	-	expression tag	UNP Q9Y230
F	469	HIS	-	expression tag	UNP Q9Y230
F	470	HIS	-	expression tag	UNP Q9Y230
F	471	HIS	-	expression tag	UNP Q9Y230
G	236	ALA	-	expression tag	UNP Q9Y230
G	237	GLY	-	expression tag	UNP Q9Y230
G	238	ALA	-	expression tag	UNP Q9Y230
G	464	LEU	-	expression tag	UNP Q9Y230
G	465	GLU	-	expression tag	UNP Q9Y230
G	466	HIS	-	expression tag	UNP Q9Y230
G	467	HIS	-	expression tag	UNP Q9Y230
G	468	HIS	-	expression tag	UNP Q9Y230
G	469	HIS	-	expression tag	UNP Q9Y230
G	470	HIS	-	expression tag	UNP Q9Y230
G	471	HIS	-	expression tag	UNP Q9Y230
H	236	ALA	-	expression tag	UNP Q9Y230
H	237	GLY	-	expression tag	UNP Q9Y230
H	238	ALA	-	expression tag	UNP Q9Y230
H	464	LEU	-	expression tag	UNP Q9Y230
H	465	GLU	-	expression tag	UNP Q9Y230
H	466	HIS	-	expression tag	UNP Q9Y230
H	467	HIS	-	expression tag	UNP Q9Y230
H	468	HIS	-	expression tag	UNP Q9Y230
H	469	HIS	-	expression tag	UNP Q9Y230
H	470	HIS	-	expression tag	UNP Q9Y230
H	471	HIS	-	expression tag	UNP Q9Y230
I	236	ALA	-	expression tag	UNP Q9Y230
I	237	GLY	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
I	238	ALA	-	expression tag	UNP Q9Y230
I	464	LEU	-	expression tag	UNP Q9Y230
I	465	GLU	-	expression tag	UNP Q9Y230
I	466	HIS	-	expression tag	UNP Q9Y230
I	467	HIS	-	expression tag	UNP Q9Y230
I	468	HIS	-	expression tag	UNP Q9Y230
I	469	HIS	-	expression tag	UNP Q9Y230
I	470	HIS	-	expression tag	UNP Q9Y230
I	471	HIS	-	expression tag	UNP Q9Y230
J	236	ALA	-	expression tag	UNP Q9Y230
J	237	GLY	-	expression tag	UNP Q9Y230
J	238	ALA	-	expression tag	UNP Q9Y230
J	464	LEU	-	expression tag	UNP Q9Y230
J	465	GLU	-	expression tag	UNP Q9Y230
J	466	HIS	-	expression tag	UNP Q9Y230
J	467	HIS	-	expression tag	UNP Q9Y230
J	468	HIS	-	expression tag	UNP Q9Y230
J	469	HIS	-	expression tag	UNP Q9Y230
J	470	HIS	-	expression tag	UNP Q9Y230
J	471	HIS	-	expression tag	UNP Q9Y230
K	236	ALA	-	expression tag	UNP Q9Y230
K	237	GLY	-	expression tag	UNP Q9Y230
K	238	ALA	-	expression tag	UNP Q9Y230
K	464	LEU	-	expression tag	UNP Q9Y230
K	465	GLU	-	expression tag	UNP Q9Y230
K	466	HIS	-	expression tag	UNP Q9Y230
K	467	HIS	-	expression tag	UNP Q9Y230
K	468	HIS	-	expression tag	UNP Q9Y230
K	469	HIS	-	expression tag	UNP Q9Y230
K	470	HIS	-	expression tag	UNP Q9Y230
K	471	HIS	-	expression tag	UNP Q9Y230
L	236	ALA	-	expression tag	UNP Q9Y230
L	237	GLY	-	expression tag	UNP Q9Y230
L	238	ALA	-	expression tag	UNP Q9Y230
L	464	LEU	-	expression tag	UNP Q9Y230
L	465	GLU	-	expression tag	UNP Q9Y230
L	466	HIS	-	expression tag	UNP Q9Y230
L	467	HIS	-	expression tag	UNP Q9Y230
L	468	HIS	-	expression tag	UNP Q9Y230
L	469	HIS	-	expression tag	UNP Q9Y230
L	470	HIS	-	expression tag	UNP Q9Y230
L	471	HIS	-	expression tag	UNP Q9Y230

- Molecule 2 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	K	1	Total 25	C 9	N 5	O 9	P 2	0	0
2	L	1	Total 27	C 10	N 5	O 10	P 2	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.

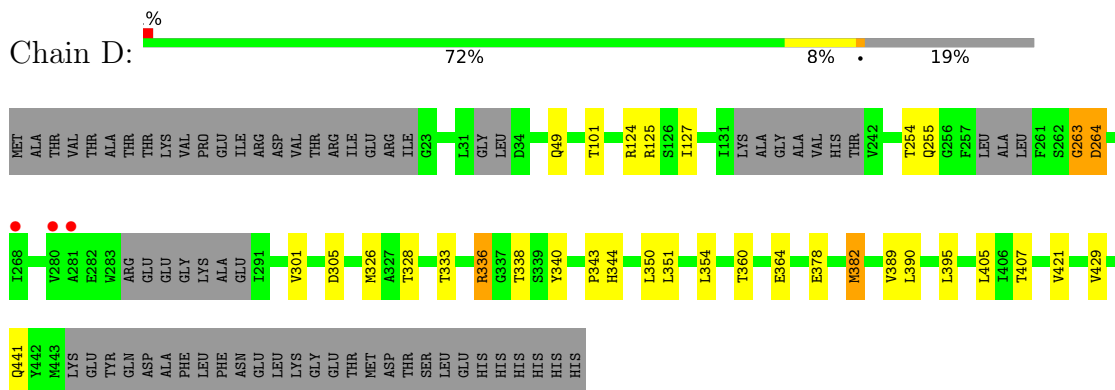• Molecule 1: RuvB-like 2

• Molecule 1: RuvB-like 2

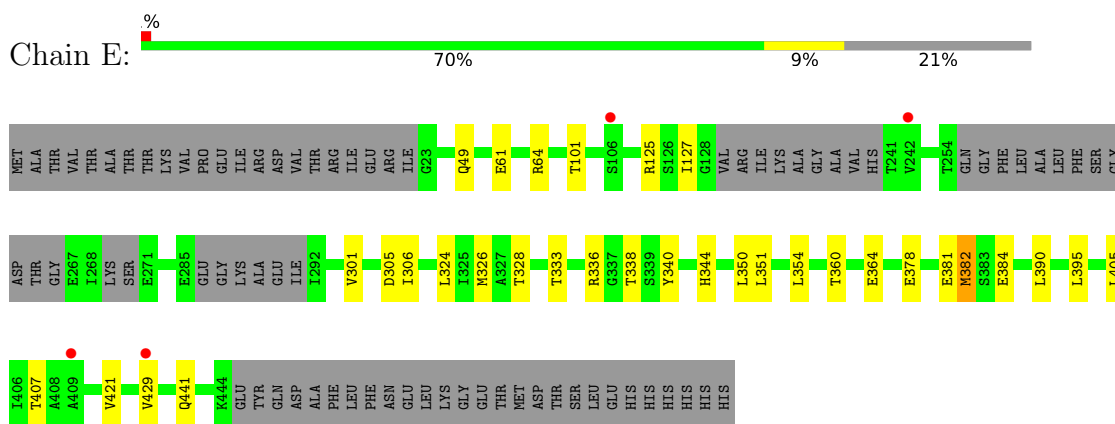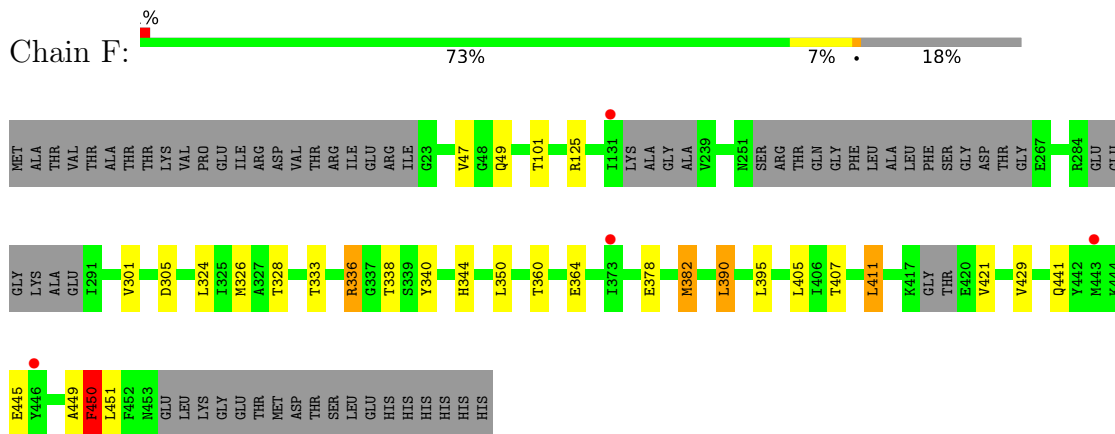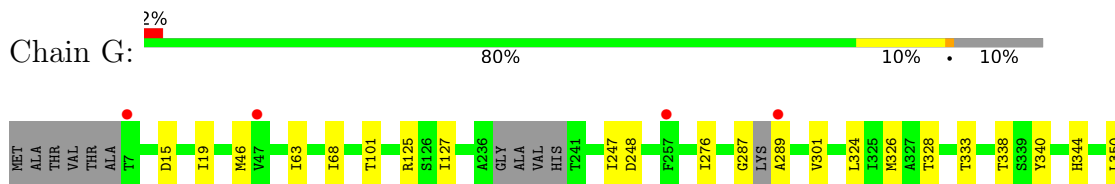• Molecule 1: RuvB-like 2

● Molecule 1: RuvB-like 2

Chain D:

● Molecule 1: RuvB-like 2

Chain E:

● Molecule 1: RuvB-like 2

Chain F:

● Molecule 1: RuvB-like 2

Chain G:

L351 L354 E364 E378 M382 A386 V389 L390 L395 L405 I406 T407 L411 V412 C413 R416 V421 V429 M443 K444 GLU TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP SER LEU GLU HIS HIS HIS HIS HIS HIS
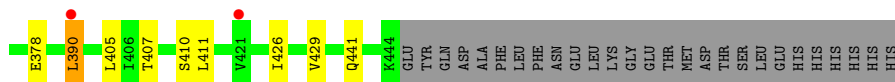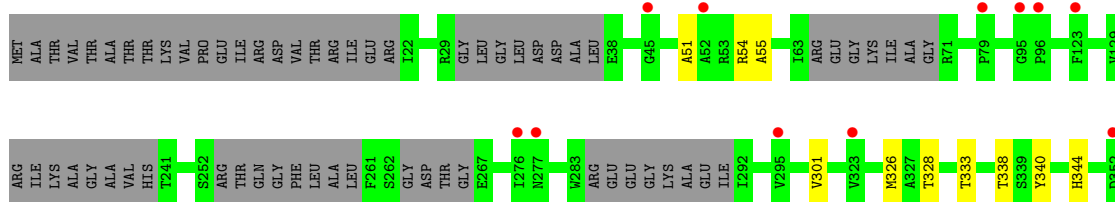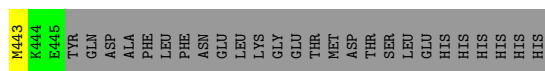
- Molecule 1: RuvB-like 2

Chain H:

4%
70%　5%　25%

MET ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG I22 R29 GLY LEU GLY LEU ASP ASP ALA LEU GLU E38 G45 A51 A52 R53 R54 A55 I63 ARG GLU GLY LYS ILE ALA GLY R71 P79 G95 P96 F123 V129

ARG ILE LYS ALA GLY ALA VAL VAL HIS T241 S252 ARG THR GLN GLY PHE LEU ALA LEU F261 S262 GLY ASP THR GLY E267 I276 N277 W283 ARG GLU GLY LYS ALA GLU ILE I292 V295 V301 V323 M326 A327 T328 T333 T338 S339 Y340 H344 D352

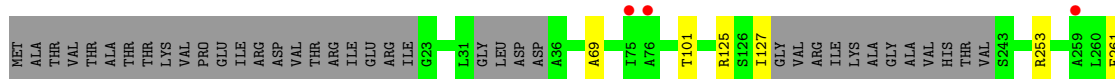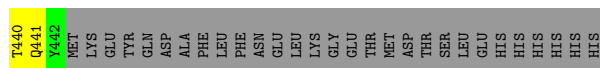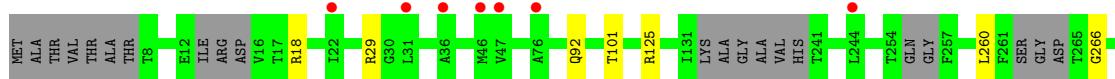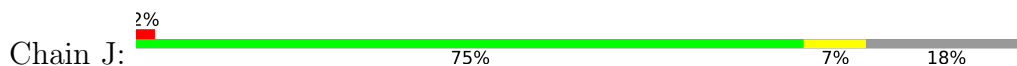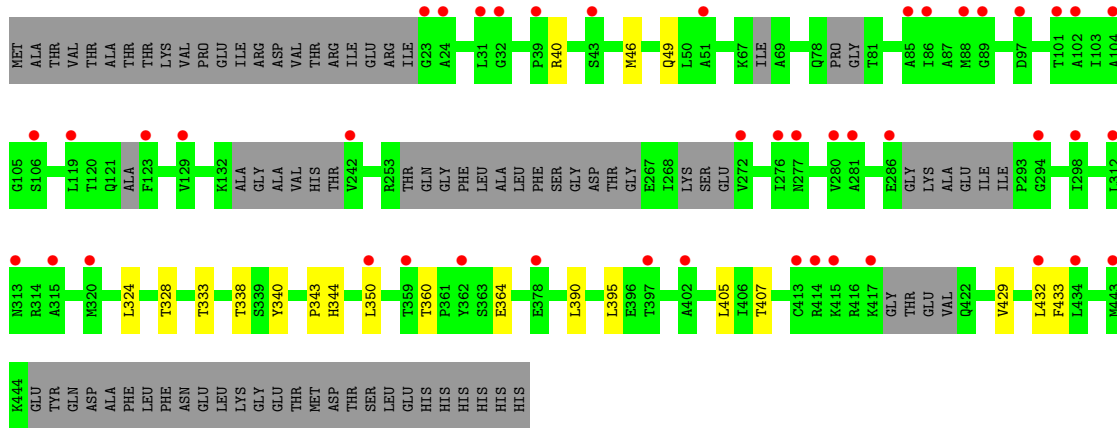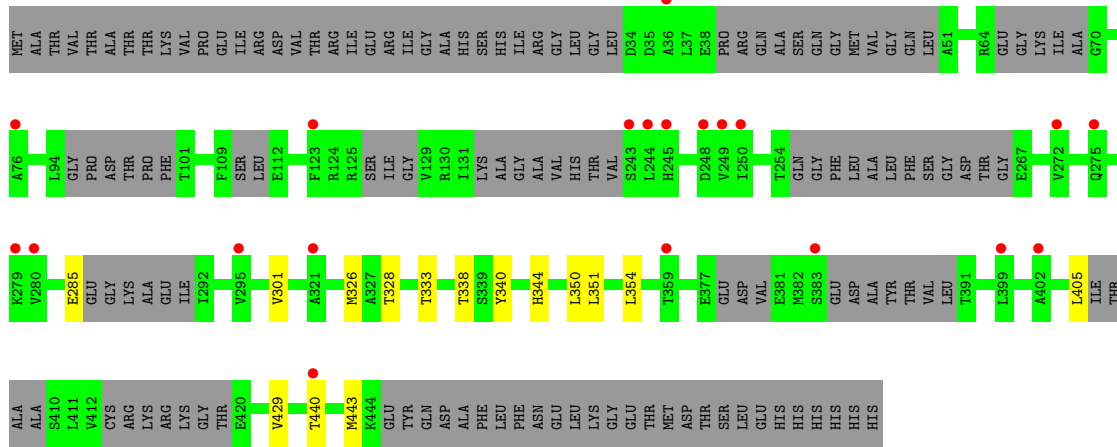E378 L390 L405 I406 T407 S410 L411 V421 I426 V429 Q441 K444 GLU TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP SER LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: RuvB-like 2

Chain I:

3%
73%　6% ·　20%

MET ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG ILE G23 L31 GLY LEU ASP ASP A36 A69 I75 A76 T101 R125 S126 I127 GLY VAL ARG ILE LYS ALA GLY ALA VAL HIS THR VAL S243 R253 A259 L260 F261

S262 G263 ASP THR G266 E267 V280 G287 LYS ALA GLU I291 V301 L324 I325 M326 A327 T328 T333 R334 I335 T338 S339 Y340 P343 H344 V357 Y362 E381 M382 D385 L390 T407 A408 V412 CYS ARG LYS ARG LYS G418 V421 T440

M443 K444 E445 TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP SER LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: RuvB-like 2

Chain J:

2%
75%　7%　18%

MET ALA THR VAL THR ALA THR T8 E12 ILE ARG ASP V16 T17 R18 I22 R29 G30 L31 A36 M46 V47 A76 Q92 T101 R125 I131 LYS ALA GLY ALA VAL HIS T241 L244 T254 GLN GLY F257 L260 F261 SER GLY ASP T265 G266

R284 GLU GLU GLY LYS ALA GLU I291 V301 D305 M326 A327 T328 T333 R336 G337 T338 S339 Y340 H344 L350 L351 L354 E364 D379 VAL GLU M382 Y387 L395 T407 R416 LYS GLY THR GLU VAL GLN VAL ASP ASP ILE K427 Y430

T440 Q441 Y442 MET LYS GLU TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP SER LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: RuvB-like 2

Chain K:

12%
71%　5%　23%

MET ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG ILE G23 A24 L31 G32 P39 R40 S43 M46 Q49 L50 A51 K67 ILE A69 Q78 PRO GLY T81 A85 I86 A87 M88 G89 D97 T101 A102 I103 A104

G105 S106 L119 T120 Q121 ALA F123 V129 K132 ALA GLY ALA VAL HIS THR V242 R253 THR GLN GLY PHE LEU ALA LEU PHE SER GLY ASP THR GLY E267 I268 LYS SER GLU V272 I276 N277 V280 A281 E286 GLY LYS ALA GLU ILE ILE P293 G294 I298 L312

N313 R314 A315 M320 L324 T328 T333 T338 S339 Y340 P343 H344 L350 T359 T360 P361 Y362 S363 E364 E378 L390 L395 E396 T397 A402 L405 I406 T407 C413 R414 K415 R416 K417 GLY THR GLU VAL Q422 V429 L432 F433 L434 M443

K444 GLU TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP THR SER LEU GLU HIS HIS HIS HIS HIS HIS

● Molecule 1: RuvB-like 2

Chain L:

5%

59%   ·   37%

MET ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG ILE GLY ALA HIS SER HIS ILE ARG GLY LEU GLY LEU D34 D35 A36 L37 E38 PRO ARG GLN ALA SER GLN GLY MET VAL GLY GLN LEU A51 R64 GLU GLY LYS ILE ALA G70

A76 L94 GLY PRO ASP THR PRO PHE T101 F109 SER LEU E112 F123 R124 R125 SER ILE GLY V129 R130 I131 LYS ALA GLY ALA VAL HIS THR VAL S243 L244 H245 D248 V249 I250 T254 GLN GLY PHE LEU ALA LEU PHE SER GLY ASP THR GLY E267 V272 Q275

K279 V280 E285 GLU GLY LYS ALA GLU ILE I292 V295 V301 A321 M326 A327 T328 T333 T338 S339 Y340 H344 L350 L351 L354 T359 E377 GLU ASP VAL E381 M382 S383 GLU ASP ALA TYR THR VAL LEU T391 L399 A402 L405 ILE THR

ALA ALA S410 L411 V412 CYS ARG LYS ARG LYS GLY THR E420 V429 T440 M443 K444 GLU TYR GLN ASP ALA PHE LEU PHE ASN GLU LEU LYS GLY GLU THR MET ASP THR SER LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.07Å 186.28Å 129.86Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	43.19 – 2.95 59.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.19-2.95) 97.1 (59.49-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.241 , 0.264 0.268 , 0.269	Depositor DCC
R_{free} test set	5179 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	80.1	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 118.3	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	0.90	EDS
Total number of atoms	22870	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.50	0/1965	0.65	0/2683
1	B	0.52	0/1985	0.70	1/2713 (0.0%)
1	C	0.54	0/2145	0.69	0/2934
1	D	0.50	0/1954	0.70	1/2671 (0.0%)
1	E	0.51	0/1907	0.67	0/2607
1	F	0.55	0/1986	0.70	0/2716
1	G	0.51	0/2210	0.70	0/3022
1	H	0.48	0/1750	0.63	0/2402
1	I	0.52	0/1850	0.71	2/2534 (0.1%)
1	J	0.50	0/1876	0.66	0/2571
1	K	0.50	0/1767	0.66	0/2426
1	L	0.49	0/1393	0.65	0/1907
All	All	0.51	0/22788	0.68	4/31186 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	69	ALA	C-N-CA	7.31	137.65	122.30
1	D	263	GLY	C-N-CA	5.89	136.43	121.70
1	B	265	THR	C-N-CA	5.41	133.66	122.30
1	I	381	GLU	N-CA-CB	5.33	120.20	110.60

There are no chirality outliers.

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	1944	0	1658	14	0
1	B	1962	0	1688	20	0
1	C	2117	0	1803	16	0
1	D	1932	0	1649	17	0
1	E	1886	0	1610	13	0
1	F	1964	0	1695	18	0
1	G	2182	0	1901	18	0
1	H	1731	0	1380	10	0
1	I	1829	0	1451	12	0
1	J	1857	0	1451	12	0
1	K	1752	0	1353	12	0
1	L	1392	0	1052	8	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
2	K	25	0	9	0	0
2	L	27	0	12	0	0
All	All	22870	0	18832	154	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 4.

All (154) 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:I:101:THR:HG21	1:I:125:ARG:HB3	1.58	0.83
1:A:101:THR:HG21	1:A:125:ARG:HB3	1.61	0.81
1:J:101:THR:HG21	1:J:125:ARG:HB3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:THR:HG21	1:E:125:ARG:HB3	1.61	0.80
1:G:101:THR:HG21	1:G:125:ARG:HB3	1.62	0.80
1:B:101:THR:HG21	1:B:125:ARG:HB3	1.63	0.80
1:F:101:THR:HG21	1:F:125:ARG:HB3	1.62	0.80
1:C:101:THR:HG21	1:C:125:ARG:HB3	1.63	0.80
1:D:101:THR:HG21	1:D:125:ARG:HB3	1.65	0.77
1:D:389:VAL:HG11	1:F:451:LEU:HD23	1.69	0.74
1:A:382:MET:HG3	1:A:421:VAL:HB	1.74	0.70
1:E:382:MET:HG3	1:E:421:VAL:HB	1.74	0.70
1:B:263:GLY:H	1:B:264:ASP:HB3	1.57	0.69
1:C:382:MET:HG3	1:C:421:VAL:HB	1.76	0.68
1:F:382:MET:HG3	1:F:421:VAL:HB	1.75	0.67
1:B:382:MET:HG3	1:B:421:VAL:HB	1.76	0.67
1:I:382:MET:HG3	1:I:421:VAL:HB	1.77	0.66
1:H:328:THR:HG21	1:H:344:HIS:HB3	1.77	0.66
1:A:328:THR:HG21	1:A:344:HIS:HB3	1.78	0.65
1:J:328:THR:HG21	1:J:344:HIS:HB3	1.78	0.65
1:D:328:THR:HG21	1:D:344:HIS:HB3	1.77	0.65
1:G:382:MET:HG3	1:G:421:VAL:HB	1.78	0.64
1:L:328:THR:HG21	1:L:344:HIS:HB3	1.79	0.64
1:D:382:MET:HG3	1:D:421:VAL:HB	1.78	0.64
1:G:248:ASP:HA	1:G:276:ILE:HD13	1.80	0.63
1:K:328:THR:HG21	1:K:344:HIS:HB3	1.78	0.63
1:G:328:THR:HG21	1:G:344:HIS:HB3	1.80	0.62
1:B:328:THR:HG21	1:B:344:HIS:HB3	1.80	0.62
1:F:328:THR:HG21	1:F:344:HIS:HB3	1.81	0.62
1:E:328:THR:HG21	1:E:344:HIS:HB3	1.80	0.62
1:F:338:THR:CG2	1:F:340:TYR:H	2.14	0.61
1:C:328:THR:HG21	1:C:344:HIS:HB3	1.81	0.61
1:A:338:THR:CG2	1:A:340:TYR:H	2.14	0.61
1:I:338:THR:CG2	1:I:340:TYR:H	2.14	0.60
1:J:338:THR:CG2	1:J:340:TYR:H	2.15	0.60
1:L:338:THR:CG2	1:L:340:TYR:H	2.15	0.60
1:C:338:THR:CG2	1:C:340:TYR:H	2.15	0.60
1:D:338:THR:CG2	1:D:340:TYR:H	2.14	0.60
1:K:405:LEU:HD22	1:K:429:VAL:HG13	1.84	0.60
1:B:338:THR:CG2	1:B:340:TYR:H	2.16	0.59
1:D:389:VAL:CG1	1:F:451:LEU:HD23	2.33	0.59
1:E:338:THR:CG2	1:E:340:TYR:H	2.14	0.59
1:I:328:THR:HG21	1:I:344:HIS:HB3	1.83	0.58
1:K:343:PRO:HB3	1:L:440:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD22	1:A:429:VAL:HG13	1.86	0.58
1:G:338:THR:CG2	1:G:340:TYR:H	2.17	0.58
1:K:338:THR:CG2	1:K:340:TYR:H	2.16	0.57
1:H:338:THR:CG2	1:H:340:TYR:H	2.17	0.56
1:B:62:MET:HG3	1:C:411:LEU:HD13	1.87	0.56
1:A:343:PRO:HB3	1:B:440:THR:CG2	2.37	0.55
1:B:405:LEU:HD22	1:B:429:VAL:HG13	1.89	0.55
1:E:61:GLU:CB	1:F:411:LEU:HD21	2.36	0.54
1:I:338:THR:HG22	1:I:340:TYR:H	1.72	0.54
1:E:405:LEU:HD22	1:E:429:VAL:HG13	1.90	0.54
1:G:247:ILE:HG22	1:G:276:ILE:HG12	1.88	0.54
1:K:49:GLN:HE22	1:K:360:THR:H	1.55	0.54
1:D:338:THR:HG22	1:D:340:TYR:H	1.73	0.54
1:D:263:GLY:HA3	1:D:264:ASP:CB	2.39	0.53
1:C:368:LYS:CB	1:C:391:THR:HG21	2.39	0.52
1:F:405:LEU:HD22	1:F:429:VAL:HG13	1.91	0.52
1:L:338:THR:HG22	1:L:340:TYR:H	1.75	0.52
1:C:49:GLN:HE22	1:C:360:THR:H	1.57	0.52
1:D:405:LEU:HD22	1:D:429:VAL:HG13	1.91	0.52
1:C:405:LEU:HD22	1:C:429:VAL:HG13	1.92	0.52
1:A:338:THR:HG22	1:A:340:TYR:H	1.75	0.51
1:F:338:THR:HG22	1:F:340:TYR:H	1.75	0.51
1:A:49:GLN:HE22	1:A:360:THR:H	1.56	0.51
1:J:338:THR:HG22	1:J:340:TYR:H	1.76	0.51
1:L:405:LEU:HD22	1:L:429:VAL:HG13	1.92	0.51
1:B:338:THR:HG22	1:B:340:TYR:H	1.75	0.51
1:A:61:GLU:CB	1:B:411:LEU:HD21	2.41	0.51
1:H:405:LEU:HD22	1:H:429:VAL:HG13	1.92	0.50
1:C:368:LYS:HA	1:C:391:THR:CG2	2.41	0.50
1:J:29:ARG:HA	1:J:92:GLN:HE21	1.76	0.50
1:K:338:THR:HG22	1:K:340:TYR:H	1.75	0.50
1:E:338:THR:HG23	1:E:340:TYR:H	1.75	0.50
1:E:49:GLN:HE22	1:E:360:THR:H	1.59	0.50
1:F:301:VAL:HG21	1:F:326:MET:CE	2.42	0.50
1:G:19:ILE:H	1:G:19:ILE:HD12	1.77	0.50
1:I:381:GLU:CD	1:I:382:MET:H	2.16	0.49
1:A:124:ARG:HD2	1:B:261:PHE:O	2.13	0.49
1:H:54:ARG:HH11	1:K:432:LEU:HD21	1.77	0.49
1:F:49:GLN:HE22	1:F:360:THR:H	1.60	0.49
1:I:343:PRO:HB3	1:J:440:THR:CG2	2.43	0.49
1:G:405:LEU:HD22	1:G:429:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:THR:HG22	1:H:340:TYR:H	1.75	0.49
1:C:338:THR:HG23	1:C:340:TYR:H	1.77	0.49
1:D:364:GLU:HA	1:D:395:LEU:HD11	1.95	0.49
1:B:301:VAL:HG21	1:B:326:MET:CE	2.43	0.48
1:C:351:LEU:HD23	1:C:354:LEU:HD12	1.96	0.48
1:G:338:THR:HG23	1:G:340:TYR:H	1.79	0.48
1:F:338:THR:HG23	1:F:340:TYR:H	1.79	0.47
1:J:364:GLU:HA	1:J:395:LEU:HD11	1.97	0.47
1:C:338:THR:HG22	1:C:340:TYR:H	1.79	0.47
1:D:49:GLN:HE22	1:D:360:THR:H	1.62	0.47
1:J:338:THR:HG23	1:J:340:TYR:H	1.80	0.46
1:E:301:VAL:HG21	1:E:326:MET:CE	2.45	0.46
1:H:390:LEU:HG	1:H:426:ILE:HD12	1.96	0.46
1:F:364:GLU:HA	1:F:395:LEU:HD11	1.98	0.46
1:L:338:THR:HG23	1:L:340:TYR:H	1.81	0.46
1:E:338:THR:HG22	1:E:340:TYR:H	1.79	0.46
1:D:343:PRO:HB3	1:I:440:THR:CG2	2.46	0.46
1:C:443:MET:CE	1:C:443:MET:HA	2.46	0.46
1:A:338:THR:HG23	1:A:340:TYR:H	1.80	0.45
1:G:338:THR:HG22	1:G:340:TYR:H	1.82	0.45
1:J:351:LEU:HD23	1:J:354:LEU:HD12	1.99	0.45
1:K:364:GLU:HA	1:K:395:LEU:HD11	1.98	0.45
1:B:49:GLN:HE22	1:B:360:THR:H	1.64	0.45
1:B:343:PRO:HB2	1:B:351:LEU:HD11	1.99	0.45
1:G:287:GLY:O	1:G:289:ALA:N	2.50	0.45
1:J:305:ASP:HA	1:J:336:ARG:HB2	1.98	0.45
1:L:351:LEU:HD23	1:L:354:LEU:HD12	1.99	0.45
1:E:364:GLU:HA	1:E:395:LEU:HD11	1.99	0.44
1:C:301:VAL:HG21	1:C:326:MET:CE	2.47	0.44
1:F:450:PHE:CD1	1:F:450:PHE:C	2.90	0.44
1:I:301:VAL:HG21	1:I:326:MET:CE	2.48	0.44
1:C:364:GLU:HA	1:C:395:LEU:HD11	1.99	0.44
1:E:305:ASP:HA	1:E:336:ARG:HB2	1.99	0.44
1:B:338:THR:HG23	1:B:340:TYR:H	1.83	0.44
1:L:301:VAL:HG21	1:L:326:MET:CE	2.48	0.43
1:A:443:MET:CE	1:A:443:MET:HA	2.48	0.43
1:D:351:LEU:HD23	1:D:354:LEU:HD12	2.00	0.43
1:G:301:VAL:HG21	1:G:326:MET:CE	2.48	0.43
1:B:305:ASP:HA	1:B:336:ARG:HB2	2.01	0.43
1:I:338:THR:HG23	1:I:340:TYR:H	1.83	0.43
1:D:305:ASP:HA	1:D:336:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:LEU:HD23	1:G:354:LEU:HD12	2.00	0.43
1:G:364:GLU:HA	1:G:395:LEU:HD11	2.00	0.43
1:I:335:ILE:O	1:I:338:THR:HB	2.19	0.43
1:A:364:GLU:HA	1:A:395:LEU:HD11	2.01	0.43
1:G:63:ILE:HG12	1:G:68:ILE:HG21	2.01	0.43
1:H:54:ARG:HD2	1:K:432:LEU:HD21	2.01	0.42
1:G:248:ASP:HA	1:G:276:ILE:CD1	2.46	0.42
1:F:301:VAL:HG21	1:F:326:MET:HE2	2.00	0.42
1:F:305:ASP:HA	1:F:336:ARG:HB2	2.00	0.42
1:B:364:GLU:HA	1:B:395:LEU:HD11	2.01	0.42
1:D:124:ARG:HD2	1:I:261:PHE:O	2.19	0.42
1:J:301:VAL:HG21	1:J:326:MET:CE	2.49	0.42
1:B:74:LEU:HB2	1:B:354:LEU:HD13	2.02	0.41
1:F:47:VAL:O	2:F:1450:ADP:N6	2.53	0.41
1:G:19:ILE:HD12	1:G:19:ILE:N	2.35	0.41
1:H:55:ALA:HB1	1:K:433:PHE:CE2	2.55	0.41
1:A:301:VAL:HG21	1:A:326:MET:CE	2.50	0.41
1:H:301:VAL:HG21	1:H:326:MET:CE	2.50	0.41
1:K:338:THR:HG23	1:K:340:TYR:H	1.84	0.41
1:J:387:TYR:HD1	1:J:387:TYR:HA	1.70	0.41
1:B:343:PRO:HB3	1:C:440:THR:CG2	2.50	0.41
1:F:390:LEU:HD23	1:F:390:LEU:HA	1.91	0.41
1:G:413:CYS:O	1:G:416:ARG:HG3	2.20	0.41
1:D:301:VAL:HG21	1:D:326:MET:CE	2.50	0.40
1:D:338:THR:HG23	1:D:340:TYR:H	1.81	0.40
1:E:351:LEU:HD23	1:E:354:LEU:HD12	2.02	0.40
1:H:51:ALA:O	1:K:432:LEU:HD22	2.22	0.40
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.92	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	288/368 (78%)	283 (98%)	5 (2%)	0	100	100
1	B	290/368 (79%)	280 (97%)	9 (3%)	1 (0%)	41	73
1	C	313/368 (85%)	304 (97%)	7 (2%)	2 (1%)	25	60
1	D	289/368 (78%)	278 (96%)	8 (3%)	3 (1%)	15	48
1	E	280/368 (76%)	275 (98%)	5 (2%)	0	100	100
1	F	291/368 (79%)	280 (96%)	8 (3%)	3 (1%)	15	48
1	G	324/368 (88%)	312 (96%)	12 (4%)	0	100	100
1	H	263/368 (72%)	259 (98%)	4 (2%)	0	100	100
1	I	282/368 (77%)	272 (96%)	9 (3%)	1 (0%)	34	69
1	J	284/368 (77%)	276 (97%)	6 (2%)	2 (1%)	22	56
1	K	265/368 (72%)	261 (98%)	4 (2%)	0	100	100
1	L	207/368 (56%)	203 (98%)	4 (2%)	0	100	100
All	All	3376/4416 (76%)	3283 (97%)	81 (2%)	12 (0%)	34	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
1	D	264	ASP
1	F	450	PHE
1	D	254	THR
1	F	445	GLU
1	J	266	GLY
1	I	253	ARG
1	C	254	THR
1	D	255	GLN
1	F	449	ALA
1	J	18	ARG
1	B	263	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	153/307 (50%)	143 (94%)	10 (6%)	17	46
1	B	155/307 (50%)	146 (94%)	9 (6%)	20	51
1	C	168/307 (55%)	156 (93%)	12 (7%)	14	43
1	D	150/307 (49%)	141 (94%)	9 (6%)	19	50
1	E	149/307 (48%)	136 (91%)	13 (9%)	10	33
1	F	156/307 (51%)	145 (93%)	11 (7%)	14	43
1	G	175/307 (57%)	162 (93%)	13 (7%)	13	41
1	H	122/307 (40%)	115 (94%)	7 (6%)	20	52
1	I	125/307 (41%)	117 (94%)	8 (6%)	17	47
1	J	122/307 (40%)	116 (95%)	6 (5%)	25	58
1	K	116/307 (38%)	109 (94%)	7 (6%)	19	50
1	L	84/307 (27%)	80 (95%)	4 (5%)	25	59
All	All	1675/3684 (46%)	1566 (94%)	109 (6%)	17	46

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	324	LEU
1	A	333	THR
1	A	350	LEU
1	A	382	MET
1	A	390	LEU
1	A	407	THR
1	A	411	LEU
1	A	441	GLN
1	A	443	MET
1	B	260	LEU
1	B	333	THR
1	B	336	ARG
1	B	350	LEU
1	B	378	GLU
1	B	382	MET
1	B	390	LEU
1	B	407	THR
1	B	411	LEU
1	C	17	THR
1	C	260	LEU
1	C	324	LEU

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Mol	Chain	Res	Type
1	C	333	THR
1	C	350	LEU
1	C	378	GLU
1	C	382	MET
1	C	390	LEU
1	C	407	THR
1	C	411	LEU
1	C	441	GLN
1	C	443	MET
1	D	127	ILE
1	D	333	THR
1	D	336	ARG
1	D	350	LEU
1	D	378	GLU
1	D	382	MET
1	D	390	LEU
1	D	407	THR
1	D	441	GLN
1	E	64	ARG
1	E	127	ILE
1	E	306	ILE
1	E	324	LEU
1	E	333	THR
1	E	350	LEU
1	E	378	GLU
1	E	381	GLU
1	E	382	MET
1	E	384	GLU
1	E	390	LEU
1	E	407	THR
1	E	441	GLN
1	F	324	LEU
1	F	333	THR
1	F	336	ARG
1	F	350	LEU
1	F	378	GLU
1	F	382	MET
1	F	390	LEU
1	F	407	THR
1	F	411	LEU
1	F	441	GLN
1	F	450	PHE

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Mol	Chain	Res	Type
1	G	15	ASP
1	G	46	MET
1	G	127	ILE
1	G	324	LEU
1	G	333	THR
1	G	350	LEU
1	G	378	GLU
1	G	382	MET
1	G	390	LEU
1	G	407	THR
1	G	411	LEU
1	G	416	ARG
1	G	443	MET
1	H	333	THR
1	H	378	GLU
1	H	390	LEU
1	H	407	THR
1	H	410	SER
1	H	411	LEU
1	H	441	GLN
1	I	127	ILE
1	I	267	GLU
1	I	324	LEU
1	I	333	THR
1	I	382	MET
1	I	390	LEU
1	I	407	THR
1	I	443	MET
1	J	260	LEU
1	J	333	THR
1	J	336	ARG
1	J	350	LEU
1	J	407	THR
1	J	441	GLN
1	K	40	ARG
1	K	46	MET
1	K	324	LEU
1	K	333	THR
1	K	350	LEU
1	K	390	LEU
1	K	407	THR
1	L	285	GLU

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Mol	Chain	Res	Type
1	L	333	THR
1	L	350	LEU
1	L	443	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	302	HIS
1	B	49	GLN
1	B	302	HIS
1	C	49	GLN
1	C	302	HIS
1	D	49	GLN
1	D	302	HIS
1	E	49	GLN
1	E	302	HIS
1	F	49	GLN
1	F	302	HIS
1	G	302	HIS
1	H	302	HIS
1	I	302	HIS
1	J	92	GLN
1	J	251	ASN
1	J	302	HIS
1	K	49	GLN
1	L	302	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands 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	ADP	D	1450	-	24,29,29	0.58	0	29,45,45	0.77	1 (3%)
2	ADP	E	1450	-	24,29,29	0.62	0	29,45,45	0.87	1 (3%)
2	ADP	G	1450	-	24,29,29	0.59	0	29,45,45	1.04	2 (6%)
2	ADP	K	1450	-	19,26,29	0.70	0	21,38,45	0.90	1 (4%)
2	ADP	H	1450	-	24,29,29	0.69	0	29,45,45	0.79	1 (3%)
2	ADP	L	1450	-	24,29,29	0.58	0	29,45,45	0.77	1 (3%)
2	ADP	B	1450	-	24,29,29	0.61	0	29,45,45	0.75	0
2	ADP	J	1450	-	24,29,29	0.65	0	29,45,45	0.80	1 (3%)
2	ADP	I	1450	-	24,29,29	0.60	0	29,45,45	0.78	1 (3%)
2	ADP	A	1450	-	24,29,29	0.61	0	29,45,45	0.75	1 (3%)
2	ADP	F	1450	-	24,29,29	0.65	0	29,45,45	0.79	0
2	ADP	C	1450	-	24,29,29	0.76	1 (4%)	29,45,45	0.77	1 (3%)

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	ADP	D	1450	-	-	4/12/32/32	0/3/3/3
2	ADP	E	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	G	1450	-	-	4/12/32/32	0/3/3/3
2	ADP	K	1450	-	-	0/2/22/32	0/3/3/3
2	ADP	H	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	L	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	J	1450	-	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	I	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1450	-	-	3/12/32/32	0/3/3/3
2	ADP	F	1450	-	-	4/12/32/32	0/3/3/3
2	ADP	C	1450	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1450	ADP	PB-O1B	2.10	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1450	ADP	PA-O3A-PB	-3.16	121.99	132.83
2	G	1450	ADP	C5-C6-N6	2.51	124.17	120.35
2	C	1450	ADP	C5-C6-N6	2.42	124.03	120.35
2	D	1450	ADP	C5-C6-N6	2.38	123.97	120.35
2	J	1450	ADP	C5-C6-N6	2.33	123.89	120.35
2	L	1450	ADP	C5-C6-N6	2.23	123.74	120.35
2	A	1450	ADP	C5-C6-N6	2.22	123.72	120.35
2	H	1450	ADP	C5-C6-N6	2.21	123.72	120.35
2	I	1450	ADP	C5-C6-N6	2.21	123.71	120.35
2	E	1450	ADP	C5-C6-N6	2.20	123.70	120.35
2	K	1450	ADP	C5-C6-N6	2.10	123.55	120.35

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1450	ADP	C5'-O5'-PA-O1A
2	A	1450	ADP	C5'-O5'-PA-O2A
2	B	1450	ADP	C5'-O5'-PA-O1A
2	B	1450	ADP	C5'-O5'-PA-O2A
2	C	1450	ADP	C5'-O5'-PA-O1A
2	C	1450	ADP	C5'-O5'-PA-O2A
2	D	1450	ADP	C5'-O5'-PA-O1A
2	D	1450	ADP	C5'-O5'-PA-O2A
2	E	1450	ADP	C5'-O5'-PA-O1A
2	E	1450	ADP	C5'-O5'-PA-O2A
2	F	1450	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	F	1450	ADP	C5'-O5'-PA-O2A
2	G	1450	ADP	C5'-O5'-PA-O1A
2	G	1450	ADP	C5'-O5'-PA-O2A
2	H	1450	ADP	C5'-O5'-PA-O2A
2	I	1450	ADP	C5'-O5'-PA-O1A
2	I	1450	ADP	C5'-O5'-PA-O2A
2	J	1450	ADP	PA-O3A-PB-O3B
2	J	1450	ADP	C5'-O5'-PA-O2A
2	L	1450	ADP	C5'-O5'-PA-O1A
2	L	1450	ADP	C5'-O5'-PA-O2A
2	J	1450	ADP	PA-O3A-PB-O2B
2	A	1450	ADP	C5'-O5'-PA-O3A
2	B	1450	ADP	C5'-O5'-PA-O3A
2	C	1450	ADP	C5'-O5'-PA-O3A
2	D	1450	ADP	C5'-O5'-PA-O3A
2	E	1450	ADP	C5'-O5'-PA-O3A
2	F	1450	ADP	C5'-O5'-PA-O3A
2	H	1450	ADP	C5'-O5'-PA-O3A
2	I	1450	ADP	C5'-O5'-PA-O3A
2	J	1450	ADP	C5'-O5'-PA-O3A
2	L	1450	ADP	C5'-O5'-PA-O3A
2	H	1450	ADP	C5'-O5'-PA-O1A
2	J	1450	ADP	C5'-O5'-PA-O1A
2	F	1450	ADP	PB-O3A-PA-O2A
2	J	1450	ADP	PA-O3A-PB-O1B
2	G	1450	ADP	C5'-O5'-PA-O3A
2	D	1450	ADP	PB-O3A-PA-O2A
2	G	1450	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1450	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 D 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP K 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP L 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP J 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP I 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 1450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 1450

Bond lengths

Bond angles

Torsions

Rings

5.7   Other polymers ⓘ

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(Å²)	Q<0.9
1	A	298/368 (80%)	-0.01	1 (0%)	94	87	53, 87, 127, 149	0
1	B	300/368 (81%)	-0.04	4 (1%)	77	61	46, 82, 118, 137	0
1	C	321/368 (87%)	-0.06	1 (0%)	94	87	46, 76, 104, 125	0
1	D	299/368 (81%)	0.10	3 (1%)	82	68	57, 90, 125, 143	0
1	E	290/368 (78%)	0.01	4 (1%)	75	59	49, 85, 140, 170	0
1	F	301/368 (81%)	0.02	4 (1%)	77	61	43, 77, 114, 147	0
1	G	330/368 (89%)	0.00	7 (2%)	63	46	46, 81, 121, 146	0
1	H	277/368 (75%)	0.25	13 (4%)	31	20	73, 112, 148, 173	0
1	I	294/368 (79%)	0.23	11 (3%)	41	27	58, 106, 139, 154	0
1	J	300/368 (81%)	0.07	8 (2%)	54	38	61, 105, 136, 155	0
1	K	283/368 (76%)	0.69	45 (15%)	1	1	75, 95, 117, 159	0
1	L	233/368 (63%)	0.38	20 (8%)	10	6	69, 123, 170, 185	0
All	All	3526/4416 (79%)	0.13	121 (3%)	45	29	43, 92, 137, 185	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	89	GLY	6.4
1	K	272	VAL	6.0
1	B	259	ALA	5.9
1	K	413	CYS	5.7
1	L	399	LEU	5.2
1	L	250	ILE	5.0
1	K	242	VAL	4.9
1	K	43	SER	4.8
1	K	51	ALA	4.5
1	L	295	VAL	4.4
1	L	36	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	280	VAL	4.1
1	K	86	ILE	4.1
1	K	402	ALA	4.1
1	L	243	SER	3.9
1	K	119	LEU	3.8
1	G	7	THR	3.7
1	K	415	LYS	3.7
1	K	104	ALA	3.6
1	L	402	ALA	3.5
1	H	421	VAL	3.4
1	H	52	ALA	3.4
1	K	106	SER	3.4
1	G	421	VAL	3.4
1	H	390	LEU	3.3
1	K	397	THR	3.1
1	K	313	ASN	3.1
1	K	276	ILE	3.1
1	L	249	VAL	3.1
1	D	268	ILE	3.1
1	L	440	THR	3.1
1	L	279	LYS	3.1
1	G	389	VAL	3.0
1	K	362	TYR	3.0
1	K	24	ALA	3.0
1	K	97	ASP	3.0
1	I	362	TYR	3.0
1	L	245	HIS	3.0
1	K	280	VAL	2.9
1	H	123	PHE	2.9
1	K	350	LEU	2.9
1	K	23	GLY	2.9
1	G	289	ALA	2.9
1	L	76	ALA	2.9
1	C	386	ALA	2.8
1	K	281	ALA	2.8
1	J	22	ILE	2.8
1	I	408	ALA	2.7
1	H	277	ASN	2.7
1	J	36	ALA	2.7
1	K	88	MET	2.7
1	H	352	ASP	2.7
1	L	280	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	106	SER	2.7
1	I	421	VAL	2.7
1	L	272	VAL	2.7
1	H	79	PRO	2.6
1	K	31	LEU	2.6
1	H	276	ILE	2.6
1	J	244	LEU	2.6
1	K	378	GLU	2.6
1	K	123	PHE	2.6
1	G	47	VAL	2.5
1	L	123	PHE	2.5
1	H	96	PRO	2.5
1	H	45	GLY	2.5
1	K	434	LEU	2.5
1	H	95	GLY	2.5
1	K	414	ARG	2.5
1	G	386	ALA	2.5
1	K	320	MET	2.5
1	B	42	ALA	2.5
1	G	257	PHE	2.5
1	K	315	ALA	2.5
1	F	443	MET	2.4
1	L	359	THR	2.4
1	K	101	THR	2.4
1	H	295	VAL	2.4
1	D	281	ALA	2.4
1	E	409	ALA	2.4
1	I	76	ALA	2.4
1	I	75	ILE	2.4
1	L	275	GLN	2.3
1	K	102	ALA	2.3
1	J	47	VAL	2.3
1	J	430	TYR	2.3
1	K	277	ASN	2.3
1	I	357	VAL	2.3
1	J	46	MET	2.3
1	K	432	LEU	2.3
1	K	443	MET	2.2
1	F	131	ILE	2.2
1	I	259	ALA	2.2
1	E	242	VAL	2.2
1	J	31	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	382	MET	2.2
1	K	129	VAL	2.2
1	I	263	GLY	2.2
1	L	321	ALA	2.2
1	B	409	ALA	2.1
1	K	312	LEU	2.1
1	K	298	ILE	2.1
1	K	417	LYS	2.1
1	F	446	TYR	2.1
1	L	383	SER	2.1
1	I	385	ASP	2.1
1	A	30	GLY	2.1
1	L	248	ASP	2.1
1	K	32	GLY	2.1
1	H	323	VAL	2.1
1	K	39	PRO	2.1
1	B	370	ILE	2.0
1	K	286	GLU	2.0
1	E	429	VAL	2.0
1	J	76	ALA	2.0
1	K	359	THR	2.0
1	D	280	VAL	2.0
1	F	373	ILE	2.0
1	K	85	ALA	2.0
1	K	294	GLY	2.0
1	L	244	LEU	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 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
2	ADP	K	1450	25/27	0.84	0.24	79,90,94,98	0
2	ADP	I	1450	27/27	0.86	0.30	110,126,135,137	0
2	ADP	L	1450	27/27	0.91	0.22	117,125,133,135	0
2	ADP	J	1450	27/27	0.93	0.19	92,113,131,133	0
2	ADP	F	1450	27/27	0.94	0.22	65,71,84,86	0
2	ADP	H	1450	27/27	0.94	0.22	94,102,116,118	0
2	ADP	C	1450	27/27	0.94	0.21	66,74,80,82	0
2	ADP	A	1450	27/27	0.95	0.18	73,78,83,84	0
2	ADP	G	1450	27/27	0.96	0.20	59,68,75,77	0
2	ADP	E	1450	27/27	0.96	0.18	74,83,88,89	0
2	ADP	B	1450	27/27	0.96	0.17	58,70,81,83	0
2	ADP	D	1450	27/27	0.97	0.19	73,78,94,101	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.
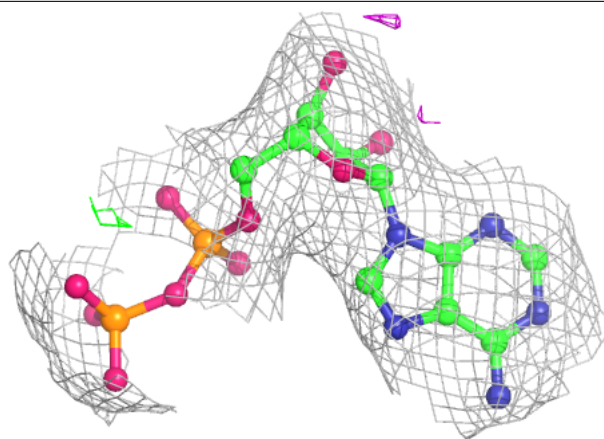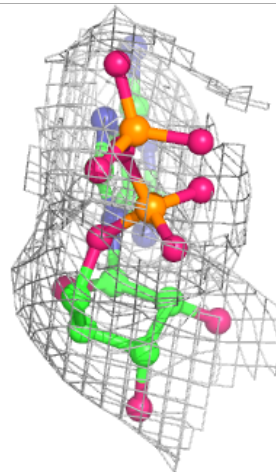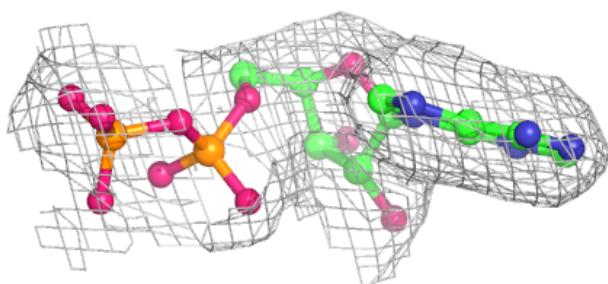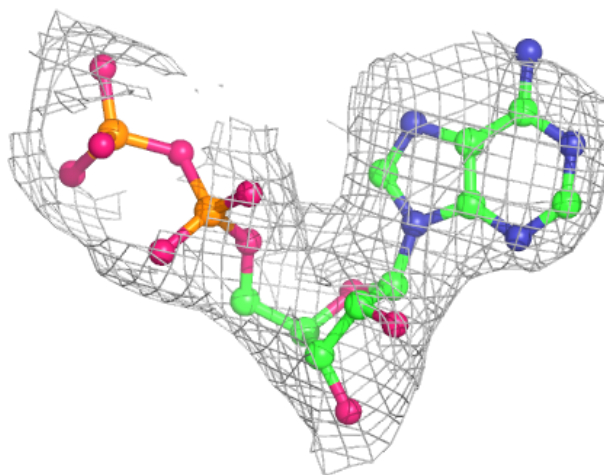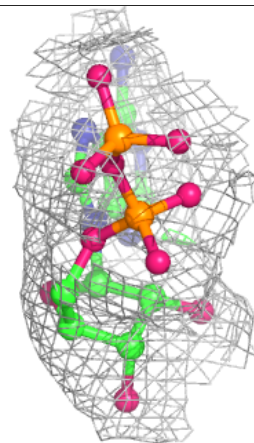

Electron density around ADP K 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
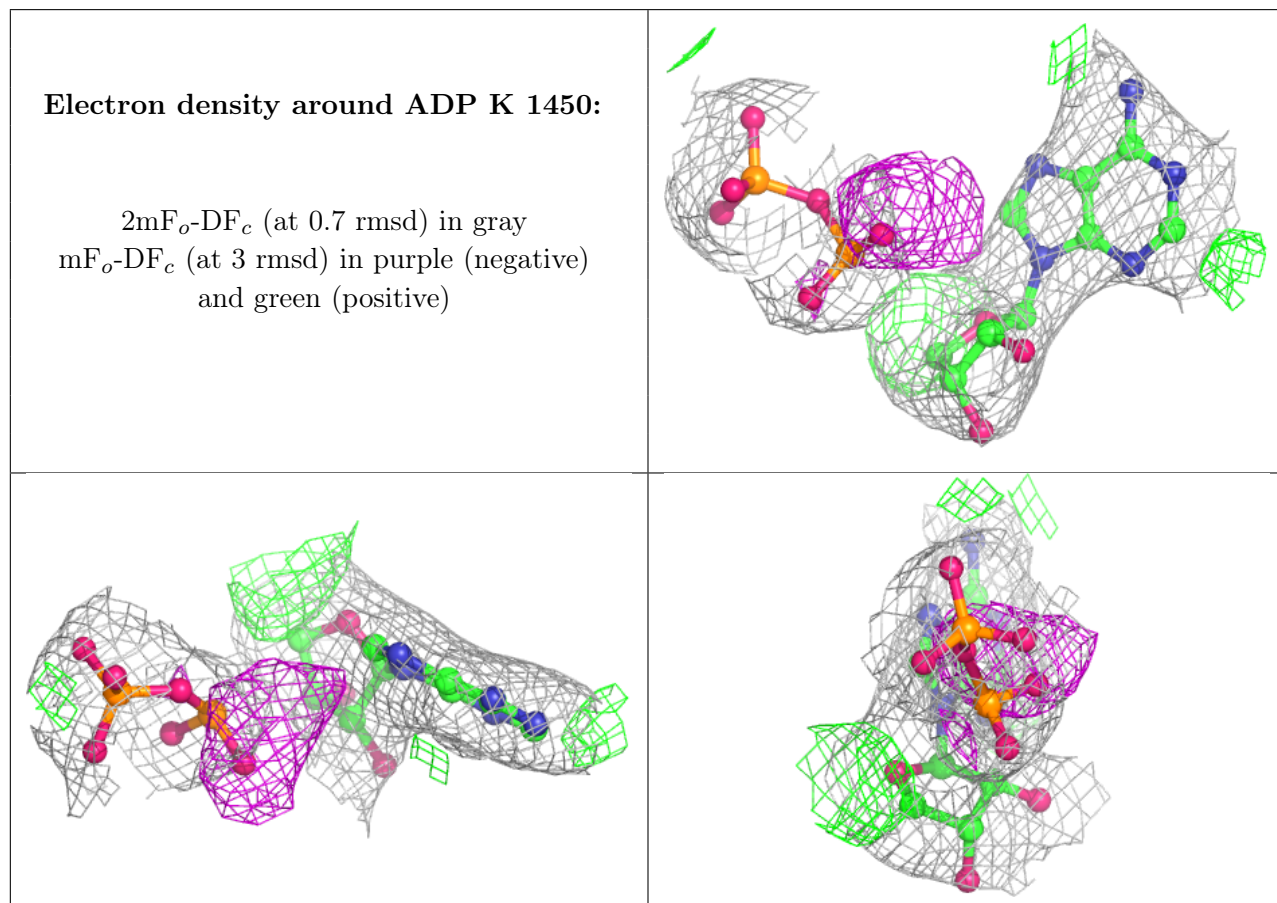
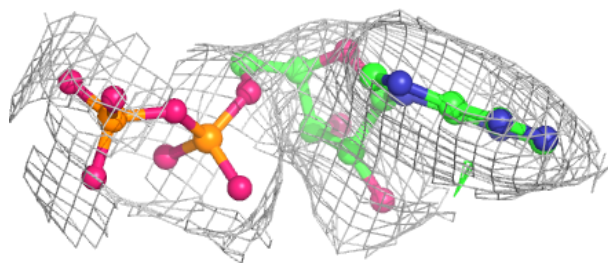**Electron density around ADP I 1450:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
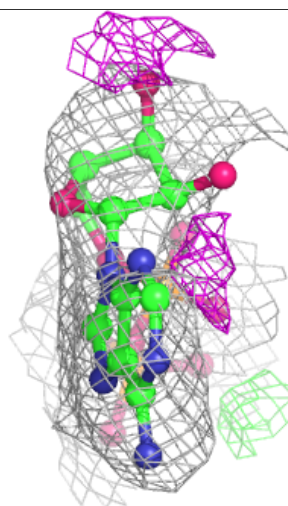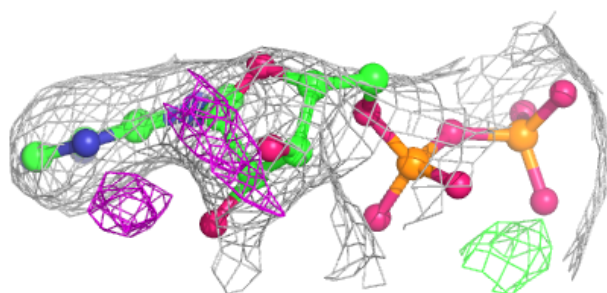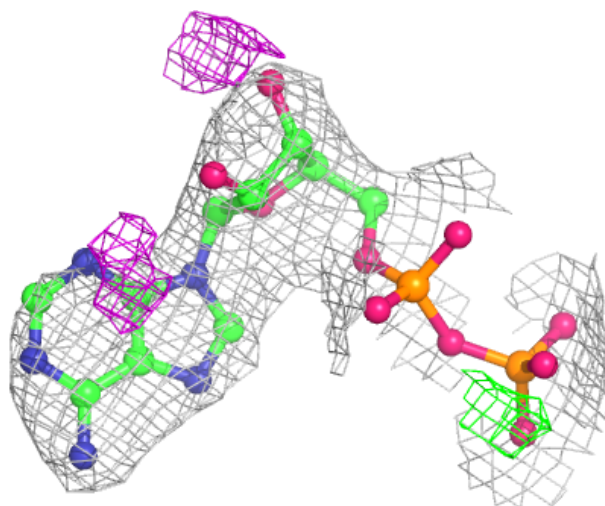
Electron density around ADP L 1450:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
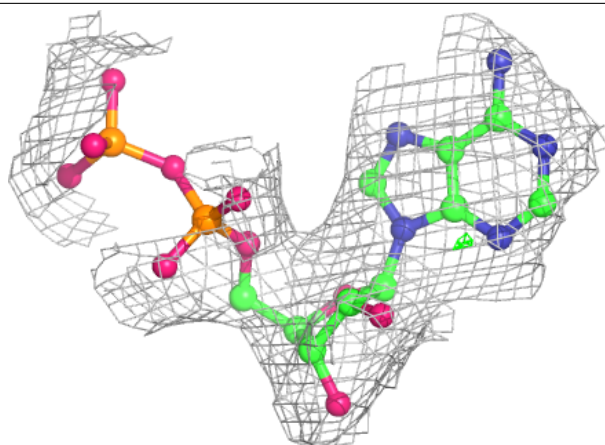and green (positive)
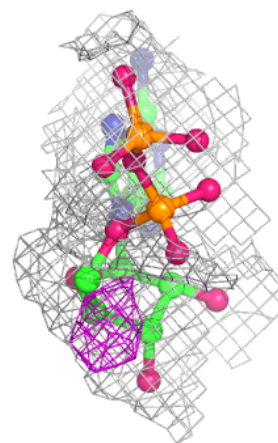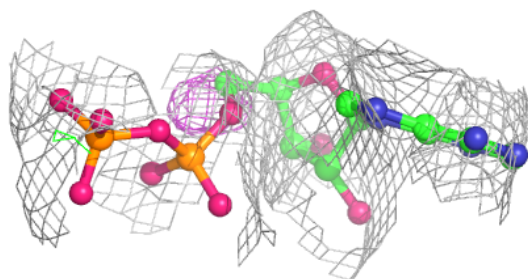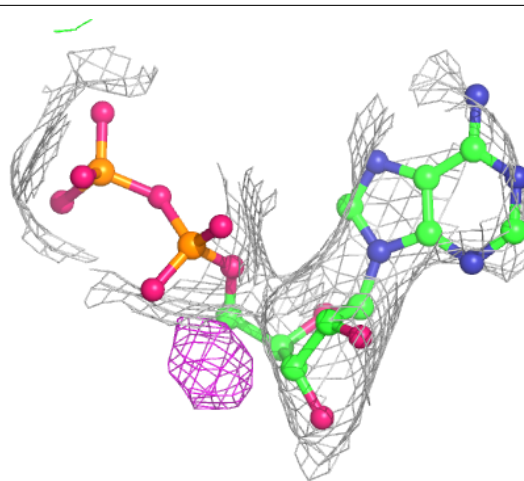
Electron density around ADP J 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
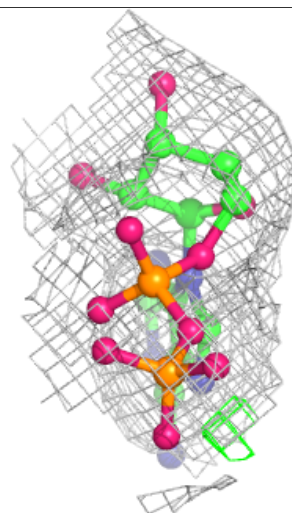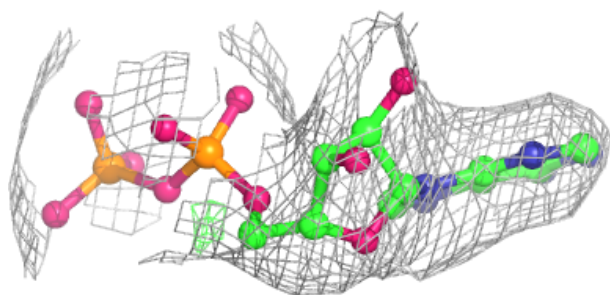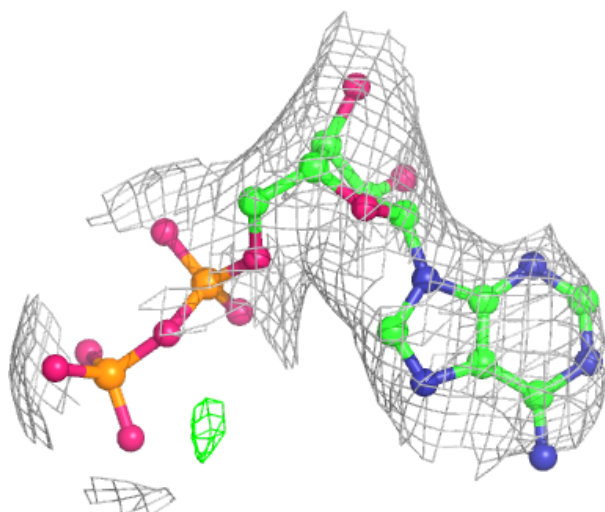
Electron density around ADP F 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
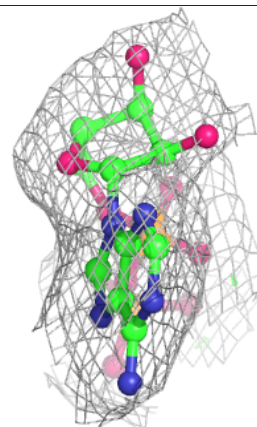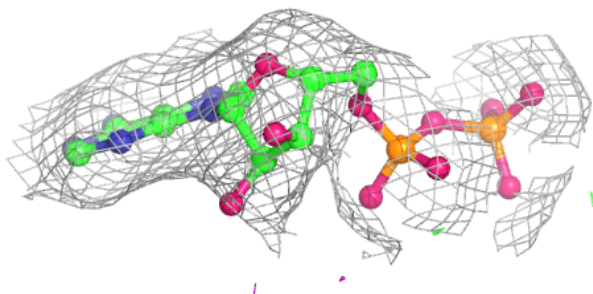and green (positive)
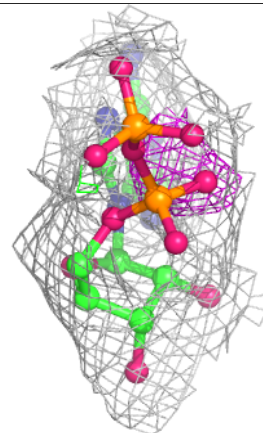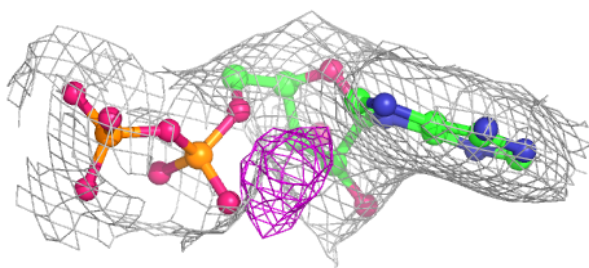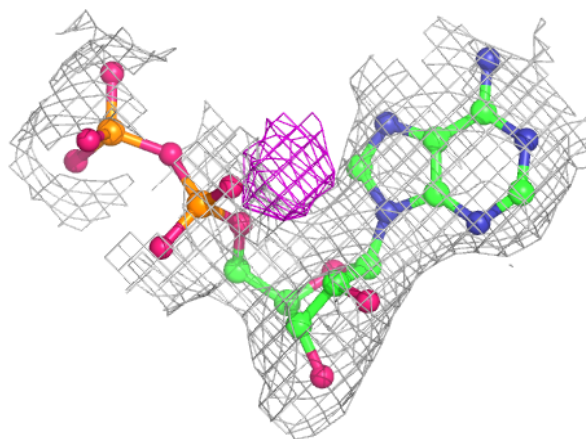
Electron density around ADP H 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
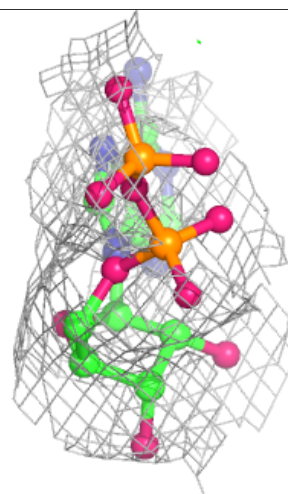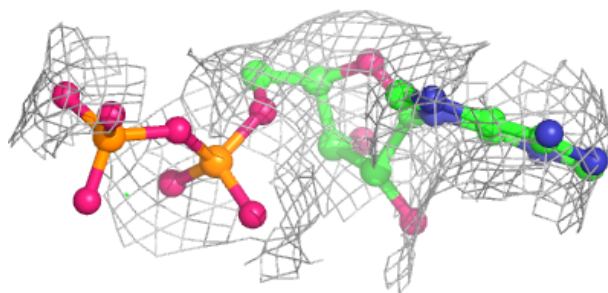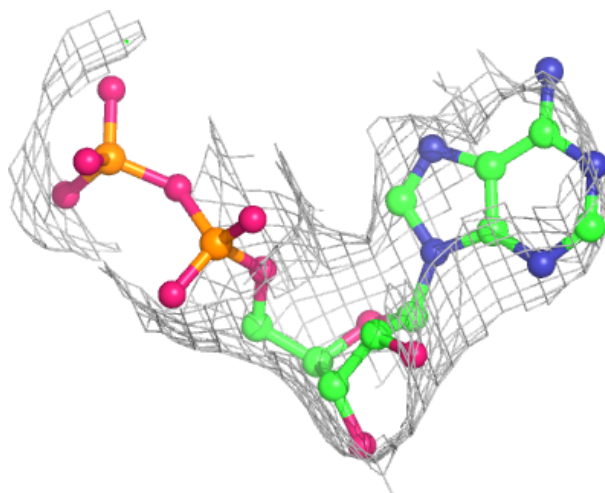
Electron density around ADP C 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
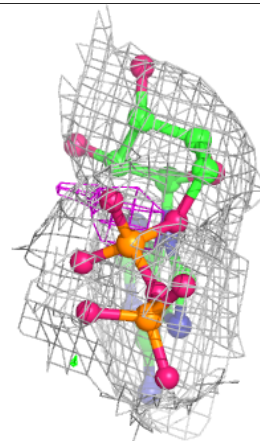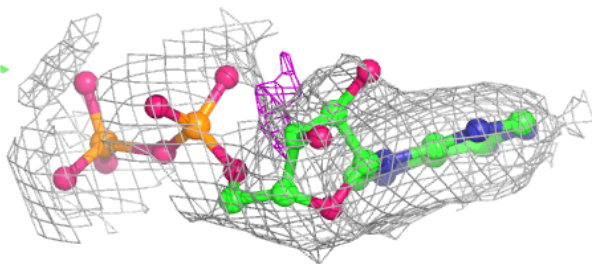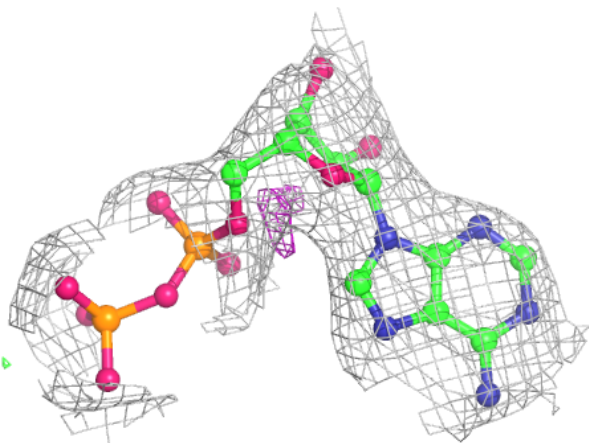
Electron density around ADP A 1450:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
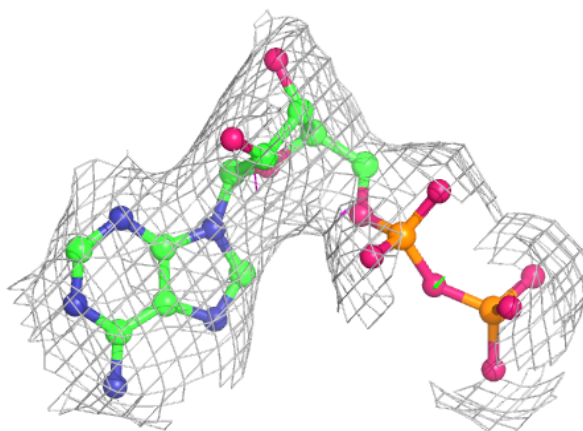and green (positive)
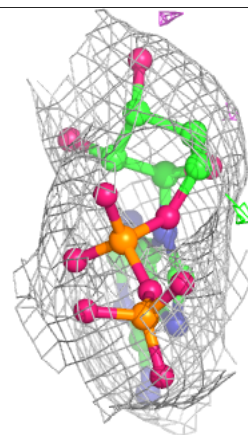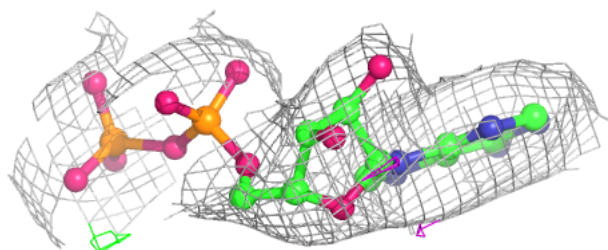
Electron density around ADP G 1450:

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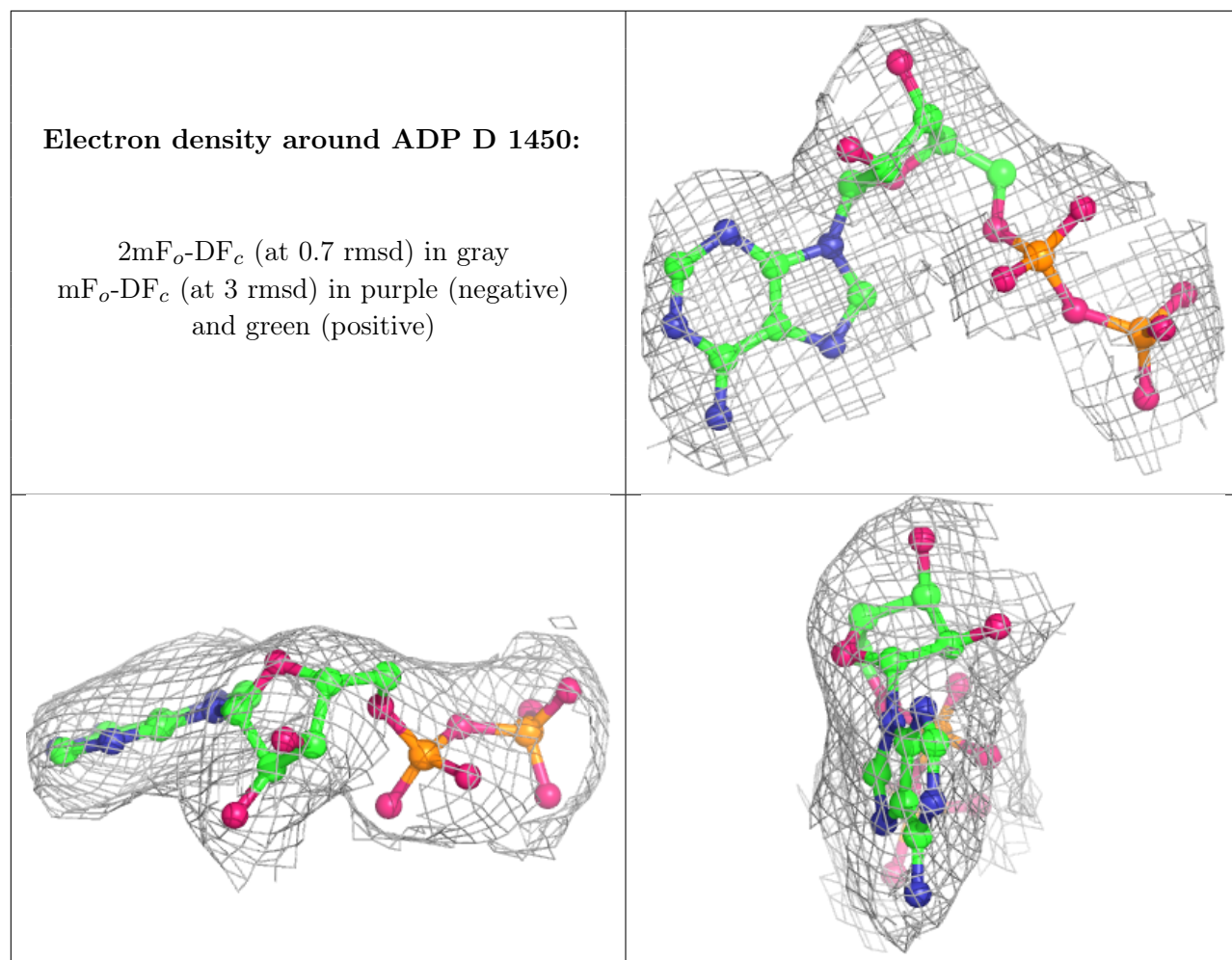and green (positive)

Electron density around ADP E 1450:

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

Electron density around ADP B 1450:

$2mF_o$-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 D 1450:

$2mF_o\text{-}DF_c$ (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.