Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:14 PM EST

PDB ID	:	7MJ1
Title	:	LarB, a carboxylase/hydrolase involved in synthesis of the cofactor for lactate racemase, in complex with NAD
Authors	:	Chatterjee, S.; Rankin, J.A.; Lagishetty, S.; Hu, J.; Hausinger, R.P.
Deposited on	:	2021-04-19
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

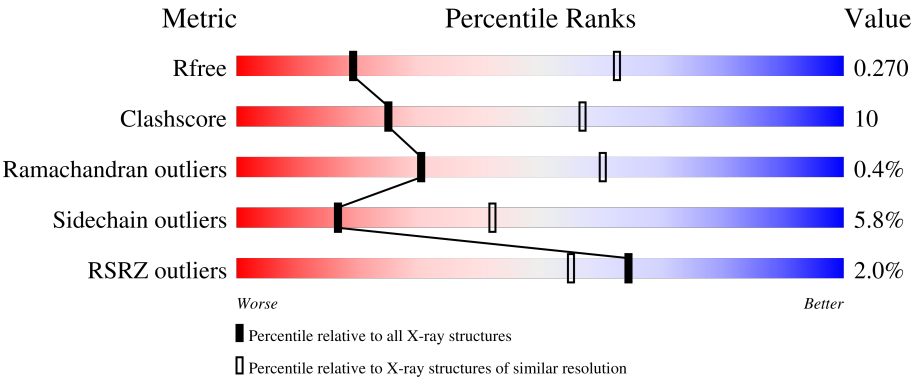
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	256	2% 55% 23% • 21%
1	B	256	2% 64% 14% 21%
1	C	256	2% 59% 19% 22%
1	D	256	2% 64% 12% • 21%
1	E	256	2% 68% 12% • 18%

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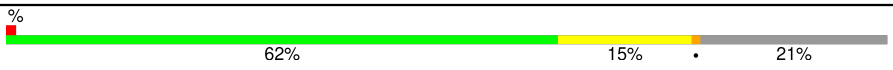
Mol	Chain	Length	Quality of chain
1	F	256	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8347 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 Pyridinium-3,5-biscarboxylic acid mononucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1377	876	234	261	6			
1	C	200	Total	C	N	O	S	0	0	0
			1358	859	231	261	7			
1	D	201	Total	C	N	O	S	0	5	0
			1347	861	226	252	8			
1	E	211	Total	C	N	O	S	0	0	0
			1419	905	236	272	6			
1	F	201	Total	C	N	O	S	0	0	0
			1365	872	225	260	8			
1	B	203	Total	C	N	O	S	0	0	0
			1389	884	234	264	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	-	expression tag	UNP F9UST0
A	248	SER	-	expression tag	UNP F9UST0
A	249	TRP	-	expression tag	UNP F9UST0
A	250	SER	-	expression tag	UNP F9UST0
A	251	HIS	-	expression tag	UNP F9UST0
A	252	PRO	-	expression tag	UNP F9UST0
A	253	GLN	-	expression tag	UNP F9UST0
A	254	PHE	-	expression tag	UNP F9UST0
A	255	GLU	-	expression tag	UNP F9UST0
A	256	LYS	-	expression tag	UNP F9UST0
C	247	ALA	-	expression tag	UNP F9UST0
C	248	SER	-	expression tag	UNP F9UST0
C	249	TRP	-	expression tag	UNP F9UST0
C	250	SER	-	expression tag	UNP F9UST0
C	251	HIS	-	expression tag	UNP F9UST0
C	252	PRO	-	expression tag	UNP F9UST0
C	253	GLN	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	254	PHE	-	expression tag	UNP F9UST0
C	255	GLU	-	expression tag	UNP F9UST0
C	256	LYS	-	expression tag	UNP F9UST0
D	247	ALA	-	expression tag	UNP F9UST0
D	248	SER	-	expression tag	UNP F9UST0
D	249	TRP	-	expression tag	UNP F9UST0
D	250	SER	-	expression tag	UNP F9UST0
D	251	HIS	-	expression tag	UNP F9UST0
D	252	PRO	-	expression tag	UNP F9UST0
D	253	GLN	-	expression tag	UNP F9UST0
D	254	PHE	-	expression tag	UNP F9UST0
D	255	GLU	-	expression tag	UNP F9UST0
D	256	LYS	-	expression tag	UNP F9UST0
E	247	ALA	-	expression tag	UNP F9UST0
E	248	SER	-	expression tag	UNP F9UST0
E	249	TRP	-	expression tag	UNP F9UST0
E	250	SER	-	expression tag	UNP F9UST0
E	251	HIS	-	expression tag	UNP F9UST0
E	252	PRO	-	expression tag	UNP F9UST0
E	253	GLN	-	expression tag	UNP F9UST0
E	254	PHE	-	expression tag	UNP F9UST0
E	255	GLU	-	expression tag	UNP F9UST0
E	256	LYS	-	expression tag	UNP F9UST0
F	247	ALA	-	expression tag	UNP F9UST0
F	248	SER	-	expression tag	UNP F9UST0
F	249	TRP	-	expression tag	UNP F9UST0
F	250	SER	-	expression tag	UNP F9UST0
F	251	HIS	-	expression tag	UNP F9UST0
F	252	PRO	-	expression tag	UNP F9UST0
F	253	GLN	-	expression tag	UNP F9UST0
F	254	PHE	-	expression tag	UNP F9UST0
F	255	GLU	-	expression tag	UNP F9UST0
F	256	LYS	-	expression tag	UNP F9UST0
B	247	ALA	-	expression tag	UNP F9UST0
B	248	SER	-	expression tag	UNP F9UST0
B	249	TRP	-	expression tag	UNP F9UST0
B	250	SER	-	expression tag	UNP F9UST0
B	251	HIS	-	expression tag	UNP F9UST0
B	252	PRO	-	expression tag	UNP F9UST0
B	253	GLN	-	expression tag	UNP F9UST0
B	254	PHE	-	expression tag	UNP F9UST0
B	255	GLU	-	expression tag	UNP F9UST0

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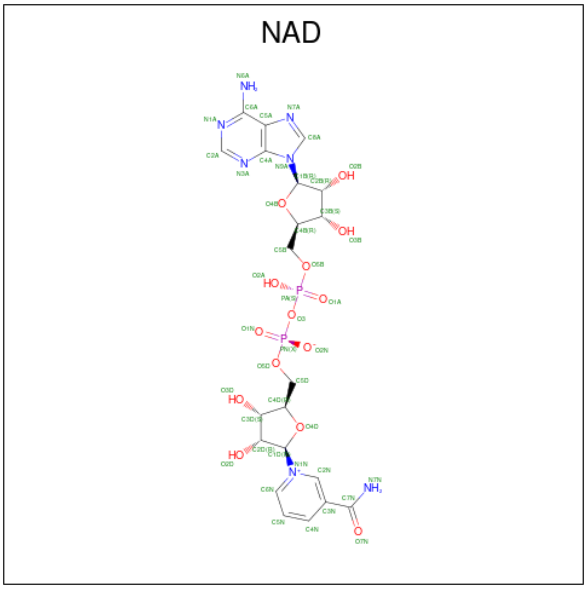
Chain	Residue	Modelled	Actual	Comment	Reference
B	256	LYS	-	expression tag	UNP F9UST0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

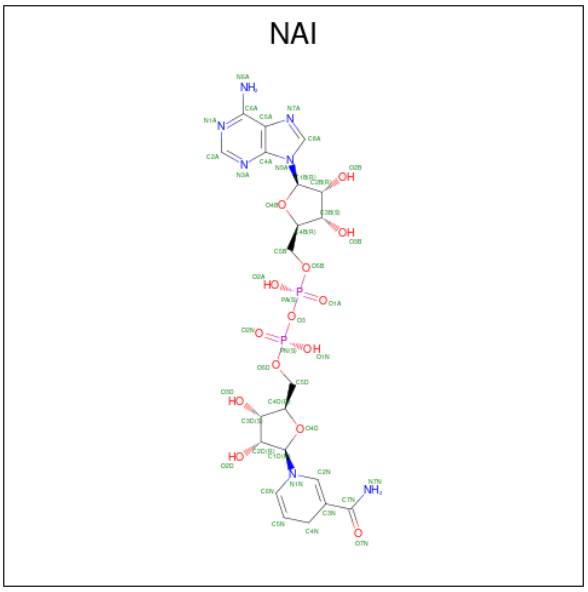
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



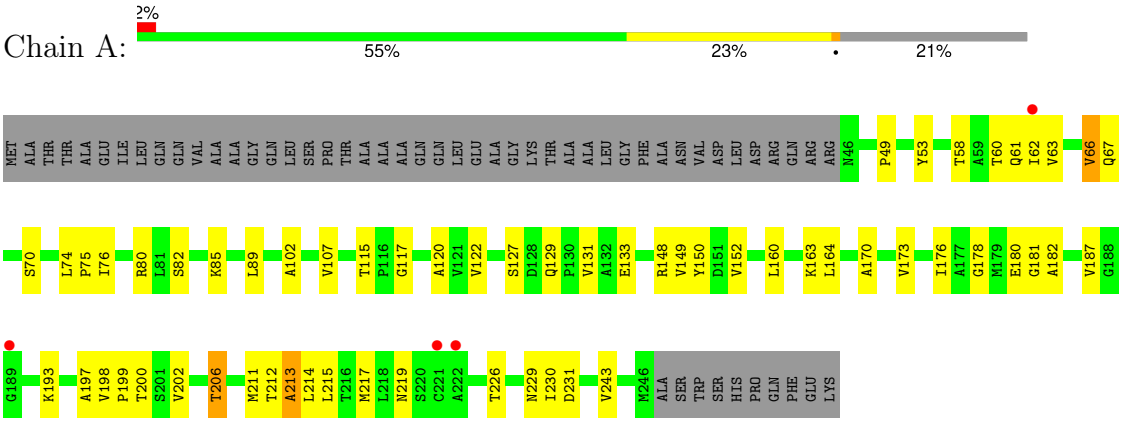
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots (i)

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.

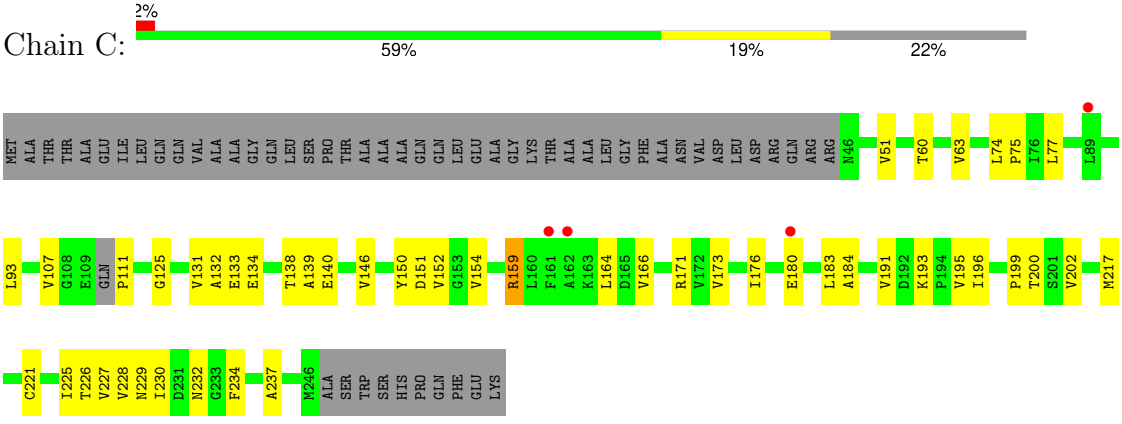
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain A:



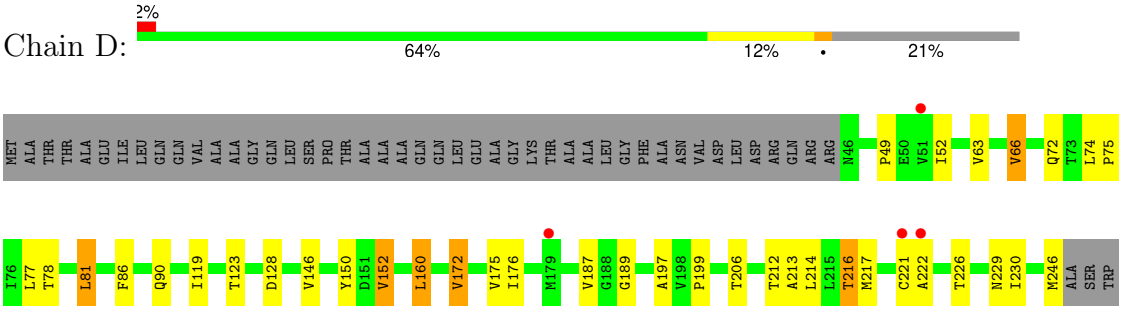
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain C:



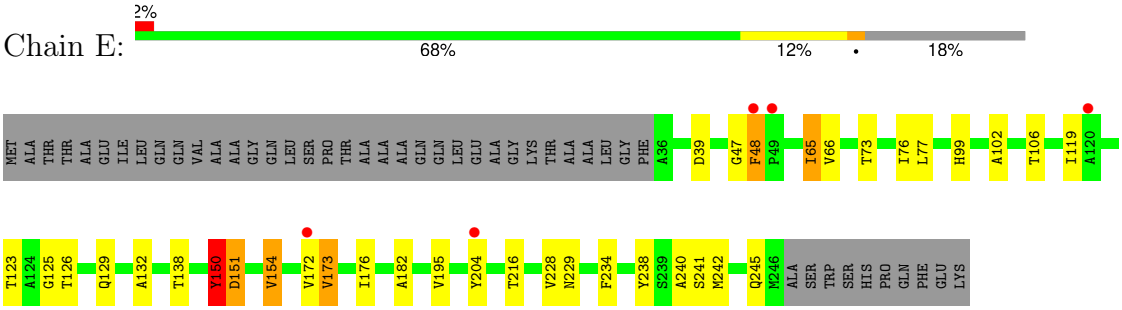
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain D:



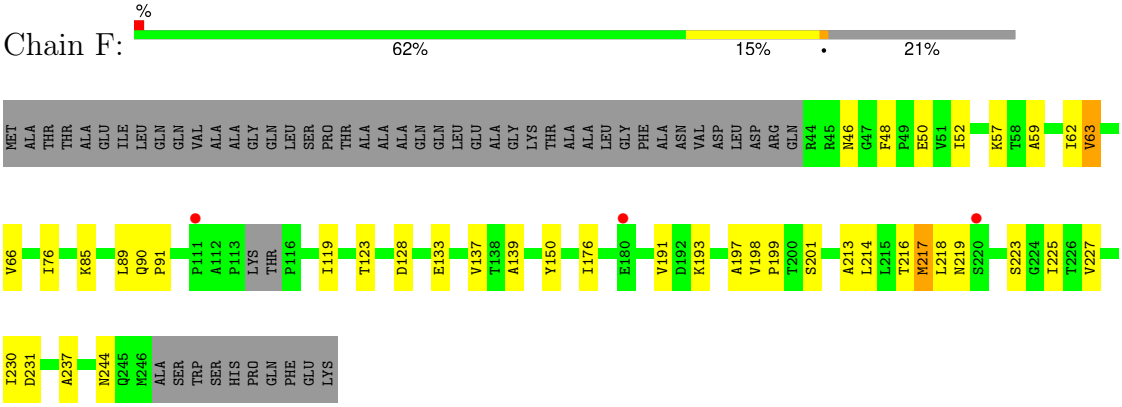
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain E:



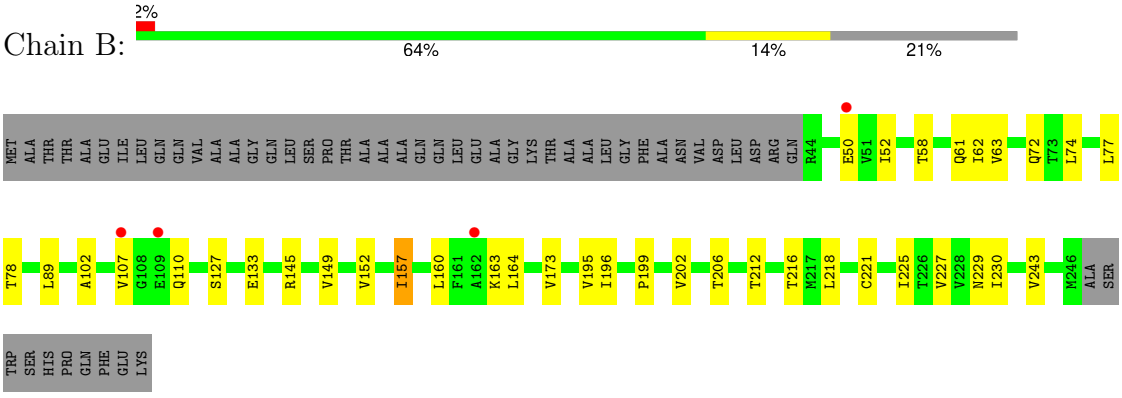
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain F:



• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.44Å 120.44Å 213.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.76 – 3.40 41.76 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.0 (41.76-3.40) 92.2 (41.76-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.243 , 0.269 0.247 , 0.270	Depositor DCC
R_{free} test set	1066 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	99.9	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 102.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8347	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAI, MG, 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	0.26	0/1399	0.49	1/1922 (0.1%)
1	B	0.26	0/1410	0.46	0/1934
1	C	0.27	0/1377	0.49	0/1889
1	D	0.25	0/1368	0.46	0/1887
1	E	0.28	0/1442	0.66	4/1985 (0.2%)
1	F	0.33	0/1385	0.50	0/1900
All	All	0.28	0/8381	0.52	5/11517 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	TYR	CA-C-N	-10.72	93.61	117.20
1	E	150	TYR	O-C-N	9.59	138.04	122.70
1	E	150	TYR	C-N-CA	-7.82	102.15	121.70
1	E	151	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	213	ALA	N-CA-CB	5.71	118.09	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	150	TYR	Mainchain

5.2 Too-close contacts (i)

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	1377	0	1365	32	0
1	B	1389	0	1378	23	0
1	C	1358	0	1319	30	0
1	D	1347	0	1281	19	1
1	E	1419	0	1360	32	1
1	F	1365	0	1332	32	1
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	E	1	0	0	0	0
3	C	44	0	25	5	0
4	E	44	0	26	9	0
All	All	8347	0	8086	158	2

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 10.

All (158) 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:F:218:LEU:HD12	1:F:227:VAL:HG11	1.36	1.07
1:F:218:LEU:HD12	1:F:227:VAL:CG1	1.92	0.98
1:E:204:TYR:OH	1:F:219:ASN:HA	1.77	0.84
1:F:218:LEU:CD1	1:F:227:VAL:HG11	2.09	0.82
1:D:199:PRO:HG2	1:D:230:ILE:HA	1.64	0.79
1:B:50:GLU:OE2	1:B:72:GLN:NE2	2.20	0.74
1:B:149:VAL:HG12	1:B:152:VAL:HG21	1.68	0.74
1:E:151:ASP:OD1	1:E:151:ASP:C	2.23	0.73
1:A:127:SER:HB3	1:A:202:VAL:HG11	1.74	0.70
3:C:302:NAD:H6N	3:C:302:NAD:H51N	1.73	0.70
1:B:149:VAL:HG13	1:B:163:LYS:HD2	1.73	0.69
1:F:57:LYS:O	1:F:85:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ALA:HB3	4:E:302:NAI:H72N	1.59	0.68
1:B:52:ILE:HB	1:B:78:THR:HG22	1.75	0.68
1:E:151:ASP:CG	1:E:151:ASP:O	2.26	0.67
1:C:191:VAL:HG12	1:C:193:LYS:H	1.60	0.66
1:E:65:ILE:HG22	1:E:66:VAL:N	2.10	0.66
1:E:123:THR:HG22	1:E:176:ILE:HB	1.78	0.65
1:A:122:VAL:HG12	1:A:149:VAL:HB	1.80	0.64
1:F:218:LEU:CD1	1:F:227:VAL:CG1	2.69	0.64
1:C:63:VAL:HG21	1:C:93:LEU:HD21	1.80	0.63
1:C:152:VAL:HG12	1:C:159:ARG:HB3	1.82	0.62
1:A:149:VAL:HG12	1:A:152:VAL:HG21	1.82	0.62
1:C:125:GLY:HA2	1:C:151:ASP:OD1	2.02	0.60
1:A:206:THR:O	1:A:212:THR:HG21	2.02	0.60
1:A:120:ALA:HB3	1:A:173:VAL:HG12	1.85	0.59
1:C:196:ILE:HD12	1:D:226:THR:HG21	1.85	0.59
1:E:228:VAL:HG22	1:E:229:ASN:H	1.67	0.58
1:C:229:ASN:OD1	1:C:230:ILE:N	2.37	0.58
1:A:229:ASN:OD1	1:A:230:ILE:N	2.38	0.57
1:F:59:ALA:HB1	1:F:89:LEU:HD21	1.87	0.57
1:B:72:GLN:HG3	1:B:74:LEU:H	1.69	0.57
1:A:243:VAL:HG13	1:B:243:VAL:HG13	1.86	0.56
1:A:211:MET:O	1:A:211:MET:HG3	2.04	0.56
1:D:52:ILE:HB	1:D:78:THR:HG22	1.88	0.56
1:E:119:ILE:HG23	1:E:172:VAL:HG12	1.85	0.56
1:E:47:GLY:O	1:E:48:PHE:HB2	2.04	0.56
1:E:150:TYR:O	1:E:151:ASP:HB3	2.03	0.56
1:F:219:ASN:O	1:F:219:ASN:OD1	2.24	0.56
1:B:127:SER:HB3	1:B:202:VAL:HG11	1.87	0.55
1:A:226:THR:HG21	1:B:196:ILE:HD12	1.88	0.55
1:A:62:ILE:O	1:A:66:VAL:HB	2.06	0.55
1:C:154:VAL:H	3:C:302:NAD:H4N	1.72	0.55
1:E:151:ASP:OD1	1:E:151:ASP:O	2.25	0.55
1:F:63:VAL:HA	1:F:66:VAL:HG12	1.89	0.54
1:D:123:THR:HG22	1:D:150:TYR:HA	1.90	0.54
1:E:182:ALA:CB	4:E:302:NAI:H72N	2.21	0.54
1:A:58:THR:HG22	1:A:61:GLN:HB2	1.87	0.54
1:D:212:THR:O	1:D:216:THR:OG1	2.25	0.54
1:D:175:VAL:HG21	1:D:187:VAL:HG21	1.90	0.54
1:B:52:ILE:HG21	1:B:62:ILE:HG22	1.89	0.54
1:C:199:PRO:HG2	1:C:230:ILE:HA	1.90	0.54
1:D:63:VAL:HA	1:D:66:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ALA:HB1	1:D:217:MET:SD	2.48	0.54
1:E:182:ALA:H	4:E:302:NAI:H72N	1.54	0.53
1:F:219:ASN:O	1:F:219:ASN:CG	2.47	0.53
1:C:221:CYS:HA	1:C:225:ILE:HB	1.91	0.53
1:B:58:THR:HG22	1:B:61:GLN:HB2	1.91	0.52
1:C:183:LEU:H	3:C:302:NAD:H72N	1.58	0.51
1:F:197:ALA:HB1	1:F:217:MET:SD	2.51	0.51
1:E:125:GLY:CA	4:E:302:NAI:O2N	2.58	0.51
1:A:74:LEU:HG	1:A:75:PRO:HD2	1.93	0.51
1:D:49:PRO:HB3	1:D:75:PRO:O	2.11	0.51
1:B:229:ASN:OD1	1:B:230:ILE:N	2.40	0.50
1:A:82:SER:HB2	1:A:85:LYS:HG3	1.94	0.50
1:E:172:VAL:HG11	1:E:240:ALA:HB1	1.94	0.50
1:C:199:PRO:HD3	1:C:217:MET:HE1	1.93	0.50
1:A:199:PRO:HG2	1:A:230:ILE:HA	1.93	0.50
1:F:191:VAL:HG12	1:F:193:LYS:H	1.77	0.50
1:A:180:GLU:O	1:A:182:ALA:N	2.40	0.50
1:E:125:GLY:HA3	4:E:302:NAI:O2N	2.12	0.50
1:C:173:VAL:HB	1:C:195:VAL:HG22	1.94	0.49
1:F:198:VAL:C	1:F:217:MET:HE1	2.33	0.49
1:F:199:PRO:HG2	1:F:230:ILE:HA	1.93	0.49
1:D:119:ILE:HG22	1:D:172:VAL:HG13	1.94	0.48
1:E:204:TYR:OH	1:F:219:ASN:CA	2.55	0.48
1:F:119:ILE:HD11	1:F:139:ALA:HB1	1.94	0.48
1:F:213:ALA:O	1:F:217:MET:HG2	2.14	0.48
1:A:170:ALA:O	1:A:193:LYS:HD3	2.12	0.48
1:C:184:ALA:O	1:C:225:ILE:HD11	2.14	0.48
1:F:198:VAL:C	1:F:217:MET:CE	2.82	0.48
1:B:221:CYS:HA	1:B:225:ILE:HB	1.94	0.48
1:E:77:LEU:HG	1:E:106:THR:HG22	1.96	0.47
1:E:138:THR:HG21	1:E:234:PHE:HD1	1.77	0.47
1:A:178:GLY:O	1:A:213:ALA:HB2	2.14	0.47
1:A:197:ALA:HB1	1:A:217:MET:SD	2.54	0.46
1:A:214:LEU:HD21	1:B:218:LEU:HD13	1.97	0.46
1:C:229:ASN:HB3	1:C:232:ASN:HB2	1.98	0.46
1:A:63:VAL:HG11	1:A:89:LEU:HD22	1.98	0.46
1:C:140:GLU:OE2	1:C:146:VAL:HG12	2.16	0.46
1:B:62:ILE:HD12	1:B:63:VAL:N	2.30	0.46
1:C:132:ALA:HA	1:C:176:ILE:HD12	1.96	0.46
1:C:138:THR:HG21	1:C:234:PHE:HA	1.97	0.46
1:A:129:GLN:HG3	1:A:150:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ALA:HB3	4:E:302:NAI:N7N	2.30	0.45
1:B:212:THR:O	1:B:216:THR:HG23	2.16	0.45
1:C:75:PRO:HG3	1:C:111:PRO:HG3	1.99	0.45
1:D:86:PHE:O	1:D:90:GLN:N	2.49	0.45
1:D:189:GLY:N	1:D:222[A]:ALA:HB1	2.32	0.45
1:E:129:GLN:HA	1:E:132:ALA:HB3	1.97	0.45
1:A:131:VAL:HG11	1:A:200:THR:HG22	1.99	0.45
1:D:152:VAL:HB	1:D:160:LEU:HD23	1.99	0.45
1:F:46:ASN:HB3	1:F:48:PHE:CD1	2.52	0.45
1:B:173:VAL:O	1:B:195:VAL:HA	2.17	0.45
1:C:138:THR:HG23	1:C:237:ALA:HB3	1.98	0.44
1:E:99:HIS:HB2	1:E:102:ALA:HB3	1.99	0.44
1:A:115:THR:HG22	1:A:117:GLY:H	1.81	0.44
1:D:123:THR:OG1	1:D:128:ASP:HB2	2.17	0.44
1:E:173:VAL:HG13	1:E:195:VAL:HG22	1.99	0.44
1:F:199:PRO:HG2	1:F:230:ILE:HG12	1.99	0.44
1:B:62:ILE:CD1	1:B:89:LEU:HD21	2.48	0.44
1:E:241:SER:O	1:E:245:GLN:HG2	2.16	0.44
1:C:166:VAL:HG22	1:B:145:ARG:NH2	2.33	0.44
1:B:50:GLU:O	1:B:77:LEU:N	2.50	0.44
1:D:81:LEU:HD11	1:D:86:PHE:HB2	2.00	0.44
1:D:213:ALA:O	1:D:217:MET:HE2	2.18	0.44
1:B:102:ALA:HB2	1:B:133:GLU:HG3	1.99	0.44
1:A:148:ARG:HB3	1:A:150:TYR:CE1	2.52	0.44
1:A:58:THR:HG23	1:A:60:THR:H	1.83	0.43
1:F:123:THR:HG22	1:F:150:TYR:HA	2.00	0.43
1:E:204:TYR:HH	1:F:219:ASN:HA	1.82	0.43
1:C:133:GLU:OE1	1:C:150:TYR:OH	2.35	0.43
1:A:102:ALA:HB2	1:A:133:GLU:HB3	2.00	0.43
1:C:199:PRO:CD	1:C:217:MET:HE1	2.48	0.43
1:F:201:SER:OG	1:F:231:ASP:OD2	2.25	0.43
1:E:154:VAL:HG12	4:E:302:NAI:H42N	2.00	0.43
1:F:139:ALA:HB2	1:F:237:ALA:HB1	2.00	0.43
1:C:139:ALA:HB2	1:C:237:ALA:HB1	2.00	0.42
1:D:72:GLN:O	1:D:74:LEU:N	2.47	0.42
1:C:51:VAL:HA	1:C:77:LEU:O	2.20	0.42
1:D:77:LEU:HD23	1:D:78:THR:N	2.35	0.42
1:C:154:VAL:N	3:C:302:NAD:H4N	2.33	0.42
1:F:198:VAL:O	1:F:217:MET:HE1	2.20	0.42
1:C:131:VAL:HG11	1:C:200:THR:HG22	2.01	0.42
1:E:216:THR:OG1	1:F:216:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:TYR:O	1:E:242:MET:HG3	2.20	0.42
1:B:77:LEU:HD23	1:B:78:THR:N	2.35	0.42
1:A:160:LEU:HD11	1:A:187:VAL:HG22	2.01	0.42
1:F:133:GLU:O	1:F:137:VAL:HG22	2.20	0.42
1:C:180:GLU:O	3:C:302:NAD:N7N	2.53	0.41
1:E:123:THR:HG21	1:E:132:ALA:HB2	2.01	0.41
1:B:157:ILE:HD13	1:B:160:LEU:HB3	2.03	0.41
1:F:123:THR:HA	1:F:176:ILE:O	2.21	0.41
1:A:211:MET:O	1:A:215:LEU:HG	2.20	0.41
1:A:215:LEU:O	1:A:219:ASN:ND2	2.53	0.41
1:C:171:ARG:NH2	1:D:246:MET:HB3	2.36	0.41
1:F:76:ILE:HD13	1:F:76:ILE:HA	1.86	0.41
1:E:126:THR:N	4:E:302:NAI:O1N	2.53	0.41
1:A:49:PRO:HB3	1:A:75:PRO:O	2.21	0.41
1:C:134:GLU:O	1:C:138:THR:HG22	2.20	0.41
1:B:199:PRO:HG2	1:B:230:ILE:HA	2.03	0.41
1:A:76:ILE:HG13	1:A:107:VAL:H	1.85	0.40
1:C:217:MET:HE3	1:C:227:VAL:HG13	2.03	0.40
1:A:131:VAL:HG21	1:A:231:ASP:HA	2.03	0.40
1:E:125:GLY:HA2	4:E:302:NAI:O2N	2.20	0.40
1:F:90:GLN:N	1:F:91:PRO:HD2	2.35	0.40
1:F:123:THR:OG1	1:F:128:ASP:HB2	2.21	0.40
1:E:204:TYR:CE1	1:F:219:ASN:HB2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:PHE:CE2	1:F:223:SER:OG[3_545]	1.65	0.55
1:D:206:THR:OG1	1:D:229:ASN:OD1[3_445]	2.11	0.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	199/256 (78%)	181 (91%)	17 (8%)	1 (0%)	25 54
1	B	201/256 (78%)	182 (90%)	19 (10%)	0	100 100
1	C	196/256 (77%)	180 (92%)	14 (7%)	2 (1%)	13 39
1	D	204/256 (80%)	178 (87%)	26 (13%)	0	100 100
1	E	209/256 (82%)	182 (87%)	25 (12%)	2 (1%)	13 39
1	F	197/256 (77%)	181 (92%)	16 (8%)	0	100 100
All	All	1206/1536 (78%)	1084 (90%)	117 (10%)	5 (0%)	30 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	LEU
1	E	48	PHE
1	E	39	ASP
1	A	181	GLY
1	C	202	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	134/191 (70%)	124 (92%)	10 (8%)	11 35
1	B	135/191 (71%)	129 (96%)	6 (4%)	24 50
1	C	128/191 (67%)	122 (95%)	6 (5%)	22 49
1	D	120/191 (63%)	109 (91%)	11 (9%)	7 26
1	E	131/191 (69%)	126 (96%)	5 (4%)	28 54
1	F	130/191 (68%)	122 (94%)	8 (6%)	15 40
All	All	778/1146 (68%)	732 (94%)	46 (6%)	17 41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	TYR
1	A	66	VAL
1	A	67	GLN
1	A	70	SER
1	A	80	ARG
1	A	163	LYS
1	A	164	LEU
1	A	176	ILE
1	A	198	VAL
1	A	206	THR
1	C	60	THR
1	C	107	VAL
1	C	159	ARG
1	C	164	LEU
1	C	226	THR
1	C	228	VAL
1	D	66	VAL
1	D	81	LEU
1	D	146	VAL
1	D	152	VAL
1	D	160	LEU
1	D	172	VAL
1	D	176	ILE
1	D	214	LEU
1	D	216	THR
1	D	221[A]	CYS
1	D	221[B]	CYS
1	E	65	ILE
1	E	73	THR
1	E	76	ILE
1	E	154	VAL
1	E	173	VAL
1	F	50	GLU
1	F	52	ILE
1	F	62	ILE
1	F	63	VAL
1	F	214	LEU
1	F	217	MET
1	F	225	ILE
1	F	244	ASN
1	B	107	VAL
1	B	110	GLN
1	B	157	ILE

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Mol	Chain	Res	Type
1	B	164	LEU
1	B	206	THR
1	B	227	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	C	302	2	42,48,48	3.94	19 (45%)	50,73,73	2.55	7 (14%)
4	NAI	E	302	2	43,48,48	0.98	2 (4%)	50,73,73	1.57	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
3	NAD	C	302	2	-	10/26/62/62	0/5/5/5
4	NAI	E	302	2	-	11/25/72/72	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	NAD	C2D-C3D	-10.87	1.23	1.53
3	C	302	NAD	C3B-C4B	-8.74	1.30	1.53
3	C	302	NAD	O4D-C1D	8.03	1.51	1.40
3	C	302	NAD	O4B-C4B	7.75	1.62	1.45
3	C	302	NAD	O4B-C1B	-7.36	1.31	1.40
3	C	302	NAD	C7N-N7N	7.22	1.46	1.33
3	C	302	NAD	O4D-C4D	-6.18	1.31	1.45
3	C	302	NAD	PA-O3	6.05	1.66	1.59
3	C	302	NAD	PN-O3	5.79	1.65	1.59
3	C	302	NAD	C3D-C4D	5.61	1.67	1.53
3	C	302	NAD	C6A-N6A	3.55	1.46	1.34
4	E	302	NAI	C6N-N1N	3.54	1.45	1.37
3	C	302	NAD	O2D-C2D	3.32	1.51	1.43
4	E	302	NAI	C4N-C3N	3.02	1.55	1.50
3	C	302	NAD	O3B-C3B	3.02	1.50	1.43
3	C	302	NAD	O2B-C2B	-2.61	1.36	1.43
3	C	302	NAD	O7N-C7N	-2.57	1.19	1.24
3	C	302	NAD	C2A-N3A	2.49	1.36	1.32
3	C	302	NAD	O3D-C3D	2.37	1.48	1.43
3	C	302	NAD	C3N-C7N	2.27	1.54	1.50
3	C	302	NAD	C4N-C3N	-2.07	1.36	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	NAD	C1B-N9A-C4A	13.29	149.99	126.64
4	E	302	NAI	C6N-N1N-C2N	-8.47	110.25	119.32
3	C	302	NAD	N3A-C2A-N1A	-6.28	120.14	128.67
3	C	302	NAD	C5A-C6A-N6A	5.93	129.34	120.31
3	C	302	NAD	N6A-C6A-N1A	-4.06	109.67	118.33
4	E	302	NAI	C1D-N1N-C2N	3.38	126.70	121.14
3	C	302	NAD	C4D-O4D-C1D	-3.31	106.89	109.92
3	C	302	NAD	C4B-O4B-C1B	-3.14	107.05	109.92
3	C	302	NAD	C6N-N1N-C2N	-2.59	119.67	121.88
4	E	302	NAI	C5A-C6A-N6A	2.09	123.49	120.31
4	E	302	NAI	C3D-C2D-C1D	2.00	105.25	101.46
4	E	302	NAI	C3N-C2N-N1N	-2.00	120.27	123.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	NAD	C5B-O5B-PA-O2A
3	C	302	NAD	C5B-O5B-PA-O3
4	E	302	NAI	C5B-O5B-PA-O1A
4	E	302	NAI	C5B-O5B-PA-O3
4	E	302	NAI	O4D-C1D-N1N-C2N
4	E	302	NAI	C2N-C3N-C7N-N7N
4	E	302	NAI	O4B-C4B-C5B-O5B
4	E	302	NAI	C3B-C4B-C5B-O5B
4	E	302	NAI	O4D-C4D-C5D-O5D
3	C	302	NAD	C4N-C3N-C7N-O7N
3	C	302	NAD	C2N-C3N-C7N-O7N
4	E	302	NAI	C2N-C3N-C7N-O7N
4	E	302	NAI	C5B-O5B-PA-O2A
3	C	302	NAD	C4N-C3N-C7N-N7N
3	C	302	NAD	C2N-C3N-C7N-N7N
4	E	302	NAI	C3D-C4D-C5D-O5D
3	C	302	NAD	PA-O3-PN-O2N
3	C	302	NAD	O4B-C4B-C5B-O5B
3	C	302	NAD	PN-O3-PA-O2A
4	E	302	NAI	PA-O3-PN-O1N
3	C	302	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

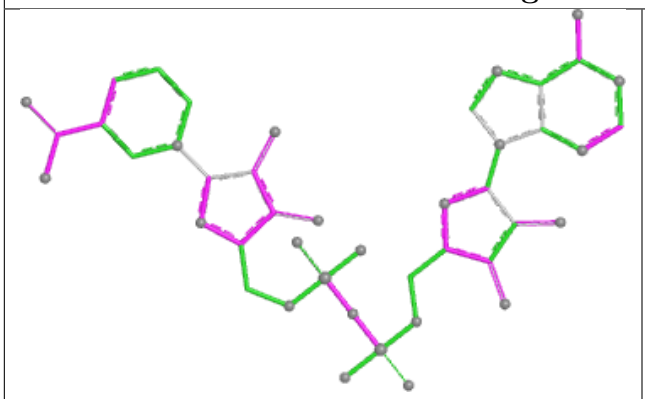
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	NAD	5	0
4	E	302	NAI	9	0

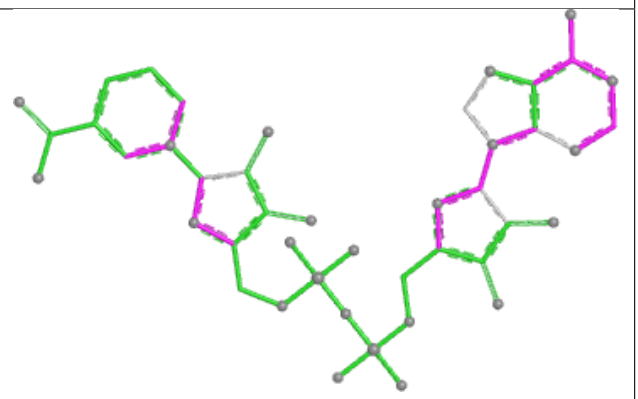
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

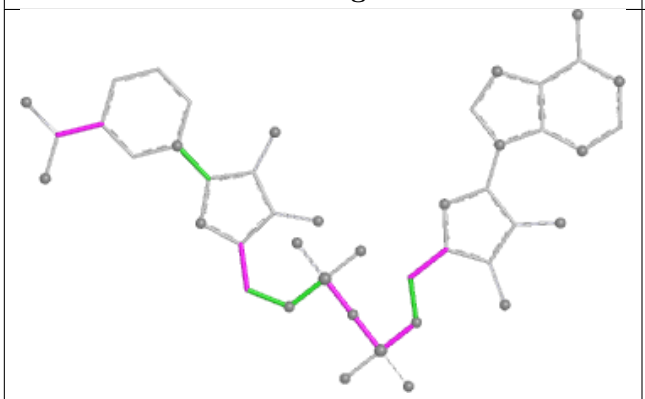
Ligand NAD C 302



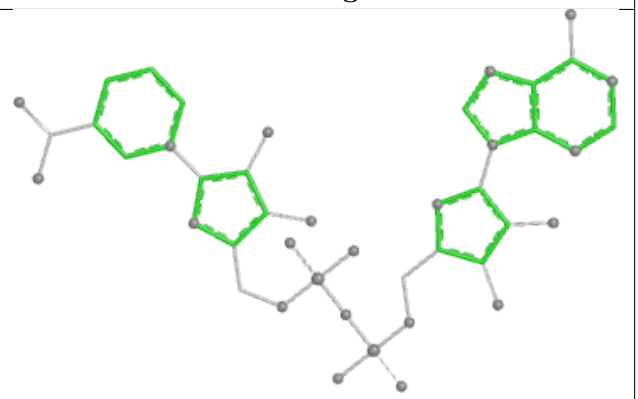
Bond lengths



Bond angles

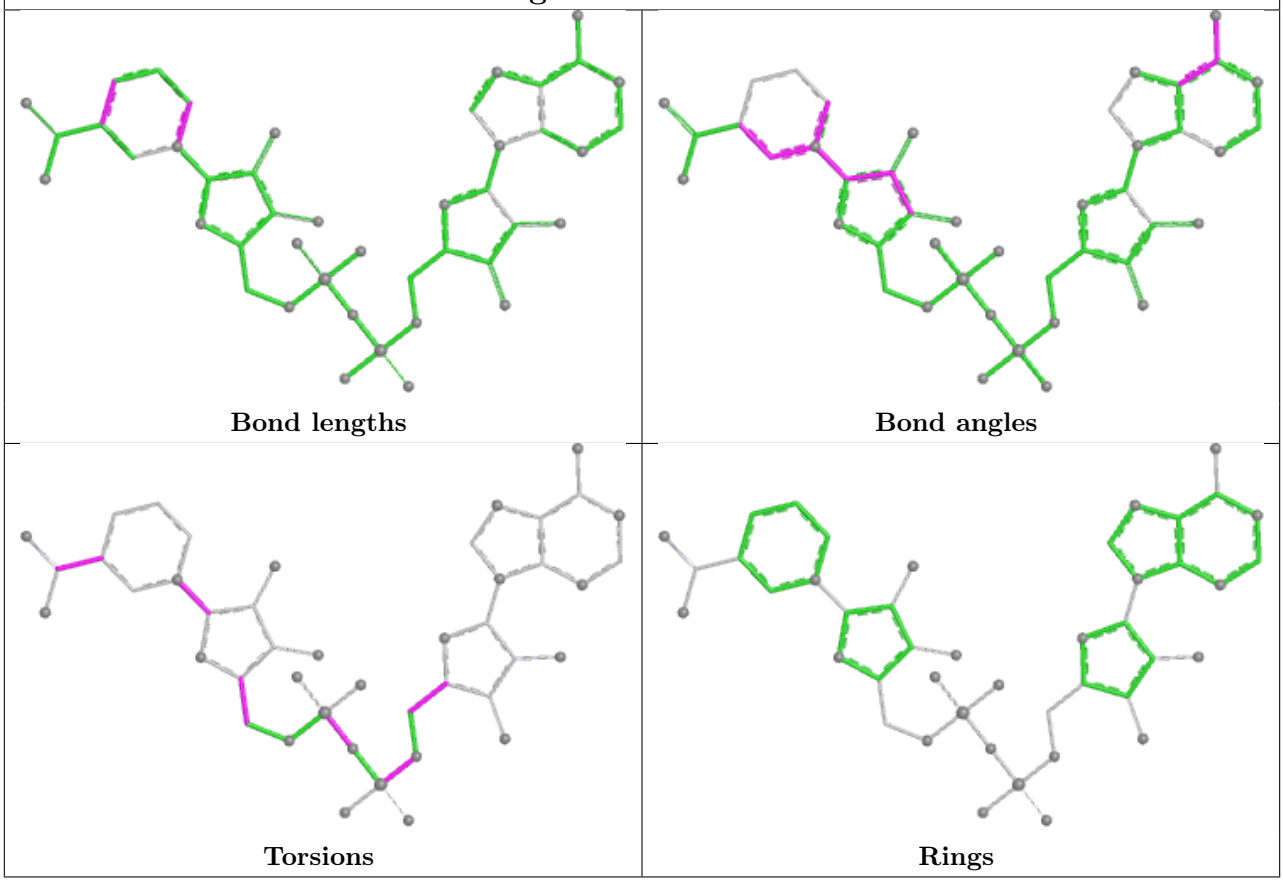


Torsions



Rings

Ligand NAI E 302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	201/256 (78%)	-0.03	4 (1%)	64	55	39, 99, 196, 262	1 (0%)
1	B	203/256 (79%)	-0.06	4 (1%)	64	55	42, 90, 159, 193	0
1	C	200/256 (78%)	0.03	4 (2%)	64	55	45, 93, 181, 255	0
1	D	201/256 (78%)	0.12	4 (1%)	64	55	31, 110, 187, 245	5 (2%)
1	E	211/256 (82%)	0.13	5 (2%)	59	51	65, 113, 173, 221	0
1	F	201/256 (78%)	0.12	3 (1%)	71	62	61, 121, 210, 294	0
All	All	1217/1536 (79%)	0.05	24 (1%)	64	55	31, 106, 189, 294	6 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222[A]	ALA	18.8
1	D	221[A]	CYS	13.8
1	A	62	ILE	3.4
1	F	220	SER	3.4
1	E	204	TYR	3.2
1	C	162	ALA	3.1
1	D	51	VAL	3.0
1	A	189	GLY	2.9
1	B	107	VAL	2.7
1	F	180	GLU	2.6
1	B	50	GLU	2.5
1	A	222	ALA	2.5
1	F	111	PRO	2.5
1	E	49	PRO	2.5
1	C	161	PHE	2.4
1	C	180	GLU	2.3
1	E	48	PHE	2.3
1	C	89	LEU	2.2
1	B	162	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	179	MET	2.1
1	E	120	ALA	2.1
1	E	172	VAL	2.0
1	A	221	CYS	2.0
1	B	109	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

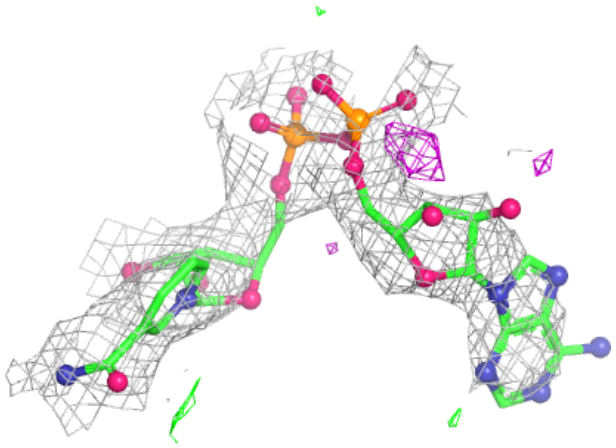
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

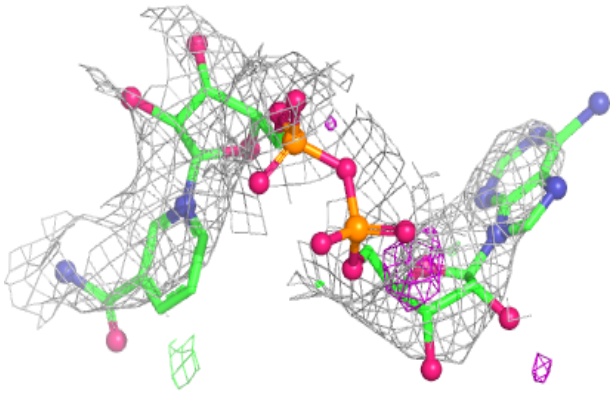
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	E	301	1/1	0.77	0.09	112,112,112,112	0
2	MG	C	303	1/1	0.78	0.09	90,90,90,90	0
2	MG	A	301	1/1	0.79	0.10	67,67,67,67	0
3	NAD	C	302	44/44	0.82	0.13	116,124,141,144	0
4	NAI	E	302	44/44	0.89	0.10	99,108,115,122	0
2	MG	C	301	1/1	0.95	0.08	76,76,76,76	0

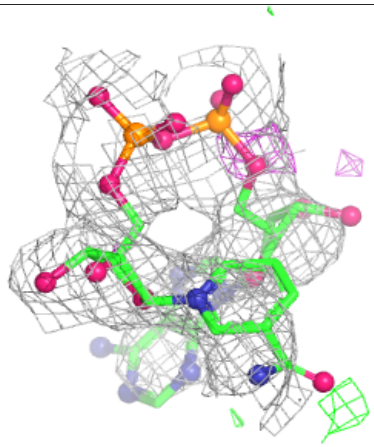
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD C 302:

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

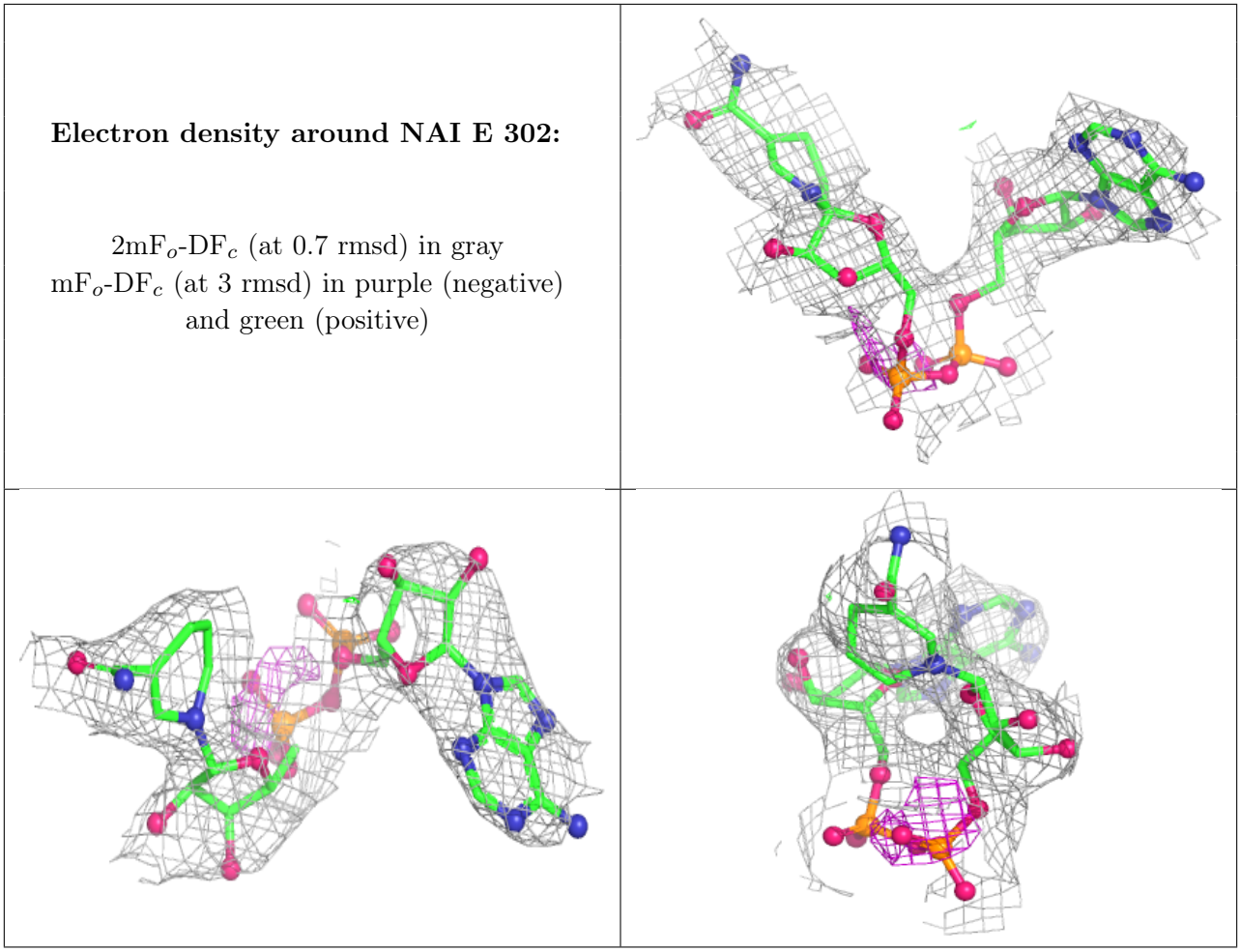






Electron density around NAI E 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.