WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 10:34 AM EDT

PDB ID	:	3OET
Title	:	D-Erythronate-4-Phosphate Dehydrogenase complexed with NAD
Authors	:	Filippova, E.V.; Wawrzak, Z.; Onopriyenko, O.; Savchenko, A.; Edwards, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on	:	2010-08-13
Resolution	:	2.36 Å(reported)

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

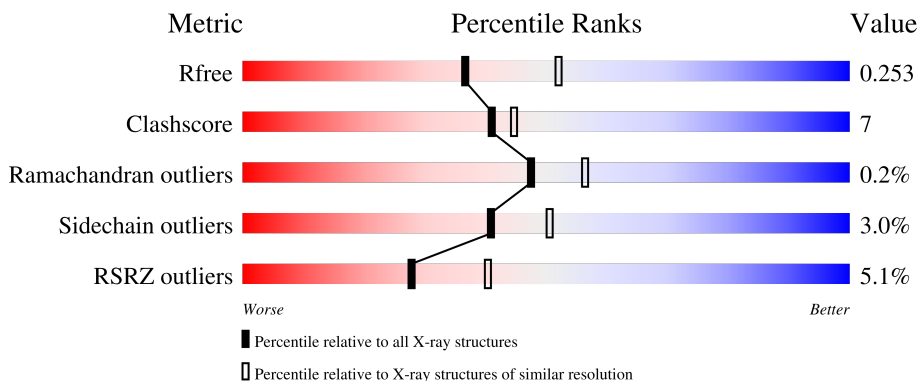|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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.
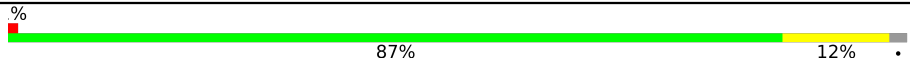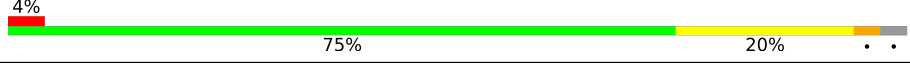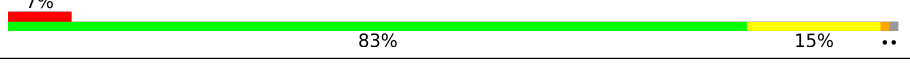
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		3.0%
RSRZ outliers		5.1%

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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	381	2% / 85% / 12% ··
1	B	381	4% / 82% / 15% ··
1	C	381	9% / 76% / 20% ··
1	D	381	4% / 88% / 10% ··

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Mol	Chain	Length	Quality of chain
1	E	381	% 87% 12%
1	F	381	8% 83% 12%
1	G	381	4% 75% 20%
1	H	381	7% 83% 15%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 23835 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 Erythronate-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	Se	0	1	0
			2888	1827	514	537	5	5			
1	B	377	Total	C	N	O	S	Se	0	1	0
			2894	1831	511	542	5	5			
1	C	372	Total	C	N	O	S	Se	0	3	0
			2865	1811	506	538	5	5			
1	D	375	Total	C	N	O	S	Se	0	0	0
			2867	1817	506	534	5	5			
1	E	375	Total	C	N	O	S	Se	0	0	0
			2880	1826	507	537	5	5			
1	F	365	Total	C	N	O	S	Se	0	0	0
			2791	1773	489	519	5	5			
1	G	370	Total	C	N	O	S	Se	0	0	0
			2843	1801	501	531	5	5			
1	H	378	Total	C	N	O	S	Se	0	0	0
			2897	1836	516	535	5	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P60802
A	-1	ASN	-	expression tag	UNP P60802
A	0	ALA	-	expression tag	UNP P60802
B	-2	SER	-	expression tag	UNP P60802
B	-1	ASN	-	expression tag	UNP P60802
B	0	ALA	-	expression tag	UNP P60802
C	-2	SER	-	expression tag	UNP P60802
C	-1	ASN	-	expression tag	UNP P60802
C	0	ALA	-	expression tag	UNP P60802
D	-2	SER	-	expression tag	UNP P60802
D	-1	ASN	-	expression tag	UNP P60802
D	0	ALA	-	expression tag	UNP P60802
E	-2	SER	-	expression tag	UNP P60802

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP P60802
E	0	ALA	-	expression tag	UNP P60802
F	-2	SER	-	expression tag	UNP P60802
F	-1	ASN	-	expression tag	UNP P60802
F	0	ALA	-	expression tag	UNP P60802
G	-2	SER	-	expression tag	UNP P60802
G	-1	ASN	-	expression tag	UNP P60802
G	0	ALA	-	expression tag	UNP P60802
H	-2	SER	-	expression tag	UNP P60802
H	-1	ASN	-	expression tag	UNP P60802
H	0	ALA	-	expression tag	UNP P60802

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)
  (formula: $C_{21}H_{27}N_7O_{14}P_2$).

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

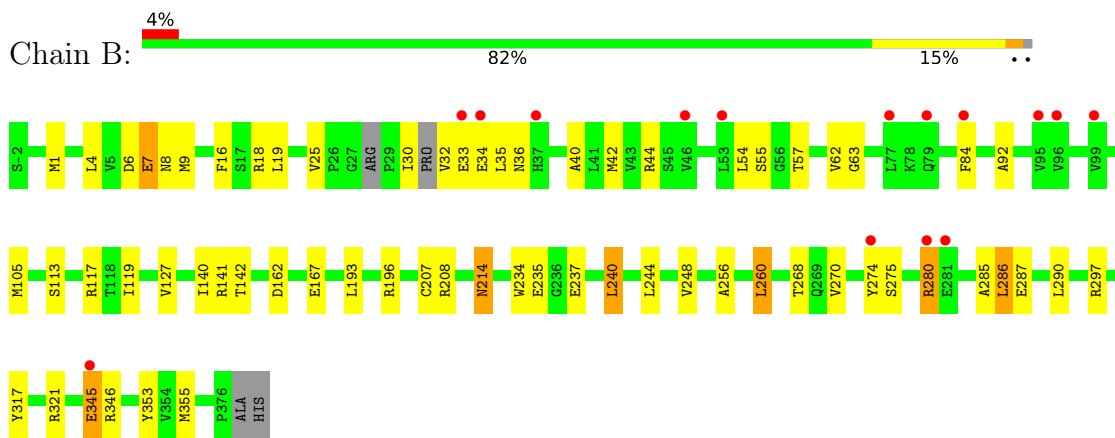| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	79	Total	O	0	3
			79	79		
3	C	78	Total	O	0	0
			78	78		
3	D	62	Total	O	0	0
			62	62		
3	E	91	Total	O	0	1
			91	91		
3	F	84	Total	O	0	1
			85	85		
3	G	47	Total	O	0	1
			48	48		
3	H	36	Total	O	0	0
			36	36		

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.
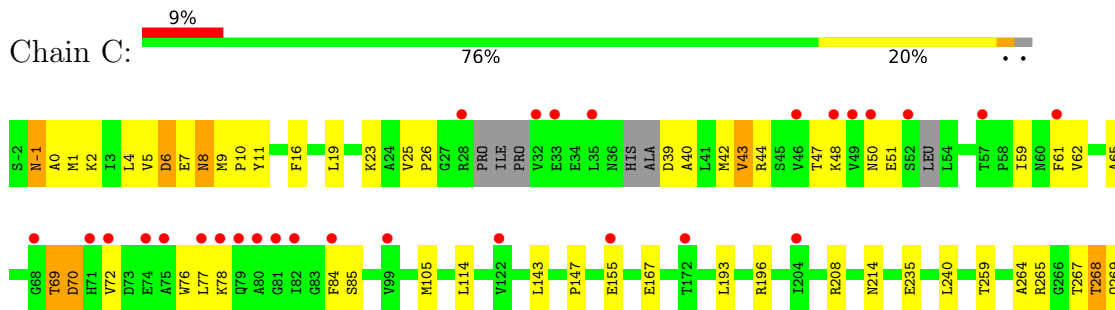
• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain A:
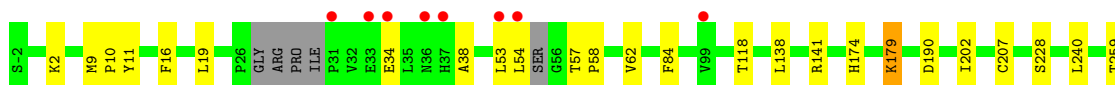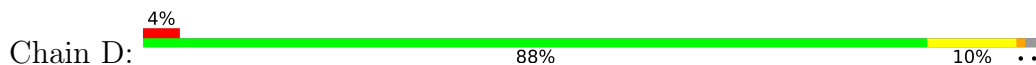
• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain B:

• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain C:

V270 F271 E272 A273 Y274 S275 A276 F277 I278 G279 ARG E281 E287 L290 P291 H301 D305 Q306 P307 Y317 R321 D322 D323 A324 P325 A330 G331 I332 E335 E345 R346 Y353 V354 M355 C356 D357 P376 ALA HIS

• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain D:

4%
88%
10%

S-2 K2 M9 P10 Y11 F16 L19 P26 GLY ARG PRO ILE P31 V32 E33 E34 L35 N36 H37 A38 L53 L54 SER G56 T57 P58 V62 F84 V99 T118 L138 R141 H174 K179 D190 I202 C207 S228 L240 T259

L260 T268 Q269 V270 A273 Y274 S275 A276 F277 I278 G279 R280 E281 Q282 R283 E287 P291 Y317 R321 P325 V329 A330 G331 I332 E335 R346 R347 Y353 V354 M355 N371 A377 HIS

• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain E:

%
87%
12%

SER ASN ALA M1 K2 I3 L4 M9 P10 L15 F16 L19 V25 P26 E34 L35 N36 H37 M42 S52 G56 T57 N91 M105 E108 S113 I119 Q132 E136 T142 P148 G153 D154 E155 V165 Y183 R196 I202

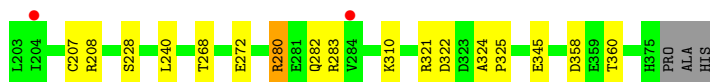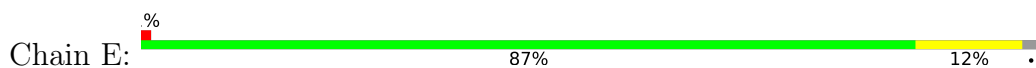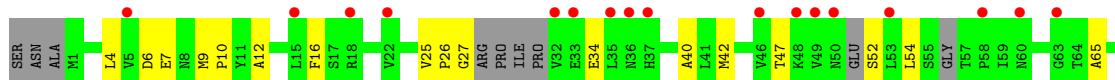L203 I204 C207 R208 S228 L240 T268 E272 V284 R280 E281 Q282 R283 K310 R321 D322 D323 A324 P325 E345 D358 S359 T360 H375 PRO ALA HIS

• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain F:

8%
83%
12%

SER ASN ALA M1 L4 V5 D6 E7 N8 M9 P10 Y11 A12 L15 F16 S17 R18 V22 V25 P26 G27 ARG PRO ILE PRO V32 E33 E34 L35 N36 H37 A40 L41 M42 V46 T47 K48 V49 N50 GLU S52 L53 L54 S55 GLY T57 P58 I59 N60 G63 T64 A65

T69 A75 W76 L77 A80 I119 V124 G128 Q132 R141 T142 L143 L144 R159 E167 Y183 I204 C207 N214 L221 V229 W234 E235 G236 E237 L240 T268 Q269 V270 F271 E272 A273 A276 F277 I278 G279 R280 GLU GLN ARG VAL

ALA L286 E287 T288 L289 R297 D318 R321 A324 P325 M355 P376 ALA HIS
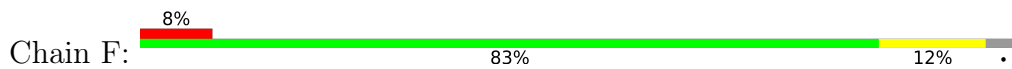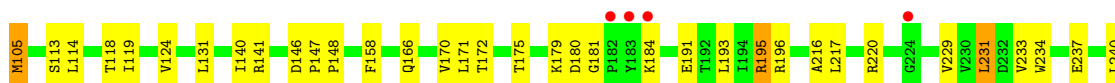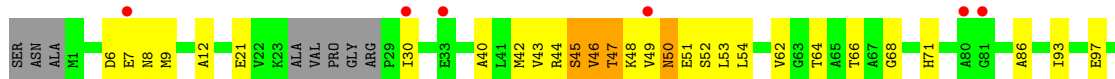
• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain G:

4%
75%
20%

SER ASN ALA M1 D6 E7 N8 M9 A12 E21 V22 K23 ALA VAL PRO GLY ARG P29 I30 E33 A40 L41 M42 V43 R44 S45 V46 T47 K48 V49 N50 E51 S52 L53 L54 V62 G63 T64 A65 T66 A67 G68 H71 A80 G81 A86 I93 E97

M105 S113 L114 T118 I119 V124 L131 I140 R141 D146 P147 P148 F158 Q166 V170 L171 T172 T175 K179 D180 D181 P182 Y183 K184 E191 T192 L193 I194 R195 R196 A216 L217 R220 G224 V229 V230 D231 D232 V233 W234 E237 L240
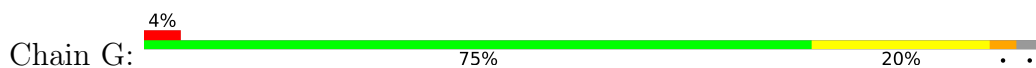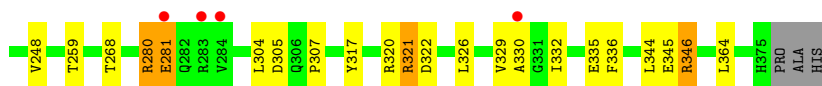
• Molecule 1: Erythronate-4-phosphate dehydrogenase

Chain H:

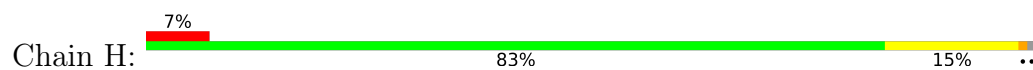# 4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.28Å　167.76Å　103.95Å 90.00°　93.88°　90.00°	Depositor
Resolution (Å)	30.19　–　2.36 30.19　–　2.36	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.19-2.36) 98.7 (30.19-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190　,　0.253 0.189　,　0.253	Depositor DCC
R_{free} test set	6469 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23835	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% 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	0.61	0/2937	0.72	0/3981
1	B	0.64	0/2942	0.74	0/3989
1	C	0.63	0/2910	0.72	0/3942
1	D	0.64	0/2915	0.71	0/3953
1	E	0.66	1/2931 (0.0%)	0.71	0/3977
1	F	0.63	0/2837	0.69	0/3846
1	G	0.57	0/2891	0.67	0/3919
1	H	0.54	0/2948	0.64	0/4000
All	All	0.61	1/23311 (0.0%)	0.70	0/31607

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	345	GLU	CG-CD	5.42	1.60	1.51

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2914	40	0
1	B	2894	0	2904	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2865	0	2863	67	0
1	D	2867	0	2883	23	0
1	E	2880	0	2906	26	0
1	F	2791	0	2803	31	0
1	G	2843	0	2864	63	0
1	H	2897	0	2929	41	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	3	0
2	F	44	0	26	1	0
2	G	44	0	26	2	0
2	H	44	0	26	2	0
3	A	79	0	0	1	0
3	B	79	0	0	2	0
3	C	78	0	0	5	0
3	D	62	0	0	2	0
3	E	91	0	0	1	0
3	F	85	0	0	3	0
3	G	48	0	0	1	0
3	H	36	0	0	1	0
All	All	23835	0	23274	329	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 7.

All (329) 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:C:43:VAL:HG22	1:C:44:ARG:H	1.07	1.17
1:H:43:VAL:HG21	1:H:47:THR:HB	1.28	1.15
1:C:4:LEU:HD22	1:C:23:LYS:HB3	1.40	1.02
1:C:9:MSE:HE3	1:C:65:ALA:HB2	1.44	0.97
1:C:265:ARG:HG2	1:C:269:GLN:HE21	1.33	0.92
1:A:43:VAL:HG21	1:A:47:THR:HB	1.52	0.90
1:G:64:THR:OG1	1:G:66:THR:HG22	1.73	0.89
1:G:43:VAL:HG22	1:G:44:ARG:O	1.72	0.88
1:F:16:PHE:HZ	1:F:270:VAL:HG12	1.38	0.88
1:C:43:VAL:HG22	1:C:44:ARG:N	1.89	0.87
1:B:32:VAL:HA	1:B:35:LEU:HD12	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:LEU:HG	1:G:345:GLU:N	1.94	0.81
1:A:259:THR:HG22	1:A:346[A]:ARG:HG2	1.64	0.79
1:G:118:THR:HG23	1:G:141:ARG:HG2	1.63	0.78
1:H:25:VAL:HG11	1:H:30:ILE:HG23	1.67	0.77
1:A:66:THR:HG22	1:A:68:GLY:H	1.48	0.76
1:D:274:TYR:CZ	1:D:278:ILE:HD11	2.20	0.76
1:B:140:ILE:O	1:B:142:THR:HG23	1.85	0.76
1:G:43:VAL:HG23	1:G:47:THR:HG23	1.66	0.75
1:B:280:ARG:HH21	1:B:280:ARG:HG3	1.52	0.74
1:A:43:VAL:HG21	1:A:47:THR:CB	2.18	0.74
1:B:317:TYR:CD1	1:B:346[B]:ARG:HD2	2.23	0.73
1:C:43:VAL:CG2	1:C:44:ARG:H	1.88	0.73
1:C:2:LYS:O	1:C:39:ASP:HB3	1.88	0.73
1:H:43:VAL:CG2	1:H:47:THR:HB	2.13	0.73
1:H:43:VAL:HG22	1:H:44:ARG:O	1.89	0.73
1:A:256:ALA:O	1:A:346[B]:ARG:NH2	2.20	0.73
1:B:285:ALA:HB1	1:B:287:GLU:OE2	1.88	0.72
1:C:259:THR:HG22	1:C:346:ARG:HG2	1.70	0.72
1:C:9:MSE:HE2	1:C:267:THR:HG23	1.69	0.72
1:H:43:VAL:HG21	1:H:47:THR:CB	2.15	0.71
1:G:259:THR:HG22	1:G:346:ARG:HG2	1.74	0.70
1:C:9:MSE:HE3	1:C:65:ALA:CB	2.20	0.69
1:A:317:TYR:CD1	1:A:346[A]:ARG:HD3	2.28	0.69
1:E:105:MSE:HE2	3:E:425:HOH:O	1.91	0.68
1:G:317:TYR:CD1	1:G:346:ARG:HD3	2.28	0.68
1:C:240:LEU:C	1:C:240:LEU:HD12	2.15	0.67
1:B:317:TYR:CD1	1:B:346[A]:ARG:HD3	2.30	0.67
1:F:324:ALA:HB3	1:F:325:PRO:HD3	1.77	0.66
1:D:291:PRO:O	1:D:347:ARG:NH2	2.29	0.65
1:B:280:ARG:HG3	1:B:280:ARG:NH2	2.11	0.65
1:C:306:GLN:HB3	1:C:307:PRO:HD3	1.78	0.65
3:C:398:HOH:O	1:F:318:ASP:HB3	1.97	0.65
1:H:43:VAL:HG22	1:H:44:ARG:N	2.12	0.65
1:C:4:LEU:CD2	1:C:23:LYS:HB3	2.21	0.65
1:G:43:VAL:CG2	1:G:47:THR:HG23	2.27	0.65
1:C:301:HIS:ND1	1:C:357:ASP:OD2	2.22	0.64
1:F:4:LEU:HD11	1:F:34:GLU:HB3	1.79	0.64
1:G:240:LEU:O	1:G:240:LEU:HD12	1.98	0.64
1:G:93:ILE:O	1:G:97:GLU:HG3	1.98	0.64
1:C:317:TYR:CG	1:C:346:ARG:HD2	2.33	0.64
1:A:75:ALA:O	1:A:79:GLN:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:THR:HG22	1:D:346:ARG:HG2	1.80	0.63
1:B:162:ASP:OD1	1:B:196:ARG:NH1	2.31	0.63
1:A:285:ALA:HB3	1:A:288:THR:HG23	1.81	0.62
1:A:180:ASP:HB3	3:A:418:HOH:O	1.98	0.62
1:E:202:ILE:HG12	1:E:228:SER:HB2	1.82	0.62
1:A:201:ALA:O	1:A:227:LEU:HD12	2.00	0.62
1:B:141:ARG:NH2	1:B:167:GLU:OE1	2.27	0.62
1:G:240:LEU:HD12	1:G:240:LEU:C	2.21	0.61
1:C:43:VAL:HG21	1:C:47:THR:OG1	2.00	0.61
1:G:64:THR:OG1	1:G:66:THR:CG2	2.47	0.61
1:A:191:GLU:OE2	1:A:195:ARG:NH2	2.23	0.61
1:A:353:TYR:HH	1:B:353:TYR:HH	1.49	0.61
1:C:69[B]:THR:O	1:C:70[B]:ASP:C	2.38	0.60
1:A:244:LEU:O	1:A:248:VAL:HG13	2.01	0.60
1:E:280:ARG:O	1:E:282:GLN:HG3	2.03	0.59
1:G:50:ASN:N	1:G:50:ASN:HD22	2.00	0.59
1:G:9:MSE:HG3	1:G:12:ALA:HB2	1.84	0.58
1:F:9:MSE:HB3	1:F:12:ALA:HB2	1.85	0.58
1:C:39:ASP:O	1:C:59:ILE:HA	2.03	0.58
1:A:49:VAL:HB	1:A:72:VAL:HG13	1.85	0.58
1:H:234:TRP:O	1:H:237:GLU:HG3	2.04	0.58
1:C:275:SER:O	1:C:281:GLU:N	2.37	0.58
1:C:51:GLU:HG3	1:C:76:TRP:CE2	2.39	0.58
1:B:42:MSE:HA	1:B:63:GLY:O	2.05	0.57
1:G:326:LEU:O	1:G:330:ALA:HB2	2.04	0.57
1:C:61:PHE:HB3	1:C:274:TYR:HE1	1.69	0.57
1:D:16:PHE:HZ	1:D:270:VAL:HG12	1.68	0.57
1:E:4:LEU:HD21	1:E:34:GLU:HG3	1.87	0.57
1:G:217:LEU:HD21	1:G:229:VAL:HG11	1.85	0.57
1:F:279:GLY:O	1:F:280:ARG:HG3	2.05	0.56
1:G:6:ASP:OD2	1:G:8:ASN:HB2	2.05	0.56
1:C:290:LEU:HB3	1:C:291:PRO:HD2	1.87	0.56
1:G:234:TRP:O	1:G:237:GLU:HG3	2.06	0.56
1:A:317:TYR:CD1	1:A:346[B]:ARG:HD2	2.41	0.56
1:G:166:GLN:HE21	1:G:196:ARG:HH22	1.53	0.56
1:C:7:GLU:N	1:C:25:VAL:O	2.37	0.56
1:G:21:GLU:OE2	1:H:23:LYS:HD3	2.06	0.56
1:B:16:PHE:HZ	1:B:270:VAL:HG12	1.71	0.55
1:H:16:PHE:HZ	1:H:270:VAL:HG12	1.72	0.55
1:H:306:GLN:HB3	1:H:307:PRO:HD3	1.89	0.55
1:E:16:PHE:CE1	1:E:42:MSE:HE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:ALA:O	1:H:96:VAL:HG23	2.07	0.55
1:F:287:GLU:O	1:F:287:GLU:HG2	2.07	0.55
1:G:166:GLN:HE21	1:G:196:ARG:NH2	2.04	0.55
1:G:231:LEU:HD22	1:G:248:VAL:HG11	1.89	0.55
1:F:286:LEU:HD23	1:F:289:LEU:HD12	1.87	0.55
1:C:9:MSE:CE	1:C:65:ALA:HB2	2.28	0.55
1:F:6:ASP:OD2	1:F:27:GLY:HA3	2.08	0.54
1:C:196:ARG:HD3	3:C:428:HOH:O	2.06	0.54
1:F:9:MSE:HE2	1:F:65:ALA:HB3	1.90	0.54
1:F:40:ALA:HB1	1:F:42:MSE:HE2	1.89	0.54
1:C:72:VAL:HG11	1:C:84:PHE:CE1	2.43	0.54
1:E:165:VAL:HG11	1:E:196:ARG:NH1	2.23	0.54
1:A:317:TYR:CE1	1:A:346[B]:ARG:HD2	2.43	0.54
1:A:242:VAL:O	1:A:246:GLU:HG2	2.07	0.53
1:B:62:VAL:O	1:B:84:PHE:HA	2.08	0.53
1:C:193:LEU:HD23	1:C:193:LEU:C	2.29	0.53
1:D:53:LEU:O	1:D:54:LEU:HG	2.08	0.53
1:B:287:GLU:CD	1:B:287:GLU:H	2.12	0.53
1:C:332:ILE:HB	1:C:335:GLU:HG3	1.90	0.53
1:G:332:ILE:HG22	1:G:335:GLU:HG2	1.91	0.53
1:G:66:THR:HG23	1:G:68:GLY:O	2.09	0.53
1:E:240:LEU:C	1:E:240:LEU:HD12	2.29	0.53
1:B:286:LEU:HD13	1:B:290:LEU:HD11	1.90	0.52
1:G:119:ILE:HG12	1:G:170:VAL:HB	1.91	0.52
1:C:48:LYS:HG3	3:C:419:HOH:O	2.08	0.52
1:H:304:LEU:HD23	1:H:364:LEU:HD23	1.91	0.52
1:F:4:LEU:CD1	1:F:34:GLU:HB3	2.39	0.52
1:C:277:PHE:C	1:C:277:PHE:CD2	2.83	0.52
1:C:51:GLU:HG3	1:C:76:TRP:NE1	2.24	0.52
1:E:240:LEU:HD12	1:E:240:LEU:O	2.10	0.52
1:G:48:LYS:O	1:G:50:ASN:ND2	2.42	0.52
1:H:25:VAL:HG12	1:H:26:PRO:O	2.09	0.52
1:A:285:ALA:CB	1:A:288:THR:HG23	2.40	0.52
1:G:105:MSE:HE2	1:G:320:ARG:HD3	1.91	0.52
1:B:260:LEU:HD13	1:B:345:GLU:HB2	1.92	0.52
1:C:77:LEU:HD23	1:C:84:PHE:HB2	1.92	0.52
1:E:324:ALA:HB3	1:E:325:PRO:HD3	1.92	0.52
1:B:4:LEU:HD21	1:B:34:GLU:CG	2.40	0.51
1:B:40:ALA:HB2	1:B:274:TYR:OH	2.09	0.51
1:G:43:VAL:HG22	1:G:44:ARG:N	2.24	0.51
1:E:108:GLU:OE2	1:E:310:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:GLU:HG3	1:H:192:THR:N	2.25	0.51
1:B:297:ARG:HB3	1:B:355:MSE:HE2	1.91	0.51
1:B:260:LEU:HD13	1:B:345:GLU:CB	2.40	0.51
1:D:2:LYS:HB3	1:D:38:ALA:HA	1.92	0.51
1:C:143:LEU:HD23	1:H:333:PRO:HG2	1.92	0.51
1:G:166:GLN:NE2	1:G:196:ARG:HH22	2.09	0.51
1:F:16:PHE:CZ	1:F:270:VAL:HG12	2.30	0.50
1:B:7:GLU:HB3	1:B:25:VAL:O	2.11	0.50
1:G:54:LEU:HD11	1:G:62:VAL:HG21	1.94	0.50
1:H:244:LEU:O	1:H:248:VAL:HG13	2.12	0.50
1:G:49:VAL:HG21	1:G:62:VAL:HG11	1.93	0.50
1:D:57:THR:HB	1:D:58:PRO:CD	2.42	0.49
1:B:244:LEU:O	1:B:248:VAL:HG13	2.12	0.49
1:C:40:ALA:HB2	1:C:274:TYR:OH	2.12	0.49
1:E:19:LEU:C	1:E:19:LEU:HD12	2.33	0.49
1:H:162:ASP:O	1:H:166:GLN:HG3	2.12	0.49
1:G:216:ALA:O	1:G:220:ARG:HG2	2.12	0.49
1:H:25:VAL:HG13	1:H:26:PRO:HD2	1.94	0.49
1:H:146:ASP:OD2	2:H:379:NAD:H1B	2.13	0.49
1:C:240:LEU:HD12	1:C:240:LEU:O	2.12	0.49
1:G:45:SER:HA	1:G:71:HIS:CE1	2.48	0.49
1:H:183:TYR:O	1:H:184:LYS:C	2.51	0.49
1:H:64:THR:HG23	1:H:66:THR:HG22	1.95	0.49
1:C:317:TYR:CD1	1:C:346:ARG:CD	2.96	0.49
1:G:30:ILE:HD11	1:G:47:THR:HG21	1.95	0.49
1:A:8:ASN:HB2	1:A:44:ARG:NH1	2.28	0.48
1:C:-1:ASN:N	1:C:-1:ASN:OD1	2.45	0.48
1:C:355:MSE:HE1	3:F:386:HOH:O	2.13	0.48
1:H:66:THR:HG23	1:H:68:GLY:O	2.13	0.48
1:H:43:VAL:CG2	1:H:44:ARG:N	2.76	0.48
1:A:285:ALA:HB3	1:A:288:THR:CG2	2.43	0.48
1:B:8:ASN:HB2	1:B:44:ARG:NH1	2.29	0.48
1:C:324:ALA:HB3	1:C:325:PRO:HD3	1.95	0.48
1:E:36:ASN:OD1	1:E:57:THR:HG22	2.14	0.48
1:G:124:VAL:HG23	1:G:146:ASP:HB2	1.96	0.48
1:G:51:GLU:C	1:G:53:LEU:H	2.17	0.48
1:G:147:PRO:HB2	1:G:148:PRO:HD3	1.96	0.48
1:B:4:LEU:HD21	1:B:34:GLU:HG3	1.95	0.48
1:C:16:PHE:HZ	1:C:270:VAL:HG12	1.79	0.47
1:C:61:PHE:HD2	1:C:277:PHE:CD1	2.32	0.47
1:C:317:TYR:CD1	1:C:346:ARG:HD3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ILE:HB	1:D:335:GLU:HG3	1.96	0.47
1:A:43:VAL:CG2	1:A:47:THR:HB	2.36	0.47
1:H:214:ASN:ND2	3:H:385:HOH:O	2.33	0.47
1:A:41:LEU:C	1:A:41:LEU:HD23	2.34	0.47
1:B:317:TYR:CE1	1:B:346[B]:ARG:HD2	2.49	0.47
1:C:48:LYS:HE3	3:C:419:HOH:O	2.13	0.47
1:C:277:PHE:HD2	1:C:278:ILE:HG23	1.80	0.47
1:D:62:VAL:O	1:D:84:PHE:HA	2.15	0.47
1:E:25:VAL:HG22	1:E:26:PRO:HD2	1.95	0.47
1:A:40:ALA:HB1	1:A:42:MSE:HE2	1.96	0.47
1:C:345:GLU:HA	3:C:436:HOH:O	2.15	0.47
1:F:9:MSE:HE2	1:F:65:ALA:CB	2.45	0.47
1:G:233:VAL:HA	1:G:237:GLU:OE2	2.15	0.47
1:A:-1:ASN:OD1	1:A:-1:ASN:N	2.39	0.47
1:C:305:ASP:OD1	1:C:307:PRO:HD2	2.15	0.47
1:C:6:ASP:OD1	1:C:8:ASN:N	2.43	0.46
1:D:274:TYR:CE2	1:D:278:ILE:HD11	2.50	0.46
1:D:317:TYR:CD1	1:D:346:ARG:HD3	2.50	0.46
1:B:54:LEU:O	1:B:55:SER:C	2.54	0.46
1:G:131:LEU:HD21	1:G:172:THR:HG21	1.97	0.46
1:G:317:TYR:CD1	1:G:346:ARG:CD	2.97	0.46
1:D:57:THR:HB	1:D:58:PRO:HD2	1.98	0.46
1:E:358:ASP:OD1	1:E:360:THR:OG1	2.30	0.46
1:B:18:ARG:O	1:B:19:LEU:HD23	2.16	0.46
1:G:44:ARG:O	1:G:46:VAL:N	2.49	0.46
1:H:43:VAL:CG2	1:H:47:THR:CB	2.86	0.46
1:C:264:ALA:HB2	1:C:290:LEU:HD21	1.98	0.46
1:A:260:LEU:HD13	1:A:345:GLU:HG3	1.96	0.46
1:A:346[A]:ARG:HG3	1:A:347:ARG:N	2.31	0.46
1:C:10:PRO:HB2	1:C:11:TYR:CD2	2.50	0.46
1:G:7:GLU:O	1:G:7:GLU:CG	2.64	0.46
1:C:279:GLY:C	1:C:281:GLU:N	2.70	0.46
1:A:332:ILE:HB	1:A:335:GLU:HG3	1.97	0.46
1:B:207:CYS:SG	1:B:208:ARG:N	2.89	0.45
1:C:61:PHE:CD1	1:C:61:PHE:C	2.89	0.45
1:C:5:VAL:HG12	1:C:42:MSE:HB2	1.98	0.45
1:E:2:LYS:HD2	1:E:37:HIS:O	2.15	0.45
1:G:329:VAL:HA	1:G:332:ILE:HD12	1.98	0.45
1:B:40:ALA:HB1	1:B:42:MSE:HE2	1.98	0.45
1:F:240:LEU:HD12	1:F:240:LEU:C	2.37	0.45
1:G:40:ALA:HB1	1:G:42:MSE:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:VAL:HG21	1:H:144:LEU:HB3	1.98	0.45
1:H:245:LEU:HD23	1:H:330:ALA:CB	2.46	0.45
1:E:207:CYS:HB2	2:E:379:NAD:H4D	1.99	0.45
1:G:280:ARG:O	1:G:281:GLU:C	2.55	0.45
1:H:66:THR:HG21	1:H:71:HIS:HE1	1.82	0.45
1:H:324:ALA:HB3	1:H:325:PRO:HD3	1.98	0.45
1:B:1:MSE:HE3	3:B:457:HOH:O	2.15	0.44
1:E:119:ILE:O	1:E:142:THR:HA	2.17	0.44
1:F:297:ARG:NH1	3:F:386:HOH:O	2.50	0.44
1:G:147:PRO:HD2	2:G:379:NAD:C2A	2.48	0.44
1:G:191:GLU:O	1:G:195:ARG:HB3	2.16	0.44
1:A:41:LEU:HD23	1:A:42:MSE:N	2.33	0.44
1:B:117:ARG:NH1	3:B:385:HOH:O	2.28	0.44
1:B:275:SER:O	1:B:280:ARG:N	2.51	0.44
1:E:132:GLN:O	1:E:136:GLU:HG3	2.17	0.44
1:F:119:ILE:O	1:F:142:THR:HA	2.17	0.44
1:E:207:CYS:SG	1:E:208:ARG:N	2.89	0.44
1:A:43:VAL:CG2	1:A:47:THR:CB	2.94	0.44
1:F:355:MSE:HE1	3:F:386:HOH:O	2.18	0.44
1:H:280:ARG:O	1:H:281:GLU:C	2.55	0.44
1:D:118:THR:HG23	1:D:141:ARG:HG2	2.00	0.44
1:F:4:LEU:HD11	1:F:34:GLU:CB	2.47	0.44
1:B:317:TYR:CG	1:B:346[A]:ARG:HD3	2.52	0.43
1:D:10:PRO:O	1:D:11:TYR:HB2	2.18	0.43
1:F:214:ASN:ND2	1:F:235:GLU:H	2.16	0.43
1:C:51:GLU:CG	1:C:76:TRP:CE2	3.01	0.43
1:D:174:HIS:HA	1:D:207:CYS:HB3	1.99	0.43
1:B:92:ALA:HA	1:B:127:VAL:HG22	2.00	0.43
1:C:214:ASN:ND2	1:C:235:GLU:H	2.17	0.43
1:G:304:LEU:HD23	1:G:364:LEU:HD23	2.00	0.43
1:C:268:THR:O	1:C:272:GLU:HG3	2.19	0.43
1:C:317:TYR:CD1	1:C:346:ARG:HD2	2.53	0.43
1:D:325:PRO:O	1:D:329:VAL:HG22	2.19	0.43
1:G:193:LEU:C	1:G:193:LEU:HD23	2.39	0.43
1:F:234:TRP:HB2	1:F:237:GLU:HG3	2.00	0.43
1:A:265:ARG:HA	1:A:268:THR:HB	2.01	0.43
1:B:214:ASN:HB2	1:B:235:GLU:OE1	2.19	0.43
1:B:256:ALA:O	1:B:346[B]:ARG:NH1	2.45	0.43
1:D:9:MSE:HA	1:D:10:PRO:HD3	1.85	0.43
1:D:190:ASP:HB2	3:D:419:HOH:O	2.19	0.43
1:E:321:ARG:HD2	1:E:322:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:GLU:CD	1:F:26:PRO:HA	2.39	0.43
1:A:66:THR:HG22	1:A:68:GLY:N	2.27	0.43
1:D:353:TYR:HA	1:D:371:ASN:O	2.19	0.43
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.89	0.43
1:G:240:LEU:C	1:G:240:LEU:CD1	2.86	0.43
1:H:245:LEU:CD2	1:H:330:ALA:CB	2.97	0.42
1:A:192:THR:O	1:A:196:ARG:HG3	2.19	0.42
1:C:155:GLU:OE1	1:H:341:LYS:NZ	2.52	0.42
1:F:279:GLY:C	1:F:280:ARG:HG3	2.38	0.42
1:G:114:LEU:HB3	1:G:140:ILE:HD11	2.00	0.42
1:C:0:ALA:C	1:C:1:MSE:HE2	2.40	0.42
1:F:54:LEU:HD12	1:F:77:LEU:HD21	2.01	0.42
1:G:7:GLU:O	1:G:7:GLU:HG3	2.20	0.42
1:G:175:THR:HG22	2:G:379:NAD:C4A	2.49	0.42
1:B:234:TRP:HB2	1:B:237:GLU:HG3	2.01	0.42
1:G:158:PHE:HB3	3:G:498:HOH:O	2.19	0.42
1:G:317:TYR:CG	1:G:346:ARG:HD2	2.54	0.42
1:B:30:ILE:HG21	1:B:35:LEU:HD21	2.01	0.42
1:E:9:MSE:HA	1:E:10:PRO:HD3	1.94	0.42
1:A:33:GLU:OE1	1:A:33:GLU:HA	2.19	0.42
1:C:274:TYR:O	1:C:278:ILE:HG12	2.19	0.42
1:F:207:CYS:HB2	2:F:379:NAD:H4D	2.02	0.42
1:H:194:ILE:CG2	1:H:220:ARG:HG3	2.49	0.42
1:A:280:ARG:O	1:A:282:GLN:HG3	2.20	0.42
1:B:193:LEU:C	1:B:193:LEU:HD23	2.40	0.42
1:E:207:CYS:HA	2:E:379:NAD:H1D	2.01	0.42
1:G:180:ASP:HB2	1:G:181:GLY:H	1.73	0.42
1:A:173:PHE:HE1	1:A:203:LEU:HD11	1.85	0.42
1:G:179:LYS:O	1:G:184:LYS:HG3	2.20	0.42
1:G:305:ASP:CG	1:G:307:PRO:HD2	2.40	0.42
1:F:159:ARG:HE	1:F:159:ARG:HB3	1.73	0.41
1:A:259:THR:HG22	1:A:346[B]:ARG:HG2	2.03	0.41
1:F:9:MSE:HA	1:F:10:PRO:HD3	1.90	0.41
1:H:51:GLU:O	1:H:55:SER:HB2	2.20	0.41
1:H:214:ASN:ND2	1:H:235:GLU:H	2.18	0.41
1:E:148:PRO:HG3	1:E:183:TYR:CG	2.55	0.41
1:F:141:ARG:NH2	1:F:167:GLU:OE1	2.47	0.41
1:A:40:ALA:HB1	1:A:42:MSE:CE	2.50	0.41
1:B:6:ASP:HB3	1:B:9:MSE:HE3	2.00	0.41
1:G:321:ARG:NH1	1:G:322:ASP:OD1	2.53	0.41
1:G:336:PHE:CD2	1:G:336:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:359:GLU:HB2	1:H:374:HIS:CE1	2.56	0.41
1:B:36:ASN:HA	1:B:57:THR:HG22	2.01	0.41
1:C:61:PHE:HB3	1:C:274:TYR:CE1	2.53	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.93	0.41
1:E:91:ASN:OD1	2:E:379:NAD:H5N	2.21	0.41
1:A:193:LEU:C	1:A:193:LEU:HD23	2.40	0.41
1:F:124:VAL:HA	1:F:128:GLY:HA3	2.02	0.41
1:A:317:TYR:CG	1:A:346[A]:ARG:CD	3.04	0.41
1:C:25:VAL:HG12	1:C:26:PRO:O	2.21	0.41
1:C:353:TYR:HE2	1:C:355:MSE:SE	2.53	0.41
1:H:15:LEU:HD12	1:H:15:LEU:HA	1.86	0.41
1:H:176:PRO:HD3	2:H:379:NAD:H52A	2.03	0.41
1:C:50:ASN:O	1:C:51:GLU:C	2.57	0.41
1:F:132:GLN:NE2	1:F:144:LEU:HD11	2.36	0.40
1:F:221:LEU:HD11	1:F:229:VAL:HG21	2.02	0.40
1:A:305:ASP:OD1	1:A:307:PRO:HD2	2.21	0.40
1:C:264:ALA:CB	1:C:290:LEU:HD21	2.52	0.40
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.92	0.40
1:G:171:LEU:HD12	1:G:171:LEU:HA	1.91	0.40
1:G:234:TRP:CD2	1:G:240:LEU:HD22	2.56	0.40
1:H:245:LEU:CD2	1:H:330:ALA:HB2	2.51	0.40
1:C:147:PRO:HD2	2:C:379:NAD:C2A	2.52	0.40
1:D:179:LYS:NZ	3:D:409:HOH:O	2.54	0.40
1:G:64:THR:HG23	1:G:86:ALA:HA	2.03	0.40
1:H:231:LEU:O	1:H:251:GLY:HA2	2.20	0.40
1:C:61:PHE:CD1	1:C:62:VAL:N	2.90	0.40
1:D:202:ILE:HG12	1:D:228:SER:HB2	2.02	0.40
1:D:353:TYR:CE2	1:D:355:MSE:HG2	2.56	0.40
1:E:272:GLU:OE2	1:E:283:ARG:HG3	2.20	0.40
1:H:28:ARG:HA	1:H:29:PRO:HA	1.85	0.40
1:B:240:LEU:HD12	1:B:240:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/381 (98%)	360 (97%)	12 (3%)	0	100	100
1	B	372/381 (98%)	352 (95%)	20 (5%)	0	100	100
1	C	365/381 (96%)	341 (93%)	21 (6%)	3 (1%)	19	20
1	D	369/381 (97%)	352 (95%)	17 (5%)	0	100	100
1	E	373/381 (98%)	358 (96%)	15 (4%)	0	100	100
1	F	355/381 (93%)	339 (96%)	16 (4%)	0	100	100
1	G	366/381 (96%)	341 (93%)	22 (6%)	3 (1%)	19	20
1	H	376/381 (99%)	354 (94%)	22 (6%)	0	100	100
All	All	2948/3048 (97%)	2797 (95%)	145 (5%)	6 (0%)	47	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	45	SER
1	C	70[A]	ASP
1	C	70[B]	ASP
1	G	52	SER
1	G	281	GLU
1	C	43	VAL

5.3.2 Protein sidechains (i)

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	303/303 (100%)	294 (97%)	9 (3%)	41	50
1	B	303/303 (100%)	290 (96%)	13 (4%)	29	35
1	C	299/303 (99%)	285 (95%)	14 (5%)	26	31
1	D	299/303 (99%)	292 (98%)	7 (2%)	50	61
1	E	303/303 (100%)	299 (99%)	4 (1%)	69	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	291/303 (96%)	285 (98%)	6 (2%)	53	65
1	G	298/303 (98%)	287 (96%)	11 (4%)	34	42
1	H	303/303 (100%)	292 (96%)	11 (4%)	35	43
All	All	2399/2424 (99%)	2324 (97%)	75 (3%)	41	48

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	43	VAL
1	A	105	MSE
1	A	155	GLU
1	A	180	ASP
1	A	281	GLU
1	A	321	ARG
1	A	346[A]	ARG
1	A	346[B]	ARG
1	B	7	GLU
1	B	33	GLU
1	B	105	MSE
1	B	113	SER
1	B	119	ILE
1	B	214	ASN
1	B	240	LEU
1	B	260	LEU
1	B	268	THR
1	B	280	ARG
1	B	286	LEU
1	B	321	ARG
1	B	345	GLU
1	C	-1	ASN
1	C	6	ASP
1	C	8	ASN
1	C	19	LEU
1	C	69[A]	THR
1	C	69[B]	THR
1	C	78	LYS
1	C	85	SER
1	C	105	MSE
1	C	167	GLU
1	C	208	ARG

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Mol	Chain	Res	Type
1	C	268	THR
1	C	321	ARG
1	C	323	ASP
1	D	19	LEU
1	D	34	GLU
1	D	179	LYS
1	D	240	LEU
1	D	268	THR
1	D	321	ARG
1	D	346	ARG
1	E	52	SER
1	E	113	SER
1	E	268	THR
1	E	280	ARG
1	F	25	VAL
1	F	47	THR
1	F	52	SER
1	F	268	THR
1	F	289	LEU
1	F	321	ARG
1	G	46	VAL
1	G	47	THR
1	G	50	ASN
1	G	105	MSE
1	G	113	SER
1	G	195	ARG
1	G	231	LEU
1	G	268	THR
1	G	280	ARG
1	G	321	ARG
1	G	346	ARG
1	H	21	GLU
1	H	66	THR
1	H	115	ARG
1	H	119	ILE
1	H	162	ASP
1	H	191	GLU
1	H	192	THR
1	H	288	THR
1	H	321	ARG
1	H	360	THR
1	H	375	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	B	166	GLN
1	C	269	GLN
1	D	269	GLN
1	E	375	HIS
1	F	214	ASN
1	G	50	ASN
1	G	166	GLN
1	G	214	ASN
1	H	166	GLN
1	H	214	ASN
1	H	374	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 ⓘ

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	$\#\|Z\| > 2$
2	NAD	A	379	-	42,48,48	1.82	4 (9%)	50,73,73	1.14	4 (8%)
2	NAD	C	379	-	42,48,48	1.85	4 (9%)	50,73,73	1.32	7 (14%)
2	NAD	F	379	-	42,48,48	1.74	4 (9%)	50,73,73	1.56	8 (16%)
2	NAD	H	379	-	42,48,48	1.80	3 (7%)	50,73,73	1.16	3 (6%)
2	NAD	B	379	-	42,48,48	1.75	4 (9%)	50,73,73	1.26	3 (6%)
2	NAD	E	379	-	42,48,48	1.82	4 (9%)	50,73,73	1.38	5 (10%)
2	NAD	D	379	-	42,48,48	1.75	3 (7%)	50,73,73	1.32	4 (8%)
2	NAD	G	379	-	42,48,48	1.93	3 (7%)	50,73,73	1.35	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
2	NAD	A	379	-	-	6/26/62/62	0/5/5/5
2	NAD	C	379	-	-	6/26/62/62	0/5/5/5
2	NAD	F	379	-	-	2/26/62/62	0/5/5/5
2	NAD	H	379	-	-	9/26/62/62	0/5/5/5
2	NAD	B	379	-	-	11/26/62/62	0/5/5/5
2	NAD	E	379	-	-	8/26/62/62	0/5/5/5
2	NAD	D	379	-	-	2/26/62/62	0/5/5/5
2	NAD	G	379	-	-	7/26/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	379	NAD	O7N-C7N	10.05	1.43	1.24
2	C	379	NAD	O7N-C7N	9.30	1.42	1.24
2	E	379	NAD	O7N-C7N	9.20	1.41	1.24
2	A	379	NAD	O7N-C7N	9.15	1.41	1.24
2	H	379	NAD	O7N-C7N	9.01	1.41	1.24
2	B	379	NAD	O7N-C7N	8.91	1.41	1.24
2	D	379	NAD	O7N-C7N	8.67	1.40	1.24
2	F	379	NAD	O7N-C7N	8.38	1.40	1.24
2	H	379	NAD	C2A-N3A	4.44	1.39	1.32
2	A	379	NAD	C2A-N3A	4.04	1.38	1.32
2	G	379	NAD	C2A-N3A	4.04	1.38	1.32
2	F	379	NAD	C2A-N3A	3.92	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	379	NAD	C2A-N3A	3.87	1.38	1.32
2	D	379	NAD	C2A-N3A	3.75	1.38	1.32
2	B	379	NAD	C2A-N3A	3.74	1.38	1.32
2	E	379	NAD	C2A-N3A	3.66	1.38	1.32
2	F	379	NAD	C2N-N1N	2.86	1.38	1.35
2	B	379	NAD	C2A-N1A	2.73	1.39	1.33
2	E	379	NAD	C2N-N1N	2.67	1.38	1.35
2	C	379	NAD	C2A-N1A	2.66	1.38	1.33
2	G	379	NAD	C2A-N1A	2.62	1.38	1.33
2	F	379	NAD	C2A-N1A	2.57	1.38	1.33
2	D	379	NAD	C2A-N1A	2.51	1.38	1.33
2	E	379	NAD	C2A-N1A	2.44	1.38	1.33
2	H	379	NAD	C2A-N1A	2.34	1.38	1.33
2	C	379	NAD	C2N-N1N	2.28	1.37	1.35
2	A	379	NAD	C2A-N1A	2.20	1.38	1.33
2	A	379	NAD	C2N-N1N	2.11	1.37	1.35
2	B	379	NAD	C2B-C1B	-2.03	1.50	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	379	NAD	N3A-C2A-N1A	-5.85	119.54	128.68
2	B	379	NAD	N3A-C2A-N1A	-5.73	119.73	128.68
2	F	379	NAD	N3A-C2A-N1A	-5.70	119.77	128.68
2	E	379	NAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	H	379	NAD	N3A-C2A-N1A	-5.21	120.53	128.68
2	D	379	NAD	N3A-C2A-N1A	-5.08	120.75	128.68
2	C	379	NAD	N3A-C2A-N1A	-4.99	120.89	128.68
2	A	379	NAD	N3A-C2A-N1A	-4.71	121.32	128.68
2	F	379	NAD	C3N-C7N-N7N	3.90	122.43	117.75
2	F	379	NAD	O7N-C7N-C3N	-3.60	115.33	119.63
2	D	379	NAD	PN-O3-PA	-3.26	121.65	132.83
2	E	379	NAD	O7N-C7N-C3N	-3.05	115.98	119.63
2	F	379	NAD	O3D-C3D-C4D	-2.91	102.63	111.05
2	E	379	NAD	C3N-C7N-N7N	2.88	121.20	117.75
2	D	379	NAD	C3N-C7N-N7N	2.87	121.20	117.75
2	G	379	NAD	PN-O3-PA	-2.87	122.99	132.83
2	D	379	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
2	E	379	NAD	PN-O3-PA	-2.79	123.26	132.83
2	F	379	NAD	PN-O3-PA	-2.76	123.36	132.83
2	G	379	NAD	C1B-N9A-C4A	-2.67	121.94	126.64
2	C	379	NAD	C4A-C5A-N7A	-2.66	106.63	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	379	NAD	C3N-C7N-N7N	2.65	120.93	117.75
2	C	379	NAD	PN-O3-PA	-2.63	123.80	132.83
2	G	379	NAD	O3D-C3D-C4D	-2.58	103.59	111.05
2	A	379	NAD	PN-O3-PA	-2.53	124.15	132.83
2	H	379	NAD	C4A-C5A-N7A	-2.47	106.83	109.40
2	E	379	NAD	C1B-N9A-C4A	-2.36	122.50	126.64
2	H	379	NAD	PN-O3-PA	-2.34	124.79	132.83
2	F	379	NAD	C4N-C3N-C7N	-2.32	114.82	121.04
2	B	379	NAD	PN-O3-PA	-2.23	125.17	132.83
2	A	379	NAD	C3N-C7N-N7N	2.19	120.38	117.75
2	C	379	NAD	O7N-C7N-C3N	-2.18	117.02	119.63
2	B	379	NAD	O3D-C3D-C4D	-2.13	104.89	111.05
2	C	379	NAD	O2N-PN-O1N	2.12	122.74	112.24
2	F	379	NAD	C1B-N9A-C4A	-2.07	123.01	126.64
2	C	379	NAD	C1B-N9A-C4A	-2.03	123.08	126.64
2	A	379	NAD	O4D-C1D-C2D	-2.02	103.97	106.93
2	F	379	NAD	O2N-PN-O1N	2.01	122.20	112.24
2	G	379	NAD	O2N-PN-O1N	2.00	122.14	112.24

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	379	NAD	O4D-C1D-N1N-C2N
2	A	379	NAD	O4D-C1D-N1N-C6N
2	B	379	NAD	O4D-C1D-N1N-C2N
2	B	379	NAD	O4D-C1D-N1N-C6N
2	B	379	NAD	C2D-C1D-N1N-C2N
2	C	379	NAD	O4D-C1D-N1N-C2N
2	C	379	NAD	O4D-C1D-N1N-C6N
2	C	379	NAD	C2D-C1D-N1N-C2N
2	D	379	NAD	O4D-C1D-N1N-C6N
2	E	379	NAD	O4D-C1D-N1N-C6N
2	F	379	NAD	O4D-C1D-N1N-C6N
2	G	379	NAD	O4D-C1D-N1N-C2N
2	G	379	NAD	O4D-C1D-N1N-C6N
2	G	379	NAD	C2D-C1D-N1N-C2N
2	G	379	NAD	C2D-C1D-N1N-C6N
2	H	379	NAD	C5B-O5B-PA-O1A
2	H	379	NAD	O4B-C4B-C5B-O5B
2	H	379	NAD	O4D-C1D-N1N-C2N
2	H	379	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	E	379	NAD	O4B-C4B-C5B-O5B
2	H	379	NAD	C3B-C4B-C5B-O5B
2	E	379	NAD	C4N-C3N-C7N-O7N
2	E	379	NAD	C4N-C3N-C7N-N7N
2	E	379	NAD	C3B-C4B-C5B-O5B
2	A	379	NAD	C4N-C3N-C7N-N7N
2	A	379	NAD	C4N-C3N-C7N-O7N
2	B	379	NAD	O4B-C4B-C5B-O5B
2	G	379	NAD	C4N-C3N-C7N-N7N
2	G	379	NAD	C4N-C3N-C7N-O7N
2	E	379	NAD	C5D-O5D-PN-O3
2	H	379	NAD	C5B-O5B-PA-O3
2	H	379	NAD	C5B-O5B-PA-O2A
2	B	379	NAD	O4D-C4D-C5D-O5D
2	D	379	NAD	O4B-C4B-C5B-O5B
2	E	379	NAD	O4D-C4D-C5D-O5D
2	B	379	NAD	C4N-C3N-C7N-N7N
2	G	379	NAD	O4B-C4B-C5B-O5B
2	B	379	NAD	C3D-C4D-C5D-O5D
2	B	379	NAD	C4N-C3N-C7N-O7N
2	C	379	NAD	O4B-C4B-C5B-O5B
2	C	379	NAD	PN-O3-PA-O1A
2	E	379	NAD	C3D-C4D-C5D-O5D
2	B	379	NAD	C3B-C4B-C5B-O5B
2	A	379	NAD	C2D-C1D-N1N-C2N
2	B	379	NAD	C5D-O5D-PN-O3
2	B	379	NAD	C2D-C1D-N1N-C6N
2	C	379	NAD	C2D-C1D-N1N-C6N
2	H	379	NAD	C2D-C1D-N1N-C2N
2	H	379	NAD	C2D-C1D-N1N-C6N
2	A	379	NAD	O4B-C4B-C5B-O5B
2	F	379	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	379	NAD	1	0
2	F	379	NAD	1	0
2	H	379	NAD	2	0
2	E	379	NAD	3	0
2	G	379	NAD	2	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 A 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD F 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD H 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD E 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 379

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD G 379

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(Å²)	Q<0.9
1	A	370/381 (97%)	0.00	8 (2%)	62	72	26, 41, 83, 116	0
1	B	372/381 (97%)	0.15	15 (4%)	38	51	22, 37, 86, 118	0
1	C	367/381 (96%)	0.30	33 (8%)	9	14	22, 37, 84, 99	0
1	D	370/381 (97%)	0.04	17 (4%)	32	45	23, 37, 91, 121	0
1	E	370/381 (97%)	-0.01	5 (1%)	75	83	23, 38, 59, 73	0
1	F	360/381 (94%)	0.38	32 (8%)	9	14	23, 39, 79, 112	0
1	G	365/381 (95%)	0.31	14 (3%)	40	53	29, 50, 76, 98	0
1	H	373/381 (97%)	0.22	25 (6%)	17	26	28, 51, 76, 95	0
All	All	2947/3048 (96%)	0.17	149 (5%)	28	40	22, 42, 80, 121	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	6.8
1	F	37	HIS	5.9
1	C	32	VAL	5.2
1	B	37	HIS	4.9
1	A	33	GLU	4.9
1	F	15	LEU	4.8
1	F	36	ASN	4.7
1	C	49	VAL	4.7
1	F	287	GLU	4.4
1	C	81	GLY	4.4
1	F	279	GLY	4.4
1	B	84	PHE	4.4
1	G	80	ALA	4.3
1	G	49	VAL	4.3
1	A	36	ASN	4.2
1	C	33	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	288	THR	4.2
1	G	30	ILE	4.1
1	D	279	GLY	4.0
1	F	77	LEU	3.9
1	F	60	ASN	3.8
1	C	79	GLN	3.8
1	C	35	LEU	3.8
1	F	35	LEU	3.8
1	D	53	LEU	3.6
1	D	287	GLU	3.6
1	C	75	ALA	3.6
1	F	58	PRO	3.5
1	H	333	PRO	3.5
1	G	183	TYR	3.5
1	H	150	ALA	3.5
1	C	80	ALA	3.4
1	C	48	LYS	3.4
1	D	33	GLU	3.4
1	F	50	ASN	3.4
1	B	281	GLU	3.3
1	F	268	THR	3.3
1	C	52	SER	3.3
1	C	57	THR	3.3
1	C	281	GLU	3.2
1	C	61	PHE	3.2
1	C	50	ASN	3.1
1	F	18	ARG	3.0
1	F	48	LYS	3.0
1	F	286	LEU	3.0
1	E	204	ILE	3.0
1	G	81	GLY	3.0
1	F	33	GLU	3.0
1	F	5	VAL	3.0
1	F	46	VAL	3.0
1	C	72	VAL	2.9
1	H	178	TYR	2.9
1	A	345	GLU	2.9
1	C	82	ILE	2.9
1	D	331	GLY	2.9
1	B	77	LEU	2.9
1	G	330	ALA	2.9
1	C	155	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	283	ARG	2.8
1	H	331	GLY	2.8
1	B	79	GLN	2.8
1	D	36	ASN	2.8
1	F	277	PHE	2.8
1	B	345	GLU	2.8
1	A	32	VAL	2.7
1	G	284	VAL	2.7
1	H	157	ASP	2.7
1	C	74	GLU	2.7
1	G	7	GLU	2.7
1	H	183	TYR	2.7
1	F	53	LEU	2.7
1	B	53	LEU	2.7
1	C	46	VAL	2.7
1	E	284	VAL	2.7
1	G	224	GLY	2.7
1	C	84	PHE	2.6
1	D	54	LEU	2.6
1	B	33	GLU	2.6
1	C	28	ARG	2.6
1	D	281	GLU	2.6
1	A	37	HIS	2.5
1	F	276	ALA	2.5
1	E	155	GLU	2.5
1	B	46	VAL	2.5
1	B	95	VAL	2.5
1	B	99	VAL	2.5
1	C	68	GLY	2.5
1	C	71[A]	HIS	2.5
1	G	33	GLU	2.5
1	C	99	VAL	2.5
1	H	151	ALA	2.5
1	H	155	GLU	2.5
1	F	49	VAL	2.4
1	F	32	VAL	2.4
1	H	180	ASP	2.4
1	H	153	GLY	2.4
1	C	122	VAL	2.4
1	C	330	ALA	2.4
1	D	34	GLU	2.4
1	C	78	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	377	ALA	2.4
1	H	288	THR	2.4
1	H	95	VAL	2.3
1	H	284	VAL	2.3
1	H	334	GLY	2.3
1	H	204	ILE	2.3
1	H	342	ASN	2.3
1	H	158	PHE	2.3
1	G	283	ARG	2.3
1	C	77	LEU	2.3
1	F	273	ALA	2.3
1	H	172	THR	2.2
1	B	96	VAL	2.2
1	H	99	VAL	2.2
1	H	152	ARG	2.2
1	G	182	PRO	2.2
1	A	35	LEU	2.2
1	F	183	TYR	2.2
1	D	273	ALA	2.2
1	F	204	ILE	2.2
1	C	172	THR	2.2
1	D	276	ALA	2.2
1	F	80	ALA	2.2
1	C	204	ILE	2.2
1	F	272	GLU	2.2
1	A	26	PRO	2.2
1	H	226	PRO	2.2
1	E	56	GLY	2.2
1	B	280	ARG	2.1
1	F	22	VAL	2.1
1	F	69	THR	2.1
1	H	182	PRO	2.1
1	C	273	ALA	2.1
1	F	75	ALA	2.1
1	H	330	ALA	2.1
1	C	287	GLU	2.1
1	G	184	LYS	2.1
1	D	99	VAL	2.1
1	D	37	HIS	2.1
1	B	34	GLU	2.1
1	E	153	GLY	2.1
1	F	63	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	31	PRO	2.1
1	D	260	LEU	2.0
1	G	281	GLU	2.0
1	A	49	VAL	2.0
1	B	274	TYR	2.0
1	H	332	ILE	2.0
1	H	283	ARG	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	NAD	E	379	44/44	0.93	0.13	40,52,68,69	0
2	NAD	H	379	44/44	0.95	0.11	49,52,61,64	0
2	NAD	G	379	44/44	0.96	0.11	42,49,55,57	0
2	NAD	F	379	44/44	0.96	0.11	38,43,50,55	0
2	NAD	A	379	44/44	0.97	0.10	33,39,45,47	0
2	NAD	C	379	44/44	0.97	0.12	32,41,46,48	0
2	NAD	B	379	44/44	0.98	0.11	36,39,51,51	0
2	NAD	D	379	44/44	0.98	0.13	29,37,47,47	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.
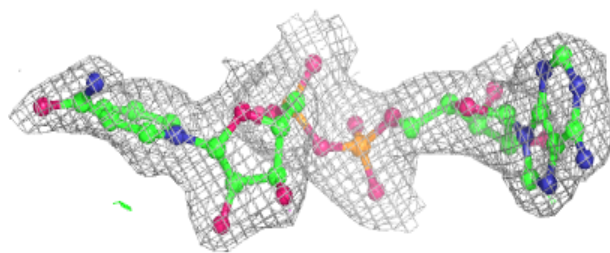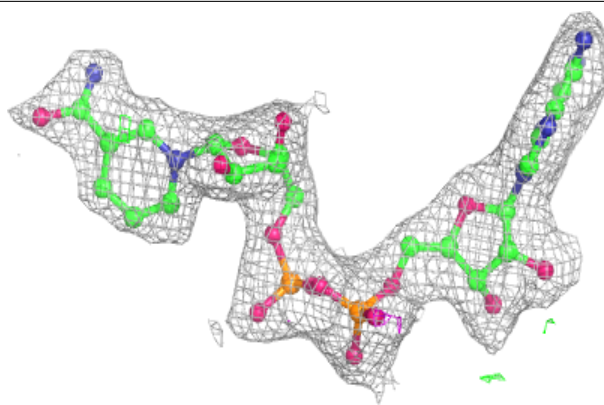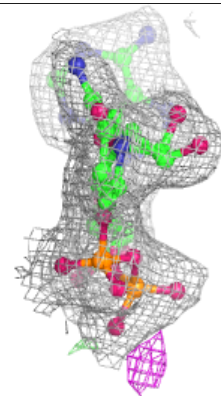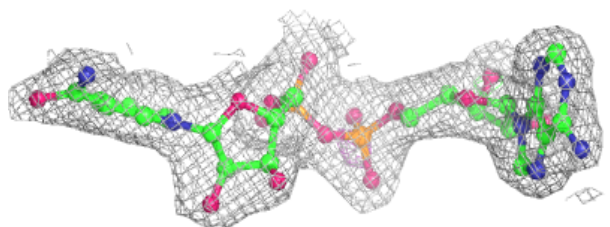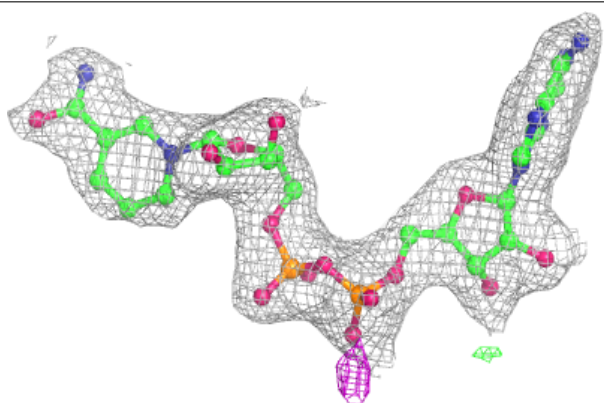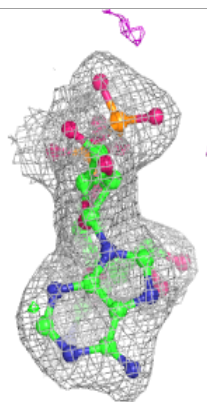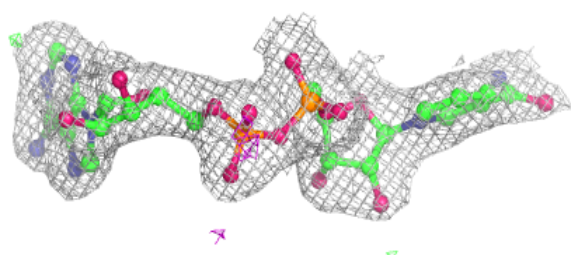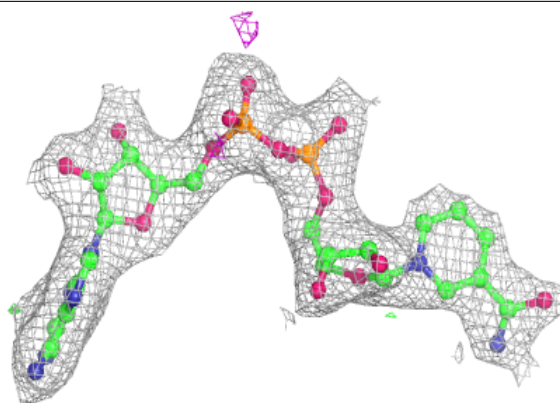
Electron density around NAD E 379:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
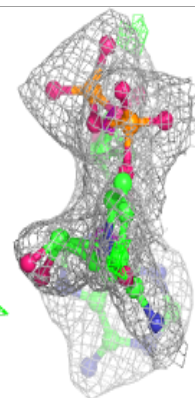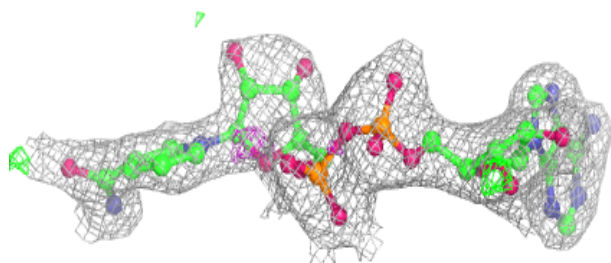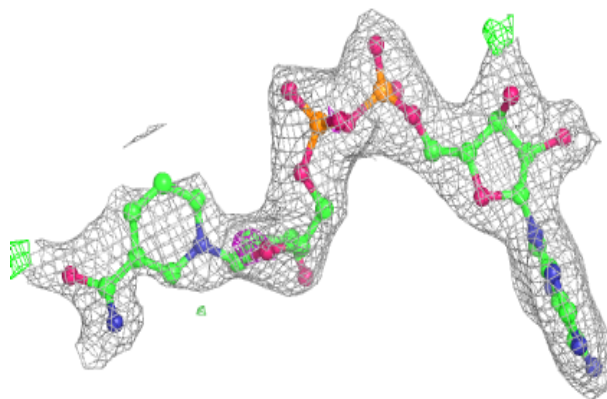
Electron density around NAD H 379:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
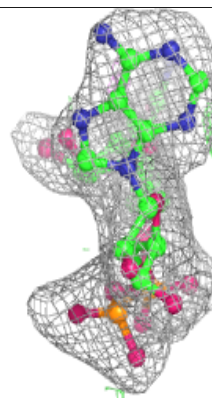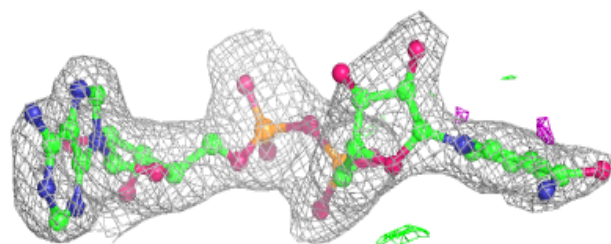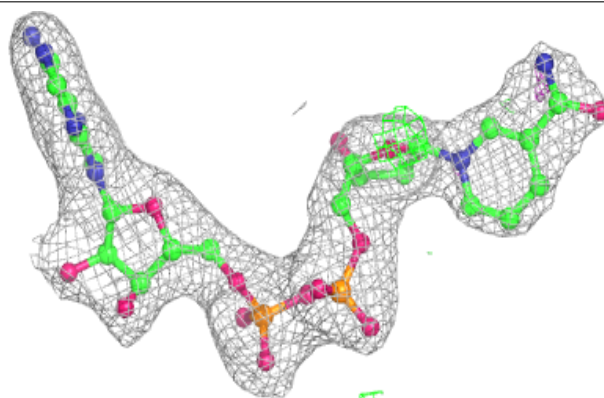
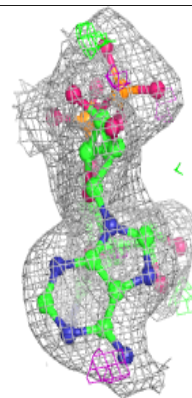**Electron density around NAD G 379:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
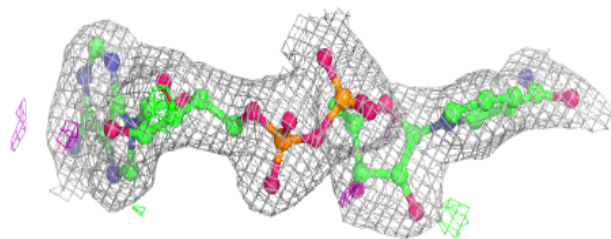and green (positive)
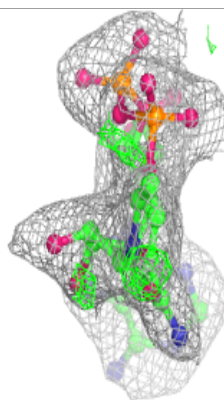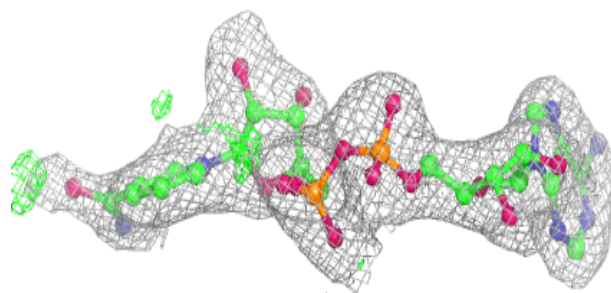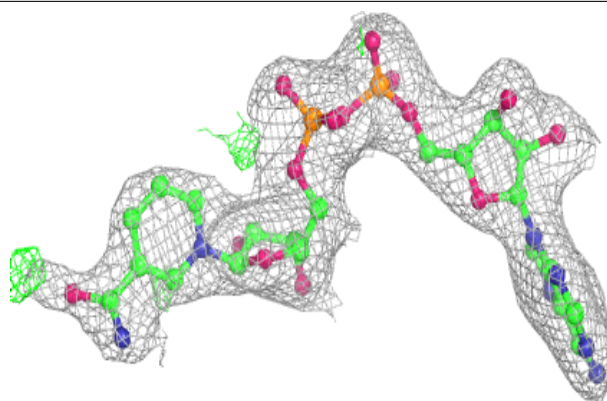
Electron density around NAD F 379:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
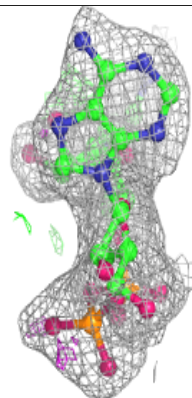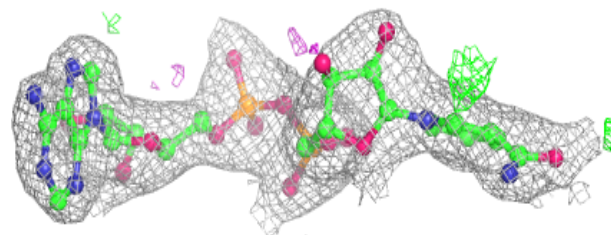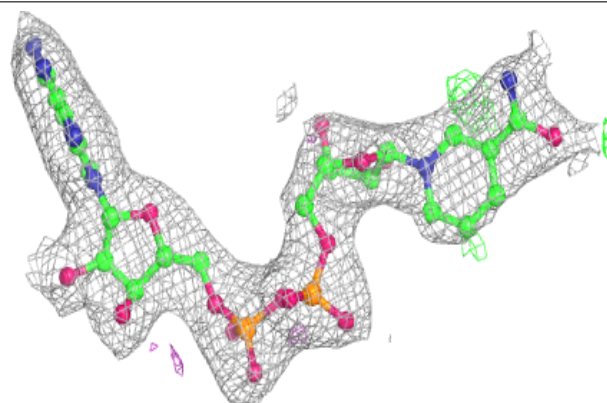
Electron density around NAD A 379:

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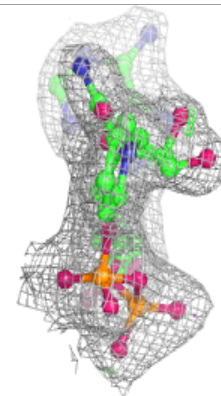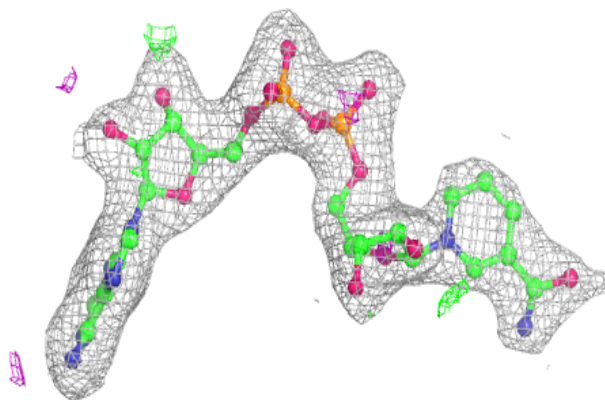

Electron density around NAD C 379:

$2mF_o$-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 379:

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

Electron density around NAD D 379:

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