Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 01:49 AM JST

PDB ID	:	6KEZ
Title	:	Crystal structure of GAPDH/CP12/PRK complex from Arabidopsis thaliana
Authors	:	Yu, A.; Xie, Y.; Li, M.
Deposited on	:	2019-07-05
Resolution	:	3.50 Å(reported)

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

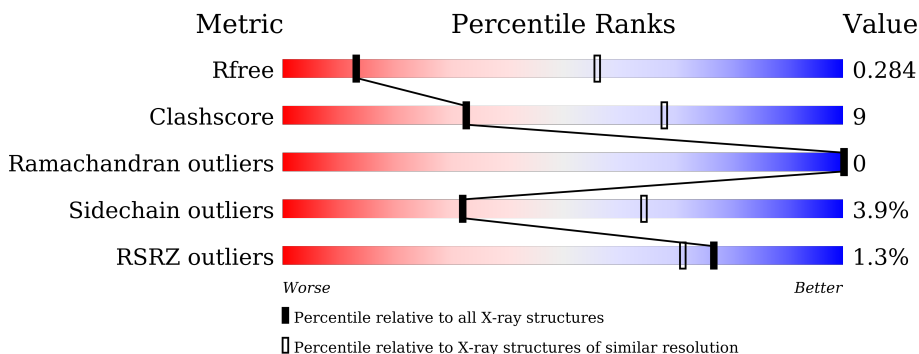|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.284
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		1.3%

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))
R$_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	339	76% 22% ••
1	B	339	73% 26% ••
1	C	339	78% 20% ••
1	D	339	80% 19% •
1	E	339	73% 25% ••
1	F	339	72% 26% ••

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WORLDWIDE wwPDB PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	G	339	80% 19%
1	H	339	76% 22%
2	I	352	% 75% 21%
2	J	352	3% 76% 20%
2	K	352	2% 76% 20%
2	L	352	4% 72% 24%
3	M	80	11% 68% 22% 9%
3	N	80	10% 62% 24% 5% 9%
3	O	80	2% 75% 14% 10%
3	P	80	2% 78% 11% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33826 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 Glyceraldehyde-3-phosphate dehydrogenase GAPA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	B	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	C	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	D	335	Total	C	N	O	S	0	0	0
			2542	1606	442	485	9			
1	E	336	Total	C	N	O	S	0	0	0
			2551	1612	444	486	9			
1	F	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	G	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	H	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P25856
A	-1	ASN	-	expression tag	UNP P25856
A	0	ALA	-	expression tag	UNP P25856
B	-2	SER	-	expression tag	UNP P25856
B	-1	ASN	-	expression tag	UNP P25856
B	0	ALA	-	expression tag	UNP P25856
C	-2	SER	-	expression tag	UNP P25856
C	-1	ASN	-	expression tag	UNP P25856
C	0	ALA	-	expression tag	UNP P25856
D	-2	SER	-	expression tag	UNP P25856
D	-1	ASN	-	expression tag	UNP P25856
D	0	ALA	-	expression tag	UNP P25856
E	-2	SER	-	expression tag	UNP P25856

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP P25856
E	0	ALA	-	expression tag	UNP P25856
F	-2	SER	-	expression tag	UNP P25856
F	-1	ASN	-	expression tag	UNP P25856
F	0	ALA	-	expression tag	UNP P25856
G	-2	SER	-	expression tag	UNP P25856
G	-1	ASN	-	expression tag	UNP P25856
G	0	ALA	-	expression tag	UNP P25856
H	-2	SER	-	expression tag	UNP P25856
H	-1	ASN	-	expression tag	UNP P25856
H	0	ALA	-	expression tag	UNP P25856

- Molecule 2 is a protein called Phosphoribulokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	342	Total 2713	C 1730	N 452	O 520	S 11	0	0	0
2	K	342	Total 2713	C 1730	N 452	O 520	S 11	0	0	0
2	J	342	Total 2713	C 1730	N 452	O 520	S 11	0	0	0
2	L	342	Total 2710	C 1729	N 452	O 518	S 11	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP P25697
I	1	ASN	-	expression tag	UNP P25697
I	2	ALA	-	expression tag	UNP P25697
K	0	SER	-	expression tag	UNP P25697
K	1	ASN	-	expression tag	UNP P25697
K	2	ALA	-	expression tag	UNP P25697
J	0	SER	-	expression tag	UNP P25697
J	1	ASN	-	expression tag	UNP P25697
J	2	ALA	-	expression tag	UNP P25697
L	0	SER	-	expression tag	UNP P25697
L	1	ASN	-	expression tag	UNP P25697
L	2	ALA	-	expression tag	UNP P25697

- Molecule 3 is a protein called Calvin cycle protein CP12-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	73	Total	C	N	O	S	0	0	0
			550	328	92	126	4			
3	N	73	Total	C	N	O	S	0	0	0
			550	328	92	126	4			
3	O	72	Total	C	N	O	S	0	0	0
			540	324	91	121	4			
3	P	72	Total	C	N	O	S	0	0	0
			543	325	91	123	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	SER	-	expression tag	UNP Q9LZP9
M	0	ASN	-	expression tag	UNP Q9LZP9
M	1	ALA	-	expression tag	UNP Q9LZP9
N	-1	SER	-	expression tag	UNP Q9LZP9
N	0	ASN	-	expression tag	UNP Q9LZP9
N	1	ALA	-	expression tag	UNP Q9LZP9
O	-1	SER	-	expression tag	UNP Q9LZP9
O	0	ASN	-	expression tag	UNP Q9LZP9
O	1	ALA	-	expression tag	UNP Q9LZP9
P	-1	SER	-	expression tag	UNP Q9LZP9
P	0	ASN	-	expression tag	UNP Q9LZP9
P	1	ALA	-	expression tag	UNP Q9LZP9

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

NAD
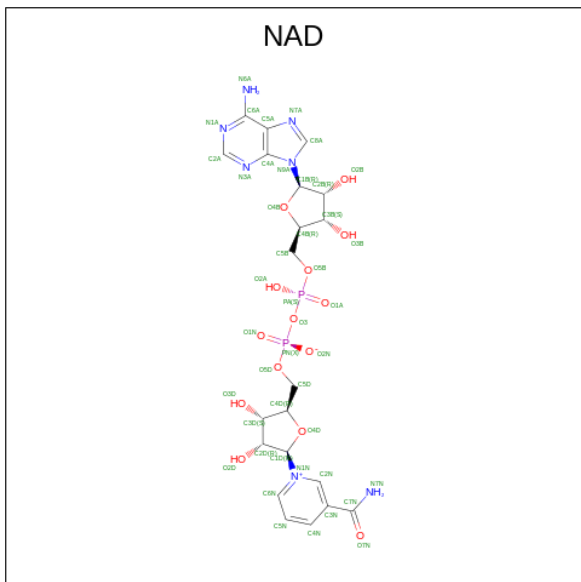
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	F	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	G	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	H	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	O 2	0	0
5	B	9	Total 9	O 9	0	0
5	C	7	Total 7	O 7	0	0
5	D	1	Total 1	O 1	0	0
5	E	4	Total 4	O 4	0	0
5	F	2	Total 2	O 2	0	0
5	G	6	Total 6	O 6	0	0
5	H	2	Total 2	O 2	0	0
5	I	1	Total 1	O 1	0	0
5	K	1	Total 1	O 1	0	0
5	N	2	Total 2	O 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 i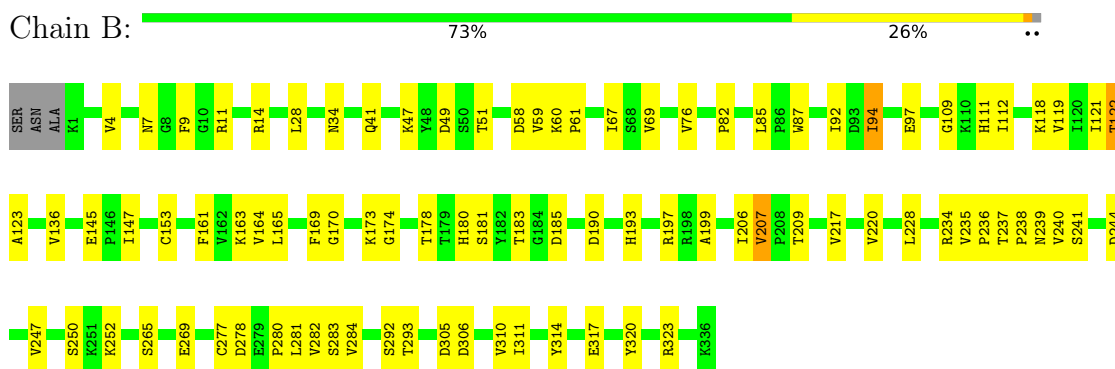n geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches 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.
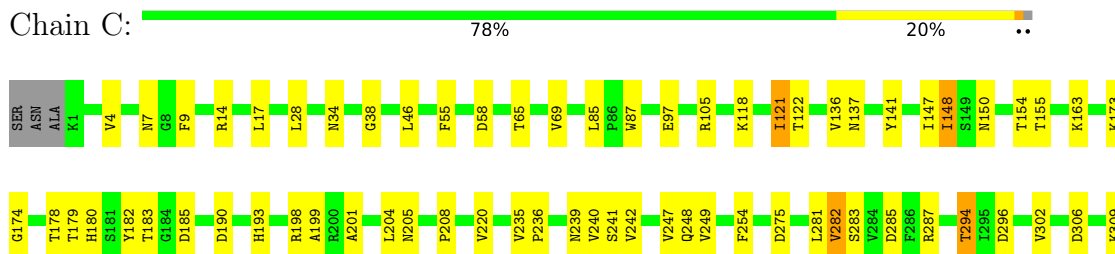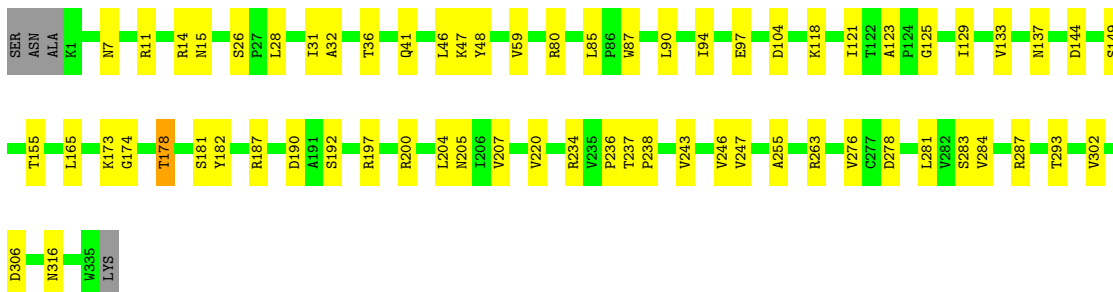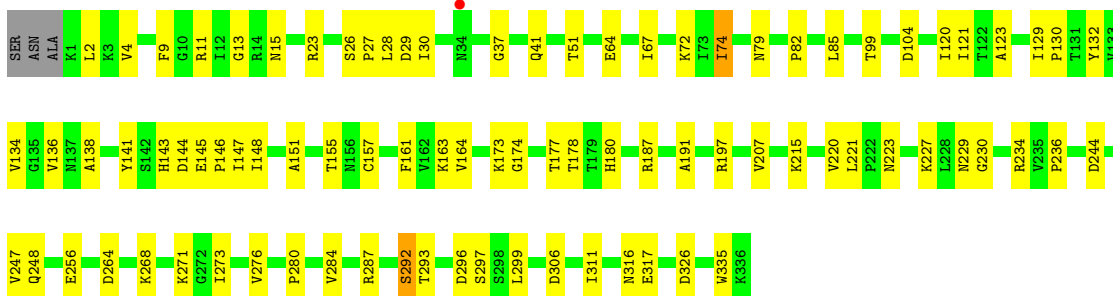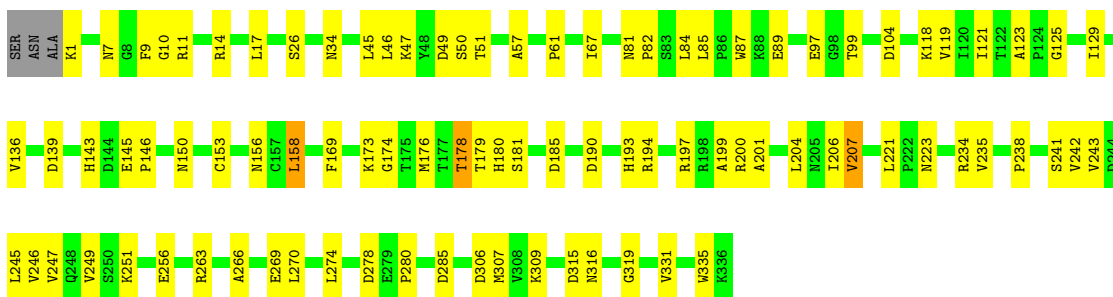
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain A:

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain B:

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain C:

V310 I311 A312 W313 Y314 D315 N316 E317 K336

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain D:

80%　　19%

SER ASN ALA K1 N7 R11 R14 N15 S26 P27 L28 I31 A32 T36 Q41 L46 K47 Y48 V59 R80 L85 P86 W87 L90 I94 E97 D104 K118 I121 T122 A123 P124 G125 I129 V133 N137 D144 S149

T155 L165 K173 G174 T178 S181 Y182 R187 D190 A191 S192 R197 R200 L204 N205 I206 V207 V220 R234 V235 P236 T237 P238 V243 V246 V247 A255 R263 V276 C277 D278 L281 V282 S283 V284 R287 T293 V302

D306 N316 W335 LYS

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain E:

73%　　25%

SER ASN ALA K1 L2 K3 V4 F9 G10 R11 I12 G13 R14 N15 R23 S26 P27 L28 D29 I30 N34 G37 Q41 T51 E64 I67 K72 I73 I74 N79 P82 L85 T99 D104 I120 I121 T122 A123 I129 P130 T131 Y132 V133

V134 G135 V136 N137 A138 Y141 S142 H143 D144 E145 P146 I147 I148 A151 T155 N156 C157 F161 V162 K163 V164 K173 G174 T177 T178 T179 H180 R187 A191 R197 V207 K215 V220 L221 P222 N223 L228 N229 G230 R234 V235 P236 D244

V247 Q248 E256 D264 K268 K271 G272 I273 V276 P280 V284 R287 S292 T293 D296 S297 S298 L299 D306 I311 N316 E317 D326 W335 K336

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain F:

72%　　26%

SER ASN ALA K1 N7 G8 F9 G10 R11 R14 L17 S26 N34 L45 L46 K47 Y48 D49 S50 T51 A57 P61 I67 N81 P82 S83 L84 L85 P86 W87 K88 E89 E97 Q98 T99 D104 K118 V119 I120 I121 T122 A123 P124 G125 I129

V136 D139 H143 D144 E145 P146 N150 C153 N156 C157 L158 F169 K173 G174 T175 M176 T177 T178 T179 H180 S181 D185 D190 H193 R194 R197 R198 A199 R200 A201 L204 N205 I206 V207 L221 P222 N223 R234 V235 P238 S241 V242 V243 D244

L245 V246 V247 Q248 V249 S250 K251 E256 R263 A266 E269 L270 L274 D278 E279 P280 D285 D306 M307 V308 K309 D315 N316 G319 V331 W335 K336

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain G:

80%　　19%

SER ASN ALA K1 V4 R14 K24 L28 D35 T36 G37 L85 P86 E97 I112 A116 K117 K118 I121 T131 H143 D144 A151 N156 G170 I171 I172 K173 G174 T178 T179 H180 S181 Y182 Q186 R187 L188 L189 D190 H193 R194 D195

L196 R197 R198 A199 L204 V207 I231 R234 V235 P236 T237 V240 S241 V242 V247 Q248 V249 S250 R263 D264 K268 V276 C277 D278 L281 V282 S283 V284 D285 F286 S292 T293 D306 K309 N316 Y320 R323 K336

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPA1

Chain H:

76%   22%
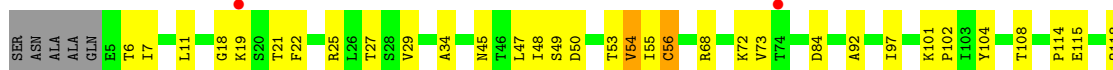
SER ASN ALA K1 L2 K3 V4 A5 F9 I12 L28 I31 D35 S50 P82 L85 P86 W87 I92 D93 I94 D104 K118 V119 I120 I121 T122 A123 K126 I129 Y132 V133 V136 N137 H143 D144 E145 I148 A151 S152 C153 T154

T155 N156 C157 F169 K173 T178 T179 H180 S181 Q186 L196 R197 R200 A201 A202 N205 I206 V207 P208 V217 L221 L224 L228 R234 V235 S241 V242 V243 D244 V249 F254 F262 A266 D275 V276 L281 V282 S283 V284 D285

D290 T293 V302 D306 K309 A312 N316 E317 D326 I330 K336

• Molecule 2: Phosphoribulokinase

Chain I:

%

75%   21%

SER ASN ALA ALA GLN E5 T6 I7 L11 G18 K19 S20 T21 F22 R25 L26 T27 S28 V29 A34 N45 T46 L47 I48 S49 D50 T53 V54 I55 C56 R68 K72 V73 T74 D84 A92 I97 K101 P102 I103 Y104 T108 P114 E115 Q118

V124 I125 E134 R135 V136 R137 L140 I144 Y145 I148 V152 I158 Q159 M162 R165 G166 H167 S168 L169 D188 Q192 V197 T203 T204 L205 D208 E211 R218 L219 I220 M221 K222 K248 L249 T250 N259 F266 V270 S271 V272

L273 E274 R281 L295 S296 Y300 V303 Q306 D312 Q324 V327 I331 R332 L334 Y335 R346 ALA GLU ALA LYS ALA

• Molecule 2: Phosphoribulokinase

Chain K:

2%

76%   20%

SER ASN ALA ALA GLN E5 I9 G10 L11 A12 K19 R25 K35 N45 I48 S49 D50 L57 H61 S62 L63 D64 R65 R68 K69 K72 L76 K94 Y104 N105 H106 V107 T108 G109 L110 L111 D112 P113 P114 I117 V124 I125 E126 G127

L139 L140 S143 I144 Y145 S149 V152 E164 H167 D184 K191 D195 A196 V197 V200 I206 P207 V214 L215 I220 M221 K222 E223 Y227 P230 G237 S238 T239 I240 R247 K248 Y253 P254 D263 S264 Y265 V270 L282 T297

L308 K309 H310 F313 S316 N317 N318 G319 T320 I331 L334 A343 T344 A345 R346 ALA GLU ALA LYS ALA

• Molecule 2: Phosphoribulokinase

Chain J:
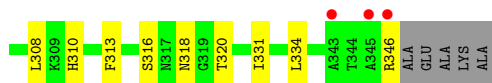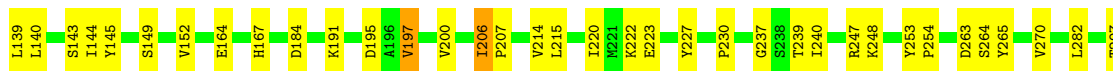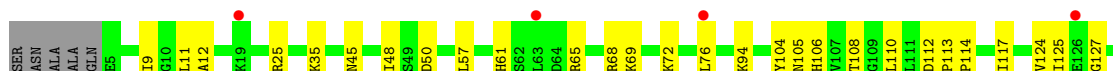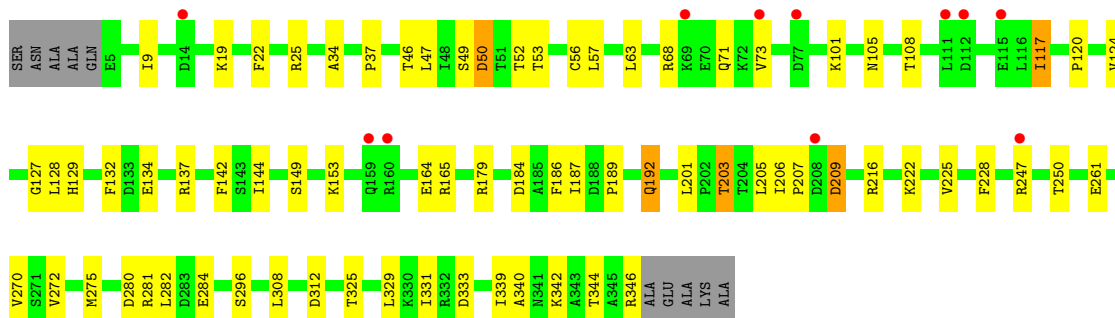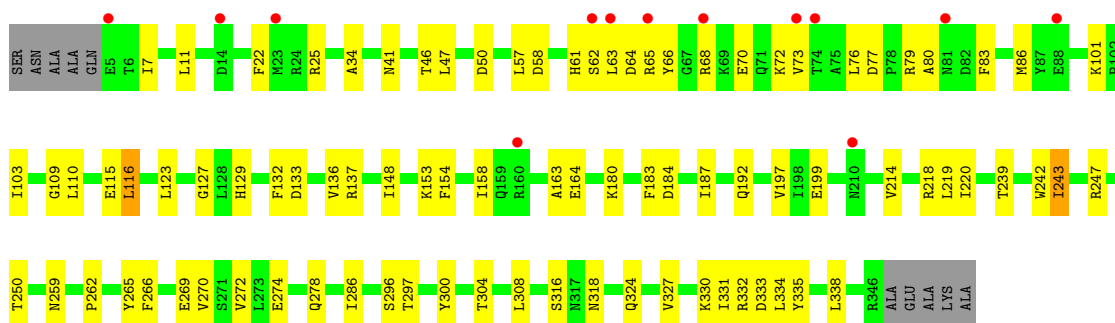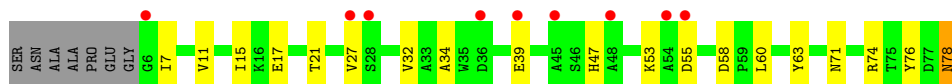
3%

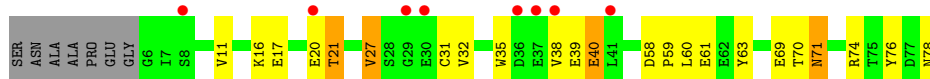76%   20%

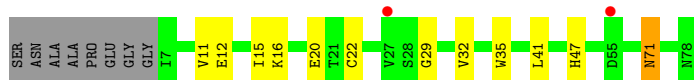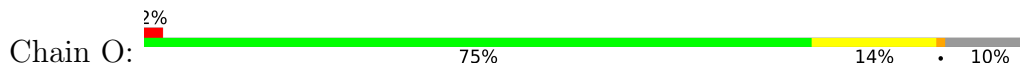• Molecule 2: Phosphoribulokinase

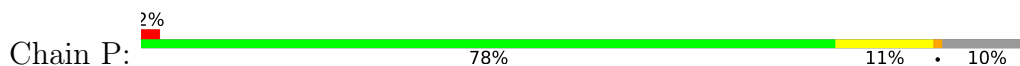Chain L:

• Molecule 3: Calvin cycle protein CP12-2

Chain M:

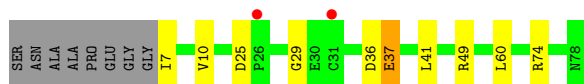• Molecule 3: Calvin cycle protein CP12-2

Chain N:

• Molecule 3: Calvin cycle protein CP12-2

Chain O:

• Molecule 3: Calvin cycle protein CP12-2

Chain P:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.81Å 204.73Å 157.04Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.09 – 3.50	Depositor EDS
% Data completeness (in resolution range)	87.3 (50.00-3.50) 86.9 (50.09-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.246 , 0.287 0.247 , 0.284	Depositor DCC
R_{free} test set	2956 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , -10.0	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	33826	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: NAD

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	0.25	0/2596	0.45	0/3523
1	B	0.25	0/2596	0.45	0/3523
1	C	0.25	0/2596	0.44	0/3523
1	D	0.24	0/2586	0.44	0/3512
1	E	0.38	0/2595	0.48	0/3523
1	F	0.25	0/2596	0.45	0/3523
1	G	0.25	0/2596	0.45	0/3523
1	H	0.26	0/2596	0.45	0/3523
2	I	0.27	0/2772	0.50	0/3754
2	J	0.26	0/2772	0.45	0/3754
2	K	0.25	0/2772	0.44	0/3754
2	L	0.25	0/2769	0.45	0/3750
3	M	0.26	0/557	0.43	0/753
3	N	0.24	0/557	0.42	0/753
3	O	0.24	0/547	0.38	0/740
3	P	0.26	0/550	0.43	0/744
All	All	0.27	0/34053	0.45	0/46175

There are no bond length outliers.

There are no bond angle outliers.

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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2552	0	2593	54	0
1	B	2552	0	2593	61	0
1	C	2552	0	2593	50	0
1	D	2542	0	2580	42	0
1	E	2551	0	2593	57	0
1	F	2552	0	2593	61	0
1	G	2552	0	2593	46	0
1	H	2552	0	2593	57	0
2	I	2713	0	2687	50	0
2	J	2713	0	2687	42	0
2	K	2713	0	2689	44	0
2	L	2710	0	2685	58	0
3	M	550	0	496	14	0
3	N	550	0	496	19	0
3	O	540	0	489	16	0
3	P	543	0	491	7	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
4	C	44	0	26	5	0
4	D	44	0	26	1	0
4	E	44	0	26	1	0
4	F	44	0	26	1	0
4	G	44	0	26	2	0
4	H	44	0	26	2	0
5	A	2	0	0	1	0
5	B	9	0	0	1	0
5	C	7	0	0	2	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	2	0	0	1	0
5	G	6	0	0	0	0
5	H	2	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	N	2	0	0	0	0
All	All	33826	0	33659	588	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 9.

All (588) 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:B:240:VAL:HG11	1:B:283:SER:HB3	1.54	0.87
1:F:10:GLY:HA2	5:F:501:HOH:O	1.73	0.86
1:G:187:ARG:HH22	3:N:74:ARG:HH12	1.24	0.82
1:C:183:THR:HG22	4:C:401:NAD:H72N	1.43	0.80
3:O:12:GLU:CG	3:O:16:LYS:HE3	2.14	0.78
2:I:19:LYS:HG3	3:O:47:HIS:CD2	2.18	0.78
1:B:240:VAL:CG1	1:B:283:SER:HB3	2.14	0.78
2:I:134:GLU:HA	2:I:137:ARG:HE	1.51	0.75
3:O:12:GLU:HG2	3:O:16:LYS:HE3	1.68	0.75
2:J:101:LYS:HE3	2:J:117:ILE:HD11	1.69	0.74
2:K:48:ILE:HD11	2:K:117:ILE:HD11	1.70	0.74
1:D:263:ARG:HG2	1:D:276:VAL:HG11	1.68	0.74
1:F:158:LEU:HD11	1:F:176:MET:HG3	1.72	0.72
2:I:18:GLY:O	2:I:19:LYS:HG3	1.90	0.72
1:F:153:CYS:SG	3:N:78:ASN:ND2	2.63	0.71
1:C:183:THR:CG2	4:C:401:NAD:H72N	2.04	0.70
1:G:263:ARG:HG2	1:G:276:VAL:HG11	1.74	0.70
1:H:5:ALA:HB2	1:H:92:ILE:HG12	1.72	0.69
1:E:177:THR:HG1	1:G:309:LYS:HZ1	1.40	0.69
1:G:97:GLU:HB3	1:G:121:ILE:HA	1.74	0.69
1:C:137:ASN:HB2	1:C:220:VAL:HG13	1.76	0.68
2:L:103:ILE:HD11	2:L:115:GLU:HB3	1.75	0.67
2:L:65:ARG:CD	2:L:109:GLY:HA3	2.24	0.67
2:I:47:LEU:HB2	2:I:54:VAL:HG13	1.77	0.67
1:E:64:GLU:HG2	3:M:53:LYS:HE2	1.76	0.66
1:B:207:VAL:HG13	1:B:234:ARG:HB2	1.76	0.66
1:C:183:THR:CG2	4:C:401:NAD:N7N	2.59	0.65
2:L:286:ILE:HG22	2:L:304:THR:HG21	1.77	0.65
2:J:57:LEU:HB2	2:J:127:GLY:HA3	1.79	0.65
1:G:151:ALA:O	1:G:156:ASN:ND2	2.29	0.64
2:I:48:ILE:HG12	2:I:53:THR:HG23	1.79	0.64
3:M:21:THR:HG22	3:M:34:ALA:HB3	1.77	0.64
1:A:185:ASP:OD2	1:A:198:ARG:NH1	2.31	0.64
1:B:118:LYS:NZ	1:B:145:GLU:O	2.30	0.64
2:L:57:LEU:HB2	2:L:127:GLY:HA3	1.78	0.64
1:C:201:ALA:O	1:C:205:ASN:ND2	2.26	0.64
2:L:64:ASP:O	2:L:68:ARG:N	2.31	0.64
1:E:4:VAL:HB	1:E:30:ILE:HG13	1.81	0.63
2:K:197:VAL:HG13	2:K:220:ILE:HB	1.79	0.63
1:C:309:LYS:HE3	1:C:311:ILE:HD11	1.81	0.63
1:A:23:ARG:NH2	1:A:326:ASP:OD1	2.31	0.63
1:A:176:MET:HB2	1:A:245:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:ARG:HD2	2:L:109:GLY:HA3	1.81	0.63
2:L:62:SER:N	2:L:80:ALA:O	2.27	0.62
1:C:7:ASN:OD1	1:C:34:ASN:ND2	2.33	0.62
1:E:177:THR:OG1	1:G:309:LYS:NZ	2.27	0.62
1:F:197:ARG:NH1	1:H:281:LEU:O	2.30	0.62
2:K:9:ILE:HB	2:K:124:VAL:HG12	1.79	0.62
1:H:254:PHE:HA	1:H:302:VAL:HG21	1.81	0.62
1:E:280:PRO:HA	1:G:197:ARG:HH21	1.65	0.62
2:I:18:GLY:O	2:I:19:LYS:CG	2.48	0.62
2:I:167:HIS:HB3	3:O:15:ILE:HD13	1.82	0.62
1:E:11:ARG:O	1:E:15:ASN:ND2	2.32	0.62
1:G:207:VAL:HB	1:G:234:ARG:HB2	1.82	0.61
2:L:214:VAL:HG12	2:L:278:GLN:HB3	1.82	0.61
1:D:7:ASN:ND2	1:D:97:GLU:OE2	2.33	0.61
1:G:292:SER:OG	1:G:323:ARG:NH1	2.32	0.61
1:H:153:CYS:SG	3:M:78:ASN:ND2	2.68	0.61
2:L:83:PHE:HA	2:L:86:MET:HB3	1.81	0.61
1:F:9:PHE:HZ	1:F:46:LEU:HD12	1.65	0.61
1:C:7:ASN:ND2	1:C:97:GLU:OE2	2.34	0.61
1:F:173:LYS:NZ	1:H:306:ASP:OD1	2.31	0.61
1:D:11:ARG:HH11	1:D:14:ARG:HH21	1.48	0.60
1:H:207:VAL:HB	1:H:234:ARG:HB2	1.82	0.60
1:B:217:VAL:HG21	1:B:228:LEU:HD12	1.83	0.60
1:C:174:GLY:HA3	1:C:247:VAL:HG12	1.84	0.60
1:E:29:ASP:OD1	1:E:72:LYS:NZ	2.33	0.60
1:H:186:GLN:HB2	1:H:202:ALA:HB2	1.82	0.60
1:F:207:VAL:HG13	1:F:234:ARG:HB2	1.84	0.60
1:H:169:PHE:HB3	1:H:249:VAL:HG21	1.84	0.60
2:K:206:ILE:HG12	2:K:207:PRO:HD2	1.84	0.60
2:I:203:THR:HG22	2:I:205:LEU:H	1.67	0.60
2:I:159:GLN:NE2	2:I:211:GLU:O	2.32	0.60
2:L:218:ARG:HG2	2:L:274:GLU:HG3	1.83	0.59
1:B:153:CYS:HB3	4:B:401:NAD:H4N	1.84	0.59
2:J:9:ILE:HG23	2:J:142:PHE:HB3	1.84	0.59
2:I:19:LYS:HG3	3:O:47:HIS:NE2	2.16	0.59
2:L:163:ALA:O	2:L:164:GLU:CD	2.40	0.59
1:A:276:VAL:HG12	1:A:295:ILE:HB	1.83	0.59
1:C:183:THR:HG21	4:C:401:NAD:N7N	2.17	0.59
1:E:134:VAL:HA	1:E:138:ALA:HB2	1.85	0.59
1:H:181:SER:H	1:H:241:SER:HB3	1.67	0.59
2:I:296:SER:O	2:I:296:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:PHE:HB3	1:F:249:VAL:HG21	1.84	0.58
2:J:144:ILE:HD11	2:J:331:ILE:HD11	1.84	0.58
2:I:19:LYS:HD2	3:O:47:HIS:NE2	2.19	0.58
2:J:34:ALA:HB1	2:J:47:LEU:HB3	1.85	0.58
1:F:179:THR:HB	1:F:242:VAL:HG22	1.84	0.58
1:E:187:ARG:HE	1:E:191:ALA:HB3	1.68	0.58
1:F:150:ASN:OD1	1:F:156:ASN:ND2	2.36	0.58
2:L:65:ARG:NH1	3:N:40:GLU:OE2	2.37	0.58
1:A:290:ASP:O	1:A:323:ARG:NH2	2.37	0.58
1:H:180:HIS:HE1	1:H:316:ASN:HD22	1.51	0.58
2:K:223:GLU:OE1	2:L:247:ARG:NH1	2.36	0.58
1:B:180:HIS:HA	1:B:241:SER:HB3	1.85	0.58
2:L:25:ARG:NH2	2:L:316:SER:OG	2.36	0.58
2:I:125:ILE:HD11	2:I:140:LEU:HD21	1.84	0.58
1:H:121:ILE:HG22	1:H:123:ALA:H	1.67	0.57
2:I:68:ARG:NH1	2:I:104:TYR:OH	2.37	0.57
1:A:184:GLY:O	3:P:74:ARG:NH2	2.36	0.57
2:K:222:LYS:HA	2:K:270:VAL:HG12	1.85	0.57
1:C:173:LYS:NZ	1:C:248:GLN:OE1	2.36	0.57
2:K:227:TYR:HB2	2:K:334:LEU:HD12	1.86	0.57
2:J:282:LEU:HD13	2:J:308:LEU:HD11	1.87	0.57
1:A:299:LEU:HD21	1:C:208:PRO:HB2	1.85	0.57
1:A:209:THR:HG22	1:A:232:ALA:HB3	1.87	0.57
1:C:180:HIS:HA	1:C:241:SER:HB3	1.87	0.57
1:A:173:LYS:NZ	1:C:306:ASP:OD1	2.29	0.56
1:D:187:ARG:NH1	1:D:192:SER:O	2.38	0.56
1:G:170:GLY:O	1:G:250:SER:N	2.27	0.56
2:K:247:ARG:NH2	2:L:269:GLU:OE1	2.36	0.56
2:L:63:LEU:CD1	2:L:79:ARG:HG3	2.35	0.56
1:B:11:ARG:NH1	1:B:49:ASP:OD1	2.38	0.56
1:B:119:VAL:HG22	1:B:147:ILE:HG13	1.86	0.56
1:B:183:THR:OG1	1:B:234:ARG:NH2	2.38	0.56
1:D:316:ASN:N	1:D:316:ASN:OD1	2.38	0.56
1:E:223:ASN:O	1:E:227:LYS:NZ	2.36	0.56
1:F:47:LYS:NZ	1:F:57:ALA:O	2.38	0.56
2:K:65:ARG:NH1	2:K:106:HIS:O	2.38	0.56
1:D:123:ALA:O	1:D:149:SER:OG	2.22	0.56
1:B:190:ASP:O	1:C:14:ARG:NH2	2.37	0.56
1:D:94:ILE:HG22	1:D:118:LYS:HB3	1.87	0.56
2:K:223:GLU:HG3	2:K:230:PRO:HG2	1.86	0.56
2:L:58:ASP:HA	2:L:61:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:LEU:HD11	2:L:79:ARG:HG3	1.88	0.56
1:B:41:GLN:NE2	1:C:193:HIS:O	2.34	0.56
1:C:254:PHE:HA	1:C:302:VAL:HG21	1.86	0.56
2:I:102:PRO:HA	2:I:114:PRO:HA	1.88	0.56
2:K:45:ASN:OD1	2:K:106:HIS:NE2	2.39	0.56
1:D:26:SER:HB2	1:D:28:LEU:HD12	1.88	0.55
1:B:153:CYS:SG	1:B:180:HIS:NE2	2.73	0.55
1:F:181:SER:OG	1:F:316:ASN:ND2	2.40	0.55
2:L:66:TYR:O	2:L:70:GLU:N	2.39	0.55
1:B:173:LYS:NZ	1:D:306:ASP:OD1	2.39	0.55
1:B:240:VAL:HG11	1:B:283:SER:CB	2.31	0.55
1:F:190:ASP:O	1:G:14:ARG:NH2	2.40	0.55
2:J:71:GLN:HB2	2:J:73:VAL:HG23	1.88	0.55
1:D:41:GLN:HE22	3:P:60:LEU:HD22	1.72	0.55
1:B:235:VAL:HG23	1:B:237:THR:HG22	1.89	0.55
1:E:207:VAL:HG12	1:G:282:VAL:HG11	1.89	0.55
2:J:296:SER:O	2:J:296:SER:OG	2.20	0.55
2:L:46:THR:OG1	2:L:101:LYS:NZ	2.40	0.55
2:L:164:GLU:HG2	3:N:11:VAL:HG11	1.89	0.55
1:E:273:ILE:HG23	1:E:292:SER:HB2	1.88	0.54
2:K:25:ARG:NH2	2:K:316:SER:OG	2.40	0.54
1:E:143:HIS:HD2	1:E:335:TRP:HA	1.71	0.54
1:F:238:PRO:HG3	1:G:204:LEU:HD21	1.90	0.54
2:I:27:THR:HG21	2:I:34:ALA:HB2	1.88	0.54
2:K:144:ILE:HD11	2:K:331:ILE:HD11	1.89	0.54
2:K:263:ASP:OD1	2:K:264:SER:N	2.40	0.54
2:J:203:THR:HA	2:J:216:ARG:HB2	1.88	0.54
1:A:313:TRP:HZ2	1:C:208:PRO:HG3	1.73	0.54
1:F:269:GLU:HG2	1:F:270:LEU:HG	1.89	0.54
1:B:209:THR:HG21	1:B:234:ARG:HH11	1.71	0.54
2:I:259:ASN:HB3	2:I:274:GLU:HB2	1.89	0.54
2:I:312:ASP:OD1	2:I:312:ASP:N	2.41	0.54
1:A:263:ARG:HG3	1:A:276:VAL:HG21	1.89	0.54
1:B:164:VAL:HG21	1:B:265:SER:HB2	1.90	0.54
2:I:222:LYS:HA	2:I:270:VAL:HG12	1.90	0.54
1:D:121:ILE:HG22	1:D:123:ALA:H	1.72	0.54
1:E:248:GLN:OE1	1:G:248:GLN:NE2	2.41	0.54
2:L:163:ALA:C	2:L:164:GLU:OE1	2.46	0.54
3:N:27:VAL:HG23	3:N:32:VAL:HG21	1.90	0.53
2:K:105:ASN:ND2	2:K:112:ASP:OD2	2.42	0.53
1:B:51:THR:HG21	1:B:239:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:SER:HG	1:D:237:THR:HG1	1.55	0.53
1:G:264:ASP:HB3	1:G:268:LYS:HE2	1.90	0.53
1:G:284:VAL:HG11	1:H:50:SER:HA	1.90	0.53
1:B:174:GLY:HA3	1:B:247:VAL:HG22	1.89	0.53
3:M:27:VAL:HG11	3:M:32:VAL:HG23	1.88	0.53
1:B:11:ARG:NH2	1:B:317:GLU:OE2	2.41	0.53
2:K:282:LEU:HD13	2:K:308:LEU:HD11	1.90	0.53
1:A:11:ARG:NE	1:A:317:GLU:OE1	2.39	0.53
1:H:94:ILE:HG22	1:H:118:LYS:HB3	1.91	0.53
1:A:316:ASN:OD1	1:A:317:GLU:N	2.41	0.53
2:I:192:GLN:HB3	2:I:266:PHE:HD2	1.72	0.53
2:L:58:ASP:HA	2:L:61:HIS:HD2	1.74	0.53
1:D:178:THR:HB	1:D:243:VAL:HG23	1.91	0.52
1:H:35:ASP:OD1	4:H:401:NAD:O2B	2.27	0.52
2:K:125:ILE:HD11	2:K:140:LEU:HD11	1.90	0.52
2:L:73:VAL:HG13	2:L:77:ASP:HB3	1.90	0.52
1:F:266:ALA:HB2	1:F:274:LEU:HD12	1.90	0.52
1:H:180:HIS:CE1	1:H:316:ASN:HD22	2.27	0.52
2:J:164:GLU:HG2	2:J:165:ARG:HE	1.74	0.52
1:B:7:ASN:OD1	1:B:34:ASN:ND2	2.42	0.52
2:J:165:ARG:HD3	3:M:7:ILE:HG21	1.91	0.52
1:H:4:VAL:HG13	1:H:94:ILE:HG13	1.92	0.52
1:F:185:ASP:HB2	3:N:76:TYR:HB2	1.90	0.52
1:F:249:VAL:HG22	1:F:251:LYS:H	1.74	0.52
1:C:118:LYS:NZ	1:C:141:TYR:OH	2.40	0.52
1:C:239:ASN:HD22	1:C:287:ARG:HD3	1.74	0.52
1:E:130:PRO:HB2	1:E:148:ILE:HG22	1.91	0.52
1:A:95:VAL:HB	1:A:119:VAL:HG22	1.92	0.52
1:F:200:ARG:NH1	1:H:285:ASP:OD2	2.42	0.52
1:B:58:ASP:OD1	1:B:60:LYS:NZ	2.42	0.52
1:F:194:ARG:NH1	3:N:61:GLU:OE2	2.42	0.51
2:K:108:THR:HG22	2:K:110:LEU:HD12	1.91	0.51
1:A:158:LEU:HA	1:A:161:PHE:HE1	1.74	0.51
1:A:295:ILE:HD13	1:A:312:ALA:HB2	1.93	0.51
2:K:346:ARG:C	2:J:346:ARG:HB3	2.30	0.51
1:B:236:PRO:HG2	1:D:236:PRO:HG2	1.93	0.51
1:B:94:ILE:HD12	1:B:118:LYS:HB2	1.93	0.51
1:B:206:ILE:HG13	1:D:237:THR:HG21	1.93	0.51
1:B:244:ASP:HB3	1:B:311:ILE:HD13	1.93	0.51
2:J:179:ARG:NH2	3:M:39:GLU:HG3	2.26	0.51
1:A:168:LYS:NZ	1:A:264:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASP:OD1	1:D:173:LYS:NZ	2.35	0.51
1:E:256:GLU:N	1:E:256:GLU:OE1	2.43	0.51
2:J:280:ASP:N	2:J:284:GLU:OE2	2.38	0.51
2:I:7:ILE:HD12	2:I:335:TYR:HD1	1.74	0.51
1:F:125:GLY:HA3	1:F:129:ILE:HG21	1.92	0.51
1:F:246:VAL:HG22	1:F:309:LYS:HG3	1.92	0.51
2:K:68:ARG:NH2	3:P:36:ASP:OD2	2.43	0.51
1:A:4:VAL:HG11	1:A:28:LEU:HB3	1.93	0.51
2:I:250:THR:O	2:I:281:ARG:NH2	2.42	0.51
1:B:282:VAL:HG22	1:D:200:ARG:HD3	1.93	0.50
1:C:136:VAL:HG13	1:C:163:LYS:HD2	1.93	0.50
1:F:1:LYS:NZ	1:F:26:SER:O	2.40	0.50
1:F:285:ASP:OD1	1:H:200:ARG:NH1	2.44	0.50
2:K:164:GLU:OE2	3:P:49:ARG:NH2	2.43	0.50
2:J:222:LYS:HA	2:J:270:VAL:HG12	1.93	0.50
1:H:221:LEU:HD23	1:H:224:LEU:HD13	1.93	0.50
2:L:163:ALA:O	2:L:164:GLU:CG	2.59	0.50
1:E:174:GLY:HA3	1:E:247:VAL:HG12	1.93	0.50
2:L:197:VAL:HG22	2:L:220:ILE:HB	1.93	0.50
1:B:97:GLU:OE2	1:B:111:HIS:NE2	2.41	0.50
1:C:296:ASP:HB2	1:C:313:TRP:HE1	1.77	0.50
1:G:37:GLY:HA2	3:N:60:LEU:HB2	1.93	0.50
2:I:327:VAL:O	2:I:331:ILE:HG12	2.12	0.50
1:A:235:VAL:HG11	1:C:235:VAL:HG11	1.94	0.49
1:E:180:HIS:CE1	1:E:316:ASN:HD22	2.30	0.49
1:E:229:ASN:OD1	1:E:230:GLY:N	2.45	0.49
1:F:206:ILE:HD11	1:H:235:VAL:HG21	1.94	0.49
2:I:220:ILE:HG23	2:I:272:VAL:HG12	1.93	0.49
1:B:206:ILE:HB	1:D:283:SER:HB3	1.93	0.49
1:F:180:HIS:CE1	1:F:316:ASN:HD22	2.31	0.49
1:A:103:VAL:HG12	1:A:125:GLY:HA2	1.94	0.49
1:B:284:VAL:HG13	1:D:205:ASN:HB3	1.95	0.49
1:D:11:ARG:O	1:D:15:ASN:ND2	2.32	0.49
1:E:120:ILE:HG12	1:E:148:ILE:HD11	1.94	0.49
1:H:275:ASP:OD1	1:H:276:VAL:N	2.46	0.49
1:B:161:PHE:CZ	1:B:310:VAL:HB	2.48	0.49
1:D:47:LYS:HD3	1:D:59:VAL:HB	1.93	0.49
1:F:153:CYS:H	3:N:78:ASN:HD21	1.59	0.49
2:J:9:ILE:HB	2:J:124:VAL:HG12	1.94	0.49
1:B:292:SER:HB3	1:B:323:ARG:HH11	1.78	0.49
1:C:275:ASP:HB3	1:C:294:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:PRO:HA	1:F:85:LEU:HG	1.94	0.48
2:L:199:GLU:OE1	2:L:218:ARG:NH1	2.46	0.48
3:M:60:LEU:HA	3:M:63:TYR:HB3	1.94	0.48
2:K:50:ASP:OD1	2:K:50:ASP:N	2.42	0.48
1:A:204:LEU:HD11	1:D:238:PRO:HB3	1.94	0.48
1:A:238:PRO:HG3	1:D:204:LEU:HD21	1.94	0.48
1:C:7:ASN:HA	1:C:34:ASN:HB3	1.95	0.48
2:K:68:ARG:NH1	2:K:104:TYR:OH	2.46	0.48
2:L:163:ALA:C	2:L:164:GLU:CD	2.72	0.48
3:N:71:ASN:OD1	3:N:71:ASN:N	2.45	0.48
1:F:153:CYS:HB3	4:F:401:NAD:H5N	1.95	0.48
1:F:280:PRO:HB2	1:H:197:ARG:HG3	1.94	0.48
1:E:132:TYR:CE2	1:E:141:TYR:HD1	2.30	0.48
2:L:11:LEU:HD22	2:L:22:PHE:HE2	1.79	0.48
1:D:306:ASP:OD1	1:D:306:ASP:N	2.46	0.48
1:F:14:ARG:NH2	1:G:190:ASP:O	2.38	0.48
1:H:217:VAL:HG11	1:H:228:LEU:HD12	1.95	0.48
2:K:12:ALA:HB3	2:K:145:TYR:HD1	1.78	0.48
3:O:29:GLY:HA2	3:O:32:VAL:HG22	1.95	0.48
1:F:158:LEU:HD21	1:F:245:LEU:HD13	1.95	0.48
2:K:72:LYS:HG3	3:P:29:GLY:HA3	1.95	0.48
1:E:306:ASP:OD1	1:G:173:LYS:NZ	2.38	0.48
1:A:138:ALA:HB3	5:A:502:HOH:O	2.12	0.47
1:F:118:LYS:HE2	1:F:146:PRO:HA	1.96	0.47
2:L:163:ALA:N	2:L:164:GLU:OE1	2.47	0.47
2:L:259:ASN:HB2	2:L:274:GLU:HB3	1.96	0.47
1:F:153:CYS:SG	1:F:180:HIS:NE2	2.73	0.47
1:H:151:ALA:HB1	1:H:155:THR:HB	1.96	0.47
1:H:306:ASP:OD1	1:H:306:ASP:N	2.45	0.47
2:I:19:LYS:CG	3:O:47:HIS:NE2	2.77	0.47
1:D:255:ALA:HB2	1:D:302:VAL:HG12	1.95	0.47
1:F:118:LYS:NZ	1:F:143:HIS:O	2.48	0.47
1:F:307:MET:HG3	1:H:173:LYS:HD2	1.97	0.47
2:K:69:LYS:HG2	3:P:37:GLU:OE2	2.13	0.47
1:B:122:THR:HG22	1:B:320:TYR:HE2	1.79	0.47
1:B:161:PHE:HZ	1:B:310:VAL:HB	1.80	0.47
1:B:121:ILE:HG22	1:B:123:ALA:H	1.79	0.47
1:E:173:LYS:HE3	1:G:306:ASP:OD1	2.14	0.47
1:C:105:ARG:HG3	1:C:147:ILE:HD12	1.96	0.47
1:D:263:ARG:NH2	1:D:278:ASP:OD1	2.47	0.47
1:E:143:HIS:CD2	1:E:335:TRP:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:VAL:HG11	1:G:28:LEU:HD23	1.97	0.47
1:H:244:ASP:OD2	1:H:309:LYS:NZ	2.48	0.47
2:I:92:ALA:HB1	2:I:97:ILE:HB	1.96	0.47
2:J:132:PHE:HE2	2:J:186:PHE:HB3	1.79	0.47
1:G:180:HIS:HA	1:G:241:SER:HB3	1.97	0.47
2:K:215:LEU:HD11	2:K:320:THR:HG23	1.97	0.47
1:C:182:TYR:HD2	1:C:236:PRO:HA	1.80	0.47
1:E:236:PRO:HG2	1:G:236:PRO:HG2	1.96	0.47
1:H:12:ILE:HD11	4:H:401:NAD:C7N	2.44	0.47
2:J:25:ARG:HE	2:J:325:THR:HG23	1.78	0.47
2:L:192:GLN:HB3	2:L:266:PHE:HD2	1.80	0.47
3:N:63:TYR:CE2	3:N:70:THR:HG21	2.49	0.47
1:A:174:GLY:HA3	1:A:247:VAL:HG12	1.97	0.46
1:B:136:VAL:HG13	1:B:163:LYS:HD2	1.97	0.46
1:B:252:LYS:HG2	1:B:305:ASP:HB3	1.97	0.46
1:H:336:LYS:HD2	1:H:336:LYS:HA	1.78	0.46
1:H:143:HIS:ND1	1:H:143:HIS:O	2.48	0.46
1:A:143:HIS:O	1:A:143:HIS:ND1	2.48	0.46
1:B:4:VAL:HG21	1:B:28:LEU:HB3	1.96	0.46
1:D:32:ALA:HB2	1:D:90:LEU:HD22	1.97	0.46
1:H:118:LYS:NZ	1:H:145:GLU:O	2.41	0.46
2:K:164:GLU:HB2	2:K:167:HIS:HD2	1.79	0.46
2:L:50:ASP:OD1	2:L:50:ASP:N	2.48	0.46
1:E:41:GLN:HG2	1:H:196:LEU:HD21	1.96	0.46
1:E:287:ARG:NH2	5:E:501:HOH:O	2.38	0.46
1:H:3:LYS:HD3	1:H:31:ILE:HD13	1.98	0.46
2:I:55:ILE:HD12	2:I:101:LYS:HE2	1.98	0.46
2:K:149:SER:HB2	2:K:152:VAL:HG12	1.96	0.46
2:J:149:SER:HB3	2:J:201:LEU:HD23	1.97	0.46
2:L:76:LEU:HD22	2:L:187:ILE:HD11	1.98	0.46
1:B:185:ASP:OD1	1:B:193:HIS:NE2	2.48	0.46
1:E:9:PHE:HA	1:E:13:GLY:HA3	1.98	0.46
1:H:133:VAL:HG23	1:H:136:VAL:HB	1.98	0.46
1:H:316:ASN:OD1	1:H:317:GLU:N	2.49	0.46
2:J:206:ILE:HG23	2:J:209:ASP:H	1.80	0.46
1:A:7:ASN:OD1	1:A:34:ASN:ND2	2.38	0.46
1:B:241:SER:HB2	1:B:314:TYR:CZ	2.50	0.46
3:M:71:ASN:OD1	3:M:74:ARG:NH1	2.49	0.46
1:A:20:TRP:NE1	1:A:28:LEU:O	2.43	0.46
1:A:180:HIS:CE1	1:A:316:ASN:HD22	2.34	0.46
1:B:197:ARG:NH2	1:D:281:LEU:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:HB	1:D:234:ARG:HB2	1.98	0.46
2:J:312:ASP:N	2:J:312:ASP:OD1	2.49	0.46
1:E:151:ALA:HB1	1:E:155:THR:HB	1.97	0.45
2:I:248:LYS:HD3	2:I:248:LYS:HA	1.77	0.45
1:A:200:ARG:NH2	1:C:285:ASP:OD2	2.47	0.45
1:A:313:TRP:CZ2	1:C:208:PRO:HG3	2.51	0.45
1:E:11:ARG:NH2	1:E:317:GLU:OE1	2.41	0.45
1:G:181:SER:HB2	1:G:237:THR:O	2.16	0.45
2:I:84:ASP:OD1	2:I:135:ARG:NH2	2.44	0.45
2:K:143:SER:HB2	2:K:195:ASP:H	1.81	0.45
2:J:189:PRO:O	2:J:192:GLN:HG2	2.17	0.45
1:F:235:VAL:HG11	1:H:235:VAL:HG11	1.96	0.45
1:A:143:HIS:CD2	1:A:336:LYS:H	2.33	0.45
1:D:133:VAL:HG23	1:D:220:VAL:HG11	1.97	0.45
1:F:81:ASN:HB3	1:F:84:LEU:HD13	1.99	0.45
1:G:85:LEU:HA	1:G:86:PRO:HD3	1.84	0.45
1:C:240:VAL:HB	1:C:283:SER:HB2	1.99	0.45
1:D:125:GLY:HA3	1:D:129:ILE:HG21	1.98	0.45
2:J:206:ILE:HG13	2:J:207:PRO:HD2	1.97	0.45
2:L:116:LEU:HD23	2:L:116:LEU:H	1.82	0.45
2:L:296:SER:HB3	2:L:333:ASP:HB2	1.99	0.45
1:E:82:PRO:HA	1:E:85:LEU:HG	1.98	0.45
1:E:143:HIS:O	1:E:143:HIS:CG	2.70	0.45
1:E:197:ARG:NH1	1:G:281:LEU:O	2.50	0.45
1:F:61:PRO:HA	1:F:67:ILE:HA	1.99	0.45
1:F:89:GLU:OE1	1:F:89:GLU:N	2.46	0.45
1:H:243:VAL:HG22	1:H:312:ALA:HB3	1.99	0.45
2:I:49:SER:OG	2:I:50:ASP:N	2.49	0.45
2:J:49:SER:N	2:J:52:THR:O	2.49	0.45
1:D:174:GLY:HA3	1:D:247:VAL:HG12	1.99	0.45
1:H:201:ALA:O	1:H:205:ASN:ND2	2.45	0.45
2:L:163:ALA:O	2:L:164:GLU:HG3	2.17	0.45
1:B:82:PRO:HA	1:B:85:LEU:HG	1.98	0.45
1:B:170:GLY:O	1:B:250:SER:N	2.48	0.45
1:E:129:ILE:CG2	1:E:147:ILE:HG22	2.47	0.45
1:F:85:LEU:HD13	1:F:87:TRP:CZ2	2.52	0.45
2:I:29:VAL:HG22	2:I:306:GLN:HG2	1.98	0.45
2:J:261:GLU:HG3	2:J:272:VAL:HB	1.99	0.45
2:L:180:LYS:HA	2:L:183:PHE:HB3	1.98	0.45
1:D:36:THR:HB	1:D:80:ARG:NH1	2.32	0.45
1:E:220:VAL:HG23	1:E:221:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ASP:HB3	1:E:311:ILE:HG12	1.99	0.45
2:I:148:ILE:HG22	2:I:152:VAL:HG13	1.99	0.45
2:L:332:ARG:HA	2:L:335:TYR:CE2	2.51	0.45
1:A:193:HIS:NE2	3:P:74:ARG:O	2.45	0.44
1:E:143:HIS:O	1:E:143:HIS:ND1	2.50	0.44
1:G:174:GLY:HA3	1:G:247:VAL:HG23	1.98	0.44
1:H:9:PHE:HB3	1:H:35:ASP:HB2	1.98	0.44
2:I:144:ILE:HD11	2:I:331:ILE:HD11	1.98	0.44
1:A:59:VAL:HG22	1:A:69:VAL:HG12	2.00	0.44
1:H:157:CYS:HA	1:H:293:THR:HG22	2.00	0.44
1:B:153:CYS:HB3	4:B:401:NAD:C4N	2.46	0.44
2:I:145:TYR:HB3	2:I:197:VAL:HG12	1.98	0.44
2:K:253:TYR:CG	2:K:254:PRO:HA	2.52	0.44
1:B:47:LYS:HD3	1:B:59:VAL:HB	1.99	0.44
1:F:121:ILE:HG22	1:F:123:ALA:H	1.81	0.44
1:F:256:GLU:OE2	1:F:256:GLU:N	2.50	0.44
2:L:34:ALA:HB1	2:L:47:LEU:HD13	1.99	0.44
1:B:238:PRO:HG3	1:C:204:LEU:HD11	1.99	0.44
1:C:185:ASP:OD2	1:C:198:ARG:NH2	2.50	0.44
1:F:180:HIS:HA	1:F:241:SER:HB3	1.99	0.44
1:G:263:ARG:NH2	1:G:278:ASP:OD1	2.46	0.44
1:F:7:ASN:HA	1:F:34:ASN:HB3	1.99	0.44
1:F:17:LEU:HD12	1:F:46:LEU:HD11	1.98	0.44
1:F:306:ASP:OD1	1:H:173:LYS:HE3	2.18	0.44
2:I:296:SER:OG	2:I:333:ASP:HB2	2.18	0.44
1:E:79:ASN:HB3	1:E:85:LEU:HD21	2.00	0.44
2:I:50:ASP:N	2:I:50:ASP:OD1	2.50	0.44
2:K:318:ASN:OD1	2:K:320:THR:OG1	2.35	0.44
3:N:17:GLU:O	3:N:21:THR:OG1	2.30	0.44
1:B:193:HIS:HB3	1:B:199:ALA:HB2	1.99	0.44
1:E:264:ASP:HB2	1:E:268:LYS:NZ	2.33	0.44
1:H:197:ARG:HD3	1:H:208:PRO:O	2.18	0.44
4:E:401:NAD:H2D	4:E:401:NAD:H2N	1.52	0.44
1:F:104:ASP:OD1	1:F:104:ASP:N	2.50	0.44
1:H:82:PRO:HA	1:H:85:LEU:HG	2.00	0.44
2:I:21:THR:O	2:I:25:ARG:HG3	2.17	0.44
2:I:22:PHE:HD2	2:I:324:GLN:HG2	1.82	0.44
2:I:68:ARG:NH1	2:I:104:TYR:HH	2.13	0.44
1:A:50:SER:HA	1:B:284:VAL:HG21	1.99	0.43
1:B:280:PRO:HB2	1:D:197:ARG:HG3	1.99	0.43
1:C:182:TYR:CD2	1:C:236:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:HIS:ND1	1:E:143:HIS:C	2.72	0.43
1:E:284:VAL:HG21	1:F:50:SER:HA	1.99	0.43
2:I:72:LYS:HB3	3:O:29:GLY:HA3	1.99	0.43
1:B:269:GLU:HB3	5:B:502:HOH:O	2.17	0.43
4:C:401:NAD:H2D	4:C:401:NAD:H2N	1.74	0.43
1:E:67:ILE:HG12	1:E:74:ILE:HG22	1.99	0.43
1:G:240:VAL:HG11	1:G:286:PHE:HB2	2.00	0.43
2:K:237:GLY:HA2	2:L:247:ARG:HH21	1.83	0.43
2:K:248:LYS:HD3	2:K:248:LYS:HA	1.71	0.43
2:L:132:PHE:O	2:L:137:ARG:NH2	2.51	0.43
3:M:17:GLU:O	3:M:21:THR:HG23	2.19	0.43
1:A:254:PHE:HB3	2:I:300:TYR:O	2.18	0.43
1:E:161:PHE:HA	1:E:164:VAL:HG12	2.00	0.43
1:E:276:VAL:HG12	1:E:297:SER:HB3	2.00	0.43
1:E:299:LEU:HD11	1:G:197:ARG:HH12	1.83	0.43
1:H:169:PHE:HB3	1:H:249:VAL:CG2	2.46	0.43
1:A:85:LEU:HD13	1:A:87:TRP:CZ2	2.53	0.43
1:H:4:VAL:HG21	1:H:28:LEU:HB3	1.99	0.43
2:I:165:ARG:HA	2:I:165:ARG:HD3	1.70	0.43
2:I:250:THR:OG1	2:I:281:ARG:NH2	2.50	0.43
2:J:128:LEU:HB3	2:J:187:ILE:HD11	2.00	0.43
3:O:12:GLU:OE2	3:O:16:LYS:NZ	2.49	0.43
1:B:87:TRP:CE3	1:B:92:ILE:HG13	2.53	0.43
1:C:121:ILE:HG12	1:C:122:THR:N	2.34	0.43
1:D:284:VAL:HG23	1:D:287:ARG:HE	1.83	0.43
1:E:145:GLU:HA	1:E:146:PRO:HD3	1.60	0.43
1:H:120:ILE:HG12	1:H:148:ILE:HD11	1.99	0.43
2:L:65:ARG:HD3	2:L:109:GLY:HA3	1.99	0.43
1:G:131:THR:HG23	1:G:151:ALA:HB2	2.00	0.43
1:G:151:ALA:O	1:G:320:TYR:HE2	2.02	0.43
1:H:126:LYS:NZ	2:J:50:ASP:OD2	2.52	0.43
2:K:239:THR:OG1	2:L:243:ILE:HG23	2.19	0.43
3:O:11:VAL:HG12	3:O:41:LEU:HB3	2.00	0.43
1:A:34:ASN:HA	1:A:77:VAL:O	2.19	0.43
1:F:193:HIS:HB3	1:F:199:ALA:HB2	2.00	0.43
1:C:38:GLY:HA2	5:C:503:HOH:O	2.17	0.43
1:E:271:LYS:HE3	1:E:271:LYS:HB3	1.85	0.43
1:H:262:PHE:O	1:H:266:ALA:N	2.47	0.43
1:A:177:THR:HG1	1:C:309:LYS:HZ1	1.56	0.43
1:A:224:LEU:HA	1:A:227:LYS:HD2	2.01	0.43
1:F:263:ARG:NH1	1:F:278:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:ASP:OD1	1:H:104:ASP:N	2.49	0.43
2:I:295:LEU:HD13	2:I:303:VAL:HG21	2.00	0.43
2:K:117:ILE:HD12	2:K:117:ILE:HA	1.76	0.43
2:L:154:PHE:CZ	2:L:158:ILE:HD11	2.54	0.43
2:L:327:VAL:O	2:L:331:ILE:HG12	2.19	0.43
1:B:61:PRO:HA	1:B:67:ILE:HA	2.00	0.43
4:D:401:NAD:H6N	4:D:401:NAD:H2D	1.81	0.43
1:F:178:THR:HA	1:F:243:VAL:HA	2.01	0.43
2:I:18:GLY:C	2:I:19:LYS:HG3	2.39	0.43
2:J:63:LEU:HD22	2:J:73:VAL:HG11	2.00	0.43
2:L:22:PHE:HD1	2:L:324:GLN:HG2	1.84	0.43
1:C:85:LEU:HD13	1:C:87:TRP:CZ2	2.54	0.42
1:E:2:LEU:HD12	1:E:2:LEU:H	1.84	0.42
1:E:11:ARG:HH22	1:E:51:THR:HB	1.83	0.42
1:F:315:ASP:HB3	1:F:319:GLY:H	1.85	0.42
1:G:180:HIS:CD2	1:G:316:ASN:HD22	2.37	0.42
1:G:193:HIS:HB3	1:G:199:ALA:HB2	2.01	0.42
2:K:57:LEU:HB2	2:K:127:GLY:HA3	2.00	0.42
2:K:240:ILE:HG12	2:L:242:TRP:CD1	2.54	0.42
1:E:23:ARG:NH2	1:E:326:ASP:OD1	2.52	0.42
1:E:26:SER:HA	1:E:27:PRO:HD3	1.93	0.42
1:G:118:LYS:NZ	1:G:143:HIS:O	2.49	0.42
2:I:19:LYS:CD	3:O:47:HIS:NE2	2.82	0.42
2:K:113:PRO:HA	2:K:114:PRO:HD3	1.89	0.42
3:O:12:GLU:O	3:O:16:LYS:HG3	2.19	0.42
1:C:4:VAL:HG11	1:C:28:LEU:HB3	2.00	0.42
1:G:144:ASP:OD1	1:G:144:ASP:N	2.52	0.42
1:C:118:LYS:HE3	1:C:118:LYS:HB2	1.85	0.42
1:E:4:VAL:HG21	1:E:28:LEU:HB3	2.00	0.42
2:K:191:LYS:HE2	2:K:265:TYR:OH	2.19	0.42
3:M:58:ASP:OD1	3:M:58:ASP:N	2.52	0.42
1:C:249:VAL:O	1:C:306:ASP:HB2	2.20	0.42
1:F:206:ILE:HB	1:H:283:SER:HB3	2.00	0.42
2:J:68:ARG:HA	2:J:73:VAL:HB	2.02	0.42
2:J:250:THR:O	2:J:281:ARG:NH1	2.45	0.42
3:N:58:ASP:N	3:N:58:ASP:OD1	2.53	0.42
1:A:178:THR:HA	1:A:243:VAL:HA	2.01	0.42
1:A:335:TRP:CD1	1:A:336:LYS:HG3	2.55	0.42
1:B:277:CYS:SG	1:B:278:ASP:N	2.93	0.42
1:F:97:GLU:OE2	1:F:99:THR:OG1	2.32	0.42
1:A:153:CYS:HB3	4:A:401:NAD:H5N	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:SER:HB2	1:D:205:ASN:HB2	2.02	0.42
1:F:145:GLU:HA	1:F:146:PRO:HD3	1.92	0.42
1:F:174:GLY:HA3	1:F:247:VAL:HG12	2.02	0.42
1:G:182:TYR:CD2	1:G:236:PRO:HA	2.55	0.42
1:G:187:ARG:HH22	3:N:74:ARG:NH1	2.04	0.42
1:H:178:THR:HA	1:H:243:VAL:HA	2.01	0.42
3:O:22:CYS:SG	3:O:35:TRP:NE1	2.89	0.42
1:A:121:ILE:HG22	1:A:123:ALA:H	1.85	0.42
1:C:281:LEU:HD11	1:D:48:TYR:CE2	2.55	0.42
1:E:121:ILE:HG22	1:E:123:ALA:H	1.83	0.42
2:J:153:LYS:HB3	2:J:153:LYS:HE2	1.89	0.42
2:L:65:ARG:HD2	2:L:109:GLY:CA	2.47	0.42
1:A:323:ARG:NH1	1:A:326:ASP:OD2	2.53	0.42
1:C:118:LYS:HD3	1:C:148:ILE:HD11	2.01	0.42
1:D:182:TYR:HD2	1:D:236:PRO:HA	1.84	0.42
2:I:197:VAL:HG22	2:I:220:ILE:HB	2.02	0.42
2:J:296:SER:OG	2:J:333:ASP:HB2	2.20	0.42
2:J:340:ALA:O	2:J:344:THR:HG22	2.20	0.42
2:L:265:TYR:HB2	2:L:270:VAL:HG21	2.00	0.42
1:A:14:ARG:NH2	1:D:190:ASP:O	2.53	0.41
1:H:132:TYR:HA	1:H:137:ASN:HD21	1.85	0.41
2:I:101:LYS:O	2:I:115:GLU:N	2.42	0.41
2:I:158:ILE:HD13	2:I:169:LEU:HD22	2.02	0.41
2:J:225:VAL:HB	2:J:228:PHE:HB3	2.01	0.41
1:A:254:PHE:HE2	1:A:256:GLU:HB2	1.84	0.41
1:A:323:ARG:HD3	1:A:323:ARG:HA	1.90	0.41
1:B:118:LYS:HE3	1:B:118:LYS:HB3	1.87	0.41
1:C:17:LEU:HD13	1:C:46:LEU:HD11	2.02	0.41
1:C:316:ASN:OD1	1:C:317:GLU:N	2.53	0.41
1:G:186:GLN:OE1	1:G:234:ARG:NH1	2.48	0.41
1:G:195:ASP:HB3	1:G:198:ARG:HD2	2.01	0.41
2:K:310:HIS:HB3	2:K:313:PHE:HD2	1.84	0.41
2:L:239:THR:HG22	2:L:262:PRO:HD2	2.02	0.41
2:J:37:PRO:HD3	2:J:46:THR:O	2.20	0.41
1:G:320:TYR:CD1	4:G:401:NAD:H5N	2.55	0.41
1:H:326:ASP:O	1:H:330:ILE:HG12	2.21	0.41
2:K:35:LYS:HD3	2:K:35:LYS:HA	1.86	0.41
2:K:94:LYS:HD2	2:K:139:LEU:HD22	2.02	0.41
2:J:105:ASN:ND2	2:J:108:THR:H	2.18	0.41
3:O:71:ASN:OD1	3:O:71:ASN:N	2.53	0.41
1:A:304:GLY:HA3	1:C:173:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ALA:HB1	1:F:204:LEU:HD13	2.02	0.41
1:G:24:LYS:HD3	1:G:24:LYS:HA	1.89	0.41
2:K:152:VAL:HG11	2:K:200:VAL:HG23	2.03	0.41
2:J:19:LYS:HA	3:M:47:HIS:CE1	2.56	0.41
1:A:154:THR:O	1:A:158:LEU:N	2.52	0.41
1:A:170:GLY:O	1:A:250:SER:N	2.45	0.41
1:B:181:SER:HB2	1:B:237:THR:O	2.20	0.41
1:C:179:THR:HB	1:C:242:VAL:HG22	2.03	0.41
1:C:241:SER:HB2	1:C:314:TYR:CZ	2.55	0.41
1:G:171:ILE:HD11	1:G:247:VAL:HG21	2.02	0.41
2:L:72:LYS:HD2	3:N:27:VAL:HG22	2.03	0.41
1:C:287:ARG:NH1	5:C:501:HOH:O	2.53	0.41
1:E:215:LYS:HE3	1:E:229:ASN:ND2	2.35	0.41
2:L:63:LEU:HD13	2:L:79:ARG:HG3	2.03	0.41
3:M:11:VAL:O	3:M:15:ILE:HG22	2.20	0.41
1:H:126:LYS:HB3	1:H:126:LYS:HE3	1.91	0.41
2:L:133:ASP:HB3	2:L:136:VAL:HG12	2.01	0.41
2:L:148:ILE:HB	2:L:153:LYS:HE3	2.03	0.41
1:E:163:LYS:HB2	1:E:221:LEU:HD21	2.03	0.41
1:G:35:ASP:OD1	4:G:401:NAD:O2B	2.29	0.41
2:J:53:THR:HB	2:J:120:PRO:HG3	2.03	0.41
2:J:247:ARG:HA	2:J:247:ARG:HD3	1.79	0.41
3:N:16:LYS:O	3:N:20:GLU:HG2	2.21	0.41
1:A:205:ASN:HB3	1:C:282:VAL:HG22	2.03	0.41
1:C:193:HIS:HB3	1:C:199:ALA:HB2	2.03	0.41
1:D:104:ASP:OD1	1:D:104:ASP:N	2.42	0.41
2:J:129:HIS:HB3	2:J:132:PHE:HB2	2.03	0.41
2:J:339:ILE:HA	2:J:342:LYS:HB2	2.02	0.41
1:A:130:PRO:HG3	1:A:145:GLU:HG2	2.02	0.40
1:B:109:GLY:O	1:B:112:ILE:HG12	2.20	0.40
1:B:240:VAL:HG13	1:B:283:SER:HB3	2.01	0.40
2:I:45:ASN:HB3	2:I:56:CYS:HB3	2.02	0.40
2:J:134:GLU:HA	2:J:137:ARG:HG2	2.03	0.40
3:N:63:TYR:HE2	3:N:70:THR:HG21	1.84	0.40
1:A:193:HIS:O	1:D:41:GLN:NE2	2.54	0.40
1:B:9:PHE:O	1:B:14:ARG:NH2	2.54	0.40
1:F:143:HIS:CD2	1:F:335:TRP:HA	2.56	0.40
3:N:35:TRP:HA	3:N:38:VAL:HG12	2.02	0.40
1:F:238:PRO:HB3	1:G:204:LEU:HD11	2.04	0.40
1:H:87:TRP:HA	1:H:92:ILE:HD13	2.04	0.40
3:O:16:LYS:O	3:O:20:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HD3	1:A:115:GLY:HA3	2.02	0.40
1:D:85:LEU:HD13	1:D:87:TRP:CZ2	2.56	0.40
1:E:37:GLY:HA2	3:M:60:LEU:HD11	2.03	0.40
1:F:11:ARG:HH12	1:F:49:ASP:CG	2.24	0.40
1:G:112:ILE:HA	1:G:116:ALA:O	2.21	0.40
1:H:1:LYS:HE2	1:H:1:LYS:HB2	1.91	0.40
2:L:41:ASN:HD21	2:L:103:ILE:HD12	1.86	0.40
2:L:220:ILE:HG12	2:L:272:VAL:HG13	2.03	0.40
3:M:74:ARG:HB3	3:M:76:TYR:CE2	2.56	0.40
1:E:30:ILE:HG22	1:E:74:ILE:HD11	2.02	0.40
1:H:153:CYS:HG	1:H:180:HIS:HE2	1.67	0.40
2:L:7:ILE:HD11	2:L:338:LEU:HD22	2.01	0.40
3:N:58:ASP:HA	3:N:59:PRO:HD3	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	334/339 (98%)	319 (96%)	15 (4%)	0	100	100
1	B	334/339 (98%)	320 (96%)	14 (4%)	0	100	100
1	C	334/339 (98%)	326 (98%)	8 (2%)	0	100	100
1	D	333/339 (98%)	324 (97%)	9 (3%)	0	100	100
1	E	334/339 (98%)	321 (96%)	13 (4%)	0	100	100
1	F	334/339 (98%)	325 (97%)	9 (3%)	0	100	100
1	G	334/339 (98%)	324 (97%)	10 (3%)	0	100	100
1	H	334/339 (98%)	324 (97%)	10 (3%)	0	100	100
2	I	340/352 (97%)	324 (95%)	16 (5%)	0	100	100
2	J	340/352 (97%)	326 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
2	L	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
3	M	71/80 (89%)	69 (97%)	2 (3%)	0	100	100
3	N	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
3	O	70/80 (88%)	69 (99%)	1 (1%)	0	100	100
3	P	70/80 (88%)	70 (100%)	0	0	100	100
All	All	4313/4440 (97%)	4176 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	279/281 (99%)	266 (95%)	13 (5%)	26	60
1	B	279/281 (99%)	268 (96%)	11 (4%)	32	64
1	C	279/281 (99%)	265 (95%)	14 (5%)	24	58
1	D	278/281 (99%)	269 (97%)	9 (3%)	39	69
1	E	279/281 (99%)	268 (96%)	11 (4%)	32	64
1	F	279/281 (99%)	268 (96%)	11 (4%)	32	64
1	G	279/281 (99%)	272 (98%)	7 (2%)	47	75
1	H	279/281 (99%)	273 (98%)	6 (2%)	52	78
2	I	300/305 (98%)	287 (96%)	13 (4%)	29	62
2	J	300/305 (98%)	289 (96%)	11 (4%)	34	65
2	K	300/305 (98%)	292 (97%)	8 (3%)	44	73
2	L	299/305 (98%)	285 (95%)	14 (5%)	26	60
3	M	60/64 (94%)	58 (97%)	2 (3%)	38	68
3	N	60/64 (94%)	53 (88%)	7 (12%)	5	26
3	O	58/64 (91%)	57 (98%)	1 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	59/64 (92%)	54 (92%)	5 (8%)	10	39
All	All	3667/3724 (98%)	3524 (96%)	143 (4%)	32	64

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	17	LEU
1	A	55	PHE
1	A	87	TRP
1	A	103	VAL
1	A	144	ASP
1	A	171	ILE
1	A	176	MET
1	A	178	THR
1	A	221	LEU
1	A	247	VAL
1	A	293	THR
1	A	311	ILE
1	B	69	VAL
1	B	76	VAL
1	B	94	ILE
1	B	122	THR
1	B	165	LEU
1	B	169	PHE
1	B	178	THR
1	B	207	VAL
1	B	220	VAL
1	B	281	LEU
1	B	293	THR
1	C	9	PHE
1	C	55	PHE
1	C	58	ASP
1	C	65	THR
1	C	69	VAL
1	C	121	ILE
1	C	148	ILE
1	C	150	ASN
1	C	154	THR
1	C	155	THR
1	C	178	THR
1	C	190	ASP

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Mol	Chain	Res	Type
1	C	282	VAL
1	C	294	THR
1	D	31	ILE
1	D	46	LEU
1	D	137	ASN
1	D	144	ASP
1	D	155	THR
1	D	165	LEU
1	D	178	THR
1	D	246	VAL
1	D	293	THR
1	E	74	ILE
1	E	99	THR
1	E	104	ASP
1	E	136	VAL
1	E	144	ASP
1	E	157	CYS
1	E	178	THR
1	E	234	ARG
1	E	292	SER
1	E	293	THR
1	E	296	ASP
1	F	45	LEU
1	F	51	THR
1	F	119	VAL
1	F	136	VAL
1	F	139	ASP
1	F	158	LEU
1	F	178	THR
1	F	207	VAL
1	F	221	LEU
1	F	223	ASN
1	F	331	VAL
1	G	178	THR
1	G	188	LEU
1	G	231	ILE
1	G	242	VAL
1	G	264	ASP
1	G	277	CYS
1	G	293	THR
1	H	129	ILE
1	H	143	HIS

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Mol	Chain	Res	Type
1	H	154	THR
1	H	284	VAL
1	H	290	ASP
1	H	293	THR
2	I	6	THR
2	I	11	LEU
2	I	54	VAL
2	I	56	CYS
2	I	73	VAL
2	I	108	THR
2	I	118	GLN
2	I	124	VAL
2	I	162	MET
2	I	188	ASP
2	I	192	GLN
2	I	218	ARG
2	I	219	LEU
2	K	11	LEU
2	K	61	HIS
2	K	76	LEU
2	K	184	ASP
2	K	197	VAL
2	K	206	ILE
2	K	214	VAL
2	K	297	THR
2	J	22	PHE
2	J	50	ASP
2	J	56	CYS
2	J	117	ILE
2	J	184	ASP
2	J	192	GLN
2	J	203	THR
2	J	205	LEU
2	J	209	ASP
2	J	275	MET
2	J	329	LEU
2	L	110	LEU
2	L	116	LEU
2	L	123	LEU
2	L	129	HIS
2	L	184	ASP
2	L	219	LEU

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Mol	Chain	Res	Type
2	L	243	ILE
2	L	250	THR
2	L	297	THR
2	L	300	TYR
2	L	308	LEU
2	L	318	ASN
2	L	330	LYS
2	L	334	LEU
3	M	55	ASP
3	M	78	ASN
3	N	21	THR
3	N	27	VAL
3	N	31	CYS
3	N	39	GLU
3	N	40	GLU
3	N	69	GLU
3	N	71	ASN
3	O	71	ASN
3	P	7	ILE
3	P	10	VAL
3	P	25	ASP
3	P	37	GLU
3	P	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	316	ASN
1	C	150	ASN
1	C	156	ASN
1	D	41	GLN
1	D	111	HIS
1	F	316	ASN
1	G	248	GLN
3	M	78	ASN
3	N	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	#$|Z| > 2$
4	NAD	B	401	-	42,48,48	0.80	1 (2%)	50,73,73	1.19	5 (10%)
4	NAD	E	401	-	42,48,48	0.81	1 (2%)	50,73,73	1.25	5 (10%)
4	NAD	F	401	-	42,48,48	0.81	1 (2%)	50,73,73	1.23	5 (10%)
4	NAD	A	401	-	42,48,48	0.82	1 (2%)	50,73,73	1.26	5 (10%)
4	NAD	C	401	-	42,48,48	2.59	24 (57%)	50,73,73	2.57	18 (36%)
4	NAD	H	401	-	42,48,48	0.81	1 (2%)	50,73,73	1.08	4 (8%)
4	NAD	G	401	-	42,48,48	0.81	1 (2%)	50,73,73	1.20	4 (8%)
4	NAD	D	401	-	42,48,48	0.81	1 (2%)	50,73,73	1.25	5 (10%)

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
4	NAD	B	401	-	-	6/26/62/62	0/5/5/5
4	NAD	E	401	-	-	8/26/62/62	0/5/5/5
4	NAD	F	401	-	-	10/26/62/62	0/5/5/5
4	NAD	A	401	-	-	11/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	C	401	-	-	11/26/62/62	0/5/5/5
4	NAD	H	401	-	-	3/26/62/62	0/5/5/5
4	NAD	G	401	-	-	11/26/62/62	0/5/5/5
4	NAD	D	401	-	-	11/26/62/62	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NAD	C2D-C1D	-6.90	1.43	1.53
4	C	401	NAD	O7N-C7N	-4.39	1.15	1.24
4	C	401	NAD	O4D-C4D	-4.14	1.35	1.45
4	C	401	NAD	PN-O1N	-3.99	1.36	1.50
4	C	401	NAD	C4A-N3A	-3.96	1.30	1.35
4	C	401	NAD	PN-O2N	-3.84	1.37	1.55
4	C	401	NAD	C4N-C3N	-3.45	1.33	1.39
4	C	401	NAD	C3D-C4D	-3.39	1.44	1.53
4	C	401	NAD	O4D-C1D	-3.09	1.36	1.41
4	C	401	NAD	C5A-N7A	-2.96	1.29	1.39
4	C	401	NAD	PN-O5D	-2.96	1.47	1.59
4	C	401	NAD	C2N-N1N	-2.85	1.31	1.35
4	C	401	NAD	C7N-N7N	-2.64	1.27	1.33
4	C	401	NAD	C6N-N1N	-2.63	1.29	1.35
4	C	401	NAD	C2B-C3B	-2.63	1.46	1.53
4	C	401	NAD	O4B-C4B	-2.61	1.39	1.45
4	C	401	NAD	C3N-C7N	-2.60	1.46	1.50
4	C	401	NAD	PA-O5B	-2.60	1.48	1.59
4	C	401	NAD	C2B-C1B	-2.55	1.49	1.53
4	C	401	NAD	O3D-C3D	-2.53	1.37	1.43
4	A	401	NAD	C5A-C4A	2.52	1.47	1.40
4	F	401	NAD	C5A-C4A	2.48	1.47	1.40
4	E	401	NAD	C5A-C4A	2.48	1.47	1.40
4	D	401	NAD	C5A-C4A	2.47	1.47	1.40
4	G	401	NAD	C5A-C4A	2.45	1.47	1.40
4	H	401	NAD	C5A-C4A	2.45	1.47	1.40
4	B	401	NAD	C5A-C4A	2.44	1.47	1.40
4	C	401	NAD	O5B-C5B	-2.42	1.35	1.44
4	C	401	NAD	O5D-C5D	-2.13	1.36	1.44
4	C	401	NAD	O4B-C1B	-2.11	1.38	1.41
4	C	401	NAD	C3B-C4B	-2.01	1.47	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	NAD	O4B-C1B-C2B	-7.86	95.45	106.93
4	C	401	NAD	O3D-C3D-C4D	-7.24	90.13	111.05
4	C	401	NAD	O4D-C1D-C2D	-6.98	96.73	106.93
4	C	401	NAD	O7N-C7N-N7N	-4.65	115.97	122.58
4	C	401	NAD	N3A-C2A-N1A	-4.10	122.27	128.68
4	D	401	NAD	PN-O3-PA	-3.70	120.13	132.83
4	C	401	NAD	PN-O3-PA	-3.65	120.29	132.83
4	C	401	NAD	O4D-C4D-C3D	-3.47	98.25	105.11
4	F	401	NAD	PN-O3-PA	-3.34	121.36	132.83
4	E	401	NAD	N3A-C2A-N1A	-3.33	123.47	128.68
4	A	401	NAD	PN-O3-PA	-3.31	121.45	132.83
4	F	401	NAD	C3B-C2B-C1B	3.28	105.92	100.98
4	A	401	NAD	N3A-C2A-N1A	-3.25	123.59	128.68
4	A	401	NAD	C3D-C2D-C1D	3.24	105.86	100.98
4	B	401	NAD	N3A-C2A-N1A	-3.23	123.62	128.68
4	C	401	NAD	C3N-C7N-N7N	3.23	121.63	117.75
4	B	401	NAD	PN-O3-PA	-3.23	121.75	132.83
4	B	401	NAD	C3D-C2D-C1D	3.22	105.83	100.98
4	G	401	NAD	N3A-C2A-N1A	-3.22	123.65	128.68
4	D	401	NAD	N3A-C2A-N1A	-3.21	123.66	128.68
4	F	401	NAD	N3A-C2A-N1A	-3.19	123.69	128.68
4	H	401	NAD	N3A-C2A-N1A	-3.14	123.77	128.68
4	G	401	NAD	PN-O3-PA	-3.14	122.06	132.83
4	H	401	NAD	C3B-C2B-C1B	3.12	105.67	100.98
4	E	401	NAD	PN-O3-PA	-3.01	122.48	132.83
4	C	401	NAD	C4A-C5A-N7A	-2.99	106.29	109.40
4	C	401	NAD	C5B-C4B-C3B	-2.98	104.01	115.18
4	C	401	NAD	O2B-C2B-C1B	2.91	121.61	110.85
4	F	401	NAD	C3D-C2D-C1D	2.90	105.34	100.98
4	A	401	NAD	C4A-C5A-N7A	-2.89	106.39	109.40
4	C	401	NAD	C2B-C3B-C4B	-2.82	97.15	102.64
4	E	401	NAD	C3D-C2D-C1D	2.79	105.18	100.98
4	A	401	NAD	C3B-C2B-C1B	2.76	105.14	100.98
4	G	401	NAD	C4A-C5A-N7A	-2.74	106.54	109.40
4	E	401	NAD	C4A-C5A-N7A	-2.74	106.55	109.40
4	B	401	NAD	C4A-C5A-N7A	-2.73	106.56	109.40
4	D	401	NAD	C4A-C5A-N7A	-2.69	106.59	109.40
4	H	401	NAD	PN-O3-PA	-2.69	123.58	132.83
4	C	401	NAD	O5B-C5B-C4B	-2.69	99.75	108.99
4	D	401	NAD	C3B-C2B-C1B	2.66	104.98	100.98
4	F	401	NAD	C4A-C5A-N7A	-2.65	106.63	109.40
4	E	401	NAD	C3B-C2B-C1B	2.59	104.89	100.98
4	G	401	NAD	C3B-C2B-C1B	2.58	104.86	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	NAD	C2D-C3D-C4D	2.57	107.64	102.64
4	H	401	NAD	C4A-C5A-N7A	-2.54	106.75	109.40
4	C	401	NAD	O2D-C2D-C1D	-2.35	102.18	110.85
4	C	401	NAD	C5A-C6A-N6A	2.34	123.90	120.35
4	C	401	NAD	O7N-C7N-C3N	2.28	122.36	119.63
4	C	401	NAD	O2N-PN-O1N	2.19	123.06	112.24
4	B	401	NAD	C3B-C2B-C1B	2.08	104.12	100.98
4	D	401	NAD	C5D-C4D-C3D	-2.08	107.39	115.18

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAD	C5B-O5B-PA-O3
4	A	401	NAD	C5D-O5D-PN-O1N
4	A	401	NAD	O4D-C1D-N1N-C2N
4	A	401	NAD	O4D-C1D-N1N-C6N
4	A	401	NAD	C2D-C1D-N1N-C2N
4	A	401	NAD	C2D-C1D-N1N-C6N
4	B	401	NAD	C5B-O5B-PA-O1A
4	B	401	NAD	C5B-O5B-PA-O2A
4	B	401	NAD	C3B-C4B-C5B-O5B
4	B	401	NAD	O4D-C1D-N1N-C2N
4	C	401	NAD	C5B-O5B-PA-O1A
4	C	401	NAD	O4D-C1D-N1N-C2N
4	C	401	NAD	O4D-C1D-N1N-C6N
4	C	401	NAD	C2D-C1D-N1N-C2N
4	C	401	NAD	C2D-C1D-N1N-C6N
4	C	401	NAD	C2N-C3N-C7N-N7N
4	D	401	NAD	C5D-O5D-PN-O3
4	D	401	NAD	C2D-C1D-N1N-C2N
4	D	401	NAD	C2D-C1D-N1N-C6N
4	D	401	NAD	C2N-C3N-C7N-O7N
4	D	401	NAD	C2N-C3N-C7N-N7N
4	E	401	NAD	C5D-O5D-PN-O3
4	E	401	NAD	C5D-O5D-PN-O2N
4	E	401	NAD	O4D-C1D-N1N-C6N
4	E	401	NAD	C2D-C1D-N1N-C6N
4	F	401	NAD	C5B-O5B-PA-O2A
4	F	401	NAD	C5B-O5B-PA-O3
4	F	401	NAD	C5D-O5D-PN-O1N
4	F	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	F	401	NAD	O4D-C1D-N1N-C6N
4	G	401	NAD	O4D-C1D-N1N-C2N
4	G	401	NAD	O4D-C1D-N1N-C6N
4	G	401	NAD	C2D-C1D-N1N-C2N
4	G	401	NAD	C2D-C1D-N1N-C6N
4	G	401	NAD	C2N-C3N-C7N-O7N
4	G	401	NAD	C2N-C3N-C7N-N7N
4	C	401	NAD	C4N-C3N-C7N-O7N
4	D	401	NAD	C4N-C3N-C7N-O7N
4	D	401	NAD	C4N-C3N-C7N-N7N
4	C	401	NAD	C4N-C3N-C7N-N7N
4	C	401	NAD	C2N-C3N-C7N-O7N
4	A	401	NAD	O4D-C4D-C5D-O5D
4	E	401	NAD	O4B-C4B-C5B-O5B
4	H	401	NAD	O4B-C4B-C5B-O5B
4	H	401	NAD	C3B-C4B-C5B-O5B
4	G	401	NAD	C4N-C3N-C7N-O7N
4	G	401	NAD	C4N-C3N-C7N-N7N
4	A	401	NAD	C3D-C4D-C5D-O5D
4	B	401	NAD	O4B-C4B-C5B-O5B
4	E	401	NAD	C3B-C4B-C5B-O5B
4	A	401	NAD	C3B-C4B-C5B-O5B
4	F	401	NAD	PN-O3-PA-O1A
4	F	401	NAD	C5D-O5D-PN-O3
4	C	401	NAD	O4B-C4B-C5B-O5B
4	C	401	NAD	C3B-C4B-C5B-O5B
4	A	401	NAD	C5B-O5B-PA-O2A
4	D	401	NAD	C5D-O5D-PN-O1N
4	D	401	NAD	C3D-C4D-C5D-O5D
4	F	401	NAD	C3B-C4B-C5B-O5B
4	E	401	NAD	O4D-C4D-C5D-O5D
4	D	401	NAD	O4B-C4B-C5B-O5B
4	B	401	NAD	C5B-O5B-PA-O3
4	E	401	NAD	C2D-C1D-N1N-C2N
4	F	401	NAD	C2D-C1D-N1N-C6N
4	A	401	NAD	O4B-C4B-C5B-O5B
4	D	401	NAD	PA-O3-PN-O1N
4	F	401	NAD	PN-O3-PA-O2A
4	G	401	NAD	PN-O3-PA-O2A
4	G	401	NAD	C5B-O5B-PA-O1A
4	G	401	NAD	O4B-C4B-C5B-O5B
4	H	401	NAD	C2N-C3N-C7N-N7N

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAD	2	0
4	E	401	NAD	1	0
4	F	401	NAD	1	0
4	A	401	NAD	1	0
4	C	401	NAD	5	0
4	H	401	NAD	2	0
4	G	401	NAD	2	0
4	D	401	NAD	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 NAD B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD H 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	336/339 (99%)	-0.22	1 (0%)	94	91	21, 35, 52, 79	0
1	B	336/339 (99%)	-0.17	0	100	100	20, 32, 48, 72	0
1	C	336/339 (99%)	-0.16	0	100	100	22, 36, 55, 66	0
1	D	335/339 (98%)	-0.11	0	100	100	19, 39, 60, 83	0
1	E	336/339 (99%)	-0.04	1 (0%)	94	91	22, 50, 78, 92	0
1	F	336/339 (99%)	-0.17	0	100	100	19, 37, 52, 69	0
1	G	336/339 (99%)	-0.17	0	100	100	17, 31, 46, 64	0
1	H	336/339 (99%)	-0.15	0	100	100	23, 40, 59, 79	0
2	I	342/352 (97%)	0.02	3 (0%)	84	79	37, 64, 91, 155	0
2	J	342/352 (97%)	0.27	11 (3%)	47	42	35, 82, 124, 142	0
2	K	342/352 (97%)	0.09	7 (2%)	65	60	33, 68, 99, 112	0
2	L	342/352 (97%)	0.26	13 (3%)	40	36	38, 87, 127, 168	3 (0%)
3	M	73/80 (91%)	0.66	9 (12%)	4	5	42, 148, 174, 188	0
3	N	73/80 (91%)	0.69	8 (10%)	5	6	30, 138, 169, 174	0
3	O	72/80 (90%)	0.22	2 (2%)	53	47	26, 91, 121, 176	0
3	P	72/80 (90%)	0.21	2 (2%)	53	47	42, 101, 135, 162	2 (2%)
All	All	4345/4440 (97%)	-0.01	57 (1%)	77	71	17, 45, 114, 188	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	63	LEU	5.7
3	N	37	GLU	5.6
2	I	19	LYS	4.9
2	J	73	VAL	4.2
3	N	29	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	K	346	ARG	4.2
2	L	74	THR	4.2
2	L	62	SER	4.1
3	M	28	SER	3.9
3	N	36	ASP	3.9
3	M	55	ASP	3.7
3	N	20	GLU	3.6
2	L	14	ASP	3.4
3	N	38	VAL	3.3
2	J	112	ASP	3.2
3	M	6	GLY	3.1
2	I	74	THR	3.0
3	P	31	CYS	3.0
3	N	41	LEU	2.8
2	J	14	ASP	2.8
2	K	343	ALA	2.7
2	K	126	GLU	2.6
2	L	65	ARG	2.6
2	L	160	ARG	2.6
3	M	54	ALA	2.5
2	J	69	LYS	2.5
3	M	39	GLU	2.5
3	M	36	ASP	2.4
2	J	208	ASP	2.4
2	L	68	ARG	2.4
2	K	19	LYS	2.4
2	L	88	GLU	2.3
2	J	115	GLU	2.3
2	L	5	GLU	2.3
2	K	345	ALA	2.2
2	L	210	ASN	2.2
2	J	111	LEU	2.2
2	K	76	LEU	2.2
3	N	8	SER	2.2
3	N	30	GLU	2.1
3	M	27	VAL	2.1
2	L	23	MET	2.1
3	O	55	ASP	2.1
2	J	159	GLN	2.1
2	J	160	ARG	2.1
2	J	77	ASP	2.1
3	O	27	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	34	ASN	2.0
2	J	247	ARG	2.0
2	L	81	ASN	2.0
3	P	26	PRO	2.0
2	I	208	ASP	2.0
3	M	48	ALA	2.0
1	A	304	GLY	2.0
2	L	73	VAL	2.0
3	M	45	ALA	2.0
2	K	63	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
4	NAD	D	401	44/44	0.89	0.33	45,52,61,65	0
4	NAD	E	401	44/44	0.91	0.30	58,66,72,76	0
4	NAD	G	401	44/44	0.92	0.26	31,31,39,43	0
4	NAD	B	401	44/44	0.94	0.20	32,32,38,45	0
4	NAD	A	401	44/44	0.94	0.26	34,34,41,44	0
4	NAD	H	401	44/44	0.94	0.27	37,40,50,53	0
4	NAD	C	401	44/44	0.95	0.21	30,30,43,47	0
4	NAD	F	401	44/44	0.95	0.21	32,32,32,43	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.
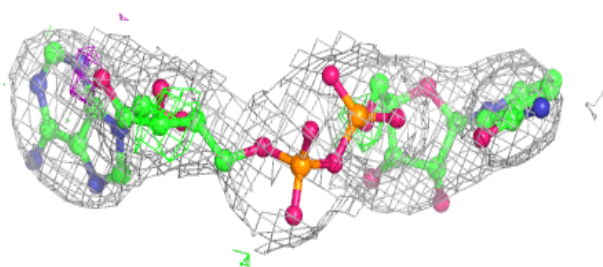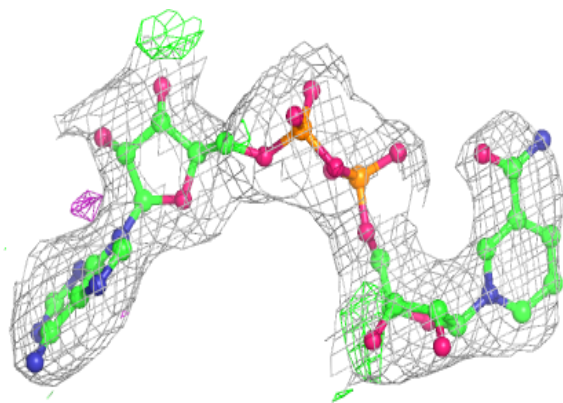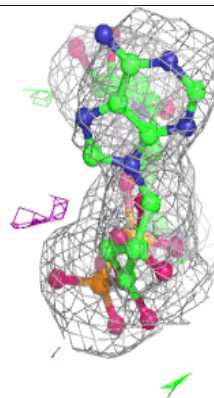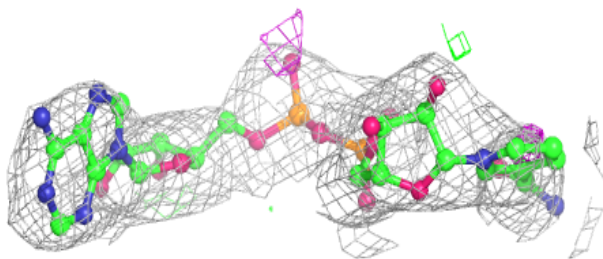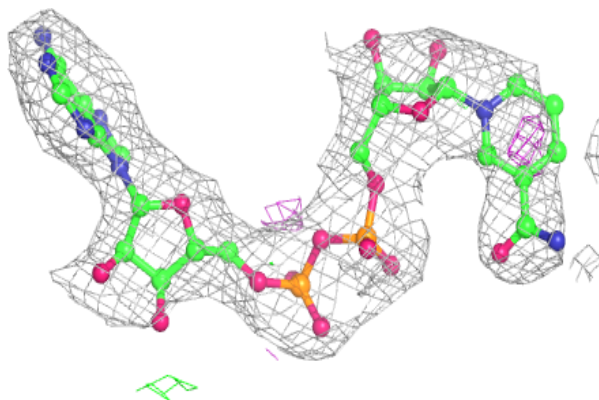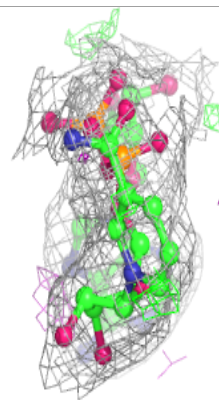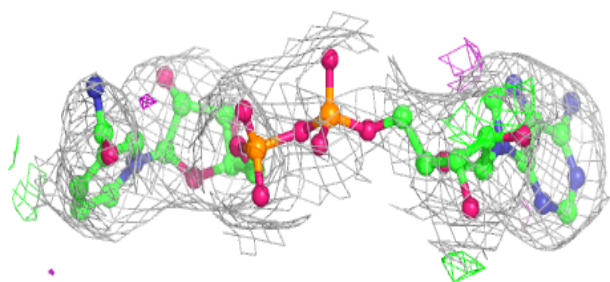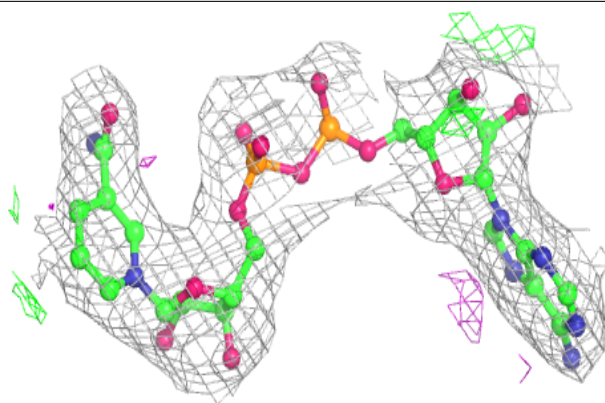
Electron density around NAD D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
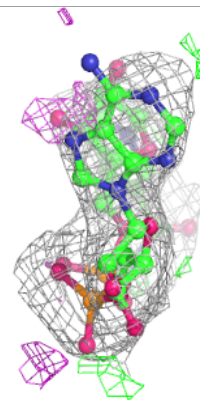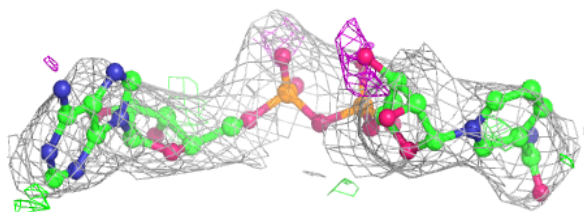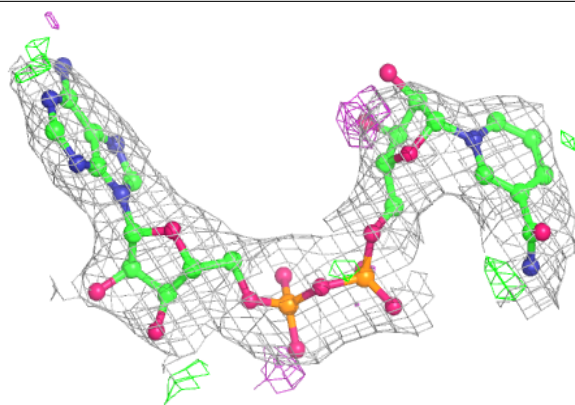
Electron density around NAD E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
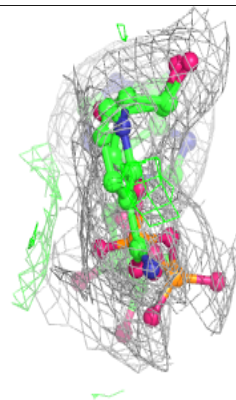mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
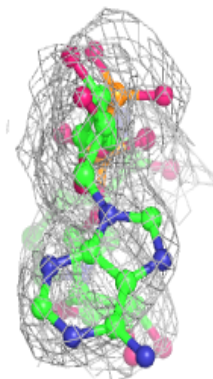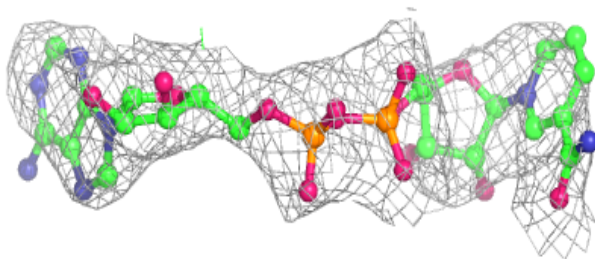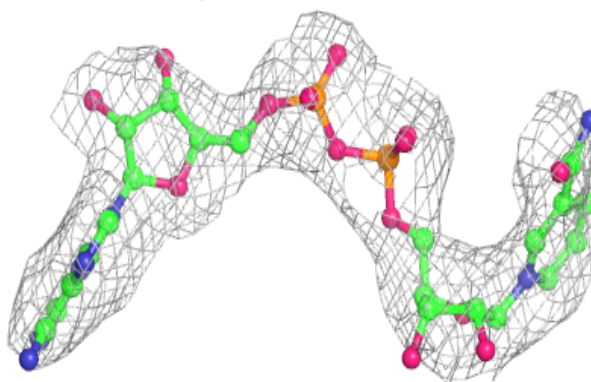
Electron density around NAD G 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
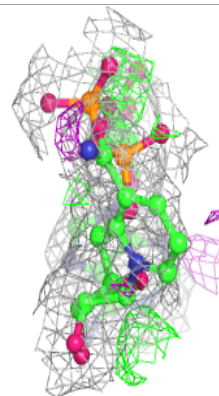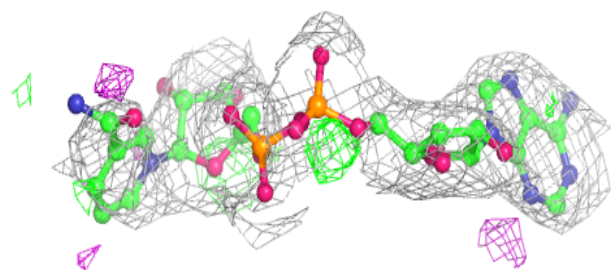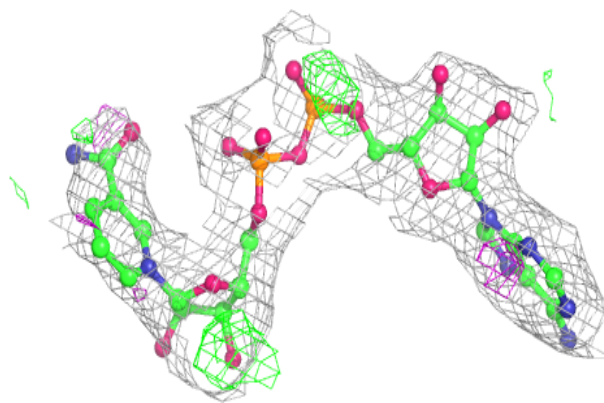
Electron density around NAD B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
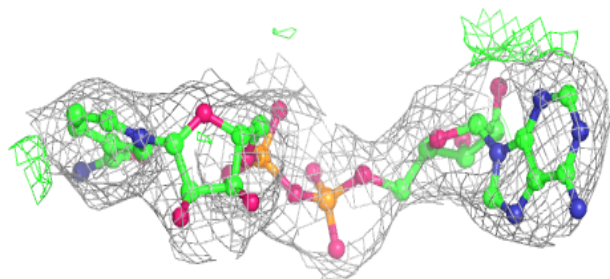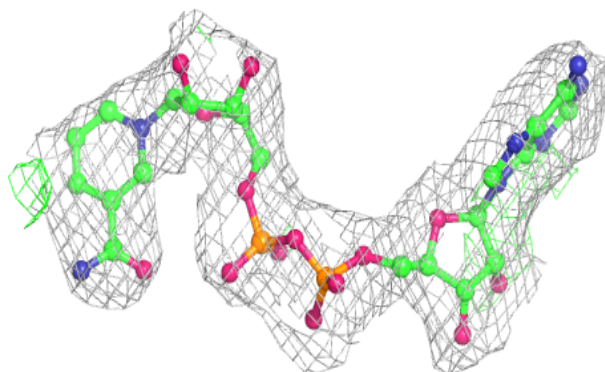and green (positive)
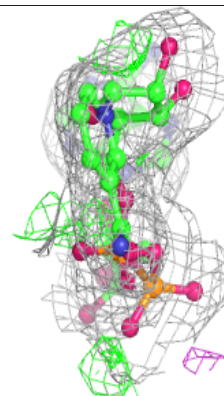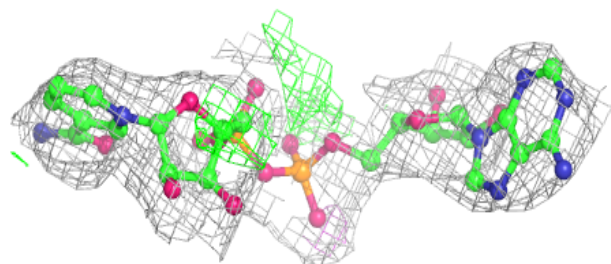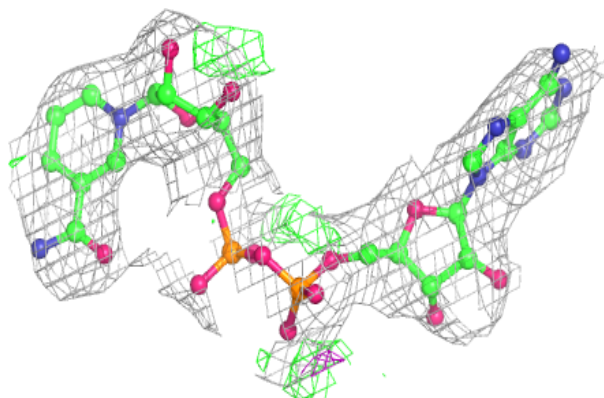
Electron density around NAD A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
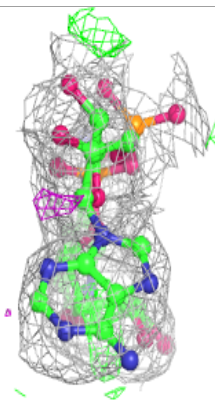
Electron density around NAD H 401:

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

Electron density around NAD C 401:

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

Electron density around NAD F 401:

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