



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:20 am BST

PDB ID : 3GNQ
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase, type I from Burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-03-17
Resolution : 2.40 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 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 : 2.11
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) : 2.11

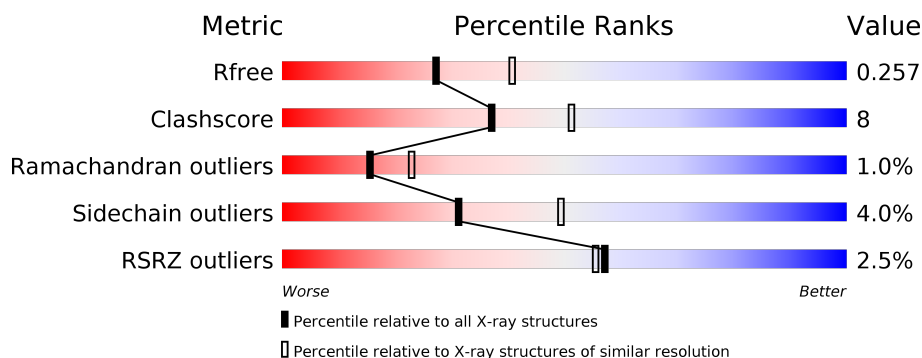
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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 $\leq 5\%$. 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	344	
1	B	344	
1	C	344	
1	D	344	
1	E	344	
1	F	344	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	344	
1	H	344	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21007 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, type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2529	1587	445	490	7			
1	B	334	Total	C	N	O	S	0	0	0
			2500	1567	439	487	7			
1	C	335	Total	C	N	O	S	0	0	0
			2521	1582	444	488	7			
1	D	335	Total	C	N	O	S	0	0	0
			2515	1579	441	488	7			
1	E	335	Total	C	N	O	S	0	0	0
			2515	1579	441	488	7			
1	F	335	Total	C	N	O	S	0	0	0
			2525	1584	444	490	7			
1	G	335	Total	C	N	O	S	0	0	0
			2523	1584	442	490	7			
1	H	335	Total	C	N	O	S	0	0	0
			2533	1590	446	490	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
A	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
A	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
A	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
A	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
A	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
A	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
A	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
B	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
B	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
B	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
B	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
B	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6

Continued on next page...

Continued from previous page...

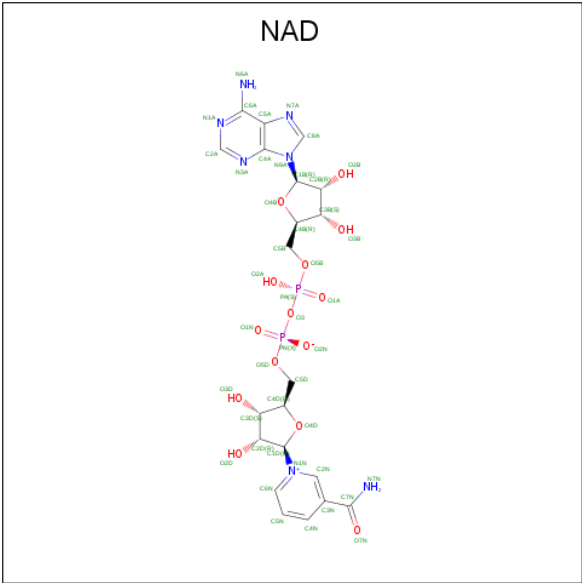
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
B	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
B	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
C	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
C	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
C	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
D	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
D	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
D	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
E	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
E	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
E	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
F	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
F	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
F	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
G	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
G	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
G	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
G	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
G	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
G	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
G	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-8	MET	-	EXPRESSION TAG	UNP Q3JNL6
H	-7	ALA	-	EXPRESSION TAG	UNP Q3JNL6
H	-6	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-5	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-4	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-3	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-2	HIS	-	EXPRESSION TAG	UNP Q3JNL6
H	-1	HIS	-	EXPRESSION TAG	UNP Q3JNL6

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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		

Continued on next page...

Continued from previous page...

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

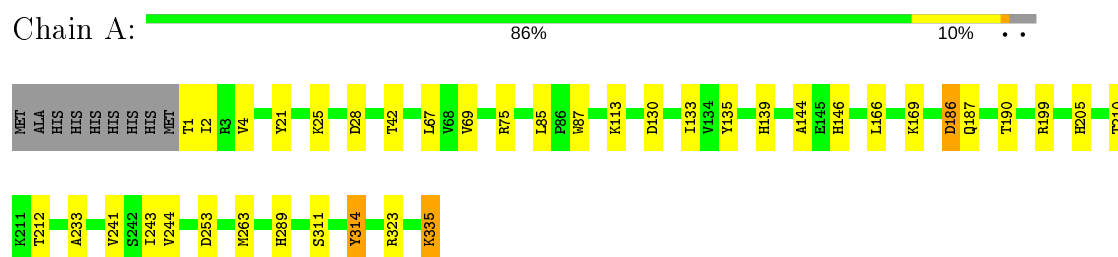
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	60	Total	O	0	0
			60	60		
3	C	81	Total	O	0	0
			81	81		
3	D	40	Total	O	0	0
			40	40		
3	E	53	Total	O	0	0
			53	53		
3	F	52	Total	O	0	0
			52	52		
3	G	33	Total	O	0	0
			33	33		
3	H	86	Total	O	0	0
			86	86		

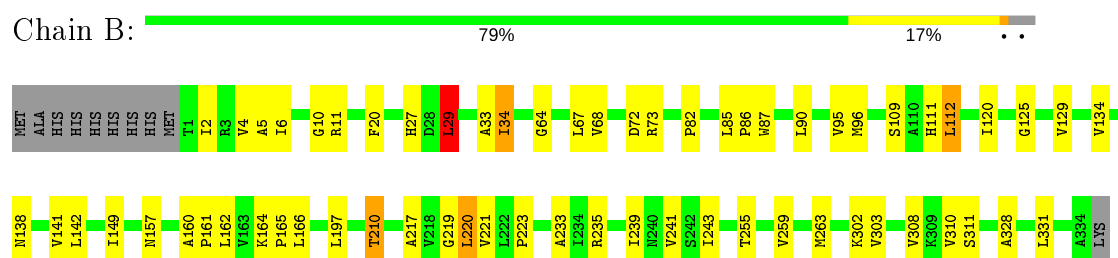
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

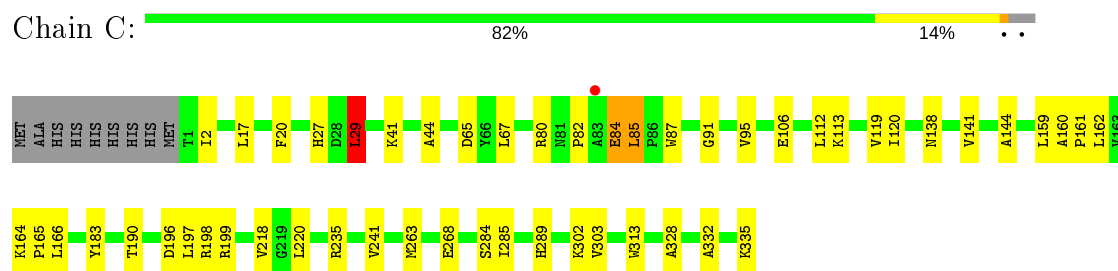
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I



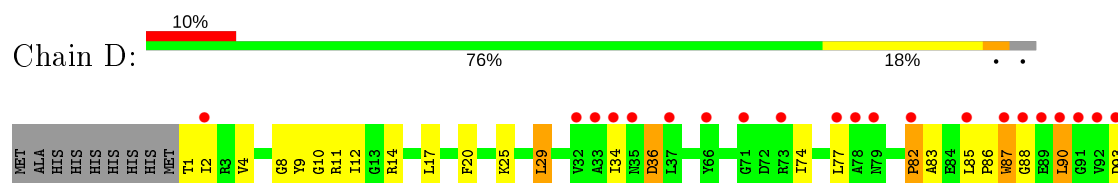
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

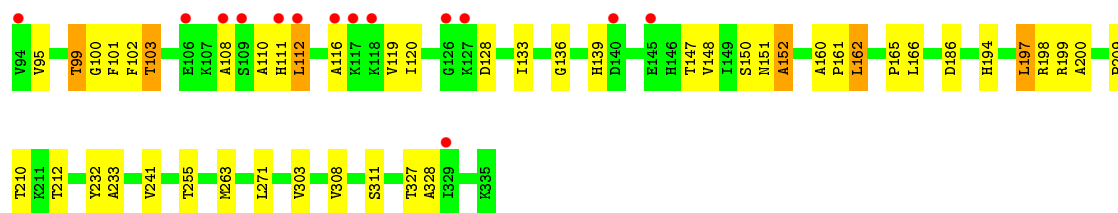


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

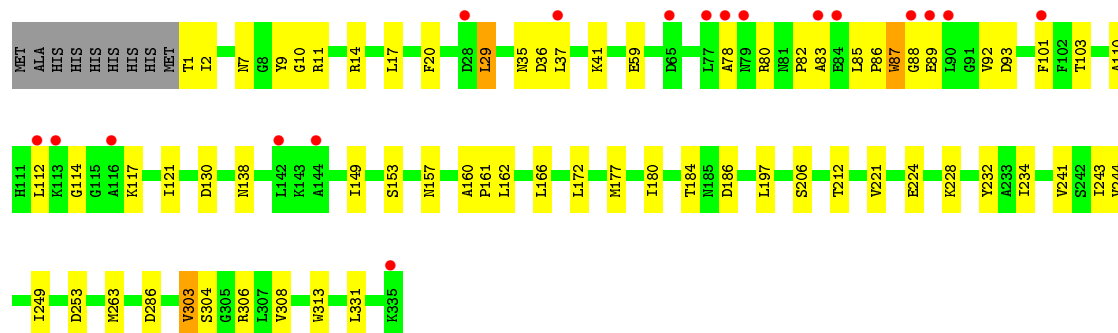
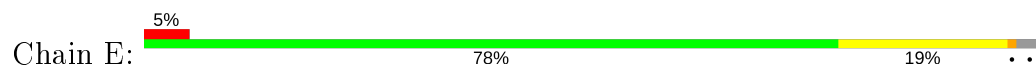


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

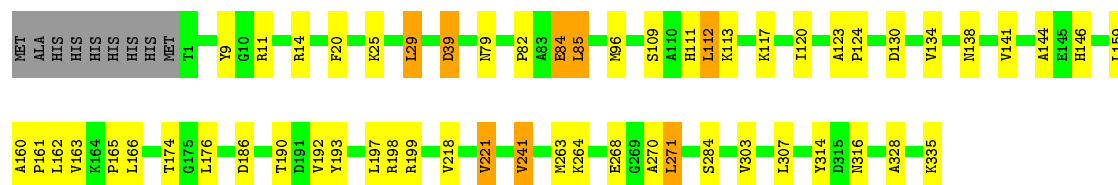
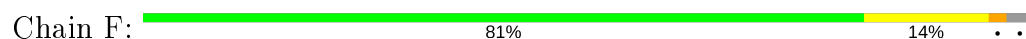




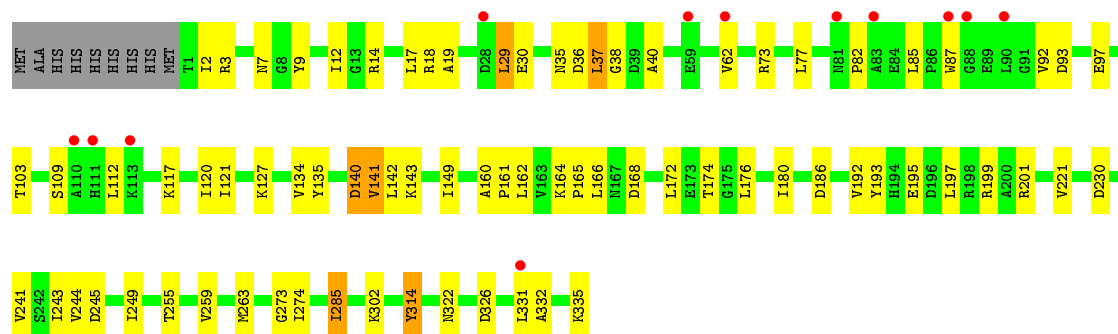
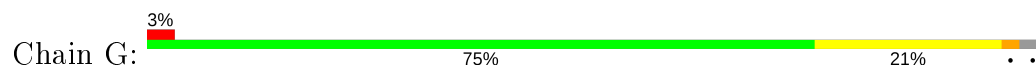
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I



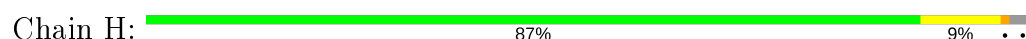
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

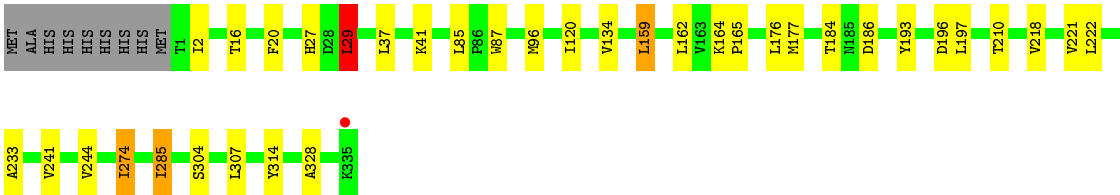


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.93Å 173.80Å 93.50Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	48.84 – 2.40 48.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.84-2.40) 99.7 (48.84-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.263 0.202 , 0.257	Depositor DCC
R_{free} test set	5649 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21007	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/2573	0.68	0/3498
1	B	0.52	0/2544	0.64	1/3466 (0.0%)
1	C	0.54	0/2565	0.65	2/3489 (0.1%)
1	D	0.50	0/2559	0.62	0/3482
1	E	0.48	0/2559	0.59	0/3482
1	F	0.52	0/2569	0.66	1/3494 (0.0%)
1	G	0.48	0/2567	0.60	0/3491
1	H	0.58	0/2577	0.68	1/3502 (0.0%)
All	All	0.53	0/20513	0.64	5/27904 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	LEU	CA-CB-CG	5.71	128.44	115.30
1	C	29	LEU	CA-CB-CG	5.41	127.74	115.30
1	C	198	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	198	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	29	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2529	0	2528	28	0
1	B	2500	0	2467	46	0
1	C	2521	0	2513	26	0
1	D	2515	0	2502	62	0
1	E	2515	0	2502	53	0
1	F	2525	0	2517	42	0
1	G	2523	0	2517	55	0
1	H	2533	0	2539	23	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	6	0
2	E	44	0	26	3	0
2	F	44	0	26	2	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	133	0	0	1	0
3	B	60	0	0	1	0
3	C	81	0	0	2	0
3	D	40	0	0	1	0
3	E	53	0	0	2	0
3	F	52	0	0	0	0
3	G	33	0	0	1	0
3	H	86	0	0	0	0
All	All	21007	0	20267	319	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 8.

All (319) 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:A:166:LEU:HG	1:A:263:MET:CE	1.89	1.02
1:G:166:LEU:HG	1:G:263:MET:HE3	1.43	0.99
1:E:162:LEU:HD12	1:E:263:MET:HE3	1.44	0.98
1:A:166:LEU:HG	1:A:263:MET:HE1	1.48	0.95
1:D:166:LEU:HG	1:D:263:MET:CE	1.98	0.94
1:F:166:LEU:HG	1:F:263:MET:CE	1.97	0.93
1:D:85:LEU:HD13	1:D:87:TRP:CZ2	2.07	0.89
1:D:120:ILE:HD13	1:D:327:THR:HG22	1.55	0.87
1:D:186:ASP:OD1	1:D:199:ARG:NH1	2.12	0.82
1:F:166:LEU:HG	1:F:263:MET:HE3	1.62	0.80
1:G:166:LEU:HG	1:G:263:MET:CE	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:LEU:C	1:G:17:LEU:HD23	2.02	0.79
1:G:149:ILE:HD13	1:G:331:LEU:HD13	1.64	0.78
1:A:166:LEU:CG	1:A:263:MET:CE	2.63	0.77
1:E:35:ASN:ND2	1:E:85:LEU:HD11	2.00	0.77
1:E:304:SER:O	1:G:174:THR:HG21	1.87	0.75
1:B:85:LEU:HD13	1:B:87:TRP:CZ2	2.22	0.74
1:E:10:GLY:HA3	2:E:901:NAD:H4B	1.71	0.72
1:D:166:LEU:HG	1:D:263:MET:HE2	1.70	0.72
1:C:82:PRO:HA	1:C:85:LEU:HD12	1.70	0.72
1:D:160:ALA:HB3	1:D:161:PRO:HD3	1.72	0.72
1:E:1:THR:C	1:E:2:ILE:HD12	2.11	0.71
1:F:120:ILE:HD11	1:F:328:ALA:HA	1.75	0.69
1:A:166:LEU:HG	1:A:263:MET:HE2	1.74	0.69
1:E:149:ILE:HD13	1:E:331:LEU:HD13	1.74	0.69
1:G:141:VAL:HG13	3:G:347:HOH:O	1.93	0.69
1:D:12:ILE:HD11	2:D:901:NAD:C2N	2.24	0.68
1:D:120:ILE:HD11	1:D:328:ALA:HA	1.75	0.68
1:B:160:ALA:HB3	1:B:161:PRO:HD3	1.76	0.68
1:D:112:LEU:HD21	1:D:147:THR:HB	1.77	0.67
1:G:186:ASP:OD1	1:G:199:ARG:NH1	2.28	0.66
1:E:37:LEU:HD13	1:E:78:ALA:HB1	1.77	0.66
1:G:82:PRO:HA	1:G:85:LEU:HD12	1.76	0.66
1:B:120:ILE:HD11	1:B:328:ALA:HA	1.78	0.66
1:E:87:TRP:HE3	1:E:92:VAL:HG21	1.61	0.66
1:E:103:THR:O	1:E:121:ILE:HD13	1.97	0.65
1:A:166:LEU:CG	1:A:263:MET:HE2	2.26	0.65
1:B:165:PRO:HB2	1:B:263:MET:HE2	1.79	0.65
1:F:166:LEU:CG	1:F:263:MET:HE3	2.27	0.64
1:F:138:ASN:O	1:F:141:VAL:HG22	1.97	0.64
1:A:42:THR:HG23	1:B:197:LEU:CD2	2.27	0.64
1:E:166:LEU:HG	1:E:263:MET:HE1	1.79	0.63
1:E:87:TRP:CE3	1:E:92:VAL:HG21	2.34	0.63
1:C:235:ARG:NH1	3:C:378:HOH:O	2.32	0.63
1:D:4:VAL:HG21	1:D:29:LEU:HD12	1.80	0.63
1:B:210:THR:HG22	1:B:233:ALA:HB3	1.79	0.63
1:G:160:ALA:HB3	1:G:161:PRO:HD3	1.79	0.63
1:E:37:LEU:HA	3:E:337:HOH:O	1.98	0.63
1:F:160:ALA:HB3	1:F:161:PRO:HD3	1.80	0.62
1:D:303:VAL:HG12	1:D:308:VAL:HG22	1.81	0.62
1:G:140:ASP:N	1:G:140:ASP:OD1	2.31	0.62
1:B:165:PRO:HB2	1:B:263:MET:CE	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ALA:HB3	1:E:161:PRO:HD3	1.81	0.62
1:A:210:THR:HG22	1:A:233:ALA:HB3	1.82	0.61
1:F:144:ALA:HB2	1:F:335:LYS:HB2	1.83	0.61
1:D:108:ALA:HB3	1:D:148:VAL:HG11	1.82	0.61
1:B:125:GLY:HA3	1:B:129:VAL:HG11	1.82	0.61
1:D:166:LEU:HG	1:D:263:MET:HE3	1.80	0.61
1:D:4:VAL:HG21	1:D:29:LEU:CD1	2.30	0.61
1:F:29:LEU:HD23	1:F:29:LEU:C	2.22	0.61
1:D:210:THR:CG2	1:D:233:ALA:HB3	2.30	0.60
1:H:159:LEU:HD13	1:H:218:VAL:HG21	1.83	0.60
1:G:273:GLY:O	1:G:274:ILE:HD12	2.02	0.60
1:A:243:ILE:HD11	1:A:311:SER:HB3	1.82	0.60
1:H:27:HIS:HB3	1:H:29:LEU:HD13	1.84	0.60
1:H:85:LEU:HD13	1:H:87:TRP:CZ2	2.37	0.59
1:E:162:LEU:CD1	1:E:263:MET:HE3	2.26	0.59
1:A:166:LEU:CD2	1:A:263:MET:HE2	2.33	0.59
1:C:190:THR:HG23	1:D:11:ARG:HD2	1.83	0.59
1:D:90:LEU:H	1:D:90:LEU:HD23	1.67	0.59
1:F:270:ALA:O	1:F:271:LEU:HB2	2.03	0.59
1:B:109:SER:HA	1:B:112:LEU:HD22	1.85	0.58
1:F:11:ARG:HG2	2:F:901:NAD:O2A	2.03	0.58
1:D:17:LEU:HD12	1:D:34:ILE:HD11	1.84	0.58
1:D:77:LEU:HD13	1:D:85:LEU:HD22	1.84	0.58
1:D:90:LEU:N	1:D:90:LEU:HD23	2.18	0.58
1:G:103:THR:O	1:G:121:ILE:HD13	2.03	0.58
1:B:82:PRO:HA	1:B:85:LEU:HD12	1.85	0.57
1:D:34:ILE:HD12	1:D:74:ILE:HG21	1.86	0.57
1:B:33:ALA:O	1:B:34:ILE:HD12	2.04	0.57
1:C:165:PRO:HB2	1:C:263:MET:HE2	1.85	0.57
1:D:210:THR:HG22	1:D:233:ALA:HB3	1.87	0.57
1:F:144:ALA:HB3	1:F:335:LYS:HD2	1.86	0.57
1:G:85:LEU:HD13	1:G:87:TRP:CZ2	2.40	0.57
1:B:142:LEU:HD22	1:B:331:LEU:HD13	1.87	0.57
1:E:304:SER:HB2	1:G:176:LEU:HD21	1.87	0.57
1:E:9:TYR:CE1	1:E:14:ARG:HG2	2.41	0.56
1:G:165:PRO:HD2	1:G:263:MET:HE1	1.87	0.56
1:D:8:GLY:HA3	1:D:99:THR:HG23	1.87	0.56
1:F:186:ASP:OD1	1:F:199:ARG:NH1	2.38	0.56
1:D:95:VAL:HB	1:D:119:VAL:HG22	1.87	0.56
1:B:95:VAL:HG11	1:B:111:HIS:CE1	2.40	0.56
1:D:162:LEU:O	1:D:263:MET:HE1	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:HD11	1:H:193:TYR:CE2	2.41	0.55
1:B:20:PHE:CE1	1:B:29:LEU:HD22	2.42	0.55
1:B:2:ILE:HD12	1:B:2:ILE:N	2.21	0.55
1:C:220:LEU:HB3	3:C:370:HOH:O	2.06	0.55
1:D:2:ILE:HG23	1:D:93:ASP:HB2	1.88	0.55
1:F:109:SER:HA	1:F:112:LEU:HD22	1.88	0.55
1:D:8:GLY:CA	1:D:99:THR:HG23	2.36	0.55
1:E:20:PHE:CE1	1:E:29:LEU:HD22	2.42	0.55
1:A:166:LEU:HD21	1:A:263:MET:HE2	1.87	0.55
1:E:112:LEU:HD11	1:E:117:LYS:O	2.06	0.55
1:C:165:PRO:HB2	1:C:263:MET:CE	2.36	0.54
1:A:130:ASP:HB3	1:A:146:HIS:CD2	2.42	0.54
1:B:166:LEU:HG	1:B:263:MET:HE1	1.88	0.54
1:E:172:LEU:C	1:E:172:LEU:HD23	2.27	0.54
1:B:27:HIS:ND1	3:B:383:HOH:O	2.34	0.54
1:B:138:ASN:O	1:B:141:VAL:HG22	2.05	0.54
1:G:109:SER:HA	1:G:112:LEU:HD13	1.90	0.54
1:G:36:ASP:O	1:G:38:GLY:N	2.40	0.54
1:D:82:PRO:HG2	1:D:110:ALA:HB3	1.90	0.54
1:B:210:THR:HG21	1:B:235:ARG:HE	1.73	0.53
1:F:82:PRO:HB3	1:F:111:HIS:CE1	2.44	0.53
1:H:285:ILE:O	1:H:285:ILE:HD13	2.08	0.53
1:G:17:LEU:C	1:G:17:LEU:CD2	2.77	0.53
1:F:159:LEU:HD23	1:F:218:VAL:HG21	1.91	0.53
1:F:166:LEU:HG	1:F:263:MET:HE1	1.88	0.53
1:F:166:LEU:CG	1:F:263:MET:CE	2.79	0.53
1:G:244:VAL:HG23	1:G:314:TYR:CE2	2.44	0.52
1:D:12:ILE:HD11	2:D:901:NAD:N1N	2.24	0.52
1:F:176:LEU:HD12	1:H:307:LEU:HG	1.91	0.52
1:H:134:VAL:HG23	1:H:221:VAL:HG11	1.91	0.52
1:E:243:ILE:HD12	1:E:313:TRP:CH2	2.44	0.52
1:G:164:LYS:NZ	1:G:168:ASP:OD2	2.43	0.52
1:G:112:LEU:N	1:G:112:LEU:HD12	2.24	0.52
1:E:303:VAL:HB	1:E:308:VAL:HG22	1.92	0.52
1:D:100:GLY:O	1:D:103:THR:HG23	2.10	0.52
1:B:162:LEU:HD21	1:B:310:VAL:CG2	2.40	0.52
1:G:192:VAL:HG22	1:G:193:TYR:H	1.74	0.52
1:B:149:ILE:CD1	1:B:331:LEU:HD22	2.40	0.51
1:B:162:LEU:HD21	1:B:310:VAL:HG21	1.92	0.51
1:A:42:THR:HG23	1:B:197:LEU:HD23	1.91	0.51
1:C:17:LEU:C	1:C:17:LEU:HD23	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:PHE:CE1	1:H:29:LEU:HD22	2.46	0.51
1:G:2:ILE:HG22	1:G:3:ARG:N	2.26	0.51
1:H:2:ILE:N	1:H:2:ILE:HD12	2.25	0.51
1:D:9:TYR:CE1	1:D:14:ARG:HG2	2.45	0.51
1:E:232:TYR:HE1	1:E:234:ILE:HD11	1.76	0.51
1:E:249:ILE:HD13	1:G:249:ILE:HG12	1.93	0.50
1:A:205:HIS:CE1	1:B:239:ILE:HB	2.46	0.50
1:B:166:LEU:HG	1:B:263:MET:CE	2.41	0.50
1:C:120:ILE:HD11	1:C:328:ALA:HA	1.94	0.50
1:D:165:PRO:HG2	1:D:263:MET:HE1	1.94	0.50
1:B:86:PRO:O	1:B:90:LEU:HD12	2.12	0.50
1:E:37:LEU:CD1	1:E:78:ALA:HB1	2.41	0.50
1:E:82:PRO:HD2	1:E:110:ALA:HB1	1.93	0.49
1:D:20:PHE:CE1	1:D:25:LYS:HA	2.47	0.49
1:F:29:LEU:HD23	1:F:29:LEU:O	2.12	0.49
1:A:190:THR:HG23	1:B:11:ARG:HD3	1.94	0.49
1:A:2:ILE:HG22	1:A:4:VAL:HG23	1.94	0.49
1:C:27:HIS:HB3	1:C:29:LEU:HD13	1.95	0.49
1:C:160:ALA:HB3	1:C:161:PRO:HD3	1.93	0.49
1:G:172:LEU:HD21	1:G:174:THR:C	2.33	0.49
1:G:192:VAL:HG22	1:G:193:TYR:N	2.28	0.49
1:B:243:ILE:HD11	1:B:311:SER:HB3	1.94	0.49
1:G:87:TRP:CE3	1:G:92:VAL:HG21	2.48	0.49
1:D:85:LEU:HD13	1:D:87:TRP:HZ2	1.74	0.48
1:H:184:THR:OG1	1:H:186:ASP:OD2	2.17	0.48
1:D:166:LEU:CG	1:D:263:MET:HE3	2.42	0.48
1:G:143:LYS:HB3	1:G:335:LYS:NZ	2.28	0.48
1:D:108:ALA:CB	1:D:148:VAL:HG11	2.44	0.48
1:D:198:ARG:HD2	1:D:209:PRO:O	2.14	0.48
1:D:194:HIS:HB3	1:D:200:ALA:HB2	1.95	0.48
1:E:180:ILE:HB	1:E:243:ILE:HG22	1.95	0.48
1:G:172:LEU:C	1:G:172:LEU:HD23	2.33	0.48
1:G:77:LEU:HD12	1:G:87:TRP:CH2	2.49	0.48
1:D:255:THR:HA	1:D:303:VAL:HG21	1.95	0.48
1:D:166:LEU:CD1	1:D:263:MET:HE3	2.44	0.48
1:E:184:THR:OG1	1:E:186:ASP:OD2	2.29	0.48
1:F:197:LEU:HD12	1:F:197:LEU:N	2.28	0.48
1:C:190:THR:HG23	1:D:11:ARG:CD	2.44	0.48
1:E:138:ASN:HD21	1:E:221:VAL:HG12	1.79	0.48
1:G:135:TYR:CE1	1:G:326:ASP:O	2.67	0.48
1:B:303:VAL:HG12	1:B:308:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:OD2	1:A:199:ARG:NH1	2.47	0.47
1:F:316:ASN:O	2:F:901:NAD:H4N	2.14	0.47
1:B:68:VAL:HG22	1:B:73:ARG:HG2	1.95	0.47
1:E:10:GLY:CA	2:E:901:NAD:H4B	2.42	0.47
1:G:85:LEU:HD13	1:G:87:TRP:HZ2	1.77	0.47
1:G:245:ASP:OD1	1:G:245:ASP:C	2.51	0.47
1:H:210:THR:HG22	1:H:233:ALA:HB3	1.97	0.47
1:B:220:LEU:C	1:B:220:LEU:HD23	2.34	0.47
1:D:111:HIS:HB2	1:D:119:VAL:HG21	1.96	0.47
1:B:95:VAL:HG11	1:B:111:HIS:ND1	2.29	0.47
1:F:241:VAL:HG11	1:F:284:SER:O	2.15	0.47
1:E:86:PRO:O	1:E:88:GLY:N	2.48	0.47
1:G:134:VAL:HG23	1:G:221:VAL:HG11	1.97	0.47
1:D:120:ILE:HD11	1:D:328:ALA:CA	2.44	0.47
1:C:84:GLU:O	1:C:85:LEU:O	2.33	0.46
1:F:270:ALA:O	1:F:271:LEU:CB	2.63	0.46
1:F:20:PHE:CE1	1:F:29:LEU:HD22	2.50	0.46
1:C:95:VAL:HB	1:C:119:VAL:HG22	1.97	0.46
1:E:35:ASN:O	1:E:36:ASP:HB2	2.14	0.46
1:A:166:LEU:CD1	1:A:263:MET:CE	2.93	0.46
1:G:17:LEU:HD23	1:G:18:ARG:N	2.30	0.46
1:G:180:ILE:HB	1:G:243:ILE:HG22	1.97	0.46
1:G:2:ILE:HG12	1:G:332:ALA:CB	2.46	0.46
1:G:19:ALA:HB1	1:G:322:ASN:OD1	2.16	0.46
1:A:210:THR:CG2	1:A:233:ALA:HB3	2.45	0.46
1:G:164:LYS:HB3	1:G:165:PRO:HD3	1.98	0.46
1:G:255:THR:O	1:G:259:VAL:HG23	2.16	0.46
1:F:264:LYS:O	1:F:268:GLU:HG2	2.15	0.45
1:G:9:TYR:CZ	1:G:14:ARG:HG2	2.50	0.45
1:A:67:LEU:CD1	1:A:69:VAL:HG23	2.46	0.45
1:C:199:ARG:HH12	1:C:235:ARG:NH1	2.14	0.45
1:C:20:PHE:CE1	1:C:29:LEU:HD22	2.51	0.45
1:D:17:LEU:C	1:D:17:LEU:HD23	2.37	0.45
1:F:20:PHE:CE1	1:F:29:LEU:CD2	3.00	0.45
1:H:196:ASP:C	1:H:196:ASP:OD1	2.53	0.45
1:A:67:LEU:CD1	1:A:69:VAL:CG2	2.94	0.45
1:F:39:ASP:N	1:F:39:ASP:OD1	2.49	0.45
1:E:153:SER:O	1:E:157:ASN:ND2	2.35	0.45
1:D:212:THR:HG22	1:D:232:TYR:HA	1.99	0.45
1:D:17:LEU:CD1	1:D:34:ILE:HD11	2.45	0.45
1:G:2:ILE:HG12	1:G:332:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ALA:HB1	1:F:124:PRO:HD2	1.99	0.45
1:F:307:LEU:HG	1:H:176:LEU:HD12	1.99	0.45
1:A:244:VAL:HG23	1:A:314:TYR:CE2	2.52	0.44
1:G:149:ILE:CD1	1:G:331:LEU:HD13	2.43	0.44
1:C:196:ASP:HB3	1:C:199:ARG:HB2	1.99	0.44
1:E:9:TYR:OH	1:E:17:LEU:HD13	2.16	0.44
1:F:84:GLU:O	1:F:85:LEU:C	2.55	0.44
1:B:217:ALA:O	1:B:220:LEU:HD22	2.17	0.44
1:E:166:LEU:HG	1:E:263:MET:CE	2.47	0.44
1:F:20:PHE:CE1	1:F:25:LYS:HA	2.52	0.44
1:A:187:GLN:HB3	3:A:365:HOH:O	2.17	0.44
1:D:197:LEU:HD13	3:D:348:HOH:O	2.18	0.44
1:D:11:ARG:HG3	2:D:901:NAD:O2A	2.18	0.44
1:G:2:ILE:H	1:G:2:ILE:HD12	1.83	0.43
1:A:85:LEU:HD13	1:A:87:TRP:CZ2	2.53	0.43
1:D:133:ILE:HD12	1:D:139:HIS:HA	2.01	0.43
1:E:83:ALA:HA	1:E:114:GLY:HA3	2.00	0.43
1:E:253:ASP:OD1	1:E:306:ARG:NH1	2.51	0.43
1:F:79:ASN:ND2	1:F:84:GLU:OE2	2.50	0.43
1:H:164:LYS:HB3	1:H:165:PRO:HD3	1.99	0.43
1:B:10:GLY:O	1:B:11:ARG:C	2.56	0.43
1:D:165:PRO:HG2	1:D:263:MET:CE	2.48	0.43
1:D:86:PRO:O	1:D:88:GLY:N	2.51	0.43
1:D:10:GLY:CA	2:D:901:NAD:H4B	2.49	0.43
1:E:10:GLY:HA3	2:E:901:NAD:C4B	2.46	0.43
1:F:165:PRO:HG2	1:F:263:MET:HE1	2.00	0.43
1:H:120:ILE:HD11	1:H:328:ALA:HA	1.98	0.43
1:E:29:LEU:HD23	1:E:29:LEU:C	2.39	0.43
1:F:9:TYR:O	1:F:14:ARG:HG3	2.18	0.43
1:A:1:THR:OG1	1:A:28:ASP:OD2	2.25	0.43
1:A:144:ALA:HB2	1:A:335:LYS:HB2	2.00	0.43
1:G:35:ASN:ND2	1:G:85:LEU:HD11	2.33	0.43
1:B:85:LEU:HD13	1:B:87:TRP:HZ2	1.76	0.43
1:C:138:ASN:O	1:C:141:VAL:HG22	2.19	0.43
1:F:29:LEU:C	1:F:29:LEU:CD2	2.87	0.43
1:G:9:TYR:CE1	1:G:14:ARG:HG2	2.54	0.43
1:F:174:THR:HB	1:H:304:SER:OG	2.19	0.43
1:B:96:MET:HE3	1:B:328:ALA:HB2	2.01	0.43
1:C:144:ALA:HB2	1:C:335:LYS:HG3	2.01	0.43
1:C:85:LEU:HD13	1:C:87:TRP:CZ2	2.54	0.43
1:E:243:ILE:HD12	1:E:313:TRP:CZ3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:PRO:O	1:E:87:TRP:C	2.56	0.43
1:H:2:ILE:CD1	1:H:2:ILE:N	2.82	0.43
1:B:4:VAL:HG21	1:B:29:LEU:HG	2.01	0.42
1:C:166:LEU:HG	1:C:263:MET:HE1	2.01	0.42
1:E:80:ARG:O	1:E:82:PRO:HD3	2.18	0.42
1:G:40:ALA:HB1	1:G:62:VAL:HG13	2.00	0.42
1:H:120:ILE:HD11	1:H:328:ALA:CB	2.49	0.42
1:D:120:ILE:HD13	1:D:327:THR:CG2	2.39	0.42
1:B:255:THR:O	1:B:259:VAL:HG23	2.18	0.42
1:F:96:MET:HE2	1:F:328:ALA:HB2	2.01	0.42
1:B:5:ALA:HB1	1:B:87:TRP:CZ3	2.55	0.42
1:C:159:LEU:HD23	1:C:218:VAL:HG21	2.00	0.42
1:E:286:ASP:OD1	1:G:201:ARG:NH1	2.45	0.42
1:G:142:LEU:HD22	1:G:331:LEU:HD12	2.01	0.42
1:B:164:LYS:HB3	1:B:165:PRO:HD3	2.02	0.42
1:E:162:LEU:O	1:E:263:MET:HE1	2.19	0.42
1:E:11:ARG:HD2	1:F:190:THR:HG23	2.01	0.42
1:A:135:TYR:HB3	1:A:323:ARG:HD3	2.02	0.42
1:B:6:ILE:HD12	1:B:34:ILE:HD11	2.01	0.42
1:C:2:ILE:HG12	1:C:332:ALA:CB	2.50	0.42
1:E:112:LEU:CD1	1:E:117:LYS:O	2.67	0.42
1:E:228:LYS:NZ	3:E:454:HOH:O	2.53	0.42
1:H:177:MET:HG3	1:H:244:VAL:HG13	2.02	0.42
1:H:120:ILE:CD1	1:H:328:ALA:HB2	2.49	0.42
1:F:192:VAL:HG22	1:F:193:TYR:H	1.84	0.42
1:E:1:THR:CG2	1:E:2:ILE:N	2.83	0.42
1:G:176:LEU:CD2	1:G:230:ASP:HB3	2.50	0.42
1:D:136:GLY:O	1:D:271:LEU:HD23	2.20	0.41
1:A:21:TYR:CE2	1:A:25:LYS:HD3	2.56	0.41
1:F:82:PRO:HA	1:F:85:LEU:HD12	2.02	0.41
1:C:164:LYS:HB3	1:C:165:PRO:HD3	2.00	0.41
1:D:100:GLY:O	1:D:102:PHE:N	2.54	0.41
1:E:82:PRO:HD2	1:E:110:ALA:CB	2.50	0.41
1:C:87:TRP:O	1:C:91:GLY:N	2.54	0.41
1:D:166:LEU:CG	1:D:263:MET:CE	2.84	0.41
1:B:219:GLY:O	1:B:223:PRO:HA	2.20	0.41
1:E:2:ILE:HD12	1:E:2:ILE:N	2.35	0.41
1:B:134:VAL:HG13	1:B:157:ASN:ND2	2.35	0.41
1:G:29:LEU:HD23	1:G:30:GLU:N	2.35	0.41
1:B:20:PHE:CE1	1:B:29:LEU:CD2	3.03	0.41
1:B:34:ILE:O	1:B:34:ILE:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:O	1:D:263:MET:CE	2.69	0.41
1:D:112:LEU:HA	1:D:116:ALA:O	2.21	0.41
1:E:243:ILE:HD12	1:E:313:TRP:CZ2	2.55	0.41
1:G:7:ASN:ND2	1:G:97:GLU:OE1	2.48	0.41
1:A:133:ILE:HD12	1:A:139:HIS:HA	2.03	0.41
1:C:44:ALA:HB2	1:C:67:LEU:HD13	2.03	0.41
1:D:12:ILE:HD12	2:D:901:NAD:O4D	2.21	0.41
1:F:134:VAL:HG23	1:F:221:VAL:HG11	2.02	0.41
1:G:12:ILE:HD11	2:G:901:NAD:C3N	2.51	0.41
1:B:149:ILE:HD13	1:B:331:LEU:HD22	2.02	0.40
1:F:130:ASP:HB3	1:F:146:HIS:CD2	2.55	0.40
1:E:206:SER:OG	1:G:285:ILE:HB	2.21	0.40
1:H:120:ILE:HD11	1:H:328:ALA:HB2	2.03	0.40
1:C:284:SER:HB3	1:C:313:TRP:CZ3	2.57	0.40
1:D:10:GLY:HA3	2:D:901:NAD:H4B	2.02	0.40
1:D:83:ALA:HA	1:D:110:ALA:O	2.22	0.40
1:E:234:ILE:N	1:E:234:ILE:HD12	2.37	0.40
1:H:164:LYS:HD2	1:H:222:LEU:HD21	2.02	0.40
1:E:177:MET:HG3	1:E:244:VAL:HG13	2.04	0.40
1:D:151:ASN:O	1:D:152:ALA:HB3	2.22	0.40
1:H:16:THR:HG21	1:H:96:MET:SD	2.62	0.40

There are no symmetry-related clashes.

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	333/344 (97%)	311 (93%)	21 (6%)	1 (0%)	41	55
1	B	332/344 (96%)	305 (92%)	25 (8%)	2 (1%)	25	36
1	C	333/344 (97%)	317 (95%)	13 (4%)	3 (1%)	17	25
1	D	333/344 (97%)	306 (92%)	21 (6%)	6 (2%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	333/344 (97%)	303 (91%)	26 (8%)	4 (1%)	13	19
1	F	333/344 (97%)	312 (94%)	18 (5%)	3 (1%)	17	25
1	G	333/344 (97%)	306 (92%)	22 (7%)	5 (2%)	10	14
1	H	333/344 (97%)	316 (95%)	15 (4%)	2 (1%)	25	36
All	All	2663/2752 (97%)	2476 (93%)	161 (6%)	26 (1%)	15	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	GLU
1	C	85	LEU
1	D	87	TRP
1	G	37	LEU
1	A	241	VAL
1	B	241	VAL
1	C	241	VAL
1	D	101	PHE
1	D	128	ASP
1	D	241	VAL
1	E	241	VAL
1	F	241	VAL
1	G	117	LYS
1	G	241	VAL
1	H	241	VAL
1	D	152	ALA
1	B	64	GLY
1	E	87	TRP
1	F	271	LEU
1	D	36	ASP
1	E	93	ASP
1	E	224	GLU
1	F	85	LEU
1	G	127	LYS
1	H	274	ILE
1	G	141	VAL

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	269/278 (97%)	260 (97%)	9 (3%)	38	57
1	B	263/278 (95%)	254 (97%)	9 (3%)	37	56
1	C	267/278 (96%)	252 (94%)	15 (6%)	21	34
1	D	266/278 (96%)	254 (96%)	12 (4%)	27	44
1	E	266/278 (96%)	256 (96%)	10 (4%)	33	51
1	F	268/278 (96%)	257 (96%)	11 (4%)	30	48
1	G	268/278 (96%)	257 (96%)	11 (4%)	30	48
1	H	270/278 (97%)	261 (97%)	9 (3%)	38	57
All	All	2137/2224 (96%)	2051 (96%)	86 (4%)	31	49

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	113	LYS
1	A	169	LYS
1	A	186	ASP
1	A	212	THR
1	A	253	ASP
1	A	289	HIS
1	A	314	TYR
1	A	335	LYS
1	B	29	LEU
1	B	34	ILE
1	B	67	LEU
1	B	72	ASP
1	B	112	LEU
1	B	210	THR
1	B	220	LEU
1	B	221	VAL
1	B	302	LYS
1	C	29	LEU
1	C	41	LYS
1	C	65	ASP
1	C	80	ARG
1	C	106	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	112	LEU
1	C	113	LYS
1	C	162	LEU
1	C	183	TYR
1	C	197	LEU
1	C	268	GLU
1	C	285	ILE
1	C	289	HIS
1	C	302	LYS
1	C	303	VAL
1	D	1	THR
1	D	29	LEU
1	D	36	ASP
1	D	82	PRO
1	D	90	LEU
1	D	99	THR
1	D	103	THR
1	D	112	LEU
1	D	150	SER
1	D	162	LEU
1	D	197	LEU
1	D	311	SER
1	E	7	ASN
1	E	29	LEU
1	E	41	LYS
1	E	59	GLU
1	E	89	GLU
1	E	101	PHE
1	E	130	ASP
1	E	197	LEU
1	E	212	THR
1	E	303	VAL
1	F	29	LEU
1	F	39	ASP
1	F	84	GLU
1	F	112	LEU
1	F	113	LYS
1	F	117	LYS
1	F	162	LEU
1	F	163	VAL
1	F	221	VAL
1	F	303	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	314	TYR
1	G	29	LEU
1	G	73	ARG
1	G	93	ASP
1	G	120	ILE
1	G	140	ASP
1	G	162	LEU
1	G	195	GLU
1	G	197	LEU
1	G	285	ILE
1	G	302	LYS
1	G	314	TYR
1	H	29	LEU
1	H	37	LEU
1	H	41	LYS
1	H	159	LEU
1	H	162	LEU
1	H	197	LEU
1	H	274	ILE
1	H	285	ILE
1	H	314	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	157	ASN
1	C	157	ASN
1	D	35	ASN
1	F	43	ASN
1	H	157	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	C	901	-	42,48,48	1.69	4 (9%)	50,73,73	1.45	8 (16%)
2	NAD	E	901	-	42,48,48	1.77	3 (7%)	50,73,73	1.26	4 (8%)
2	NAD	B	901	-	42,48,48	1.71	3 (7%)	50,73,73	1.30	4 (8%)
2	NAD	G	901	-	42,48,48	1.72	3 (7%)	50,73,73	1.24	5 (10%)
2	NAD	D	901	-	42,48,48	1.80	4 (9%)	50,73,73	1.23	4 (8%)
2	NAD	F	901	-	42,48,48	1.72	4 (9%)	50,73,73	1.29	3 (6%)
2	NAD	H	901	-	42,48,48	1.70	3 (7%)	50,73,73	1.33	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	C	901	-	-	5/26/62/62	0/5/5/5
2	NAD	E	901	-	-	2/26/62/62	0/5/5/5
2	NAD	B	901	-	-	5/26/62/62	0/5/5/5
2	NAD	G	901	-	-	5/26/62/62	0/5/5/5
2	NAD	D	901	-	-	3/26/62/62	0/5/5/5
2	NAD	F	901	-	-	5/26/62/62	0/5/5/5
2	NAD	H	901	-	-	9/26/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	NAD	O7N-C7N	9.27	1.41	1.24
2	E	901	NAD	O7N-C7N	8.91	1.41	1.24
2	G	901	NAD	O7N-C7N	8.81	1.41	1.24
2	H	901	NAD	O7N-C7N	8.59	1.40	1.24
2	F	901	NAD	O7N-C7N	8.57	1.40	1.24
2	B	901	NAD	O7N-C7N	8.56	1.40	1.24
2	C	901	NAD	O7N-C7N	8.14	1.39	1.24
2	D	901	NAD	C2A-N3A	4.27	1.39	1.32
2	F	901	NAD	C2A-N3A	4.22	1.38	1.32
2	B	901	NAD	C2A-N3A	4.21	1.38	1.32
2	G	901	NAD	C2A-N3A	4.13	1.38	1.32
2	E	901	NAD	C2A-N3A	4.10	1.38	1.32
2	C	901	NAD	C2A-N3A	3.94	1.38	1.32
2	H	901	NAD	C2A-N3A	3.45	1.37	1.32
2	E	901	NAD	C2A-N1A	2.90	1.39	1.33
2	G	901	NAD	C2A-N1A	2.85	1.39	1.33
2	B	901	NAD	C2A-N1A	2.78	1.39	1.33
2	D	901	NAD	C2A-N1A	2.75	1.39	1.33
2	C	901	NAD	C2A-N1A	2.74	1.39	1.33
2	H	901	NAD	C2A-N1A	2.55	1.38	1.33
2	F	901	NAD	C2A-N1A	2.52	1.38	1.33
2	D	901	NAD	C2N-N1N	2.29	1.37	1.35
2	F	901	NAD	C2N-N1N	2.18	1.37	1.35
2	C	901	NAD	PA-O2A	-2.16	1.45	1.55

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	NAD	N3A-C2A-N1A	-6.07	119.19	128.68
2	F	901	NAD	N3A-C2A-N1A	-5.72	119.73	128.68
2	D	901	NAD	N3A-C2A-N1A	-5.69	119.78	128.68
2	B	901	NAD	N3A-C2A-N1A	-5.63	119.88	128.68
2	G	901	NAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	C	901	NAD	N3A-C2A-N1A	-5.43	120.20	128.68
2	H	901	NAD	N3A-C2A-N1A	-5.15	120.63	128.68
2	H	901	NAD	PN-O3-PA	-3.61	120.44	132.83
2	C	901	NAD	C3N-C7N-N7N	3.34	121.76	117.75
2	B	901	NAD	PN-O3-PA	-3.32	121.42	132.83
2	F	901	NAD	PN-O3-PA	-3.08	122.27	132.83
2	C	901	NAD	C1B-N9A-C4A	-3.06	121.26	126.64
2	C	901	NAD	PN-O3-PA	-2.95	122.70	132.83
2	G	901	NAD	PN-O3-PA	-2.93	122.77	132.83
2	H	901	NAD	C2N-C3N-C4N	2.86	121.50	118.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	NAD	C2N-C3N-C4N	2.81	121.44	118.26
2	C	901	NAD	O7N-C7N-C3N	-2.65	116.46	119.63
2	B	901	NAD	C2N-C3N-C4N	2.58	121.18	118.26
2	D	901	NAD	C6N-N1N-C2N	-2.50	119.69	121.97
2	E	901	NAD	C5A-C6A-N6A	-2.38	116.74	120.35
2	B	901	NAD	O7N-C7N-C3N	-2.36	116.81	119.63
2	G	901	NAD	C1B-N9A-C4A	-2.35	122.51	126.64
2	E	901	NAD	PN-O3-PA	-2.24	125.14	132.83
2	C	901	NAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	E	901	NAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	H	901	NAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	G	901	NAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	G	901	NAD	O2N-PN-O1N	2.14	122.81	112.24
2	F	901	NAD	C3N-C7N-N7N	2.13	120.31	117.75
2	D	901	NAD	C3D-C2D-C1D	2.10	104.14	100.98
2	C	901	NAD	C6N-N1N-C2N	-2.09	120.07	121.97
2	D	901	NAD	O2N-PN-O1N	2.08	122.54	112.24
2	H	901	NAD	C1B-N9A-C4A	-2.07	123.00	126.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	NAD	O4D-C1D-N1N-C2N
2	C	901	NAD	O4D-C1D-N1N-C6N
2	C	901	NAD	C2D-C1D-N1N-C2N
2	C	901	NAD	C2D-C1D-N1N-C6N
2	E	901	NAD	O4D-C1D-N1N-C2N
2	B	901	NAD	O4D-C1D-N1N-C2N
2	B	901	NAD	O4D-C1D-N1N-C6N
2	B	901	NAD	C2D-C1D-N1N-C2N
2	B	901	NAD	C2D-C1D-N1N-C6N
2	G	901	NAD	O4D-C1D-N1N-C2N
2	G	901	NAD	O4D-C1D-N1N-C6N
2	G	901	NAD	C2D-C1D-N1N-C6N
2	D	901	NAD	O4D-C1D-N1N-C2N
2	F	901	NAD	O4D-C1D-N1N-C2N
2	F	901	NAD	O4D-C1D-N1N-C6N
2	F	901	NAD	C2D-C1D-N1N-C2N
2	F	901	NAD	C2D-C1D-N1N-C6N
2	H	901	NAD	O4D-C1D-N1N-C2N
2	H	901	NAD	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

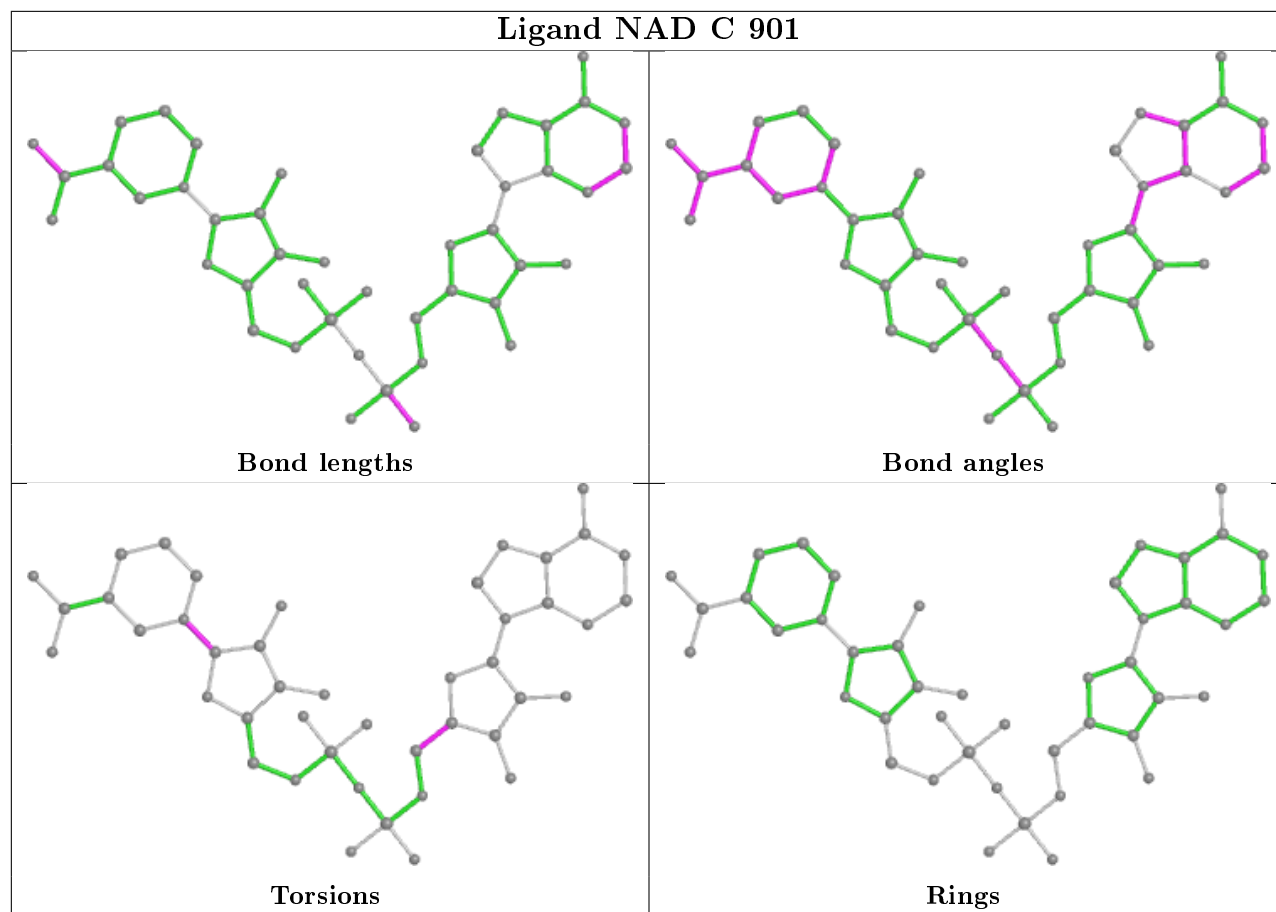
Mol	Chain	Res	Type	Atoms
2	H	901	NAD	C2D-C1D-N1N-C2N
2	H	901	NAD	C2D-C1D-N1N-C6N
2	H	901	NAD	C4N-C3N-C7N-N7N
2	H	901	NAD	C4N-C3N-C7N-O7N
2	C	901	NAD	O4B-C4B-C5B-O5B
2	D	901	NAD	PN-O3-PA-O1A
2	H	901	NAD	C2N-C3N-C7N-N7N
2	H	901	NAD	O4B-C4B-C5B-O5B
2	E	901	NAD	O4B-C4B-C5B-O5B
2	H	901	NAD	C2N-C3N-C7N-O7N
2	G	901	NAD	C2D-C1D-N1N-C2N
2	G	901	NAD	O4B-C4B-C5B-O5B
2	D	901	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	O4B-C4B-C5B-O5B
2	F	901	NAD	O4B-C4B-C5B-O5B

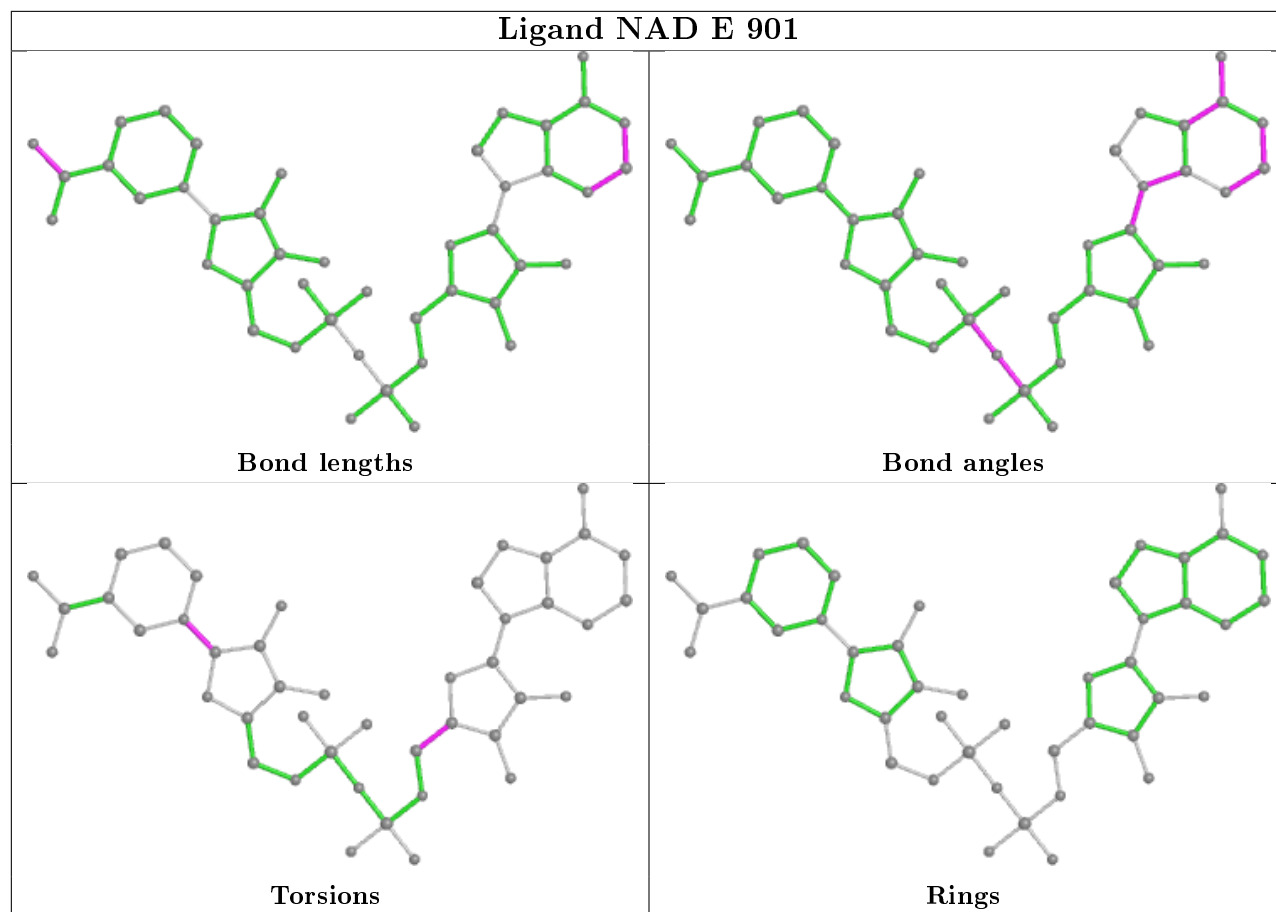
There are no ring outliers.

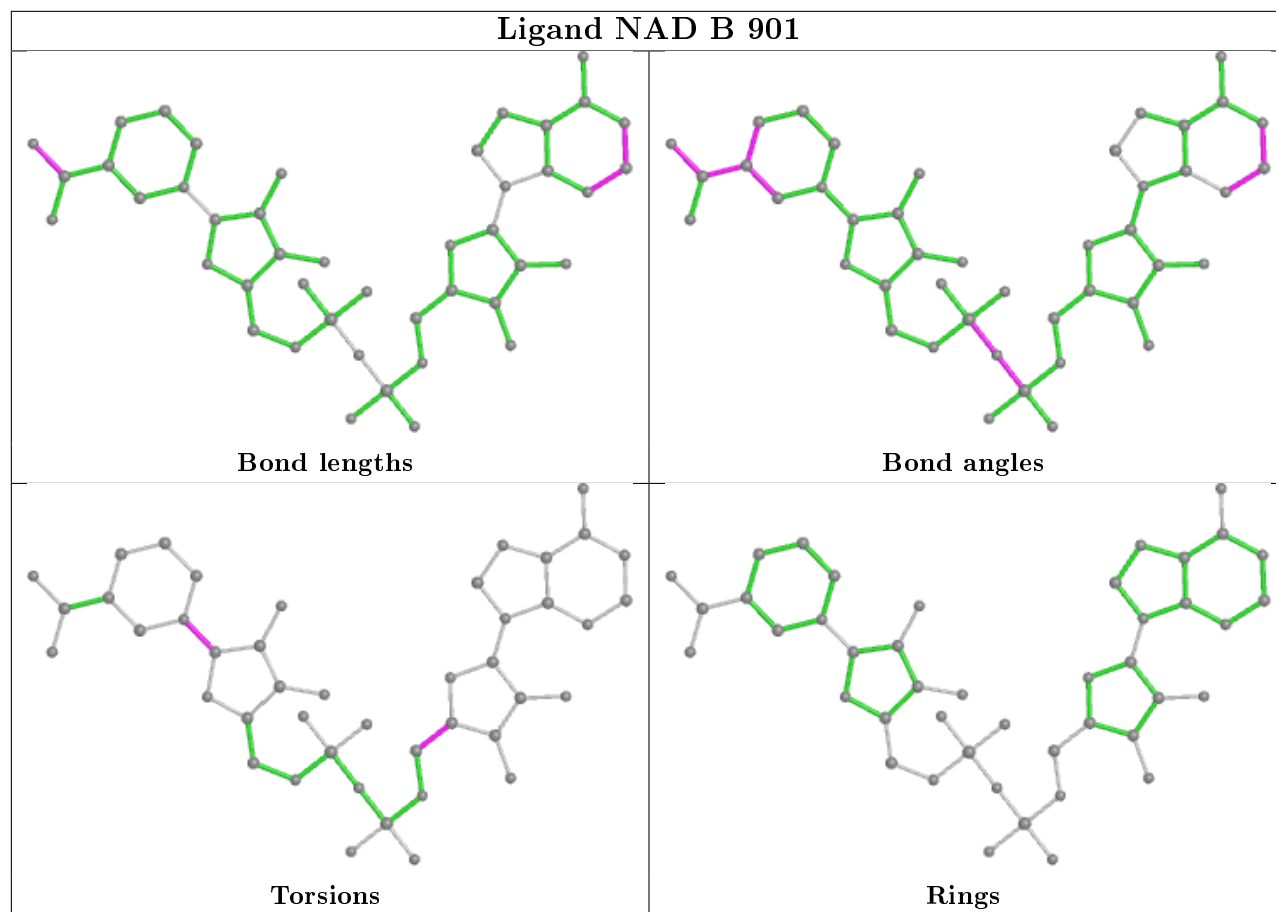
4 monomers are involved in 12 short contacts:

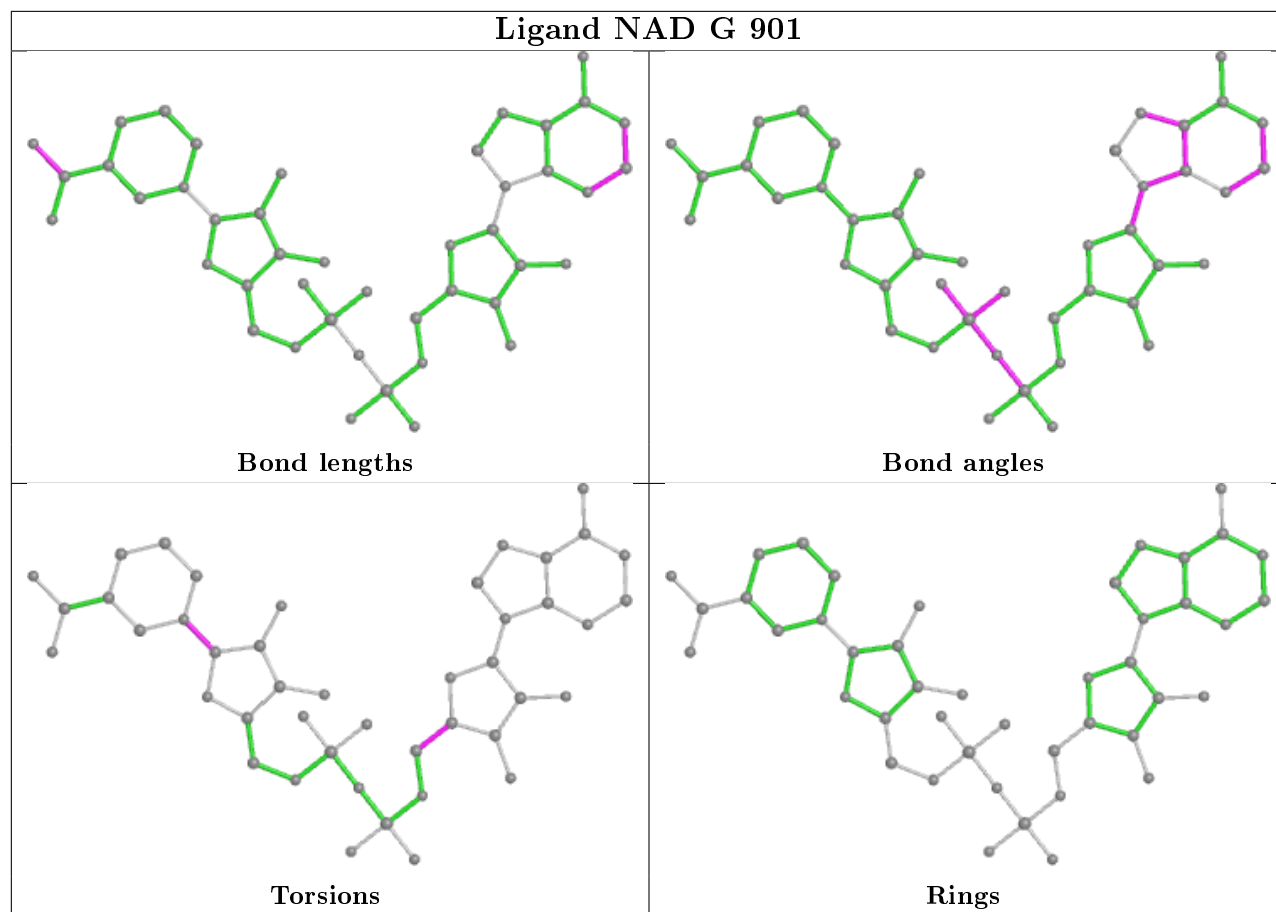
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	NAD	3	0
2	G	901	NAD	1	0
2	D	901	NAD	6	0
2	F	901	NAD	2	0

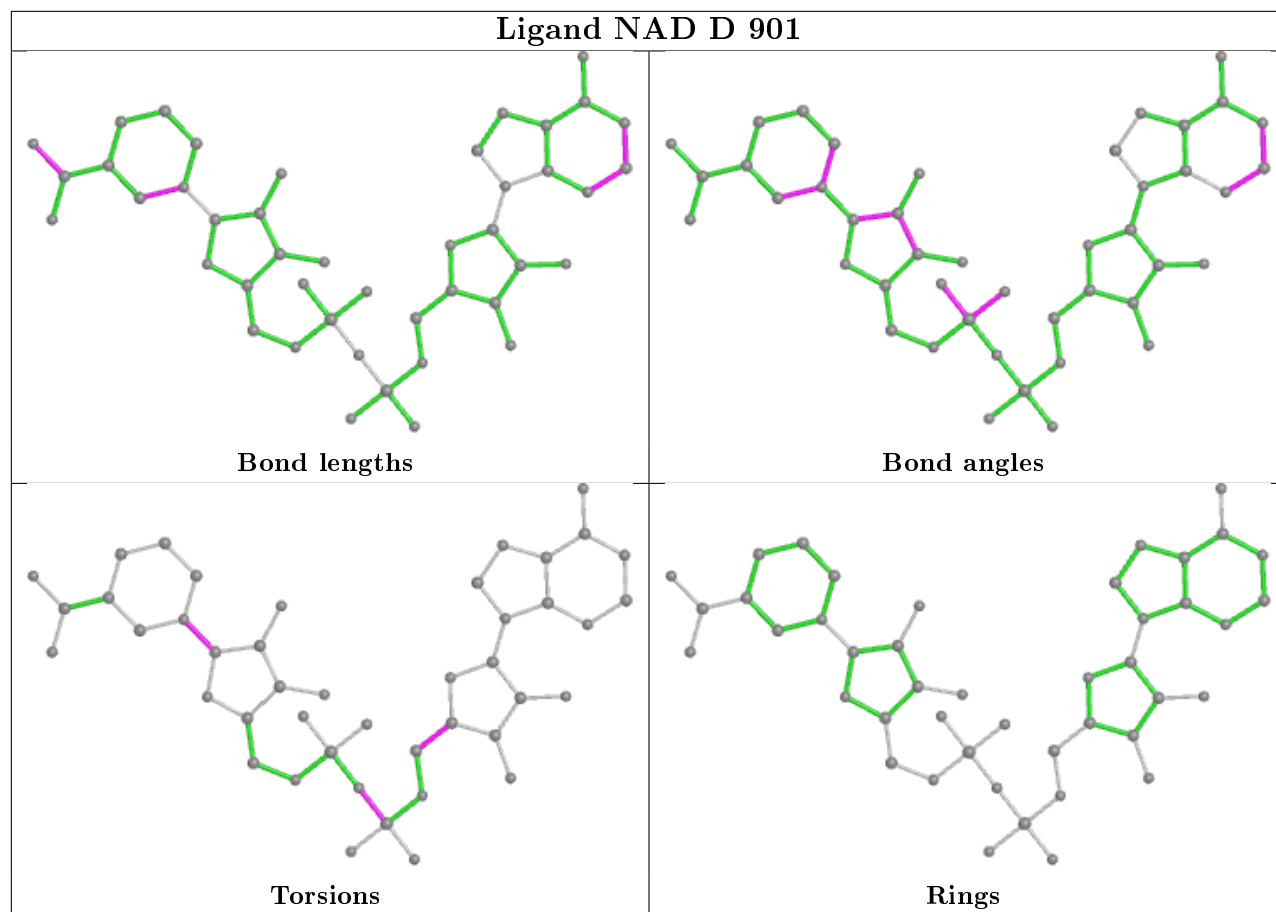
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

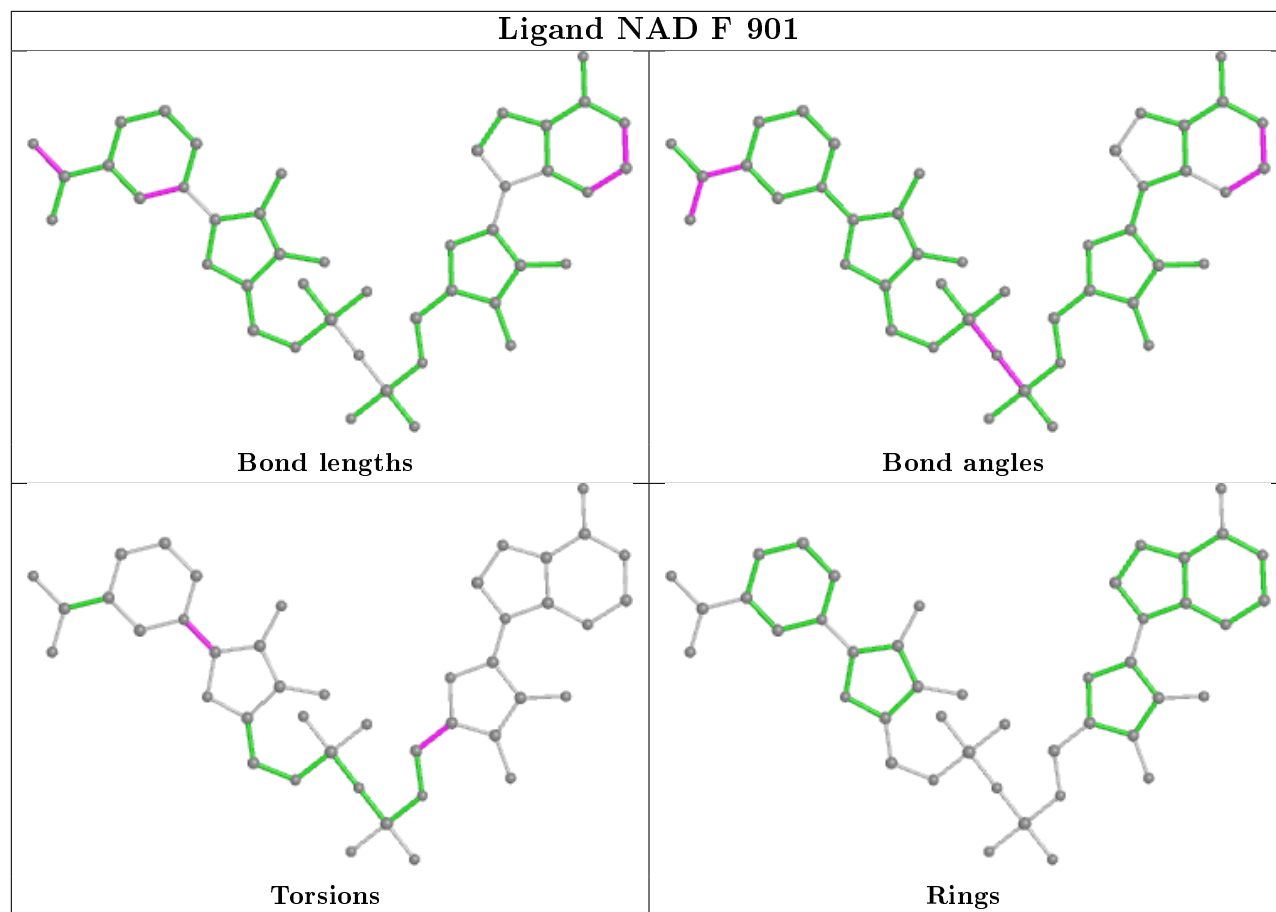


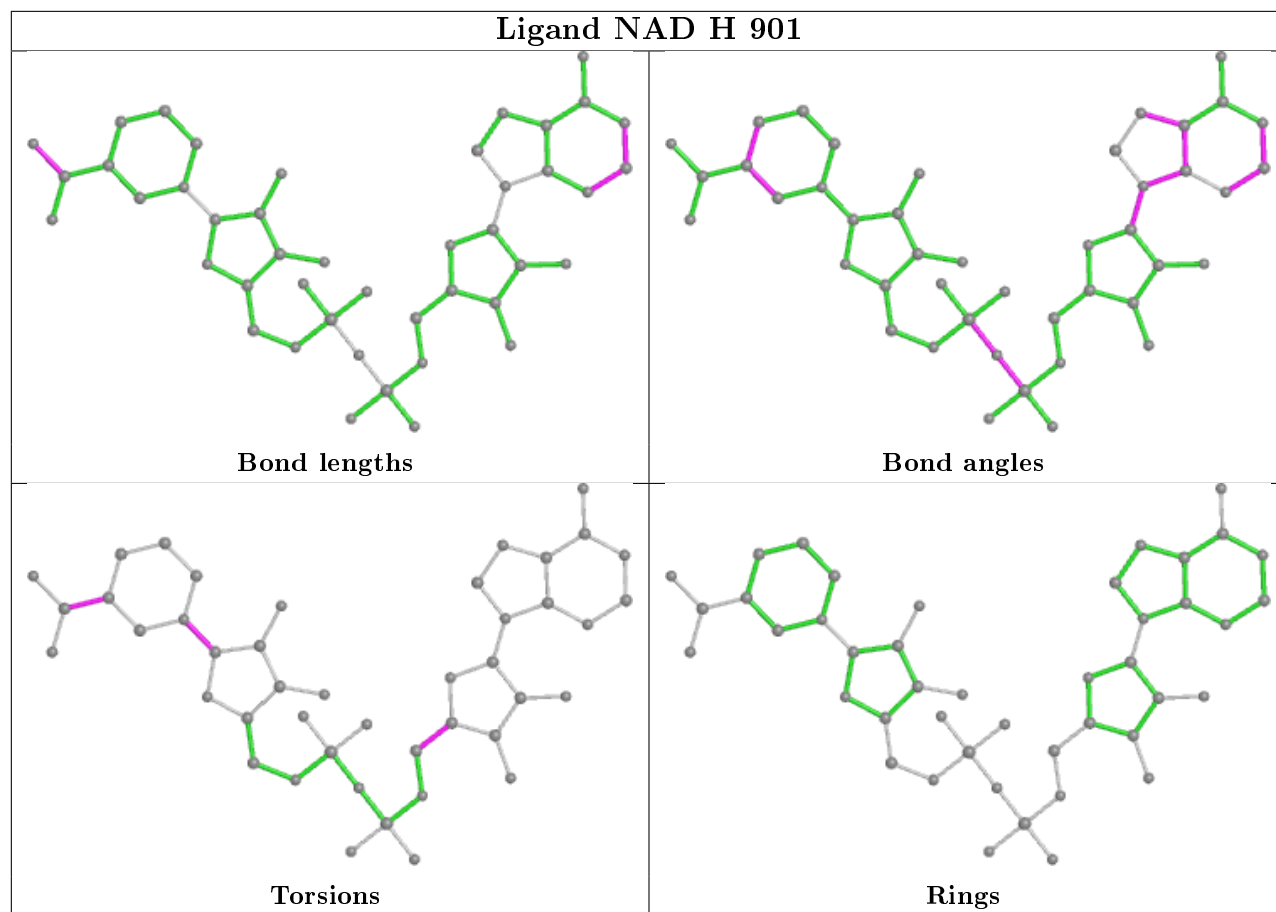












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	335/344 (97%)	-0.46	0 100 100	13, 25, 40, 50	0
1	B	334/344 (97%)	-0.18	0 100 100	15, 38, 59, 63	0
1	C	335/344 (97%)	-0.37	1 (0%) 94 93	14, 30, 44, 52	0
1	D	335/344 (97%)	0.41	35 (10%) 6 6	17, 42, 90, 94	0
1	E	335/344 (97%)	0.15	18 (5%) 25 24	17, 43, 76, 87	0
1	F	335/344 (97%)	-0.24	0 100 100	15, 35, 51, 59	0
1	G	335/344 (97%)	0.10	12 (3%) 42 42	18, 45, 73, 79	0
1	H	335/344 (97%)	-0.41	1 (0%) 94 93	12, 25, 39, 44	0
All	All	2679/2752 (97%)	-0.12	67 (2%) 57 55	12, 34, 69, 94	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	78	ALA	6.6
1	D	87	TRP	6.5
1	E	83	ALA	6.4
1	D	88	GLY	5.4
1	D	85	LEU	5.4
1	E	335	LYS	5.3
1	D	78	ALA	5.0
1	D	111	HIS	4.8
1	D	108	ALA	4.3
1	D	33	ALA	4.3
1	E	88	GLY	4.3
1	D	92	VAL	4.0
1	D	109	SER	4.0
1	D	112	LEU	3.9
1	E	79	ASN	3.8
1	G	83	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	90	LEU	3.6
1	E	77	LEU	3.6
1	D	34	ILE	3.5
1	E	84	GLU	3.5
1	D	117	LYS	3.5
1	D	66	TYR	3.5
1	E	28	ASP	3.4
1	E	89	GLU	3.4
1	E	37	LEU	3.4
1	D	89	GLU	3.4
1	D	35	ASN	3.3
1	D	37	LEU	3.3
1	E	101	PHE	3.1
1	D	90	LEU	3.1
1	G	110	ALA	3.1
1	D	106	GLU	3.0
1	D	77	LEU	2.9
1	D	93	ASP	2.9
1	G	111	HIS	2.9
1	D	32	VAL	2.9
1	C	83	ALA	2.8
1	G	331	LEU	2.8
1	D	91	GLY	2.8
1	D	127	LYS	2.8
1	G	62	VAL	2.8
1	G	113	LYS	2.7
1	E	142	LEU	2.7
1	D	118	LYS	2.7
1	E	116	ALA	2.6
1	D	145	GLU	2.6
1	D	2	ILE	2.6
1	D	329	ILE	2.6
1	E	144	ALA	2.6
1	E	90	LEU	2.6
1	D	71	GLY	2.5
1	D	82	PRO	2.5
1	D	79	ASN	2.5
1	E	112	LEU	2.5
1	D	116	ALA	2.5
1	D	94	VAL	2.4
1	D	140	ASP	2.4
1	D	126	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	65	ASP	2.4
1	G	87	TRP	2.3
1	G	88	GLY	2.2
1	H	335	LYS	2.2
1	D	73	ARG	2.2
1	E	113	LYS	2.1
1	G	81	ASN	2.0
1	G	28	ASP	2.0
1	G	59	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 carbohydrates in this entry.

6.4 Ligands [i](#)

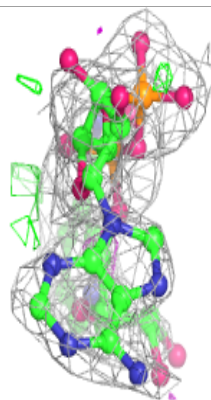
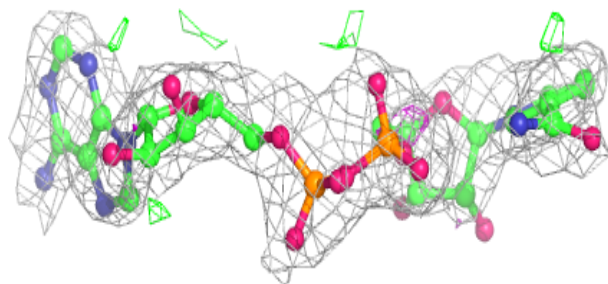
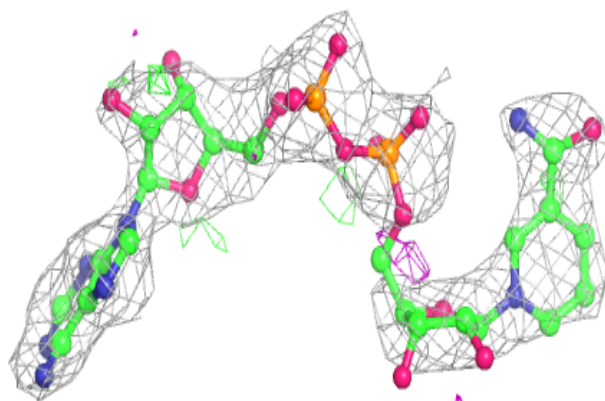
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	D	901	44/44	0.88	0.22	60,66,67,68	0
2	NAD	E	901	44/44	0.91	0.18	42,54,60,61	0
2	NAD	G	901	44/44	0.95	0.13	37,43,55,56	0
2	NAD	C	901	44/44	0.97	0.12	17,24,30,31	0
2	NAD	B	901	44/44	0.97	0.11	25,30,35,37	0
2	NAD	F	901	44/44	0.97	0.12	28,32,40,41	0
2	NAD	H	901	44/44	0.97	0.11	14,19,23,25	0

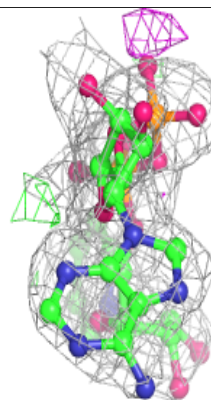
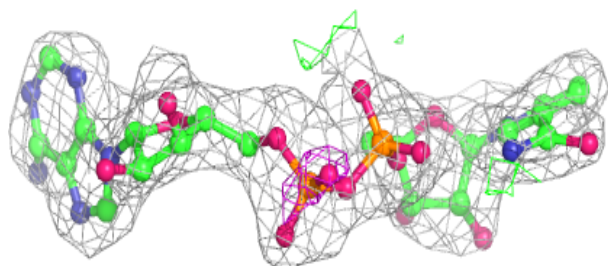
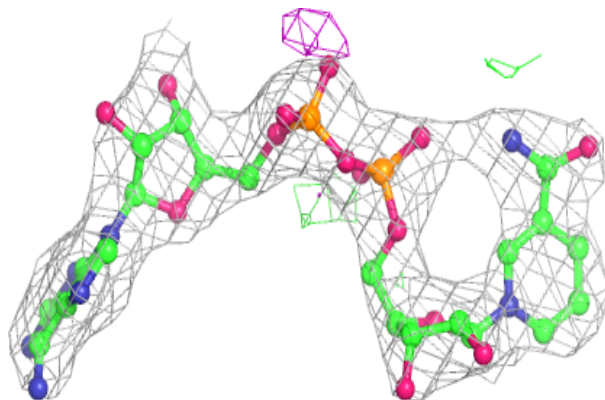
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 901:

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

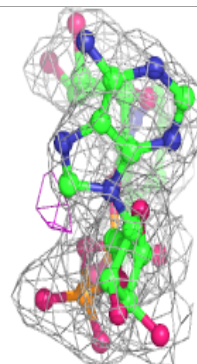
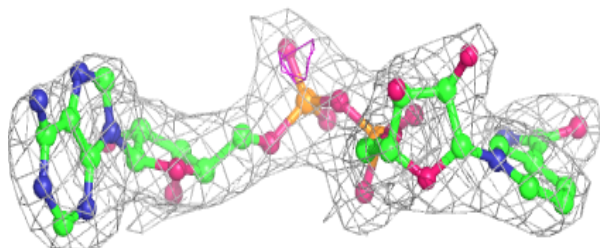
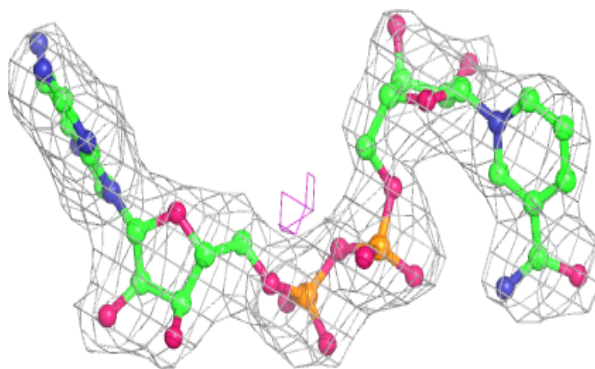
**Electron density around NAD E 901:**

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

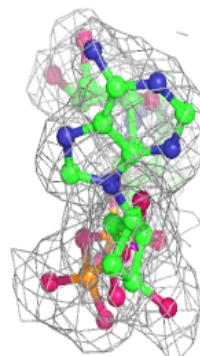
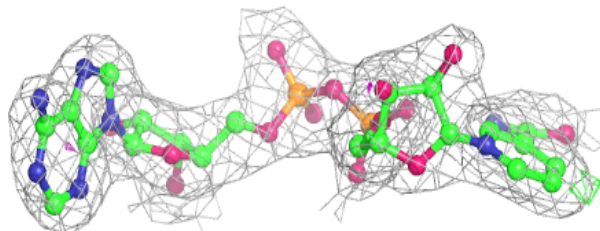
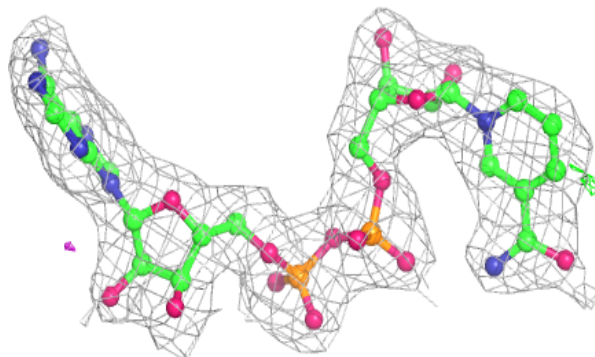


Electron density around NAD G 901:

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

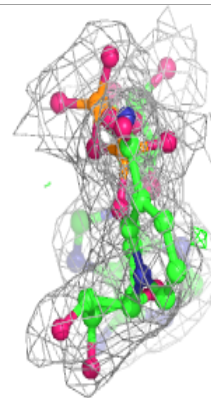
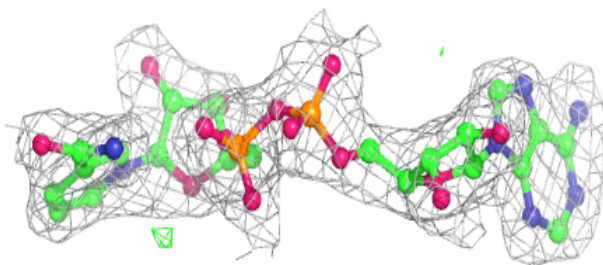
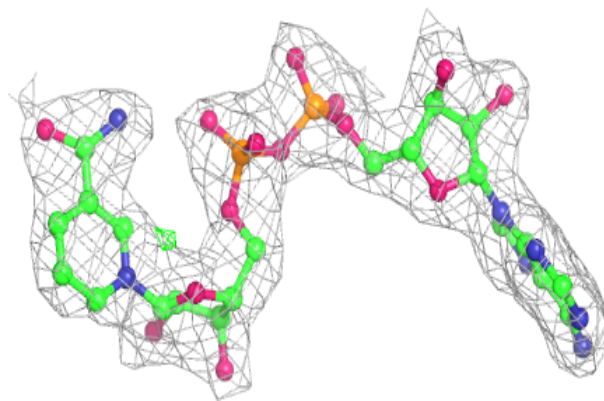
**Electron density around NAD C 901:**

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

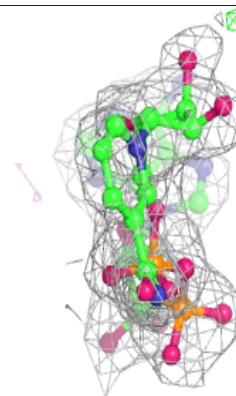
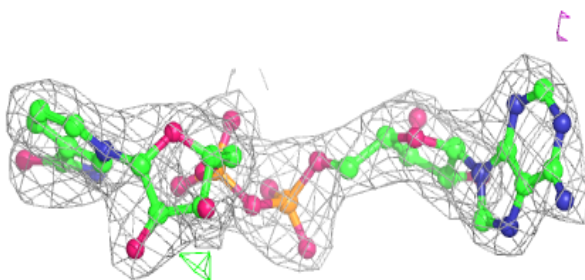
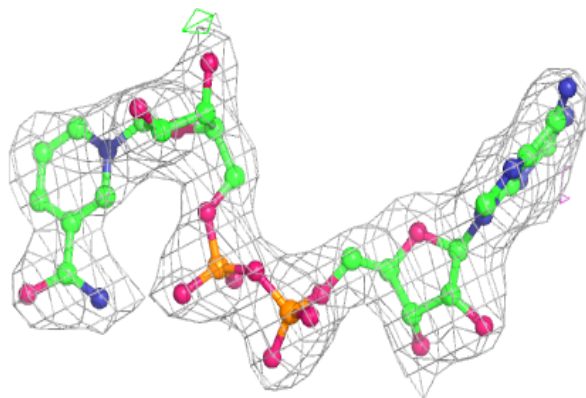


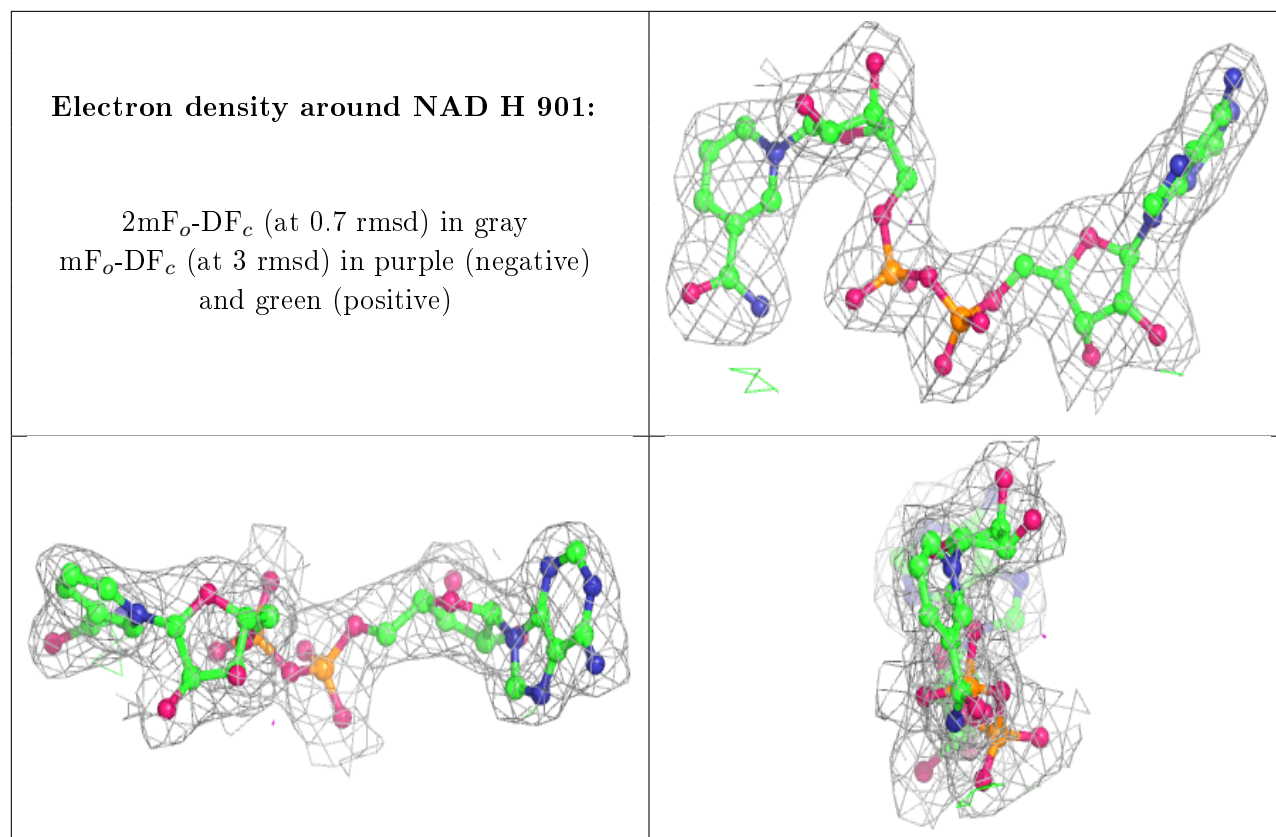
Electron density around NAD B 901:

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

**Electron density around NAD F 901:**

$2mF_o-DF_c$ (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.