Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 12:10 AM EDT

PDB ID	:	2Q2Q
Title	:	Structure of D-3-Hydroxybutyrate Dehydrogenase from Pseudomonas putida
Authors	:	Paithankar, K.S.; Feller, C.; Kuettner, E.B.; Keim, A.; Grunow, M.; Strater, N.
Deposited on	:	2007-05-29
Resolution	:	2.02 Å(reported)

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

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

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

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

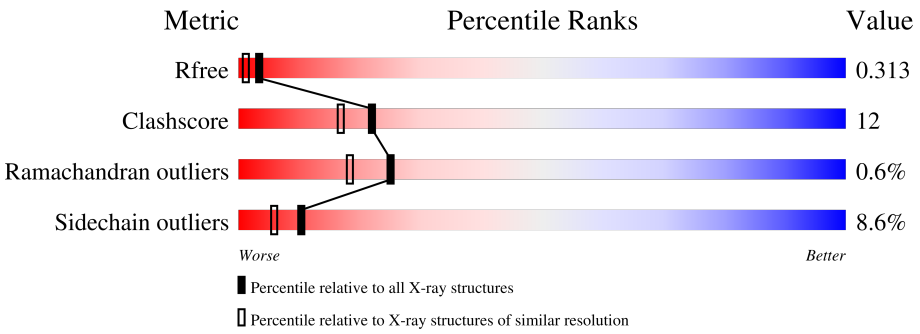
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

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%

Mol	Chain	Length	Quality of chain
1	A	255	71% 24% • •
1	B	255	76% 20% • ••
1	C	255	67% 24% 5% 5%
1	D	255	73% 22% 5%
1	E	255	68% 24% 5% • •
1	F	255	69% 20% • 7%
1	G	255	73% 22% • •

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Mol	Chain	Length	Quality of chain
1	H	255	71% 19% • • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15261 atoms, of which 0 are hydrogens and 0 are deuteriums.

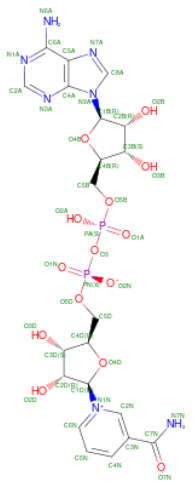
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-D-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1843	1171	330	338	4	0	0	0
1	B	252	1852	1176	332	340	4	0	0	0
1	C	243	1784	1137	319	324	4	0	0	0
1	D	255	1869	1185	336	344	4	0	0	0
1	E	249	1833	1165	329	335	4	0	0	0
1	F	238	1742	1110	311	317	4	0	0	0
1	G	251	1845	1173	331	337	4	0	0	0
1	H	240	1758	1120	314	320	4	0	0	0

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

NAD



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	61	61	61	0	0
3	B	83	83	83	0	0
3	C	37	37	37	0	0
3	D	70	70	70	0	0
3	E	55	55	55	0	0
3	F	50	50	50	0	0

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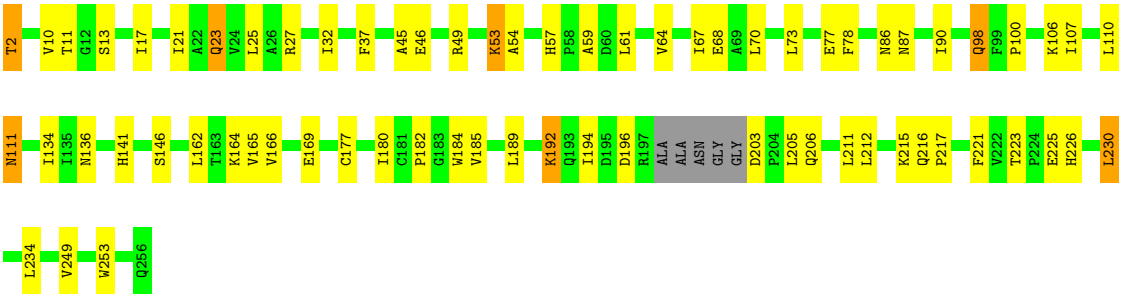
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	G	71	71	71	0	0
			Total	O		
3	H	44	44	44	0	0

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. 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. 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.

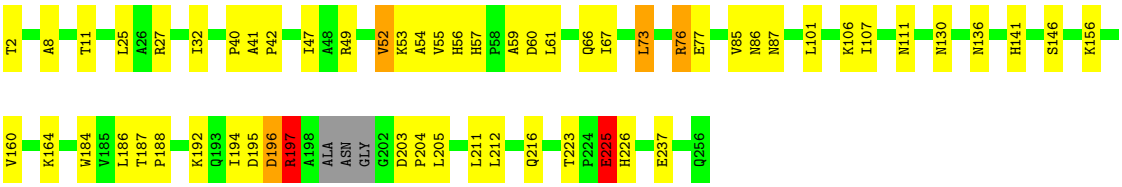
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain A:



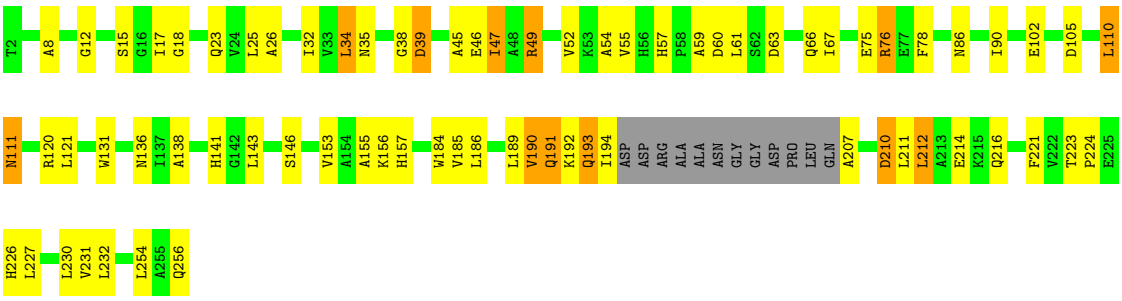
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain B:



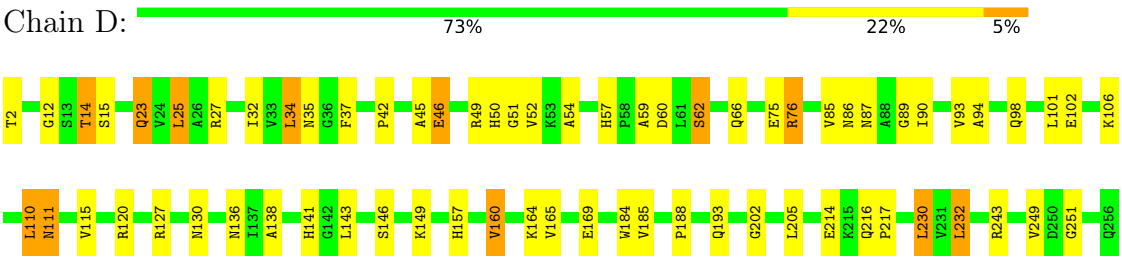
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain C:



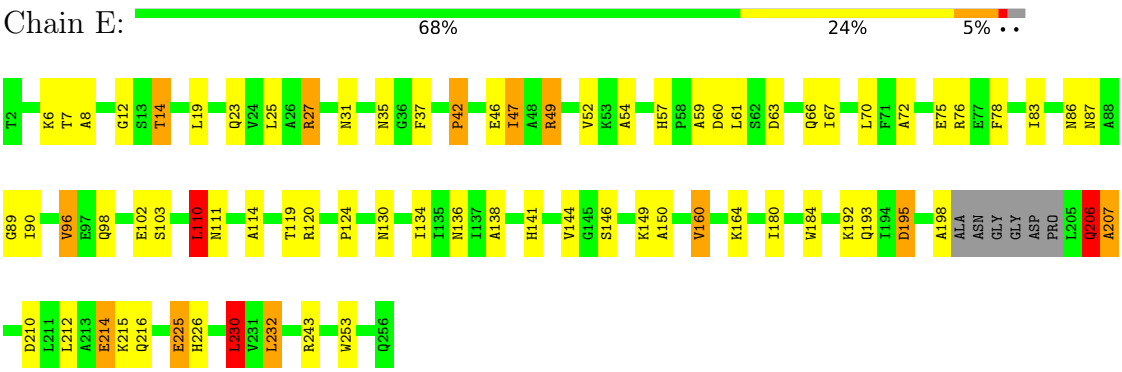
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain D:



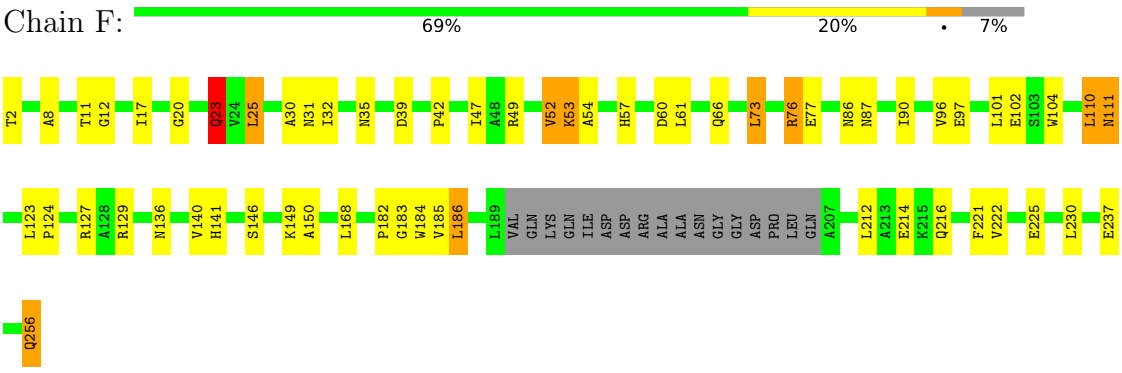
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain E:



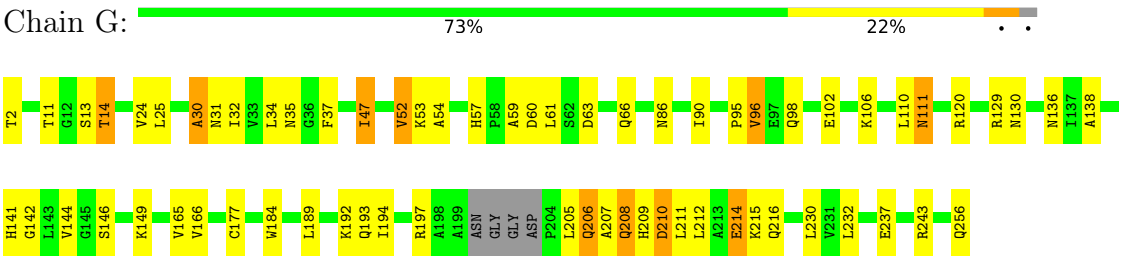
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain F:



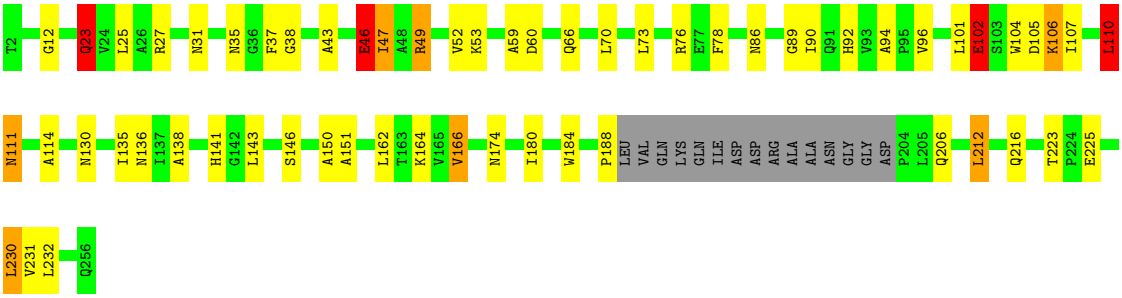
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain G:



- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain H:


T2
G12
Q23
V24
L25
A26
R27
N31
N35
G36
F37
G38
A43
E46
I47
A48
R49
V52
K53
A59
D60
Q66
L70
L73
R76
E77
F78
N86
G89
I90
Q91
H92
V93
A94
P95
V96
L101
E102
S103
W104
D105
K106
I107
L110
N111
A114
N130
I135
N136
I137
A138
H141
G142
L143
S146
A150
A151
L162
T163
K164
V165
V166
N174
I180
W184
P188
LEU
VAL
GLN
LYS
GLN
ILE
ASP
ASP
ARG
ALA
ALA
ASN
GLY
GLY
ASP
P204
L205
Q206
L212
Q216
T223
P224
E225
L230
V231
L232
Q256

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.46Å 59.91Å 116.52Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 29.96 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.02) 96.4 (29.96-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.274 0.253 , 0.313	Depositor DCC
R_{free} test set	5241 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5024e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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	1.20	4/1879 (0.2%)	0.99	1/2560 (0.0%)
1	B	1.20	5/1888 (0.3%)	1.04	5/2572 (0.2%)
1	C	1.06	2/1819 (0.1%)	1.00	2/2478 (0.1%)
1	D	1.39	12/1906 (0.6%)	1.16	15/2598 (0.6%)
1	E	1.37	8/1868 (0.4%)	1.18	11/2544 (0.4%)
1	F	1.33	8/1777 (0.5%)	1.05	5/2422 (0.2%)
1	G	1.33	14/1881 (0.7%)	1.13	10/2562 (0.4%)
1	H	1.32	8/1794 (0.4%)	1.11	7/2445 (0.3%)
All	All	1.28	61/14812 (0.4%)	1.08	56/20181 (0.3%)

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	2
1	H	0	2
All	All	0	4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	206	GLN	CD-OE1	15.60	1.58	1.24
1	G	209	HIS	CE1-NE2	14.02	1.65	1.32
1	E	206	GLN	CD-NE2	13.54	1.66	1.32
1	D	75	GLU	CG-CD	12.25	1.70	1.51
1	G	209	HIS	CG-ND1	10.21	1.61	1.38
1	D	214	GLU	CG-CD	9.54	1.66	1.51
1	F	214	GLU	CB-CG	8.57	1.68	1.52
1	F	102	GLU	CB-CG	8.56	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	23	GLN	CG-CD	8.55	1.70	1.51
1	D	115	VAL	CB-CG1	8.27	1.70	1.52
1	G	209	HIS	CG-CD2	7.61	1.48	1.35
1	F	102	GLU	CG-CD	7.44	1.63	1.51
1	F	104	TRP	CB-CG	7.31	1.63	1.50
1	D	75	GLU	CB-CG	7.25	1.66	1.52
1	D	46	GLU	CD-OE2	7.23	1.33	1.25
1	H	102	GLU	CG-CD	7.09	1.62	1.51
1	E	225	GLU	CG-CD	7.08	1.62	1.51
1	D	185	VAL	CB-CG1	6.99	1.67	1.52
1	E	160	VAL	CB-CG2	6.90	1.67	1.52
1	D	62	SER	CB-OG	-6.81	1.33	1.42
1	F	256	GLN	C-OXT	6.75	1.36	1.23
1	G	30	ALA	CA-CB	6.59	1.66	1.52
1	E	144	VAL	CB-CG2	6.59	1.66	1.52
1	G	237	GLU	CG-CD	6.52	1.61	1.51
1	B	85	VAL	CB-CG1	6.32	1.66	1.52
1	A	225	GLU	CG-CD	6.30	1.61	1.51
1	H	102	GLU	CB-CG	6.21	1.64	1.52
1	B	237	GLU	CG-CD	6.12	1.61	1.51
1	D	23	GLN	CG-CD	5.95	1.64	1.51
1	H	188	PRO	C-O	5.83	1.34	1.23
1	G	177	CYS	CB-SG	-5.74	1.72	1.81
1	H	94	ALA	CA-CB	5.67	1.64	1.52
1	F	23	GLN	CG-CD	5.64	1.64	1.51
1	E	102	GLU	CG-CD	5.63	1.60	1.51
1	C	155	ALA	CA-CB	5.61	1.64	1.52
1	G	102	GLU	CG-CD	5.61	1.60	1.51
1	A	225	GLU	CB-CG	5.60	1.62	1.52
1	E	214	GLU	CD-OE1	5.59	1.31	1.25
1	F	53	LYS	CE-NZ	5.57	1.62	1.49
1	E	96	VAL	CB-CG2	-5.54	1.41	1.52
1	B	160	VAL	CB-CG2	5.52	1.64	1.52
1	D	249	VAL	CB-CG1	5.50	1.64	1.52
1	A	98	GLN	CB-CG	-5.47	1.37	1.52
1	B	2	THR	CB-CG2	5.47	1.70	1.52
1	H	23	GLN	CB-CG	5.46	1.67	1.52
1	B	225	GLU	CG-CD	5.46	1.60	1.51
1	A	2	THR	CA-CB	5.42	1.67	1.53
1	D	76	ARG	CG-CD	5.39	1.65	1.51
1	H	166	VAL	CB-CG2	5.37	1.64	1.52
1	G	130	ASN	CB-CG	5.35	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	VAL	CB-CG1	5.32	1.64	1.52
1	D	160	VAL	CB-CG1	5.30	1.64	1.52
1	G	165	VAL	CA-CB	5.27	1.65	1.54
1	H	164	LYS	CD-CE	5.24	1.64	1.51
1	F	149	LYS	CD-CE	5.23	1.64	1.51
1	G	142	GLY	N-CA	5.22	1.53	1.46
1	G	166	VAL	CB-CG2	5.22	1.63	1.52
1	C	46	GLU	C-O	5.20	1.33	1.23
1	D	85	VAL	CB-CG2	5.10	1.63	1.52
1	G	96	VAL	CB-CG1	-5.06	1.42	1.52
1	G	24	VAL	CB-CG2	5.01	1.63	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	243	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	E	243	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	G	129	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	C	63	ASP	CB-CG-OD2	8.27	125.74	118.30
1	E	63	ASP	CB-CG-OD1	7.68	125.21	118.30
1	D	120	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	230	LEU	CB-CG-CD2	7.30	123.41	111.00
1	D	62	SER	CB-CA-C	-7.24	96.34	110.10
1	A	98	GLN	CB-CA-C	-7.20	96.01	110.40
1	D	243	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	E	230	LEU	CB-CG-CD2	7.13	123.12	111.00
1	E	195	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	H	106	LYS	CD-CE-NZ	7.02	127.85	111.70
1	D	143	LEU	CA-CB-CG	-6.94	99.34	115.30
1	H	212	LEU	CA-CB-CG	6.88	131.13	115.30
1	D	120	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	F	256	GLN	CA-C-O	-6.75	105.93	120.10
1	H	143	LEU	CB-CG-CD1	6.71	122.40	111.00
1	D	127	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	49	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	34	LEU	CA-CB-CG	6.66	130.61	115.30
1	D	76	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	F	127	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	96	VAL	CB-CA-C	-6.61	98.85	111.40
1	E	96	VAL	CG1-CB-CG2	-6.47	100.55	110.90
1	F	183	GLY	N-CA-C	-6.44	96.99	113.10
1	G	205	LEU	CA-CB-CG	6.27	129.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	120	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	E	243	ARG	CG-CD-NE	-6.07	99.05	111.80
1	B	49	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	H	110	LEU	CB-CG-CD2	5.92	121.06	111.00
1	D	34	LEU	CB-CG-CD1	5.91	121.05	111.00
1	E	110	LEU	CB-CG-CD2	5.87	120.97	111.00
1	D	243	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	E	195	ASP	CB-CG-OD1	5.81	123.53	118.30
1	G	129	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	25	LEU	CB-CG-CD1	5.72	120.72	111.00
1	E	232	LEU	CA-CB-CG	5.68	128.37	115.30
1	H	105	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	120	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	75	GLU	CA-CB-CG	5.50	125.49	113.40
1	B	76	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	243	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	243	ARG	CD-NE-CZ	5.41	131.18	123.60
1	D	232	LEU	CB-CG-CD2	5.38	120.14	111.00
1	B	27	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	129	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	105	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	52	VAL	CG1-CB-CG2	5.24	119.29	110.90
1	F	168	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	H	232	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	G	63	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	52	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	G	189	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	H	70	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	210	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	206	GLN	Sidechain
1	E	207	ALA	Peptide
1	H	38	GLY	Peptide
1	H	49	ARG	Peptide

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	1843	0	1865	57	0
1	B	1852	0	1873	35	0
1	C	1784	0	1814	56	0
1	D	1869	0	1888	43	0
1	E	1833	0	1859	51	0
1	F	1742	0	1765	46	0
1	G	1845	0	1872	33	0
1	H	1758	0	1781	38	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	26	4	0
2	F	44	0	26	3	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	61	0	0	2	0
3	B	83	0	0	2	0
3	C	37	0	0	1	0
3	D	70	0	0	4	0
3	E	55	0	0	1	1
3	F	50	0	0	1	0
3	G	71	0	0	1	1
3	H	44	0	0	2	0
All	All	15261	0	14873	350	1

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 12.

All (350) 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:32:ILE:HG22	1:C:34:LEU:HD13	1.27	1.08
1:F:186:LEU:HD23	1:F:186:LEU:H	1.19	1.07
1:C:32:ILE:HG22	1:C:34:LEU:CD1	1.90	1.01
1:E:184:TRP:H	1:E:216:GLN:HE22	1.09	1.00
1:C:32:ILE:CG2	1:C:34:LEU:CD1	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:TRP:H	1:F:216:GLN:HE22	1.08	0.98
1:F:141:HIS:HE1	1:F:146:SER:OG	1.49	0.94
1:H:184:TRP:H	1:H:216:GLN:HE22	1.10	0.94
1:D:14:THR:HG21	1:D:37:PHE:O	1.68	0.92
1:F:186:LEU:H	1:F:186:LEU:CD2	1.83	0.90
1:C:32:ILE:CG2	1:C:34:LEU:HD13	2.03	0.87
1:D:42:PRO:O	1:D:46:GLU:HG2	1.74	0.87
1:F:256:GLN:OXT	3:F:317:HOH:O	1.93	0.87
1:H:96:VAL:HG12	1:H:150:ALA:HB2	1.57	0.87
1:A:184:TRP:H	1:A:216:GLN:HE22	1.17	0.87
1:C:184:TRP:H	1:C:216:GLN:HE22	1.23	0.86
1:G:184:TRP:H	1:G:216:GLN:HE22	1.24	0.86
1:E:27:ARG:NH1	3:E:342:HOH:O	2.09	0.86
1:B:184:TRP:H	1:B:216:GLN:HE22	1.25	0.84
1:G:141:HIS:HE1	1:G:146:SER:OG	1.62	0.83
1:A:189:LEU:HD12	1:A:189:LEU:O	1.79	0.83
1:G:14:THR:HG21	1:G:37:PHE:O	1.77	0.82
1:C:45:ALA:O	1:C:49:ARG:HG2	1.80	0.81
1:A:57:HIS:CE1	1:A:59:ALA:HB2	2.15	0.81
1:D:184:TRP:H	1:D:216:GLN:HE22	1.27	0.80
1:C:32:ILE:HG21	1:C:34:LEU:CD1	2.12	0.80
1:D:51:GLY:HA2	1:F:53:LYS:HD3	1.65	0.79
1:G:57:HIS:HD2	1:G:59:ALA:H	1.31	0.79
1:E:86:ASN:HD22	1:E:136:ASN:HD21	1.32	0.78
3:D:365:HOH:O	1:H:92:HIS:HD2	1.65	0.78
1:E:90:ILE:H	1:E:111:ASN:HD21	1.33	0.77
1:C:32:ILE:HG21	1:C:34:LEU:HD11	1.68	0.76
1:G:95:PRO:HG2	1:G:98:GLN:OE1	1.86	0.75
1:A:53:LYS:HG3	1:A:78:PHE:HE1	1.52	0.75
1:E:14:THR:HG22	2:E:300:NAD:O3B	1.87	0.74
1:H:90:ILE:H	1:H:111:ASN:HD21	1.33	0.74
1:A:111:ASN:HD22	1:A:111:ASN:N	1.83	0.74
1:B:86:ASN:HD22	1:B:136:ASN:HD21	1.34	0.74
1:E:184:TRP:N	1:E:216:GLN:HE22	1.85	0.74
1:F:141:HIS:CE1	1:F:146:SER:OG	2.38	0.74
1:C:76:ARG:NE	1:C:76:ARG:HA	2.03	0.73
1:B:86:ASN:HD22	1:B:136:ASN:ND2	1.85	0.73
1:F:90:ILE:H	1:F:111:ASN:HD21	1.34	0.73
1:E:72:ALA:O	1:E:76:ARG:HG3	1.88	0.73
1:G:57:HIS:CD2	1:G:59:ALA:H	2.06	0.72
1:G:47:ILE:HD11	1:G:54:ALA:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:HB2	1:B:73:LEU:HD12	1.70	0.71
1:B:101:LEU:HD12	1:B:101:LEU:H	1.54	0.71
1:F:186:LEU:HD23	1:F:186:LEU:N	1.99	0.71
1:C:38:GLY:O	1:C:39:ASP:CB	2.38	0.71
1:G:86:ASN:HD22	1:G:136:ASN:ND2	1.88	0.71
1:D:90:ILE:H	1:D:111:ASN:HD21	1.38	0.70
1:A:184:TRP:H	1:A:216:GLN:NE2	1.90	0.69
1:E:14:THR:HG21	1:E:37:PHE:O	1.91	0.69
1:A:86:ASN:HD22	1:A:136:ASN:ND2	1.91	0.69
1:E:96:VAL:HG22	1:E:150:ALA:HB2	1.74	0.69
1:A:57:HIS:HB2	1:A:73:LEU:HD23	1.73	0.69
1:A:141:HIS:HE1	1:A:146:SER:OG	1.76	0.69
1:G:90:ILE:H	1:G:111:ASN:HD21	1.42	0.68
1:F:73:LEU:HD22	1:F:77:GLU:HG2	1.75	0.68
1:B:164:LYS:NZ	1:C:157:HIS:HE1	1.92	0.68
1:C:111:ASN:N	1:C:111:ASN:HD22	1.91	0.68
1:F:30:ALA:O	1:F:52:VAL:HG11	1.94	0.67
1:F:184:TRP:N	1:F:216:GLN:HE22	1.87	0.67
1:H:90:ILE:HG13	1:H:107:ILE:CD1	2.25	0.67
1:E:86:ASN:HD22	1:E:136:ASN:ND2	1.93	0.67
1:H:184:TRP:N	1:H:216:GLN:HE22	1.90	0.66
1:D:12:GLY:H	1:D:35:ASN:HD22	1.42	0.66
1:G:86:ASN:HD22	1:G:136:ASN:HD21	1.42	0.66
1:C:60:ASP:H	1:C:66:GLN:NE2	1.93	0.65
1:F:47:ILE:CG2	1:F:54:ALA:HB2	2.25	0.65
1:C:57:HIS:HD2	1:C:59:ALA:H	1.45	0.65
1:F:186:LEU:HD22	1:F:221:PHE:HB3	1.78	0.65
1:H:60:ASP:H	1:H:66:GLN:NE2	1.95	0.65
1:B:55:VAL:HG11	1:B:77:GLU:HG3	1.79	0.64
3:D:365:HOH:O	1:H:92:HIS:CD2	2.46	0.64
1:E:49:ARG:HD3	1:E:49:ARG:C	2.17	0.64
1:F:184:TRP:H	1:F:216:GLN:NE2	1.89	0.63
1:D:138:ALA:O	2:D:300:NAD:H6N	1.98	0.63
1:E:47:ILE:CG1	1:E:54:ALA:HB2	2.28	0.63
1:H:141:HIS:HE1	1:H:146:SER:OG	1.80	0.63
1:E:184:TRP:H	1:E:216:GLN:NE2	1.88	0.63
1:A:90:ILE:HG22	1:A:111:ASN:HD21	1.63	0.62
1:C:184:TRP:N	1:C:216:GLN:HE22	1.93	0.62
1:E:47:ILE:HD11	1:E:54:ALA:HB2	1.79	0.62
1:H:73:LEU:HD12	1:H:76:ARG:NH2	2.15	0.62
1:C:143:LEU:HD12	1:C:254:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ALA:O	1:D:49:ARG:HD2	1.99	0.62
1:G:256:GLN:OXT	3:G:310:HOH:O	2.16	0.62
1:A:90:ILE:HB	1:A:110:LEU:HD23	1.82	0.61
1:D:51:GLY:HA2	1:F:53:LYS:CD	2.29	0.61
1:H:102:GLU:O	1:H:106:LYS:HE3	2.01	0.61
1:A:86:ASN:HD22	1:A:136:ASN:HD21	1.47	0.61
1:C:61:LEU:HD22	1:C:67:ILE:HG12	1.83	0.61
1:F:47:ILE:HG22	1:F:54:ALA:HB2	1.81	0.60
1:H:86:ASN:HD22	1:H:136:ASN:HD21	1.50	0.60
1:D:141:HIS:HE1	1:D:146:SER:OG	1.83	0.60
1:E:138:ALA:O	2:E:300:NAD:H6N	2.02	0.60
1:A:164:LYS:NZ	1:D:157:HIS:HE1	2.00	0.60
1:D:57:HIS:CD2	1:D:59:ALA:HB2	2.36	0.60
1:D:60:ASP:OD1	1:D:62:SER:HB2	2.02	0.60
1:A:180:ILE:HG12	1:A:230:LEU:HD13	1.84	0.59
1:H:92:HIS:HE1	3:H:338:HOH:O	1.83	0.59
1:G:47:ILE:CD1	1:G:52:VAL:HG12	2.33	0.59
1:H:102:GLU:C	1:H:106:LYS:HE3	2.23	0.59
1:A:184:TRP:N	1:A:216:GLN:HE22	1.95	0.59
1:F:31:ASN:HA	1:F:52:VAL:HG13	1.85	0.59
1:C:110:LEU:HB3	1:C:111:ASN:HD22	1.68	0.59
1:H:184:TRP:H	1:H:216:GLN:NE2	1.92	0.58
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.66	0.58
1:C:47:ILE:HG22	1:C:54:ALA:HB2	1.84	0.58
1:B:61:LEU:O	1:B:67:ILE:HD11	2.04	0.58
1:C:38:GLY:O	1:C:39:ASP:HB3	2.03	0.58
1:D:98:GLN:HA	1:D:98:GLN:NE2	2.19	0.58
1:E:86:ASN:HB2	1:E:136:ASN:HD22	1.67	0.58
1:A:37:PHE:HB2	3:A:315:HOH:O	2.03	0.58
1:D:149:LYS:NZ	1:D:193:GLN:HE22	2.02	0.58
1:E:31:ASN:OD1	1:E:52:VAL:HG22	2.04	0.58
1:F:12:GLY:H	1:F:35:ASN:HD22	1.52	0.57
1:H:86:ASN:HD22	1:H:136:ASN:ND2	2.00	0.57
1:H:31:ASN:HA	1:H:52:VAL:HG13	1.86	0.57
1:G:206:GLN:OE1	1:G:206:GLN:HA	2.04	0.57
1:H:225:GLU:H	1:H:225:GLU:CD	2.08	0.57
1:B:184:TRP:N	1:B:216:GLN:HE22	1.97	0.57
1:B:141:HIS:HE1	1:B:146:SER:OG	1.87	0.57
1:H:12:GLY:H	1:H:35:ASN:HD22	1.51	0.57
1:D:98:GLN:NE2	1:D:98:GLN:CA	2.67	0.56
1:E:8:ALA:HA	1:E:83:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLU:O	1:H:49:ARG:HG3	2.05	0.56
1:E:149:LYS:NZ	1:E:193:GLN:HE22	2.03	0.56
1:B:60:ASP:H	1:B:66:GLN:NE2	2.03	0.56
1:D:86:ASN:HD22	1:D:136:ASN:ND2	2.03	0.56
1:F:35:ASN:HD21	2:F:300:NAD:H2A	1.71	0.56
1:C:8:ALA:HB3	1:C:32:ILE:HD13	1.88	0.55
1:E:110:LEU:HB3	1:E:111:ASN:HD22	1.70	0.55
1:H:180:ILE:HG12	1:H:230:LEU:HD13	1.88	0.55
1:E:89:GLY:HA2	1:E:110:LEU:HD13	1.88	0.55
1:A:46:GLU:OE2	1:A:49:ARG:NH1	2.40	0.55
1:C:143:LEU:HD12	1:C:254:LEU:HD13	1.89	0.55
1:C:17:ILE:HD11	1:C:185:VAL:HG21	1.88	0.55
1:G:214:GLU:HB3	1:G:215:LYS:HG2	1.89	0.55
1:C:12:GLY:H	1:C:35:ASN:HD22	1.55	0.54
1:F:17:ILE:HD11	1:F:185:VAL:HG21	1.88	0.54
1:A:45:ALA:O	1:A:49:ARG:HG2	2.08	0.54
1:B:225:GLU:CD	1:B:225:GLU:H	2.10	0.54
1:D:57:HIS:HD2	1:D:59:ALA:H	1.56	0.54
1:H:43:ALA:O	1:H:47:ILE:HG12	2.08	0.54
1:A:100:PRO:HB3	1:H:37:PHE:CD2	2.43	0.53
1:D:111:ASN:N	1:D:111:ASN:HD22	2.07	0.53
1:B:164:LYS:HZ1	1:C:157:HIS:HE1	1.55	0.53
1:A:90:ILE:HG23	1:A:107:ILE:HG12	1.90	0.53
1:E:47:ILE:CD1	1:E:54:ALA:HB2	2.39	0.53
1:B:184:TRP:H	1:B:216:GLN:NE2	2.02	0.53
1:E:207:ALA:O	1:E:210:ASP:HB2	2.09	0.53
1:A:53:LYS:HG3	1:A:78:PHE:CE1	2.38	0.53
1:C:141:HIS:HE1	1:C:146:SER:OG	1.92	0.52
1:H:89:GLY:HA2	1:H:110:LEU:HD13	1.91	0.52
1:A:23:GLN:NE2	1:A:46:GLU:HG3	2.24	0.52
1:H:223:THR:HB	1:H:225:GLU:OE1	2.09	0.52
1:C:184:TRP:H	1:C:216:GLN:NE2	2.00	0.52
1:E:42:PRO:O	1:E:46:GLU:HG2	2.09	0.52
1:A:111:ASN:N	1:A:111:ASN:ND2	2.56	0.52
1:C:138:ALA:HA	1:C:156:LYS:HD2	1.92	0.51
1:C:256:GLN:O	3:C:332:HOH:O	2.19	0.51
1:E:206:GLN:C	1:E:206:GLN:CD	2.69	0.51
1:C:184:TRP:CD1	1:C:212:LEU:HD12	2.45	0.51
1:D:86:ASN:HD22	1:D:136:ASN:HD21	1.57	0.51
1:C:26:ALA:HB2	1:C:32:ILE:HG13	1.93	0.51
1:H:135:ILE:HD12	1:H:231:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TRP:CZ3	1:A:211:LEU:HD21	2.46	0.51
1:A:57:HIS:HB3	1:A:70:LEU:HD13	1.92	0.51
1:B:107:ILE:HG23	1:B:111:ASN:HD22	1.75	0.51
1:F:90:ILE:HG12	1:F:110:LEU:HD12	1.93	0.51
1:H:53:LYS:HG2	1:H:78:PHE:CE2	2.46	0.51
1:C:17:ILE:HA	1:C:224:PRO:HB3	1.92	0.50
1:D:98:GLN:HE21	1:D:98:GLN:CA	2.24	0.50
1:F:47:ILE:HG21	1:F:54:ALA:HB2	1.92	0.50
1:A:61:LEU:O	1:A:67:ILE:HD11	2.12	0.50
1:E:141:HIS:HE1	1:E:146:SER:OG	1.94	0.50
1:D:165:VAL:O	1:D:169:GLU:HG3	2.11	0.50
1:G:11:THR:HB	1:G:61:LEU:HD11	1.93	0.50
1:E:19:LEU:O	1:E:23:GLN:HG3	2.12	0.49
1:A:141:HIS:CE1	1:A:146:SER:OG	2.62	0.49
1:C:138:ALA:O	2:C:300:NAD:H6N	2.12	0.49
1:D:184:TRP:H	1:D:216:GLN:NE2	2.03	0.49
1:H:73:LEU:HD12	1:H:76:ARG:HH21	1.75	0.49
1:C:191:GLN:HA	1:C:194:ILE:CD1	2.42	0.49
1:D:32:ILE:O	1:D:54:ALA:HA	2.12	0.49
1:A:23:GLN:NE2	1:A:46:GLU:O	2.45	0.49
1:C:55:VAL:CG2	1:C:78:PHE:HE2	2.25	0.49
1:E:207:ALA:HA	1:E:210:ASP:OD1	2.12	0.49
1:C:141:HIS:HB3	1:C:153:VAL:HG22	1.94	0.49
1:E:57:HIS:CD2	1:E:59:ALA:HB2	2.48	0.49
1:A:64:VAL:O	1:A:68:GLU:HG3	2.13	0.49
1:C:207:ALA:O	1:C:210:ASP:HB2	2.12	0.49
1:E:87:ASN:O	2:E:300:NAD:H4D	2.13	0.49
1:G:14:THR:HG22	2:G:300:NAD:O3B	2.13	0.49
1:G:184:TRP:N	1:G:216:GLN:HE22	2.02	0.49
1:D:27:ARG:HG3	1:D:50:HIS:CE1	2.48	0.48
1:D:86:ASN:HB2	1:D:136:ASN:HD22	1.77	0.48
1:B:40:PRO:HB3	1:B:56:HIS:CG	2.48	0.48
1:E:195:ASP:O	1:E:198:ALA:HB3	2.13	0.48
1:A:194:ILE:HD11	1:A:221:PHE:CZ	2.49	0.48
1:A:73:LEU:HD12	1:A:77:GLU:CG	2.43	0.48
1:A:57:HIS:HB2	1:A:73:LEU:CD2	2.43	0.48
1:E:214:GLU:HG3	1:E:215:LYS:HG2	1.96	0.48
1:E:31:ASN:OD1	1:E:52:VAL:CG2	2.62	0.48
1:A:192:LYS:O	1:A:196:ASP:OD2	2.32	0.48
1:G:57:HIS:CD2	1:G:59:ALA:HB2	2.49	0.48
1:C:191:GLN:HA	1:C:194:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:HB3	1:B:42:PRO:HD3	1.96	0.47
1:A:73:LEU:HD12	1:A:77:GLU:HG2	1.94	0.47
1:A:57:HIS:HE1	1:A:59:ALA:HB2	1.71	0.47
1:D:57:HIS:CD2	1:D:59:ALA:H	2.33	0.47
1:F:20:GLY:O	1:F:23:GLN:NE2	2.47	0.47
1:G:30:ALA:O	1:G:52:VAL:HG11	2.15	0.47
1:C:75:GLU:OE1	1:C:76:ARG:NH1	2.47	0.47
1:G:86:ASN:HB2	1:G:136:ASN:HD22	1.80	0.47
1:C:184:TRP:HD1	1:C:212:LEU:HD12	1.79	0.47
1:D:46:GLU:OE2	1:D:49:ARG:NH1	2.47	0.47
1:F:39:ASP:O	1:F:42:PRO:HD2	2.13	0.47
1:F:73:LEU:HD23	1:F:76:ARG:NH2	2.29	0.47
1:F:185:VAL:HG13	1:F:222:VAL:O	2.15	0.47
1:G:194:ILE:HG21	1:G:208:GLN:HB3	1.95	0.47
1:B:223:THR:H	1:B:226:HIS:CD2	2.33	0.47
1:D:160:VAL:HG12	1:D:164:LYS:HE3	1.96	0.47
1:F:11:THR:HB	1:F:61:LEU:HD11	1.97	0.47
1:F:86:ASN:HD22	1:F:136:ASN:ND2	2.11	0.47
1:C:12:GLY:O	1:C:18:GLY:HA3	2.15	0.47
1:C:111:ASN:N	1:C:111:ASN:ND2	2.62	0.47
1:A:86:ASN:HB2	1:A:136:ASN:HD22	1.80	0.46
1:D:87:ASN:O	2:D:300:NAD:H4D	2.16	0.46
1:E:226:HIS:HE1	1:F:237:GLU:OE1	1.98	0.46
1:A:32:ILE:O	1:A:54:ALA:HA	2.15	0.46
1:H:130:ASN:O	1:H:174:ASN:HB2	2.15	0.46
1:A:215:LYS:HB3	1:A:253:TRP:CE2	2.50	0.46
1:G:149:LYS:NZ	1:G:193:GLN:HE22	2.13	0.46
1:G:197:ARG:NH2	1:G:214:GLU:OE2	2.42	0.46
1:C:190:VAL:O	1:C:193:GLN:N	2.49	0.46
1:C:227:LEU:O	1:C:231:VAL:HG23	2.14	0.46
1:G:47:ILE:CD1	1:G:54:ALA:HB2	2.44	0.46
1:G:61:LEU:HG	2:G:300:NAD:H2A	1.98	0.46
1:A:192:LYS:N	1:A:192:LYS:HE3	2.30	0.46
1:E:47:ILE:CD1	1:E:52:VAL:HG13	2.46	0.46
1:A:17:ILE:HG22	1:A:21:ILE:HD12	1.97	0.46
1:A:90:ILE:HG22	1:A:111:ASN:ND2	2.30	0.46
1:F:87:ASN:O	2:F:300:NAD:H4D	2.16	0.46
1:A:141:HIS:HD2	3:A:316:HOH:O	1.99	0.46
1:D:57:HIS:HD2	1:D:59:ALA:HB2	1.79	0.45
1:F:60:ASP:H	1:F:66:GLN:NE2	2.14	0.45
1:A:17:ILE:HG12	1:A:185:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:HIS:HD2	1:E:59:ALA:H	1.63	0.45
1:A:90:ILE:H	1:A:111:ASN:HD21	1.63	0.45
1:C:143:LEU:CD1	1:C:254:LEU:HD13	2.46	0.45
1:F:96:VAL:HG12	1:F:150:ALA:HB2	1.99	0.45
1:C:86:ASN:HD22	1:C:136:ASN:ND2	2.14	0.45
1:G:31:ASN:OD1	1:G:53:LYS:HB2	2.17	0.45
1:H:162:LEU:O	1:H:166:VAL:HG23	2.17	0.45
1:A:73:LEU:CD1	1:A:77:GLU:HG3	2.46	0.45
1:A:134:ILE:O	1:A:177:CYS:HA	2.16	0.45
1:B:101:LEU:HD21	1:C:120:ARG:CZ	2.47	0.45
1:B:156:LYS:NZ	3:B:334:HOH:O	2.39	0.45
1:E:60:ASP:H	1:E:66:GLN:NE2	2.15	0.45
1:E:61:LEU:HG	2:E:300:NAD:H2A	1.99	0.45
1:A:203:ASP:HB3	1:A:206:GLN:HB3	1.99	0.45
1:E:49:ARG:C	1:E:49:ARG:CD	2.85	0.45
1:E:180:ILE:HG12	1:E:230:LEU:HD13	1.98	0.45
1:E:206:GLN:CD	1:E:207:ALA:N	2.70	0.44
1:F:86:ASN:HB2	1:F:136:ASN:HD22	1.82	0.44
1:B:61:LEU:HD22	1:B:67:ILE:HG12	1.99	0.44
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.83	0.44
1:D:27:ARG:CG	1:D:50:HIS:CE1	3.00	0.44
1:F:73:LEU:HD23	1:F:76:ARG:HH21	1.82	0.44
1:B:187:THR:HB	1:B:188:PRO:CD	2.47	0.44
1:D:184:TRP:N	1:D:216:GLN:HE22	2.05	0.44
1:E:12:GLY:H	1:E:35:ASN:HD22	1.64	0.44
1:E:57:HIS:HB3	1:E:70:LEU:HD13	1.99	0.44
1:B:164:LYS:HZ2	1:C:157:HIS:HE1	1.62	0.44
1:C:38:GLY:O	1:C:39:ASP:HB2	2.16	0.44
1:F:225:GLU:CD	1:F:225:GLU:H	2.21	0.44
1:H:23:GLN:OE1	1:H:27:ARG:NH2	2.51	0.44
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.83	0.44
1:C:75:GLU:HG3	1:C:76:ARG:HD2	2.00	0.44
1:B:73:LEU:CD2	1:B:77:GLU:HG2	2.49	0.43
1:F:61:LEU:HB2	1:F:110:LEU:HD23	2.00	0.43
1:F:186:LEU:HD22	1:F:221:PHE:CB	2.45	0.43
1:H:90:ILE:HG13	1:H:107:ILE:HD12	2.00	0.43
1:A:162:LEU:O	1:A:166:VAL:HG23	2.18	0.43
1:B:11:THR:O	1:B:87:ASN:HB3	2.18	0.43
1:E:216:GLN:HE21	1:E:253:TRP:HE3	1.65	0.43
1:H:104:TRP:CE3	1:H:151:ALA:HB2	2.54	0.43
1:A:90:ILE:CB	1:A:110:LEU:HD23	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:N	1:B:212:LEU:HD23	2.34	0.43
1:D:93:VAL:O	1:D:94:ALA:HB2	2.19	0.43
1:G:141:HIS:CE1	1:G:146:SER:OG	2.54	0.43
1:B:47:ILE:HG21	1:B:54:ALA:HB2	2.02	0.42
1:D:45:ALA:O	1:D:49:ARG:CD	2.66	0.42
1:H:23:GLN:HE22	1:H:225:GLU:HG3	1.84	0.42
1:A:223:THR:H	1:A:226:HIS:CD2	2.36	0.42
1:D:60:ASP:H	1:D:66:GLN:NE2	2.18	0.42
1:H:138:ALA:O	2:H:300:NAD:H6N	2.20	0.42
1:F:86:ASN:HD22	1:F:136:ASN:HD21	1.68	0.42
1:H:59:ALA:HA	1:H:66:GLN:HE21	1.84	0.42
1:B:196:ASP:O	1:B:197:ARG:HG2	2.19	0.42
1:F:8:ALA:HB3	1:F:32:ILE:HD13	2.00	0.42
1:D:89:GLY:HA2	1:D:110:LEU:HD13	2.02	0.42
1:F:12:GLY:H	1:F:35:ASN:ND2	2.18	0.42
1:A:165:VAL:O	1:A:169:GLU:HG3	2.20	0.41
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.93	0.41
1:A:11:THR:O	1:A:87:ASN:HB3	2.19	0.41
1:D:130:ASN:ND2	3:D:360:HOH:O	2.53	0.41
1:B:59:ALA:CB	1:B:66:GLN:O	2.68	0.41
1:D:217:PRO:HD2	1:D:251:GLY:O	2.21	0.41
1:E:160:VAL:HG12	1:E:164:LYS:HE3	2.02	0.41
1:G:47:ILE:HD12	1:G:47:ILE:O	2.21	0.41
1:A:10:VAL:HG12	1:A:13:SER:HB3	2.03	0.41
1:B:11:THR:HB	1:B:61:LEU:HD11	2.01	0.41
1:G:32:ILE:HG22	1:G:34:LEU:HG	2.02	0.41
1:B:141:HIS:HD2	3:B:282:HOH:O	2.02	0.41
1:C:223:THR:H	1:C:226:HIS:CD2	2.39	0.41
1:D:110:LEU:HB3	1:D:111:ASN:HD22	1.85	0.41
1:F:57:HIS:HB2	1:F:73:LEU:HD12	2.03	0.41
1:B:8:ALA:HB3	1:B:32:ILE:HD13	2.02	0.41
1:C:90:ILE:H	1:C:111:ASN:HD21	1.68	0.41
1:H:110:LEU:O	1:H:114:ALA:HB3	2.21	0.41
1:A:215:LYS:HB3	1:A:253:TRP:CZ2	2.56	0.41
1:A:73:LEU:HD11	1:A:77:GLU:HG3	2.03	0.41
1:E:7:THR:HG21	1:E:78:PHE:HB2	2.03	0.41
1:E:86:ASN:HB2	1:E:136:ASN:ND2	2.33	0.41
1:F:123:LEU:N	1:F:124:PRO:CD	2.83	0.41
1:H:92:HIS:CE1	3:H:338:HOH:O	2.64	0.41
1:B:187:THR:HB	1:B:188:PRO:HD2	2.03	0.41
1:C:186:LEU:HD22	1:C:221:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LEU:O	1:E:114:ALA:HB3	2.21	0.41
1:E:119:THR:HG23	1:E:134:ILE:HD13	2.01	0.41
1:A:182:PRO:HA	1:A:249:VAL:O	2.21	0.40
1:D:90:ILE:HD11	1:D:106:LYS:HG3	2.03	0.40
1:E:61:LEU:HD22	1:E:67:ILE:HG12	2.03	0.40
1:G:47:ILE:HD12	1:G:52:VAL:HG12	2.02	0.40
1:C:57:HIS:HD2	1:C:59:ALA:N	2.17	0.40
1:C:86:ASN:HD22	1:C:136:ASN:HD21	1.69	0.40
1:E:149:LYS:HZ1	1:E:193:GLN:HE22	1.69	0.40
1:F:111:ASN:HD22	1:F:111:ASN:N	2.19	0.40
1:G:35:ASN:HA	1:G:57:HIS:O	2.21	0.40
1:G:60:ASP:H	1:G:66:GLN:NE2	2.19	0.40
1:B:203:ASP:HA	1:B:204:PRO:HD2	1.92	0.40
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.93	0.40
1:F:182:PRO:HB2	2:F:300:NAD:C5N	2.51	0.40
1:G:14:THR:CG2	1:G:37:PHE:O	2.60	0.40
1:D:57:HIS:HE1	3:D:363:HOH:O	2.05	0.40

All (1) 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)
3:E:336:HOH:O	3:G:332:HOH:O[2_555]	1.98	0.22

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	246/255 (96%)	237 (96%)	9 (4%)	0	100 100
1	B	248/255 (97%)	230 (93%)	15 (6%)	3 (1%)	13 6
1	C	239/255 (94%)	224 (94%)	13 (5%)	2 (1%)	19 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	253/255 (99%)	244 (96%)	8 (3%)	1 (0%)	34	28
1	E	245/255 (96%)	233 (95%)	11 (4%)	1 (0%)	34	28
1	F	234/255 (92%)	226 (97%)	8 (3%)	0	100	100
1	G	247/255 (97%)	237 (96%)	7 (3%)	3 (1%)	13	6
1	H	236/255 (92%)	220 (93%)	14 (6%)	2 (1%)	19	12
All	All	1948/2040 (96%)	1851 (95%)	85 (4%)	12 (1%)	25	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ASP
1	H	46	GLU
1	H	47	ILE
1	G	207	ALA
1	B	196	ASP
1	B	130	ASN
1	B	197	ARG
1	G	138	ALA
1	C	131	TRP
1	D	202	GLY
1	E	206	GLN
1	G	206	GLN

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	188/189 (100%)	175 (93%)	13 (7%)	15	10
1	B	188/189 (100%)	175 (93%)	13 (7%)	15	10
1	C	181/189 (96%)	159 (88%)	22 (12%)	5	2
1	D	189/189 (100%)	174 (92%)	15 (8%)	12	7
1	E	186/189 (98%)	166 (89%)	20 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	176/189 (93%)	161 (92%)	15 (8%)	10 6
1	G	187/189 (99%)	169 (90%)	18 (10%)	8 4
1	H	178/189 (94%)	168 (94%)	10 (6%)	21 16
All	All	1473/1512 (97%)	1347 (91%)	126 (9%)	10 6

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	23	GLN
1	A	25	LEU
1	A	27	ARG
1	A	53	LYS
1	A	98	GLN
1	A	106	LYS
1	A	111	ASN
1	A	192	LYS
1	A	205	LEU
1	A	212	LEU
1	A	217	PRO
1	A	230	LEU
1	B	25	LEU
1	B	52	VAL
1	B	53	LYS
1	B	73	LEU
1	B	76	ARG
1	B	106	LYS
1	B	186	LEU
1	B	192	LYS
1	B	194	ILE
1	B	195	ASP
1	B	197	ARG
1	B	205	LEU
1	B	225	GLU
1	C	15	SER
1	C	23	GLN
1	C	25	LEU
1	C	34	LEU
1	C	47	ILE
1	C	49	ARG
1	C	52	VAL

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Mol	Chain	Res	Type
1	C	76	ARG
1	C	102	GLU
1	C	110	LEU
1	C	111	ASN
1	C	189	LEU
1	C	190	VAL
1	C	191	GLN
1	C	192	LYS
1	C	193	GLN
1	C	210	ASP
1	C	211	LEU
1	C	212	LEU
1	C	214	GLU
1	C	230	LEU
1	C	232	LEU
1	D	2	THR
1	D	14	THR
1	D	15	SER
1	D	23	GLN
1	D	25	LEU
1	D	34	LEU
1	D	76	ARG
1	D	101	LEU
1	D	102	GLU
1	D	110	LEU
1	D	111	ASN
1	D	188	PRO
1	D	205	LEU
1	D	230	LEU
1	D	232	LEU
1	E	6	LYS
1	E	14	THR
1	E	25	LEU
1	E	27	ARG
1	E	42	PRO
1	E	47	ILE
1	E	49	ARG
1	E	75	GLU
1	E	98	GLN
1	E	103	SER
1	E	110	LEU
1	E	120	ARG

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Mol	Chain	Res	Type
1	E	124	PRO
1	E	130	ASN
1	E	192	LYS
1	E	206	GLN
1	E	212	LEU
1	E	225	GLU
1	E	230	LEU
1	E	232	LEU
1	F	2	THR
1	F	23	GLN
1	F	25	LEU
1	F	49	ARG
1	F	52	VAL
1	F	73	LEU
1	F	76	ARG
1	F	97	GLU
1	F	101	LEU
1	F	110	LEU
1	F	111	ASN
1	F	140	VAL
1	F	186	LEU
1	F	212	LEU
1	F	230	LEU
1	G	2	THR
1	G	13	SER
1	G	14	THR
1	G	25	LEU
1	G	47	ILE
1	G	52	VAL
1	G	96	VAL
1	G	106	LYS
1	G	110	LEU
1	G	111	ASN
1	G	192	LYS
1	G	208	GLN
1	G	210	ASP
1	G	211	LEU
1	G	212	LEU
1	G	214	GLU
1	G	230	LEU
1	G	232	LEU
1	H	23	GLN

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Mol	Chain	Res	Type
1	H	25	LEU
1	H	46	GLU
1	H	101	LEU
1	H	102	GLU
1	H	110	LEU
1	H	111	ASN
1	H	206	GLN
1	H	212	LEU
1	H	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	ASN
1	A	66	GLN
1	A	111	ASN
1	A	136	ASN
1	A	141	HIS
1	A	216	GLN
1	A	226	HIS
1	A	256	GLN
1	B	35	ASN
1	B	66	GLN
1	B	111	ASN
1	B	136	ASN
1	B	141	HIS
1	B	216	GLN
1	B	226	HIS
1	B	256	GLN
1	C	35	ASN
1	C	57	HIS
1	C	66	GLN
1	C	111	ASN
1	C	136	ASN
1	C	141	HIS
1	C	157	HIS
1	C	193	GLN
1	C	216	GLN
1	D	35	ASN
1	D	57	HIS
1	D	66	GLN

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Mol	Chain	Res	Type
1	D	92	HIS
1	D	98	GLN
1	D	111	ASN
1	D	130	ASN
1	D	136	ASN
1	D	141	HIS
1	D	157	HIS
1	D	193	GLN
1	D	216	GLN
1	E	35	ASN
1	E	57	HIS
1	E	66	GLN
1	E	98	GLN
1	E	111	ASN
1	E	136	ASN
1	E	141	HIS
1	E	157	HIS
1	E	193	GLN
1	E	216	GLN
1	E	226	HIS
1	E	256	GLN
1	F	35	ASN
1	F	66	GLN
1	F	111	ASN
1	F	136	ASN
1	F	141	HIS
1	F	216	GLN
1	G	35	ASN
1	G	57	HIS
1	G	66	GLN
1	G	111	ASN
1	G	136	ASN
1	G	141	HIS
1	G	157	HIS
1	G	193	GLN
1	G	216	GLN
1	H	35	ASN
1	H	66	GLN
1	H	92	HIS
1	H	111	ASN
1	H	130	ASN
1	H	136	ASN

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Mol	Chain	Res	Type
1	H	141	HIS
1	H	216	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	D	300	-	42,48,48	1.47	6 (14%)	50,73,73	2.45	11 (22%)
2	NAD	C	300	-	42,48,48	2.00	5 (11%)	50,73,73	1.34	6 (12%)
2	NAD	G	300	-	42,48,48	1.67	5 (11%)	50,73,73	1.37	6 (12%)
2	NAD	F	300	-	42,48,48	1.82	7 (16%)	50,73,73	1.67	8 (16%)
2	NAD	H	300	-	42,48,48	1.90	7 (16%)	50,73,73	1.80	6 (12%)
2	NAD	E	300	-	42,48,48	1.65	7 (16%)	50,73,73	1.88	7 (14%)

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	D	300	-	-	5/26/62/62	0/5/5/5
2	NAD	C	300	-	-	4/26/62/62	0/5/5/5
2	NAD	G	300	-	-	6/26/62/62	0/5/5/5
2	NAD	F	300	-	-	11/26/62/62	0/5/5/5
2	NAD	H	300	-	-	7/26/62/62	0/5/5/5
2	NAD	E	300	-	-	5/26/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	O7N-C7N	9.85	1.43	1.24
2	H	300	NAD	O7N-C7N	7.95	1.39	1.24
2	F	300	NAD	O7N-C7N	7.10	1.37	1.24
2	G	300	NAD	O7N-C7N	6.43	1.36	1.24
2	E	300	NAD	O7N-C7N	6.30	1.36	1.24
2	G	300	NAD	C2A-N1A	4.40	1.42	1.33
2	H	300	NAD	C2N-N1N	4.29	1.40	1.35
2	F	300	NAD	C2A-N3A	4.16	1.38	1.32
2	C	300	NAD	C2A-N3A	4.07	1.38	1.32
2	D	300	NAD	O7N-C7N	4.03	1.31	1.24
2	D	300	NAD	C2A-N1A	3.92	1.41	1.33
2	F	300	NAD	C2N-N1N	3.83	1.39	1.35
2	H	300	NAD	C2A-N3A	3.77	1.38	1.32
2	E	300	NAD	C2N-N1N	3.57	1.39	1.35
2	F	300	NAD	C2A-N1A	3.50	1.40	1.33
2	G	300	NAD	O4B-C1B	3.34	1.45	1.41
2	E	300	NAD	C5N-C4N	3.06	1.45	1.38
2	D	300	NAD	C2N-C3N	-3.05	1.34	1.39
2	H	300	NAD	C2A-N1A	3.00	1.39	1.33
2	E	300	NAD	C2A-N3A	2.95	1.36	1.32
2	C	300	NAD	C2A-N1A	2.95	1.39	1.33
2	F	300	NAD	O4D-C1D	2.83	1.45	1.41
2	H	300	NAD	C2N-C3N	2.69	1.43	1.39
2	D	300	NAD	O4D-C1D	2.69	1.44	1.41
2	D	300	NAD	C2A-N3A	2.69	1.36	1.32
2	C	300	NAD	C2N-N1N	2.65	1.38	1.35
2	G	300	NAD	C2A-N3A	2.61	1.36	1.32
2	D	300	NAD	O4B-C1B	2.56	1.44	1.41
2	E	300	NAD	O4D-C1D	2.50	1.44	1.41
2	E	300	NAD	C3N-C7N	2.48	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	O4B-C1B	2.48	1.44	1.41
2	H	300	NAD	C4A-N3A	2.35	1.38	1.35
2	F	300	NAD	C2N-C3N	2.25	1.42	1.39
2	G	300	NAD	C2N-N1N	2.20	1.37	1.35
2	H	300	NAD	O4B-C1B	2.16	1.44	1.41
2	F	300	NAD	O4B-C1B	2.06	1.44	1.41
2	E	300	NAD	C4A-N3A	2.05	1.38	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	300	NAD	C3N-C7N-N7N	10.83	130.74	117.75
2	E	300	NAD	C3N-C7N-N7N	8.07	127.43	117.75
2	H	300	NAD	N3A-C2A-N1A	-7.08	117.61	128.68
2	D	300	NAD	O7N-C7N-N7N	-6.06	113.97	122.58
2	C	300	NAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	F	300	NAD	C3N-C7N-N7N	5.36	124.18	117.75
2	E	300	NAD	O7N-C7N-C3N	-4.98	113.67	119.63
2	E	300	NAD	N3A-C2A-N1A	-4.96	120.93	128.68
2	G	300	NAD	O7N-C7N-C3N	-4.84	113.83	119.63
2	D	300	NAD	C3B-C2B-C1B	-4.83	93.70	100.98
2	F	300	NAD	N3A-C2A-N1A	-4.75	121.25	128.68
2	H	300	NAD	C1B-N9A-C4A	-4.58	118.60	126.64
2	H	300	NAD	C3N-C7N-N7N	4.33	122.94	117.75
2	G	300	NAD	C3N-C7N-N7N	4.24	122.84	117.75
2	D	300	NAD	N3A-C2A-N1A	-4.07	122.31	128.68
2	D	300	NAD	C5A-C6A-N6A	3.79	126.11	120.35
2	D	300	NAD	O7N-C7N-C3N	-3.71	115.19	119.63
2	F	300	NAD	C6N-N1N-C2N	-3.54	118.74	121.97
2	H	300	NAD	C2A-N1A-C6A	3.47	124.70	118.75
2	D	300	NAD	O3D-C3D-C2D	-3.46	100.62	111.82
2	F	300	NAD	O7N-C7N-N7N	-3.07	118.21	122.58
2	D	300	NAD	O4D-C1D-C2D	-3.06	102.46	106.93
2	G	300	NAD	N3A-C2A-N1A	-2.97	124.03	128.68
2	D	300	NAD	O3B-C3B-C4B	-2.79	103.00	111.05
2	E	300	NAD	O7N-C7N-N7N	-2.76	118.66	122.58
2	F	300	NAD	C1B-N9A-C4A	-2.65	121.98	126.64
2	C	300	NAD	PN-O3-PA	-2.59	123.94	132.83
2	C	300	NAD	C5A-C6A-N6A	-2.50	116.55	120.35
2	E	300	NAD	C2A-N1A-C6A	2.47	122.98	118.75
2	G	300	NAD	O5B-PA-O1A	-2.44	99.55	109.07
2	G	300	NAD	C3B-C2B-C1B	-2.43	97.31	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	300	NAD	C5N-C6N-N1N	-2.42	116.94	120.40
2	E	300	NAD	O3B-C3B-C2B	-2.36	104.18	111.82
2	F	300	NAD	O5D-PN-O1N	-2.36	99.85	109.07
2	D	300	NAD	O2N-PN-O1N	2.30	123.61	112.24
2	F	300	NAD	O4D-C1D-C2D	-2.21	103.70	106.93
2	H	300	NAD	O7N-C7N-N7N	-2.20	119.45	122.58
2	F	300	NAD	O2B-C2B-C3B	2.19	118.90	111.82
2	H	300	NAD	C6N-N1N-C2N	-2.14	120.03	121.97
2	C	300	NAD	O5D-PN-O1N	2.13	117.39	109.07
2	E	300	NAD	O2B-C2B-C3B	2.12	118.69	111.82
2	G	300	NAD	C3D-C2D-C1D	-2.06	97.88	100.98
2	C	300	NAD	N6A-C6A-N1A	2.03	122.79	118.57
2	C	300	NAD	O7N-C7N-N7N	2.00	125.42	122.58

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	NAD	C5D-O5D-PN-O1N
2	D	300	NAD	C5D-O5D-PN-O2N
2	E	300	NAD	C5D-O5D-PN-O1N
2	E	300	NAD	C5D-O5D-PN-O2N
2	E	300	NAD	O4D-C1D-N1N-C2N
2	F	300	NAD	C5B-O5B-PA-O1A
2	F	300	NAD	C5B-O5B-PA-O2A
2	F	300	NAD	C5B-O5B-PA-O3
2	F	300	NAD	O4B-C4B-C5B-O5B
2	F	300	NAD	O4D-C1D-N1N-C2N
2	G	300	NAD	C5D-O5D-PN-O2N
2	G	300	NAD	O4D-C1D-N1N-C2N
2	H	300	NAD	C5D-O5D-PN-O2N
2	H	300	NAD	O4D-C1D-N1N-C2N
2	F	300	NAD	O4D-C4D-C5D-O5D
2	F	300	NAD	C3D-C4D-C5D-O5D
2	F	300	NAD	PN-O3-PA-O1A
2	C	300	NAD	C5D-O5D-PN-O3
2	D	300	NAD	C5D-O5D-PN-O3
2	E	300	NAD	C5D-O5D-PN-O3
2	G	300	NAD	C5D-O5D-PN-O3
2	C	300	NAD	PA-O3-PN-O2N
2	H	300	NAD	PA-O3-PN-O2N
2	D	300	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	H	300	NAD	C5D-O5D-PN-O1N
2	F	300	NAD	C3B-C4B-C5B-O5B
2	F	300	NAD	PA-O3-PN-O2N
2	F	300	NAD	PN-O3-PA-O2A
2	C	300	NAD	O4B-C4B-C5B-O5B
2	H	300	NAD	O4B-C4B-C5B-O5B
2	H	300	NAD	C5D-O5D-PN-O3
2	D	300	NAD	PA-O3-PN-O1N
2	G	300	NAD	PA-O3-PN-O1N
2	G	300	NAD	PA-O3-PN-O2N
2	H	300	NAD	PA-O3-PN-O1N
2	D	300	NAD	O4B-C4B-C5B-O5B
2	E	300	NAD	O4B-C4B-C5B-O5B
2	G	300	NAD	O4B-C4B-C5B-O5B

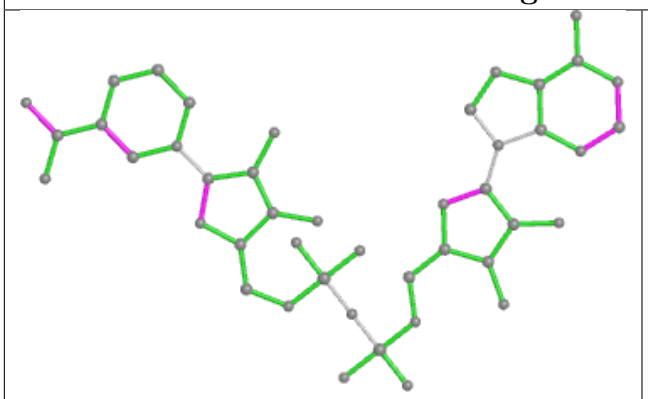
There are no ring outliers.

6 monomers are involved in 13 short contacts:

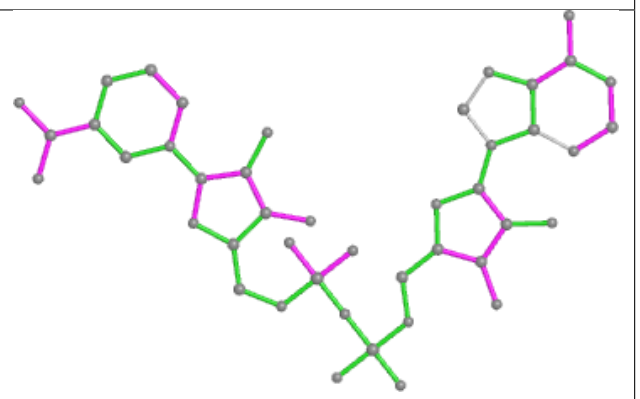
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	NAD	2	0
2	C	300	NAD	1	0
2	G	300	NAD	2	0
2	F	300	NAD	3	0
2	H	300	NAD	1	0
2	E	300	NAD	4	0

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.

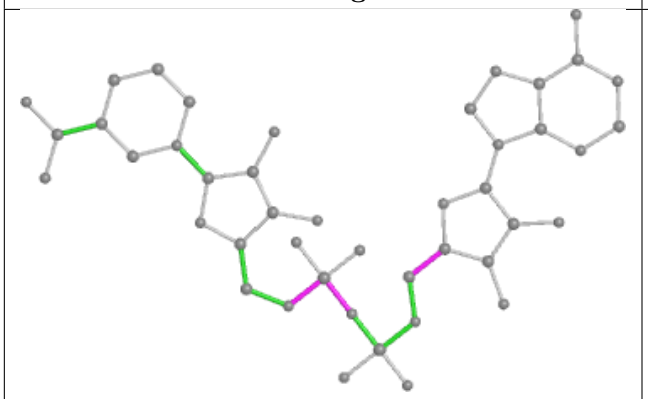
Ligand NAD D 300



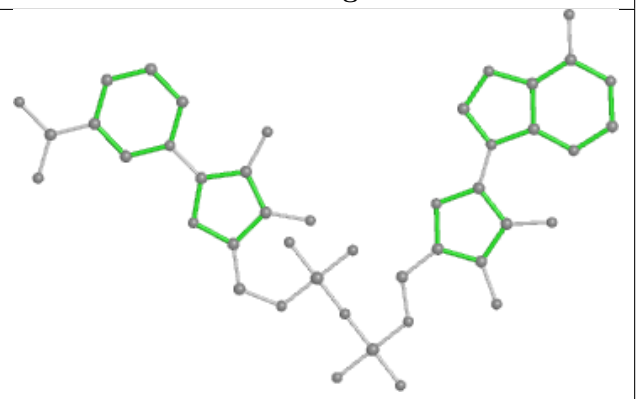
Bond lengths



Bond angles

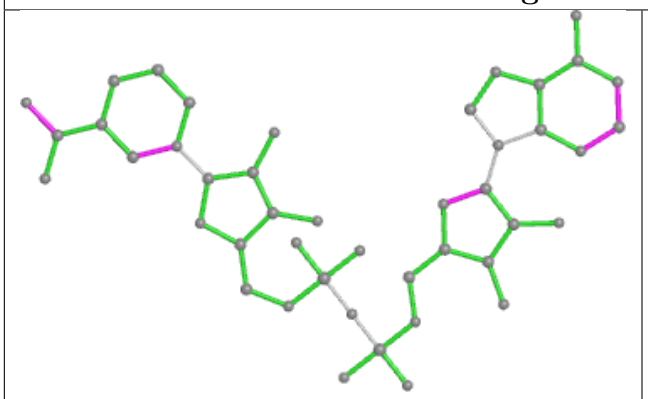


Torsions

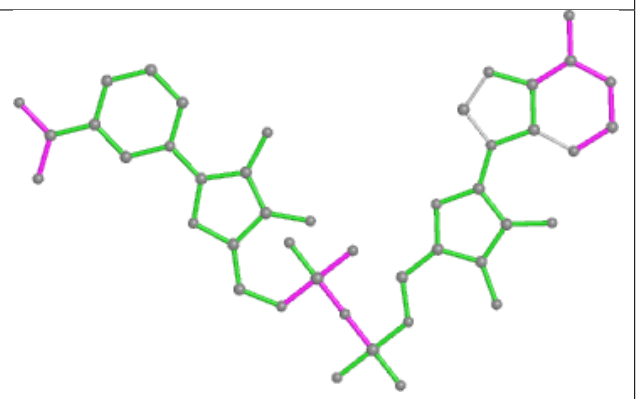


Rings

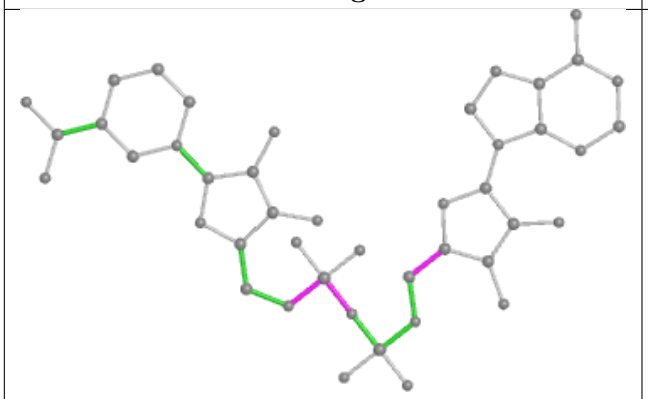
Ligand NAD C 300



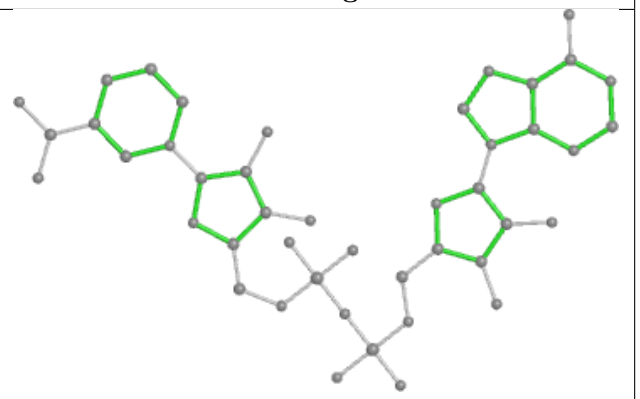
Bond lengths



Bond angles

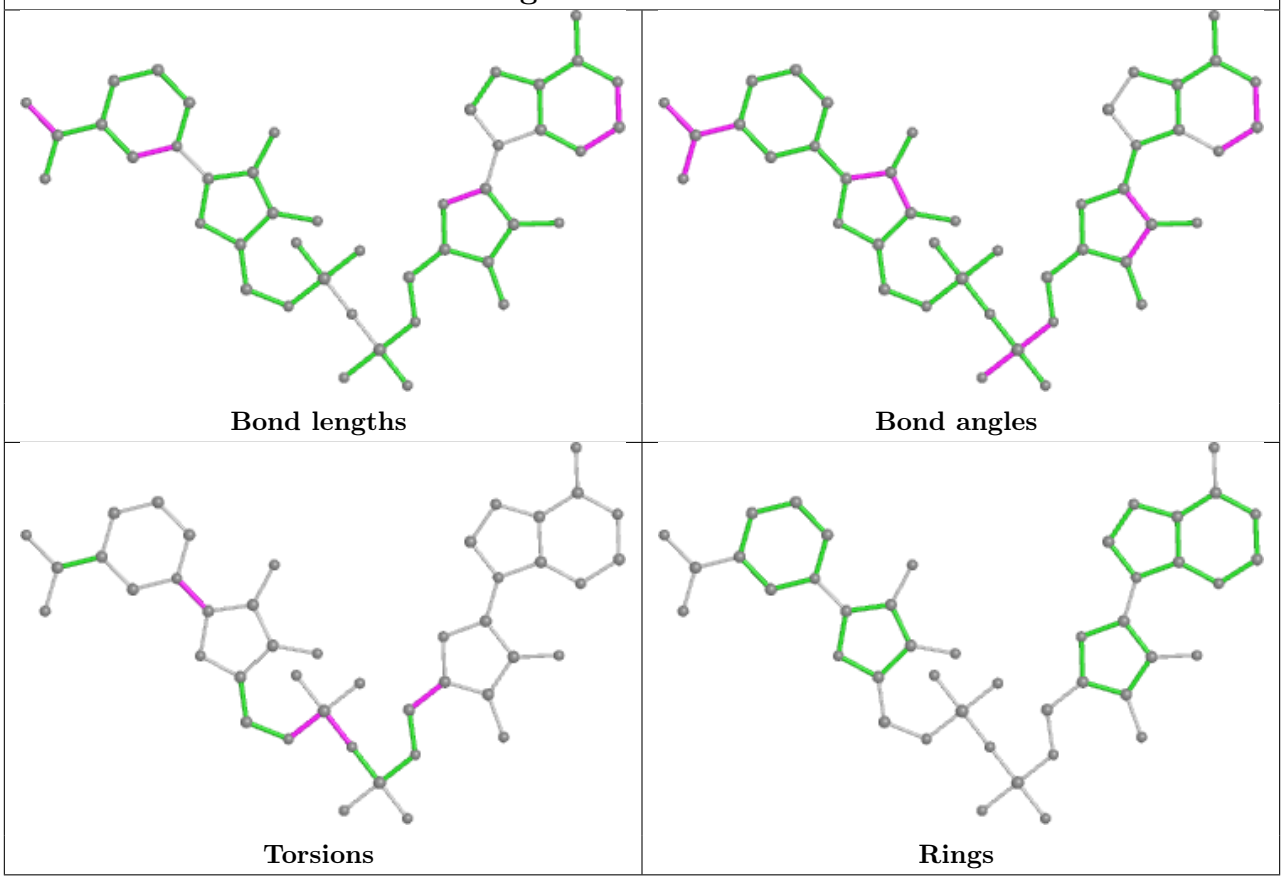


Torsions

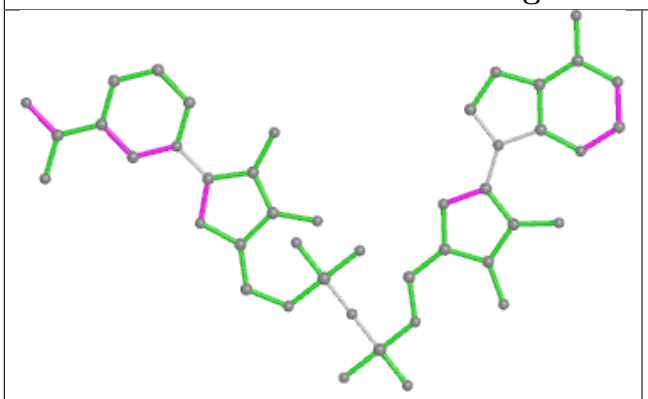


Rings

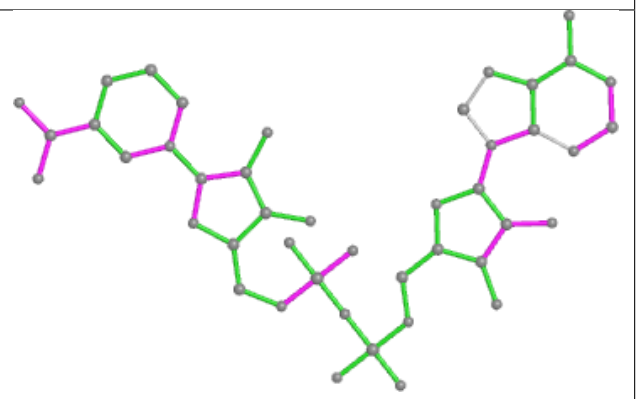
Ligand NAD G 300



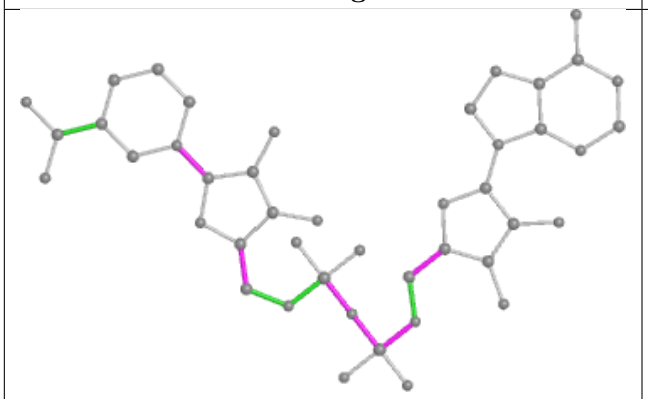
Ligand NAD F 300



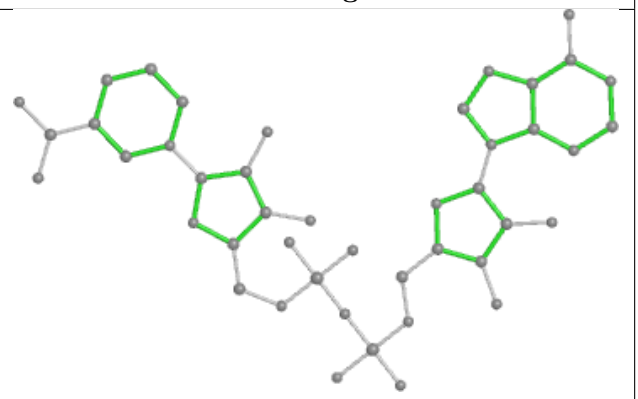
Bond lengths



Bond angles

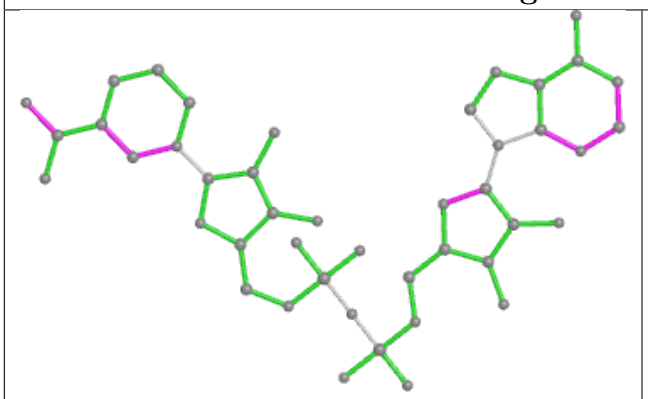


Torsions

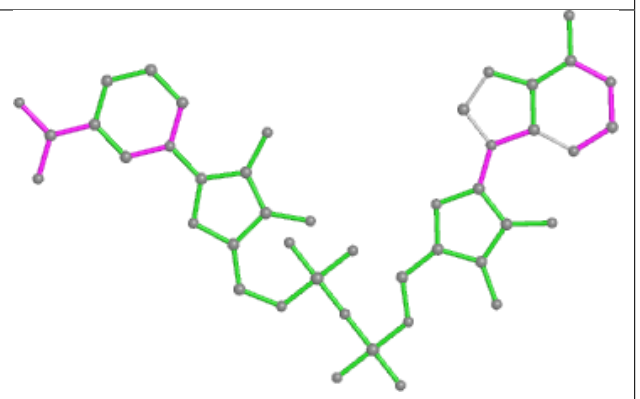


Rings

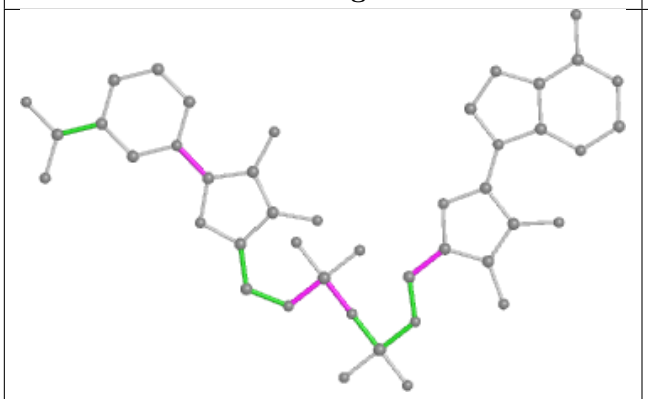
Ligand NAD H 300



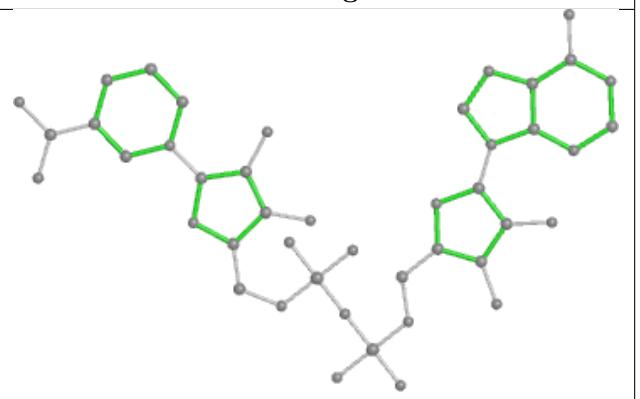
Bond lengths



Bond angles

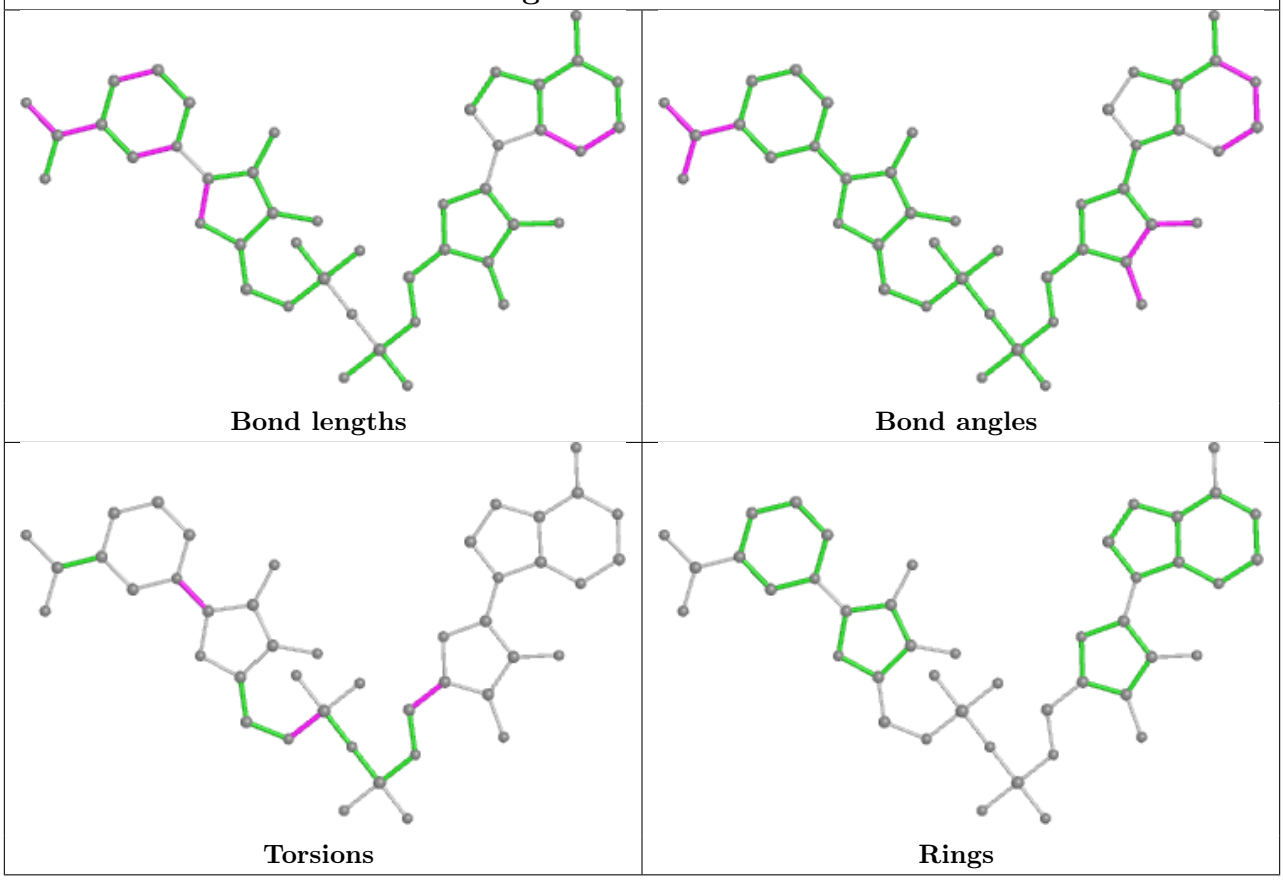


Torsions



Rings

Ligand NAD E 300



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

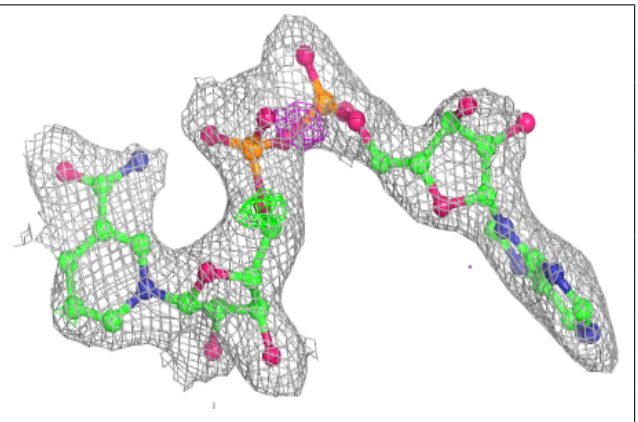
6.4 Ligands (i)

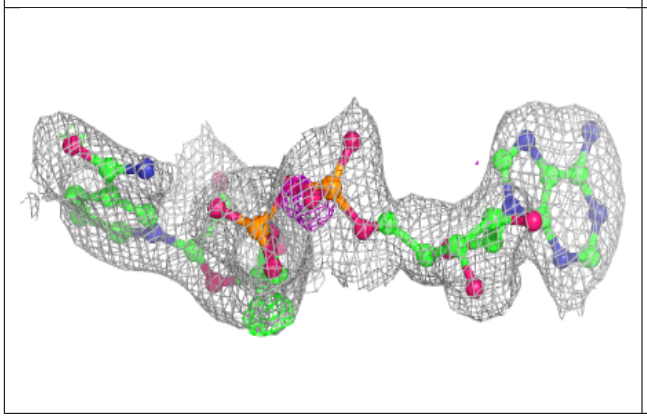
Unable to reproduce the depositors R factor - this section is therefore empty.

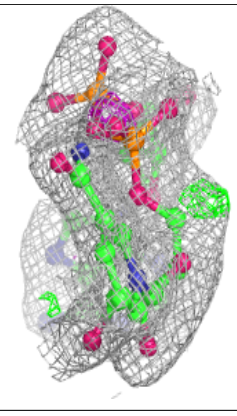
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 300:

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

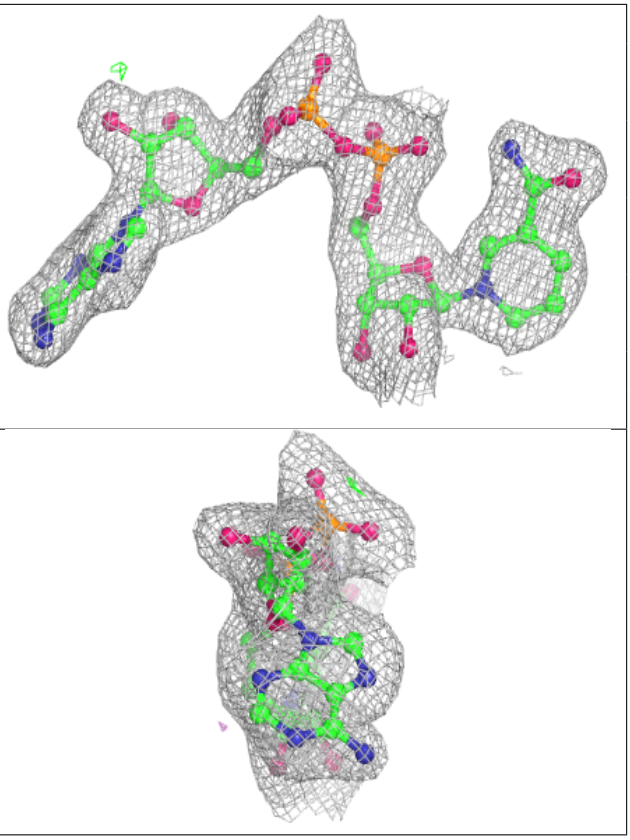






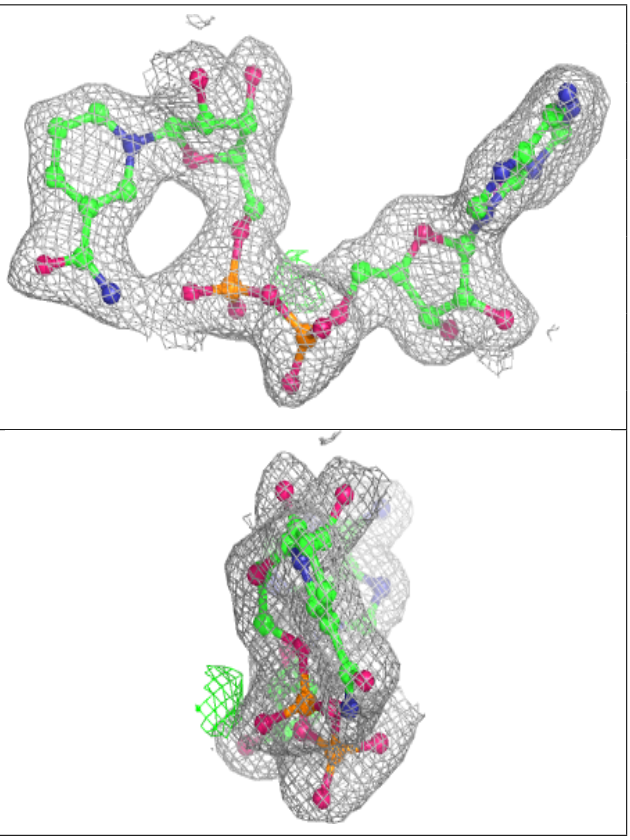
Electron density around NAD D 300:

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



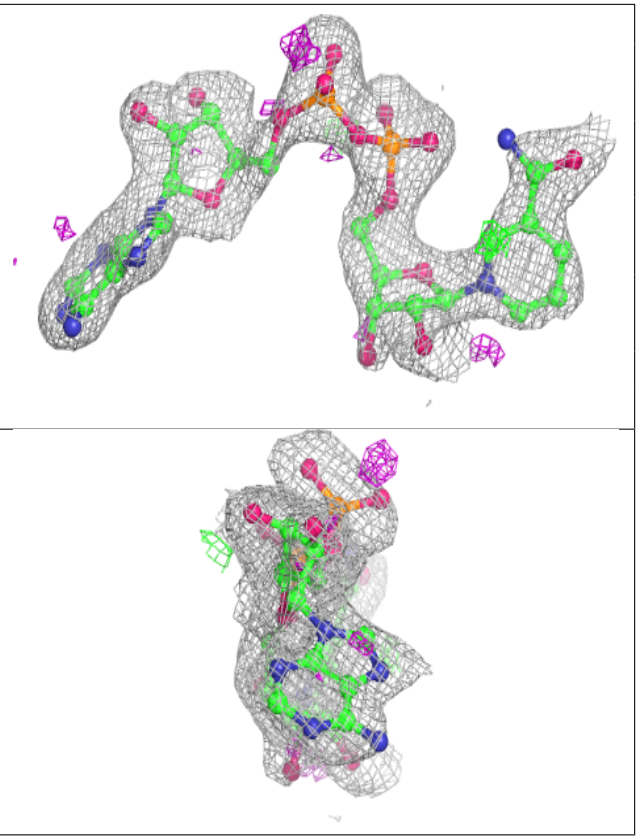
Electron density around NAD E 300:

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



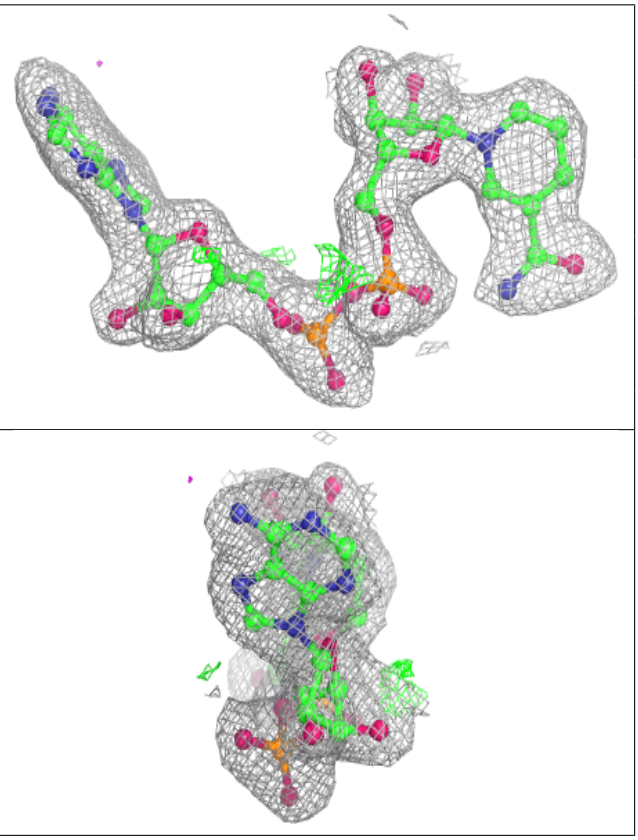
Electron density around NAD F 300:

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



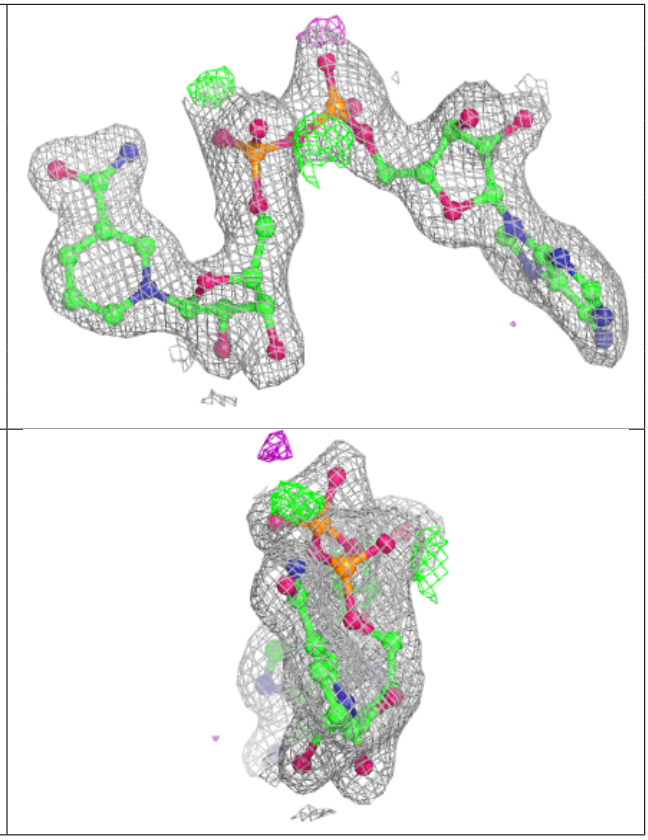
Electron density around NAD G 300:

$2mF_o$-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 300:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.