



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:31 AM UTC

PDB ID : 3GGP / pdb_00003ggp
Title : Crystal structure of prephenate dehydrogenase from *A. aeolicus* in complex with hydroxyphenyl propionate and NAD⁺
Authors : Sun, W.; Shahinas, D.; Kimber, M.S.; Christendat, D.
Deposited on : 2009-03-01
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

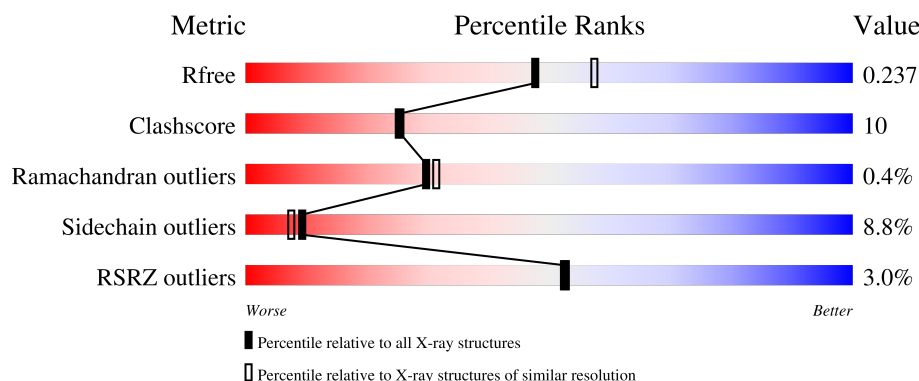
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

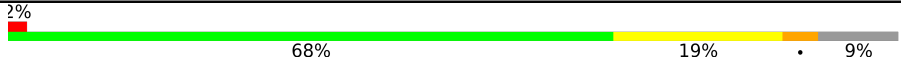
The reported resolution of this entry is 2.25 Å.

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	314	
1	B	314	
1	C	314	
1	D	314	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9369 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 Prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2260	1456	372	424	8			
1	B	284	Total	C	N	O	S	0	0	0
			2244	1446	370	420	8			
1	C	286	Total	C	N	O	S	0	0	0
			2260	1458	372	422	8			
1	D	286	Total	C	N	O	S	0	0	0
			2260	1456	372	424	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O67636
A	-1	GLY	-	expression tag	UNP O67636
A	0	SER	-	expression tag	UNP O67636
A	1	SER	-	expression tag	UNP O67636
A	2	HIS	-	expression tag	UNP O67636
A	3	HIS	-	expression tag	UNP O67636
A	4	HIS	-	expression tag	UNP O67636
A	5	HIS	-	expression tag	UNP O67636
A	6	HIS	-	expression tag	UNP O67636
A	7	HIS	-	expression tag	UNP O67636
A	8	SER	-	expression tag	UNP O67636
A	9	SER	-	expression tag	UNP O67636
A	10	GLY	-	expression tag	UNP O67636
A	11	LEU	-	expression tag	UNP O67636
A	12	VAL	-	expression tag	UNP O67636
A	13	PRO	-	expression tag	UNP O67636
A	14	ARG	-	expression tag	UNP O67636
A	15	GLY	-	expression tag	UNP O67636
A	16	SER	-	expression tag	UNP O67636
A	17	HIS	-	expression tag	UNP O67636
A	18	MET	-	expression tag	UNP O67636

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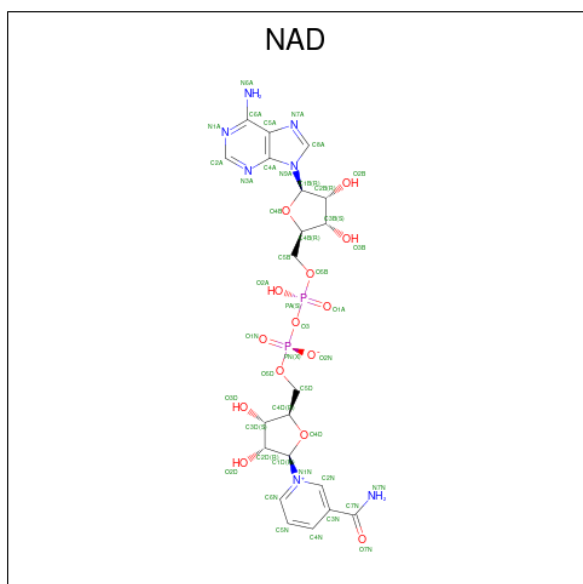
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP O67636
B	-1	GLY	-	expression tag	UNP O67636
B	0	SER	-	expression tag	UNP O67636
B	1	SER	-	expression tag	UNP O67636
B	2	HIS	-	expression tag	UNP O67636
B	3	HIS	-	expression tag	UNP O67636
B	4	HIS	-	expression tag	UNP O67636
B	5	HIS	-	expression tag	UNP O67636
B	6	HIS	-	expression tag	UNP O67636
B	7	HIS	-	expression tag	UNP O67636
B	8	SER	-	expression tag	UNP O67636
B	9	SER	-	expression tag	UNP O67636
B	10	GLY	-	expression tag	UNP O67636
B	11	LEU	-	expression tag	UNP O67636
B	12	VAL	-	expression tag	UNP O67636
B	13	PRO	-	expression tag	UNP O67636
B	14	ARG	-	expression tag	UNP O67636
B	15	GLY	-	expression tag	UNP O67636
B	16	SER	-	expression tag	UNP O67636
B	17	HIS	-	expression tag	UNP O67636
B	18	MET	-	expression tag	UNP O67636
C	-2	MET	-	expression tag	UNP O67636
C	-1	GLY	-	expression tag	UNP O67636
C	0	SER	-	expression tag	UNP O67636
C	1	SER	-	expression tag	UNP O67636
C	2	HIS	-	expression tag	UNP O67636
C	3	HIS	-	expression tag	UNP O67636
C	4	HIS	-	expression tag	UNP O67636
C	5	HIS	-	expression tag	UNP O67636
C	6	HIS	-	expression tag	UNP O67636
C	7	HIS	-	expression tag	UNP O67636
C	8	SER	-	expression tag	UNP O67636
C	9	SER	-	expression tag	UNP O67636
C	10	GLY	-	expression tag	UNP O67636
C	11	LEU	-	expression tag	UNP O67636
C	12	VAL	-	expression tag	UNP O67636
C	13	PRO	-	expression tag	UNP O67636
C	14	ARG	-	expression tag	UNP O67636
C	15	GLY	-	expression tag	UNP O67636
C	16	SER	-	expression tag	UNP O67636
C	17	HIS	-	expression tag	UNP O67636
C	18	MET	-	expression tag	UNP O67636

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP O67636
D	-1	GLY	-	expression tag	UNP O67636
D	0	SER	-	expression tag	UNP O67636
D	1	SER	-	expression tag	UNP O67636
D	2	HIS	-	expression tag	UNP O67636
D	3	HIS	-	expression tag	UNP O67636
D	4	HIS	-	expression tag	UNP O67636
D	5	HIS	-	expression tag	UNP O67636
D	6	HIS	-	expression tag	UNP O67636
D	7	HIS	-	expression tag	UNP O67636
D	8	SER	-	expression tag	UNP O67636
D	9	SER	-	expression tag	UNP O67636
D	10	GLY	-	expression tag	UNP O67636
D	11	LEU	-	expression tag	UNP O67636
D	12	VAL	-	expression tag	UNP O67636
D	13	PRO	-	expression tag	UNP O67636
D	14	ARG	-	expression tag	UNP O67636
D	15	GLY	-	expression tag	UNP O67636
D	16	SER	-	expression tag	UNP O67636
D	17	HIS	-	expression tag	UNP O67636
D	18	MET	-	expression tag	UNP O67636

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

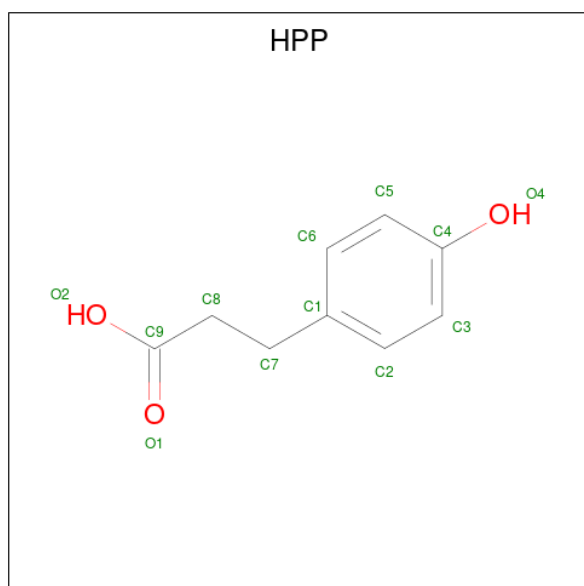


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is HYDROXYPHENYL PROPIONIC ACID (CCD ID: HPP) (formula: C₉H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	9	3		
4	C	1	Total	C	O	0	0
			12	9	3		

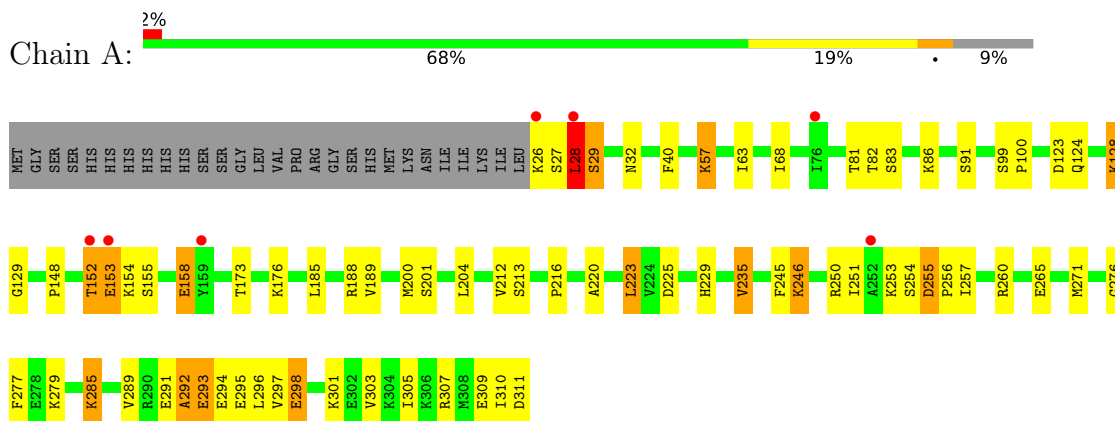
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0
5	B	40	Total 40	O 40	0	0
5	C	41	Total 41	O 41	0	0
5	D	24	Total 24	O 24	0	0

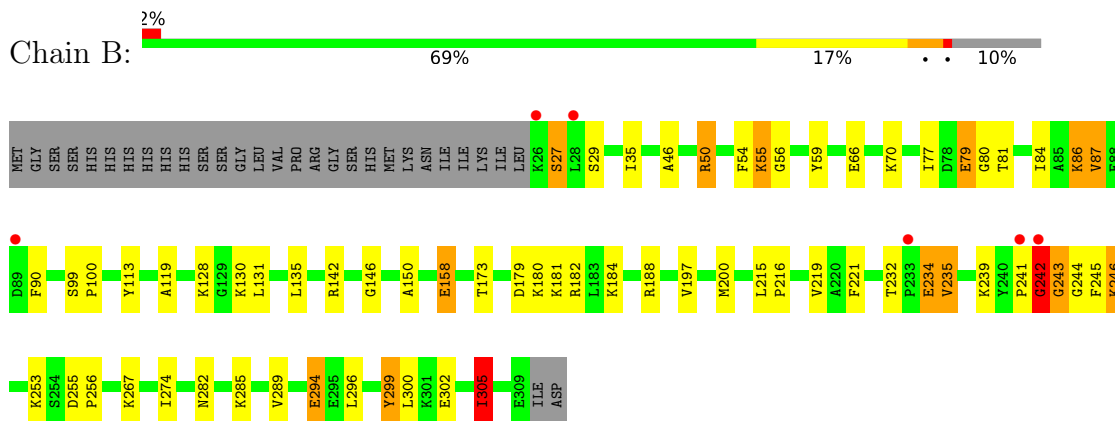
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues 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.

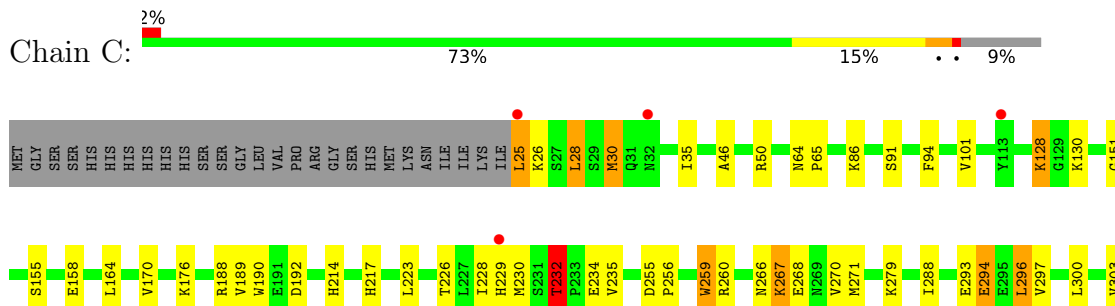
- Molecule 1: Prephenate dehydrogenase

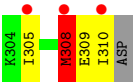


- Molecule 1: Prephenate dehydrogenase

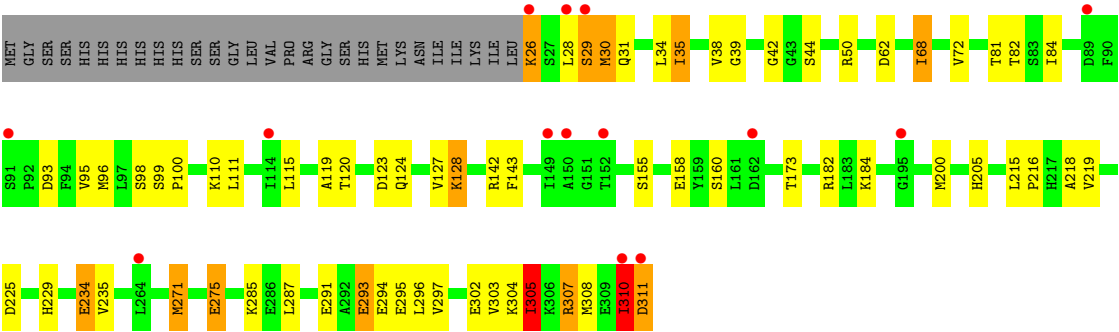


- Molecule 1: Prephenate dehydrogenase





● Molecule 1: Prephenate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.06Å 92.36Å 163.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 2.25 44.45 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.45-2.25) 97.4 (44.45-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.198 , 0.248 0.189 , 0.237	Depositor DCC
R_{free} test set	1751 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9369	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.24% 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: CL, HPP, 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	1.13	3/2303 (0.1%)	1.22	7/3098 (0.2%)
1	B	1.15	2/2287 (0.1%)	1.17	6/3076 (0.2%)
1	C	1.19	3/2303 (0.1%)	1.19	6/3098 (0.2%)
1	D	1.09	4/2303 (0.2%)	1.14	3/3098 (0.1%)
All	All	1.14	12/9196 (0.1%)	1.18	22/12370 (0.2%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	VAL	C-O	-6.16	1.16	1.24
1	A	201	SER	CA-C	6.08	1.59	1.53
1	C	91	SER	CA-C	6.05	1.60	1.52
1	C	228	ILE	CA-CB	5.89	1.61	1.54
1	D	305	ILE	CA-CB	5.85	1.61	1.54
1	D	311	ASP	N-CA	5.78	1.57	1.46
1	B	242	GLY	C-O	5.69	1.31	1.23
1	C	232	THR	C-N	5.52	1.40	1.33
1	A	212	VAL	CA-CB	5.46	1.60	1.54
1	D	218	ALA	CA-CB	5.35	1.61	1.53
1	A	152	THR	CA-CB	5.33	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	307	ARG	CA-C	5.11	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	310	ILE	N-CA-C	10.26	121.93	112.29
1	C	309	GLU	N-CA-C	8.66	121.51	110.33
1	C	28	LEU	N-CA-C	-7.75	103.80	113.18
1	A	28	LEU	N-CA-C	7.33	120.25	109.69
1	B	55	LYS	N-CA-C	-7.28	98.75	110.32
1	C	308	MET	N-CA-C	6.85	118.53	111.14
1	A	255	ASP	CA-C-N	6.52	126.45	119.28
1	A	255	ASP	C-N-CA	6.52	126.45	119.28
1	A	235	VAL	N-CA-C	6.15	116.49	106.72
1	C	259	TRP	N-CA-C	6.12	118.03	111.36
1	A	40	PHE	N-CA-C	6.05	117.55	111.07
1	D	143	PHE	N-CA-C	6.02	119.06	109.24
1	A	204	LEU	N-CA-C	-5.66	105.20	111.36
1	B	305	ILE	CB-CA-C	-5.61	102.85	111.71
1	C	293	GLU	N-CA-C	5.32	117.08	111.28
1	D	30	MET	N-CA-C	5.27	125.76	111.00
1	B	299	TYR	N-CA-C	-5.16	105.74	111.36
1	B	113	TYR	CA-C-N	-5.09	115.79	121.85
1	B	113	TYR	C-N-CA	-5.09	115.79	121.85
1	C	296	LEU	N-CA-C	-5.07	105.65	111.07
1	A	295	GLU	N-CA-C	-5.02	105.45	111.03
1	B	221	PHE	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	243	GLY	Peptide
1	C	308	MET	Peptide
1	D	310	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2260	0	2311	51	0
1	B	2244	0	2296	42	0
1	C	2260	0	2318	51	0
1	D	2260	0	2311	52	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	12	0	9	0	0
4	C	12	0	8	0	0
5	A	38	0	0	1	0
5	B	40	0	0	0	0
5	C	41	0	0	3	0
5	D	24	0	0	0	0
All	All	9369	0	9357	179	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 10.

All (179) 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:276:GLY:HA3	1:C:230:MET:CE	1.70	1.20
1:A:276:GLY:HA3	1:C:230:MET:HE2	1.22	1.16
1:D:96:MET:HE2	1:D:124:GLN:CG	1.76	1.15
1:B:50:ARG:HH11	1:B:50:ARG:HG3	1.06	1.14
1:D:96:MET:HE2	1:D:124:GLN:HG3	1.10	1.06
1:C:232:THR:HG23	1:C:234:GLU:H	1.23	1.03
1:D:307:ARG:HH12	1:D:311:ASP:C	1.74	0.94
1:B:294:GLU:H	1:B:294:GLU:CD	1.75	0.93
1:B:50:ARG:HG3	1:B:50:ARG:NH1	1.77	0.90
1:D:96:MET:CE	1:D:124:GLN:HG3	2.02	0.88
1:D:96:MET:HE1	1:D:123:ASP:C	1.97	0.88
1:B:243:GLY:HA3	1:B:245:PHE:H	1.40	0.86
1:B:50:ARG:HH11	1:B:50:ARG:CG	1.86	0.85
1:D:119:ALA:O	1:D:142:ARG:HG2	1.76	0.85
1:C:232:THR:HG22	1:C:235:VAL:H	1.41	0.82
1:D:35:ILE:HD11	1:D:42:GLY:HA3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:HG22	1:C:235:VAL:N	1.96	0.80
1:A:220:ALA:HB3	1:A:251:ILE:HD12	1.65	0.79
1:C:232:THR:HG23	1:C:234:GLU:N	1.98	0.79
1:D:310:ILE:O	1:D:310:ILE:HG22	1.82	0.77
1:D:271:MET:O	1:D:275:GLU:HG2	1.85	0.76
1:D:307:ARG:NH1	1:D:311:ASP:C	2.43	0.76
1:C:35:ILE:CD1	1:C:46:ALA:HB2	2.15	0.76
1:D:96:MET:CE	1:D:123:ASP:C	2.61	0.74
1:C:214:HIS:HD2	1:C:266:ASN:HD22	1.35	0.73
1:C:294:GLU:H	1:C:294:GLU:CD	1.96	0.72
1:A:276:GLY:CA	1:C:230:MET:CE	2.60	0.72
1:D:99:SER:HB2	1:D:100:PRO:CD	2.22	0.70
1:A:276:GLY:HA3	1:C:230:MET:HE3	1.72	0.69
1:B:35:ILE:HD13	1:B:46:ALA:HB2	1.74	0.69
1:C:30:MET:HE2	1:C:94:PHE:CG	2.27	0.69
1:B:302:GLU:O	1:B:305:ILE:HG12	1.93	0.68
1:C:151:GLY:HA2	1:C:164:LEU:HD11	1.77	0.66
1:B:84:ILE:O	1:B:87:VAL:HG13	1.96	0.66
1:B:243:GLY:HA3	1:B:245:PHE:N	2.11	0.65
1:D:308:MET:O	1:D:311:ASP:N	2.26	0.65
1:A:246:LYS:HD3	1:A:246:LYS:C	2.23	0.64
1:A:271:MET:HE3	1:C:288:ILE:CG2	2.28	0.64
1:C:30:MET:HE3	1:C:189:VAL:HG21	1.80	0.63
1:C:35:ILE:HD13	1:C:46:ALA:HB2	1.81	0.63
1:D:96:MET:HE1	1:D:123:ASP:O	1.99	0.63
1:A:276:GLY:CA	1:C:230:MET:HE2	2.12	0.62
1:B:294:GLU:CD	1:B:294:GLU:N	2.52	0.62
1:D:35:ILE:CD1	1:D:42:GLY:CA	2.78	0.61
1:D:96:MET:CE	1:D:124:GLN:CG	2.68	0.61
1:B:79:GLU:HG3	1:B:80:GLY:N	2.15	0.60
1:C:214:HIS:CD2	1:C:266:ASN:HD22	2.19	0.60
1:C:226:THR:HG23	1:C:230:MET:HE3	1.85	0.59
1:D:96:MET:HE2	1:D:124:GLN:HG2	1.75	0.59
1:A:32:ASN:OD1	1:A:57:LYS:HG3	2.03	0.59
1:C:214:HIS:HE1	5:C:1005:HOH:O	1.86	0.58
1:A:225:ASP:OD1	1:A:229:HIS:HE1	1.86	0.58
1:A:99:SER:HB2	1:A:100:PRO:CD	2.34	0.58
1:A:285:LYS:O	1:A:289:VAL:HG23	2.03	0.57
1:C:30:MET:HE2	1:C:94:PHE:CD2	2.40	0.57
1:C:232:THR:CG2	1:C:234:GLU:H	2.09	0.57
1:A:292:ALA:O	1:A:293:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:MET:HE3	1:C:288:ILE:HG22	1.87	0.56
1:D:304:LYS:O	1:D:308:MET:HG3	2.04	0.56
1:A:292:ALA:O	1:A:293:GLU:CB	2.53	0.56
1:D:35:ILE:CD1	1:D:42:GLY:HA3	2.33	0.56
1:A:153:GLU:O	1:A:153:GLU:HG2	2.05	0.56
1:A:99:SER:HB2	1:A:100:PRO:HD2	1.88	0.56
1:A:291:GLU:OE1	1:C:267:LYS:HE2	2.05	0.56
1:A:27:SER:O	1:A:28:LEU:HD13	2.06	0.56
1:A:305:ILE:O	1:A:309:GLU:HG3	2.06	0.56
1:A:271:MET:CE	1:C:288:ILE:CG2	2.84	0.55
1:A:296:LEU:HD23	1:C:260:ARG:HG2	1.88	0.55
1:C:234:GLU:HG2	1:C:234:GLU:O	2.06	0.55
1:D:308:MET:HA	1:D:311:ASP:HA	1.88	0.55
1:C:64:ASN:OD1	1:C:65:PRO:HD2	2.06	0.55
1:C:232:THR:CG2	1:C:234:GLU:N	2.70	0.54
1:B:128:LYS:HE2	1:B:146:GLY:O	2.08	0.54
1:D:99:SER:HB2	1:D:100:PRO:HD2	1.90	0.53
1:D:215:LEU:HB3	1:D:216:PRO:HD3	1.89	0.53
1:A:294:GLU:O	1:A:298:GLU:HB2	2.09	0.53
1:B:253:LYS:O	1:D:304:LYS:HE2	2.10	0.52
1:D:35:ILE:HD13	1:D:42:GLY:CA	2.40	0.52
1:B:35:ILE:CD1	1:B:46:ALA:HB2	2.39	0.51
1:B:215:LEU:HB3	1:B:216:PRO:HD3	1.92	0.51
1:B:158:GLU:H	1:B:158:GLU:CD	2.18	0.51
1:B:235:VAL:O	1:B:235:VAL:CG2	2.58	0.51
1:A:223:LEU:HD13	1:A:245:PHE:CE1	2.46	0.51
1:D:38:VAL:HG23	1:D:38:VAL:O	2.11	0.51
1:D:173:THR:HA	1:D:200:MET:O	2.11	0.50
1:A:271:MET:CE	1:C:288:ILE:HG21	2.41	0.50
1:B:239:LYS:C	1:B:241:PRO:HD3	2.38	0.49
1:A:246:LYS:HD3	1:A:246:LYS:O	2.12	0.49
1:A:307:ARG:HH12	1:A:311:ASP:HB3	1.78	0.49
1:B:79:GLU:CG	1:B:80:GLY:N	2.76	0.49
1:C:294:GLU:CD	1:C:294:GLU:N	2.69	0.49
1:D:34:LEU:HB3	1:D:95:VAL:HG22	1.95	0.49
1:B:232:THR:OG1	1:B:234:GLU:OE1	2.26	0.48
1:A:124:GLN:HE21	1:A:148:PRO:HG3	1.79	0.48
1:B:282:ASN:HA	1:B:285:LYS:HD3	1.95	0.48
1:C:267:LYS:HB3	1:C:267:LYS:HE3	1.52	0.48
1:B:241:PRO:O	1:B:242:GLY:C	2.57	0.48
1:D:291:GLU:O	1:D:293:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HG3	1:C:297:VAL:HG23	1.95	0.47
1:A:173:THR:HA	1:A:200:MET:O	2.14	0.47
1:A:276:GLY:O	1:A:279:LYS:HB3	2.14	0.47
1:B:84:ILE:O	1:B:87:VAL:CG1	2.62	0.47
1:D:111:LEU:HB3	1:D:115:LEU:HD12	1.97	0.47
1:D:287:LEU:HD22	1:D:295:GLU:HB2	1.95	0.47
1:A:152:THR:OG1	1:A:154:LYS:HE3	2.14	0.47
1:B:294:GLU:N	1:B:294:GLU:OE2	2.39	0.47
1:C:300:LEU:O	1:C:303:VAL:HG22	2.14	0.47
1:C:128:LYS:HE3	1:C:128:LYS:HA	1.97	0.47
1:A:291:GLU:O	1:A:292:ALA:O	2.33	0.47
1:B:142:ARG:HA	1:B:182:ARG:NE	2.30	0.47
1:B:131:LEU:O	1:B:135:LEU:HG	2.15	0.46
1:B:180:LYS:O	1:B:184:LYS:HG3	2.15	0.46
1:A:123:ASP:OD2	1:A:128:LYS:NZ	2.47	0.46
1:D:35:ILE:HD13	1:D:42:GLY:HA2	1.97	0.46
1:D:50:ARG:HD3	1:D:50:ARG:HA	1.73	0.46
1:D:142:ARG:HA	1:D:182:ARG:NE	2.31	0.46
1:B:119:ALA:O	1:B:142:ARG:HG2	2.16	0.46
1:B:27:SER:C	1:B:29:SER:H	2.23	0.45
1:A:152:THR:O	1:A:154:LYS:HG3	2.16	0.45
1:B:244:GLY:O	1:B:245:PHE:C	2.59	0.45
1:A:213:SER:C	1:A:216:PRO:HD2	2.41	0.45
1:B:99:SER:HB2	1:B:100:PRO:HD2	1.99	0.45
1:C:176:LYS:HG2	5:C:1094:HOH:O	2.16	0.45
1:D:84:ILE:HG12	1:D:110:LYS:HG3	1.99	0.45
1:D:123:ASP:OD2	1:D:128:LYS:NZ	2.41	0.44
1:A:225:ASP:OD1	1:A:229:HIS:CE1	2.69	0.44
1:C:188:ARG:NE	1:C:192:ASP:OD2	2.51	0.44
1:D:310:ILE:HD12	1:D:310:ILE:H	1.82	0.44
1:B:59:TYR:CD2	1:B:90:PHE:HB3	2.53	0.44
1:A:63:ILE:HG12	2:A:312:NAD:C5A	2.48	0.44
1:C:255:ASP:HA	1:C:256:PRO:HD3	1.80	0.44
1:D:234:GLU:C	1:D:235:VAL:HG23	2.42	0.44
1:B:274:ILE:HG21	1:D:285:LYS:HD2	2.00	0.43
1:D:120:THR:OG1	1:D:182:ARG:HG2	2.19	0.43
1:C:25:LEU:O	1:C:28:LEU:HG	2.18	0.43
1:D:225:ASP:O	1:D:229:HIS:HD2	2.01	0.43
1:B:54:PHE:CZ	1:B:56:GLY:HA3	2.54	0.43
1:A:176:LYS:HG2	5:A:1417:HOH:O	2.18	0.43
1:D:128:LYS:HG3	1:D:205:HIS:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:HE3	1:B:246:LYS:HB3	1.72	0.43
1:C:214:HIS:CE1	5:C:1005:HOH:O	2.68	0.43
1:D:310:ILE:HD12	1:D:310:ILE:N	2.34	0.43
1:A:128:LYS:O	1:A:129:GLY:C	2.62	0.42
1:D:26:LYS:C	1:D:28:LEU:H	2.27	0.42
1:C:217:HIS:CD2	1:C:259:TRP:CZ2	3.07	0.42
1:D:96:MET:CE	1:D:124:GLN:N	2.83	0.42
1:B:81:THR:HG21	1:B:86:LYS:HB3	2.02	0.42
1:B:173:THR:HA	1:B:200:MET:O	2.19	0.42
1:D:39:GLY:HA3	2:D:312:NAD:O5B	2.19	0.42
1:D:128:LYS:HE3	1:D:128:LYS:HA	2.01	0.42
1:A:152:THR:O	1:A:154:LYS:N	2.52	0.42
1:A:271:MET:HE1	1:C:288:ILE:HB	2.01	0.42
1:D:310:ILE:O	1:D:310:ILE:CG2	2.56	0.42
1:A:153:GLU:HG3	1:A:253:LYS:HB2	2.02	0.41
1:D:62:ASP:O	1:D:82:THR:HA	2.20	0.41
1:A:158:GLU:H	1:A:158:GLU:CD	2.29	0.41
1:D:44:SER:N	1:D:160:SER:HB2	2.35	0.41
1:D:68:ILE:HD11	1:D:81:THR:O	2.20	0.41
1:A:285:LYS:HB2	1:C:271:MET:HE1	2.03	0.41
1:A:57:LYS:HB3	1:A:57:LYS:NZ	2.36	0.41
1:A:277:PHE:HA	1:C:226:THR:OG1	2.21	0.41
1:A:255:ASP:HA	1:A:256:PRO:HD3	1.75	0.41
1:A:81:THR:OG1	1:A:82:THR:N	2.53	0.41
1:B:255:ASP:HA	1:B:256:PRO:HD3	1.81	0.41
1:C:30:MET:HE2	1:C:94:PHE:CD1	2.56	0.41
1:C:30:MET:CE	1:C:189:VAL:HG21	2.50	0.41
1:A:185:LEU:O	1:A:189:VAL:HG23	2.20	0.41
1:B:66:GLU:O	1:B:70:LYS:HG3	2.21	0.41
1:C:170:VAL:HG11	1:C:190:TRP:CG	2.56	0.41
1:C:234:GLU:O	1:C:235:VAL:HB	2.20	0.41
1:A:28:LEU:HB3	1:A:29:SER:H	1.76	0.41
1:B:179:ASP:OD1	1:B:179:ASP:C	2.63	0.41
1:C:266:ASN:O	1:C:270:VAL:HG23	2.21	0.41
1:B:150:ALA:O	2:B:312:NAD:H4N	2.21	0.40
1:D:302:GLU:HA	1:D:305:ILE:HG12	2.04	0.40
1:B:296:LEU:O	1:B:300:LEU:HG	2.22	0.40
1:D:30:MET:HA	1:D:93:ASP:OD2	2.22	0.40
1:C:50:ARG:HA	1:C:50:ARG:HD3	1.85	0.40
1:C:155:SER:OG	1:C:255:ASP:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/314 (90%)	272 (96%)	10 (4%)	2 (1%)	18	17
1	B	282/314 (90%)	265 (94%)	16 (6%)	1 (0%)	30	31
1	C	284/314 (90%)	270 (95%)	14 (5%)	0	100	100
1	D	284/314 (90%)	269 (95%)	14 (5%)	1 (0%)	30	31
All	All	1134/1256 (90%)	1076 (95%)	54 (5%)	4 (0%)	30	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ALA
1	A	293	GLU
1	B	242	GLY
1	D	29	SER

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	250/275 (91%)	224 (90%)	26 (10%)	7	5
1	B	248/275 (90%)	228 (92%)	20 (8%)	11	9
1	C	250/275 (91%)	231 (92%)	19 (8%)	12	10
1	D	250/275 (91%)	227 (91%)	23 (9%)	8	6
All	All	998/1100 (91%)	910 (91%)	88 (9%)	9	7

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	28	LEU
1	A	29	SER
1	A	57	LYS
1	A	68	ILE
1	A	83	SER
1	A	86	LYS
1	A	91	SER
1	A	128	LYS
1	A	153	GLU
1	A	155	SER
1	A	158	GLU
1	A	188	ARG
1	A	223	LEU
1	A	235	VAL
1	A	246	LYS
1	A	250	ARG
1	A	254	SER
1	A	257	ILE
1	A	265	GLU
1	A	285	LYS
1	A	297	VAL
1	A	298	GLU
1	A	301	LYS
1	A	303	VAL
1	A	310	ILE
1	B	27	SER
1	B	50	ARG
1	B	55	LYS
1	B	77	ILE
1	B	79	GLU
1	B	86	LYS
1	B	87	VAL
1	B	130	LYS
1	B	158	GLU
1	B	181	LYS
1	B	188	ARG
1	B	219	VAL
1	B	234	GLU
1	B	235	VAL
1	B	246	LYS
1	B	267	LYS

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Mol	Chain	Res	Type
1	B	289	VAL
1	B	294	GLU
1	B	299	TYR
1	B	305	ILE
1	C	25	LEU
1	C	26	LYS
1	C	30	MET
1	C	86	LYS
1	C	101	VAL
1	C	128	LYS
1	C	130	LYS
1	C	158	GLU
1	C	223	LEU
1	C	229	HIS
1	C	232	THR
1	C	267	LYS
1	C	268	GLU
1	C	279	LYS
1	C	294	GLU
1	C	296	LEU
1	C	305	ILE
1	C	308	MET
1	C	310	ILE
1	D	26	LYS
1	D	29	SER
1	D	31	GLN
1	D	35	ILE
1	D	68	ILE
1	D	72	VAL
1	D	98	SER
1	D	127	VAL
1	D	128	LYS
1	D	155	SER
1	D	158	GLU
1	D	184	LYS
1	D	219	VAL
1	D	234	GLU
1	D	271	MET
1	D	275	GLU
1	D	293	GLU
1	D	294	GLU
1	D	296	LEU

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Mol	Chain	Res	Type
1	D	297	VAL
1	D	303	VAL
1	D	305	ILE
1	D	310	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	229	HIS
1	B	31	GLN
1	B	32	ASN
1	B	283	HIS
1	C	214	HIS
1	D	229	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HPP	B	313	-	12,12,12	1.27	1 (8%)	15,15,15	1.38	3 (20%)
2	NAD	A	312	-	46,48,48	2.19	7 (15%)	64,73,73	1.95	13 (20%)
2	NAD	C	312	-	46,48,48	2.23	9 (19%)	64,73,73	1.91	18 (28%)
2	NAD	B	312	-	46,48,48	1.96	8 (17%)	64,73,73	1.84	13 (20%)
2	NAD	D	312	-	46,48,48	2.24	8 (17%)	64,73,73	1.60	10 (15%)
4	HPP	C	313	-	12,12,12	1.79	2 (16%)	15,15,15	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HPP	B	313	-	-	2/5/5/5	0/1/1/1
2	NAD	A	312	-	-	4/30/62/62	0/5/5/5
2	NAD	C	312	-	-	5/30/62/62	0/5/5/5
2	NAD	B	312	-	-	5/30/62/62	0/5/5/5
2	NAD	D	312	-	-	6/30/62/62	0/5/5/5
4	HPP	C	313	-	-	2/5/5/5	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	312	NAD	O7N-C7N	10.05	1.42	1.24
2	D	312	NAD	O7N-C7N	9.57	1.42	1.24
2	A	312	NAD	O7N-C7N	9.27	1.41	1.24
2	D	312	NAD	PN-O3	7.08	1.67	1.59
2	B	312	NAD	O7N-C7N	6.84	1.36	1.24
2	B	312	NAD	PA-O3	5.95	1.65	1.59
2	A	312	NAD	C2N-N1N	5.69	1.41	1.35
2	C	312	NAD	PN-O3	5.58	1.65	1.59
2	A	312	NAD	PN-O3	5.30	1.65	1.59
2	B	312	NAD	C2N-N1N	4.59	1.40	1.35
2	B	312	NAD	C2A-N3A	3.99	1.41	1.33
4	C	313	HPP	C3-C2	3.99	1.45	1.38
2	D	312	NAD	C2N-N1N	3.81	1.39	1.35
2	C	312	NAD	PA-O3	3.58	1.63	1.59
2	A	312	NAD	C2N-C3N	3.54	1.44	1.39
2	D	312	NAD	PA-O3	3.45	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	312	NAD	C5A-N7A	-3.30	1.33	1.39
2	C	312	NAD	C2N-N1N	3.22	1.38	1.35
2	A	312	NAD	PA-O3	3.09	1.62	1.59
2	B	312	NAD	C2A-N1A	3.05	1.39	1.33
2	A	312	NAD	C2A-N3A	2.98	1.39	1.33
2	C	312	NAD	C8A-N7A	2.85	1.37	1.31
2	D	312	NAD	C2A-N1A	2.81	1.38	1.33
2	D	312	NAD	C2A-N3A	2.76	1.38	1.33
2	A	312	NAD	C2A-N1A	2.61	1.38	1.33
2	D	312	NAD	C8A-N7A	2.55	1.36	1.31
2	C	312	NAD	PA-O2A	-2.21	1.45	1.55
2	B	312	NAD	C7N-N7N	-2.20	1.28	1.33
4	C	313	HPP	C6-C5	2.16	1.42	1.38
2	C	312	NAD	C6N-N1N	2.14	1.40	1.35
2	B	312	NAD	C4A-N3A	2.14	1.38	1.34
4	B	313	HPP	C6-C5	2.09	1.42	1.38
2	B	312	NAD	PA-O2A	-2.09	1.45	1.55
2	C	312	NAD	O4B-C4B	-2.09	1.40	1.45
2	D	312	NAD	C5A-N7A	-2.02	1.35	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	312	NAD	N3A-C2A-N1A	-7.08	117.86	128.58
2	A	312	NAD	N3A-C2A-N1A	-6.84	118.23	128.58
2	D	312	NAD	N3A-C2A-N1A	-6.05	119.43	128.58
2	A	312	NAD	O2A-PA-O3	5.91	123.25	107.27
2	B	312	NAD	N3A-C2A-N1A	-5.67	120.00	128.58
2	B	312	NAD	N9A-C8A-N7A	-4.87	107.02	113.94
2	B	312	NAD	O3-PA-O1A	-4.78	96.32	110.70
2	A	312	NAD	C5A-C4A-N3A	-4.65	120.32	126.72
2	C	312	NAD	O2A-PA-O3	4.53	119.53	107.27
2	B	312	NAD	C4A-N9A-C8A	4.51	110.48	105.74
2	C	312	NAD	O7N-C7N-C3N	4.26	124.80	119.60
2	D	312	NAD	N9A-C8A-N7A	-3.94	108.35	113.94
2	A	312	NAD	O5B-C5B-C4B	-3.86	95.86	108.99
2	A	312	NAD	C2A-N3A-C4A	3.85	121.24	111.83
2	C	312	NAD	O7N-C7N-N7N	-3.44	117.65	122.62
2	B	312	NAD	O7N-C7N-N7N	-3.34	117.80	122.62
2	B	312	NAD	C4A-N9A-C1B	-3.19	119.18	126.63
2	C	312	NAD	C2A-N1A-C6A	3.18	123.95	118.73
2	A	312	NAD	N3A-C4A-N9A	3.14	132.51	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	312	NAD	O2N-PN-O1N	3.14	127.05	112.44
2	B	312	NAD	C5A-N7A-C8A	3.14	108.38	103.45
2	D	312	NAD	C5A-C4A-N3A	-3.13	122.40	126.72
2	C	312	NAD	C5A-C4A-N3A	-3.13	122.41	126.72
2	D	312	NAD	C2A-N3A-C4A	3.01	119.18	111.83
2	A	312	NAD	N9A-C8A-N7A	-3.00	109.67	113.94
2	B	312	NAD	C5A-C4A-N3A	-3.00	122.59	126.72
2	C	312	NAD	C2A-N3A-C4A	2.94	119.00	111.83
2	D	312	NAD	C5A-N7A-C8A	2.93	108.05	103.45
2	A	312	NAD	O3-PA-O1A	-2.84	102.17	110.70
4	B	313	HPP	C7-C8-C9	-2.70	106.56	113.83
2	C	312	NAD	O2N-PN-O1N	2.69	124.98	112.44
2	B	312	NAD	N3A-C4A-N9A	2.67	131.71	127.17
4	B	313	HPP	C6-C5-C4	-2.67	117.06	119.88
2	A	312	NAD	O4B-C1B-N9A	2.63	113.14	108.09
2	A	312	NAD	O2A-PA-O5B	-2.62	95.71	107.57
2	B	312	NAD	O2A-PA-O3	2.59	114.27	107.27
2	C	312	NAD	C5A-C4A-N9A	2.52	108.56	105.81
2	C	312	NAD	N9A-C8A-N7A	-2.47	110.44	113.94
2	D	312	NAD	O5D-PN-O1N	-2.44	99.26	108.94
2	B	312	NAD	C6A-C5A-C4A	2.44	120.50	117.18
2	C	312	NAD	C6N-C5N-C4N	2.44	122.96	119.45
4	B	313	HPP	C2-C3-C4	2.42	122.44	119.88
2	A	312	NAD	C6N-N1N-C2N	-2.39	119.85	121.88
2	C	312	NAD	O3-PA-O1A	-2.36	103.62	110.70
2	C	312	NAD	C1B-N9A-C8A	2.34	132.30	127.09
2	D	312	NAD	C4A-N9A-C8A	2.22	108.07	105.74
2	C	312	NAD	C2D-C3D-C4D	2.19	106.83	102.61
2	D	312	NAD	O2A-PA-O3	2.18	113.16	107.27
2	C	312	NAD	C5N-C4N-C3N	-2.13	118.27	120.36
2	C	312	NAD	C4A-N9A-C1B	-2.13	121.65	126.63
2	D	312	NAD	O2N-PN-O1N	2.12	122.32	112.44
2	B	312	NAD	O7N-C7N-C3N	2.10	122.17	119.60
2	A	312	NAD	C2N-C3N-C4N	2.07	120.66	118.26
2	B	312	NAD	O5B-C5B-C4B	-2.05	102.01	108.99
2	C	312	NAD	O5B-C5B-C4B	-2.03	102.07	108.99
2	D	312	NAD	C4A-C5A-N7A	-2.03	108.26	110.58
2	C	312	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	312	NAD	O4D-C1D-N1N-C2N
2	B	312	NAD	O4D-C1D-N1N-C2N
2	B	312	NAD	O4D-C1D-N1N-C6N
2	B	312	NAD	C2D-C1D-N1N-C2N
2	B	312	NAD	C2D-C1D-N1N-C6N
2	C	312	NAD	O4D-C1D-N1N-C2N
2	C	312	NAD	O4D-C1D-N1N-C6N
2	D	312	NAD	C5D-O5D-PN-O3
2	D	312	NAD	C5D-O5D-PN-O2N
2	C	312	NAD	C5B-O5B-PA-O1A
2	D	312	NAD	C5D-O5D-PN-O1N
2	A	312	NAD	PN-O3-PA-O2A
2	D	312	NAD	PA-O3-PN-O2N
2	C	312	NAD	C2D-C1D-N1N-C6N
4	C	313	HPP	C7-C8-C9-O2
4	C	313	HPP	C7-C8-C9-O1
4	B	313	HPP	C7-C8-C9-O1
4	B	313	HPP	C7-C8-C9-O2
2	A	312	NAD	O4D-C1D-N1N-C6N
2	A	312	NAD	PN-O3-PA-O1A
2	D	312	NAD	O4B-C4B-C5B-O5B
2	D	312	NAD	PA-O3-PN-O1N
2	C	312	NAD	O4B-C4B-C5B-O5B
2	B	312	NAD	C2B-C1B-N9A-C8A

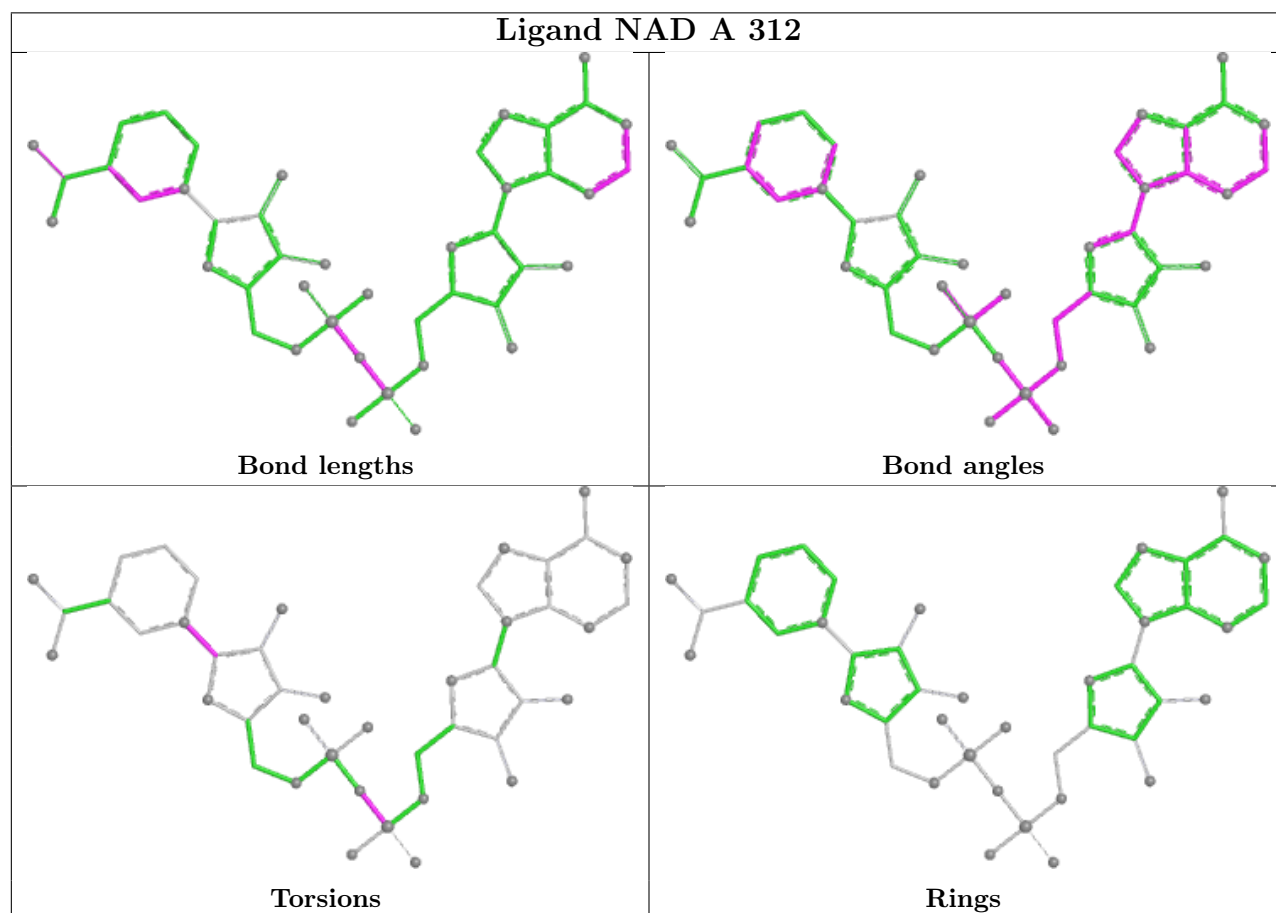
There are no ring outliers.

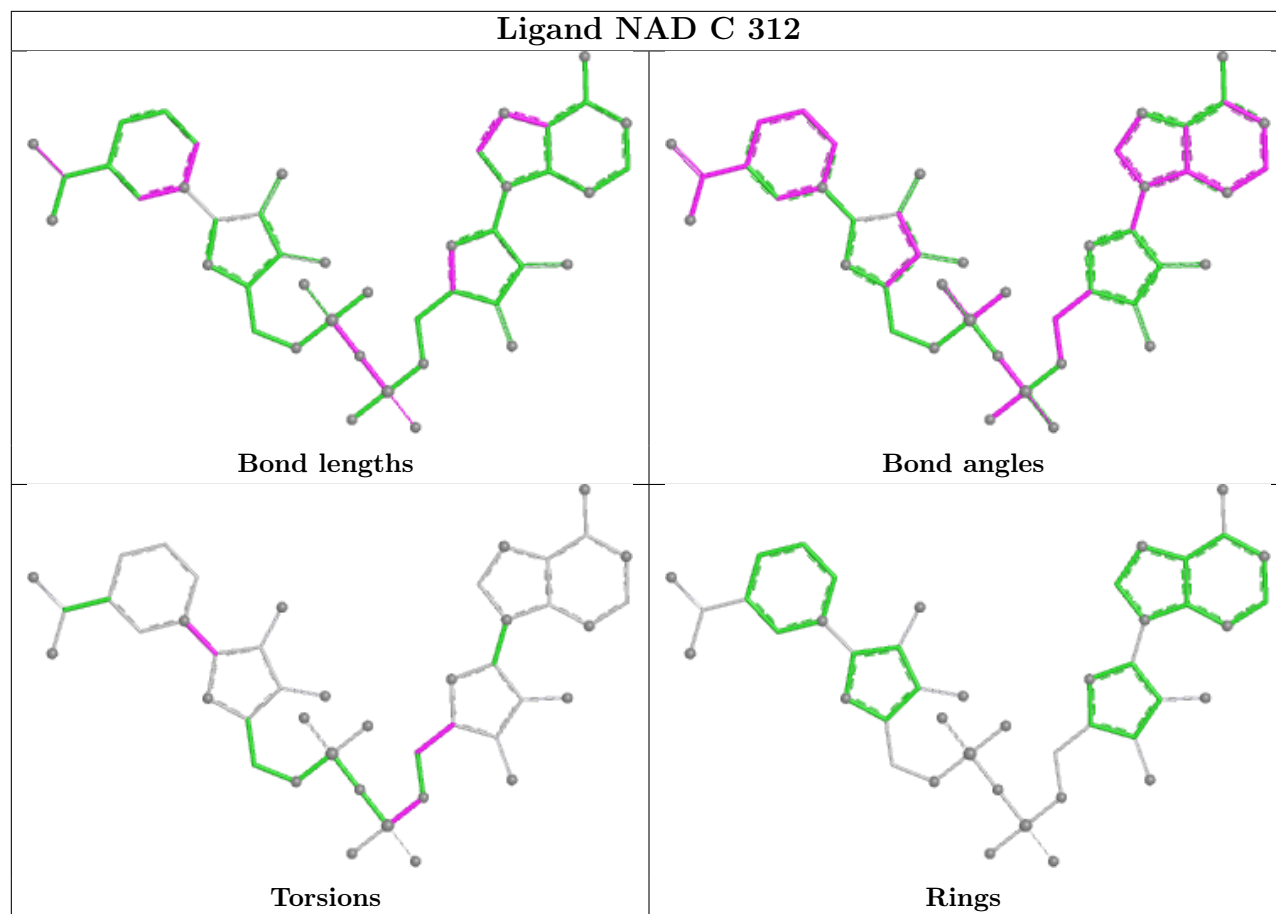
3 monomers are involved in 3 short contacts:

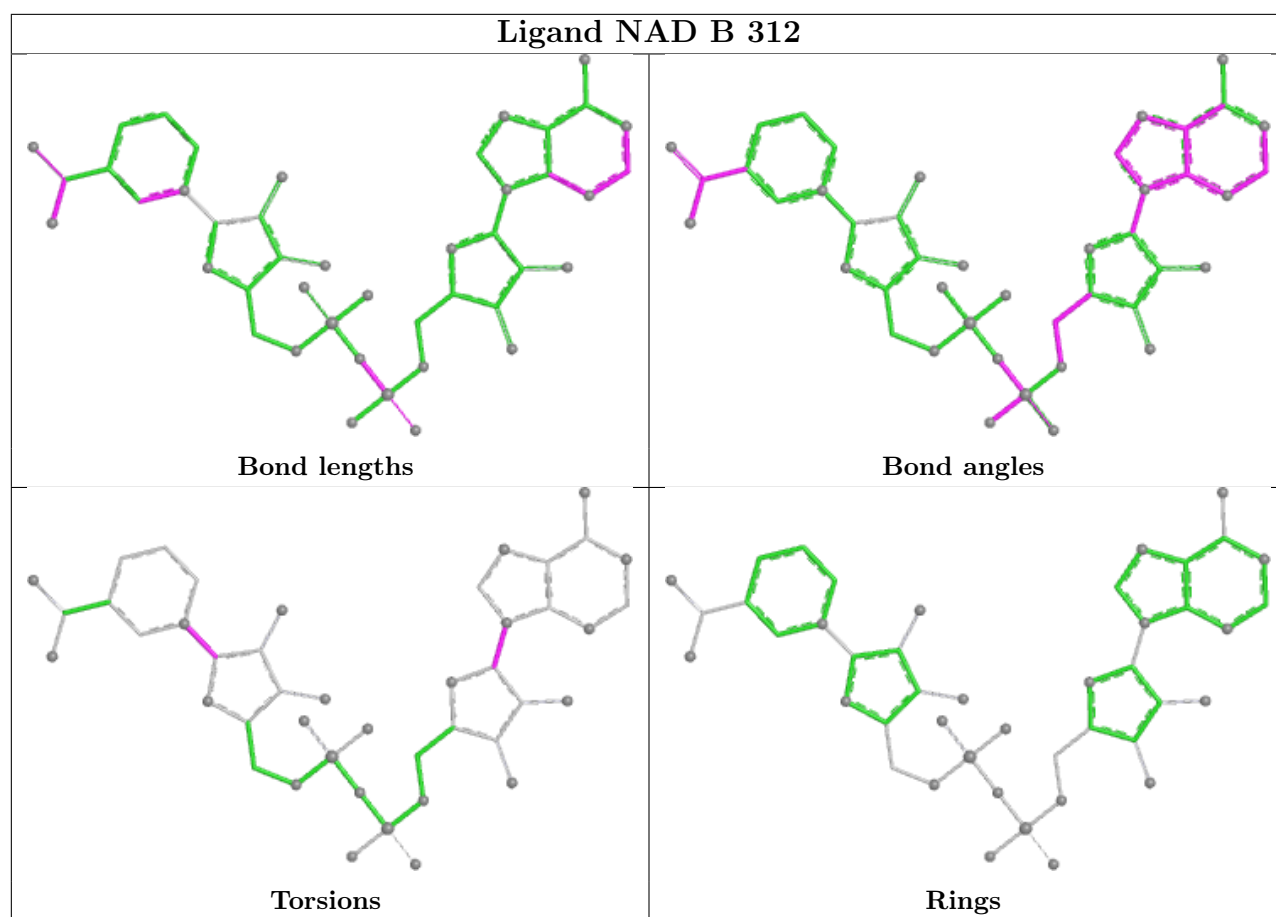
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	312	NAD	1	0
2	B	312	NAD	1	0
2	D	312	NAD	1	0

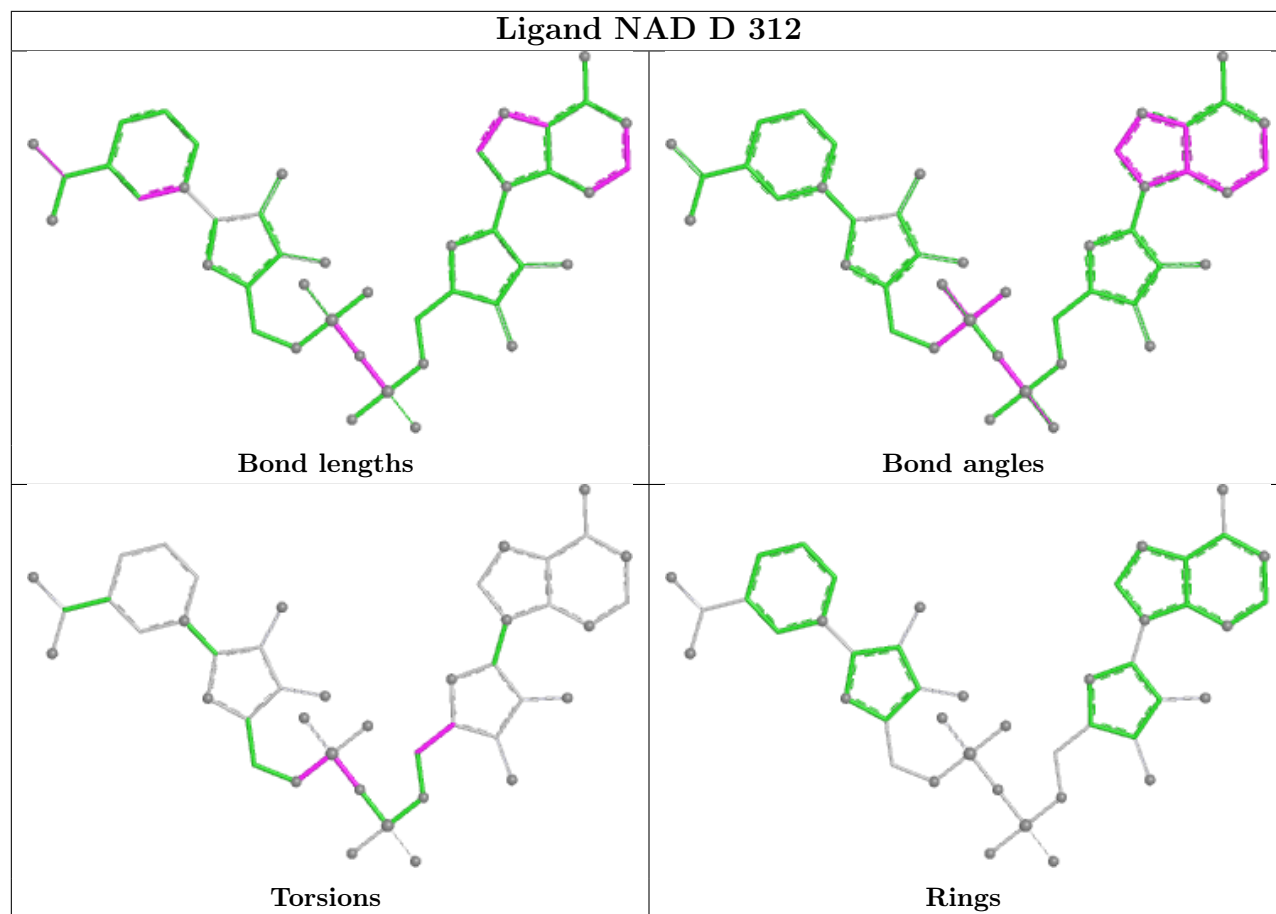
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	286/314 (91%)	0.48	7 (2%) 59 61	43, 58, 73, 86	0
1	B	284/314 (90%)	0.47	6 (2%) 63 64	43, 55, 67, 87	0
1	C	286/314 (91%)	0.22	7 (2%) 59 61	47, 54, 74, 111	0
1	D	286/314 (91%)	0.63	14 (4%) 35 34	47, 61, 80, 91	0
All	All	1142/1256 (90%)	0.45	34 (2%) 52 53	43, 57, 76, 111	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LEU	4.4
1	C	310	ILE	3.8
1	A	152	THR	3.7
1	D	26	LYS	3.7
1	C	25	LEU	3.6
1	D	310	ILE	3.6
1	D	152	THR	3.4
1	A	252	ALA	3.4
1	B	242	GLY	3.4
1	C	229	HIS	3.3
1	C	308	MET	3.0
1	D	150	ALA	2.8
1	B	26	LYS	2.8
1	C	305	ILE	2.7
1	D	28	LEU	2.7
1	A	153	GLU	2.6
1	B	28	LEU	2.6
1	D	29	SER	2.6
1	B	233	PRO	2.5
1	A	76	ILE	2.5
1	C	113	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	LYS	2.5
1	B	241	PRO	2.4
1	D	311	ASP	2.3
1	D	114	ILE	2.3
1	D	264	LEU	2.2
1	D	195	GLY	2.2
1	D	149	ILE	2.1
1	D	89	ASP	2.1
1	A	159	TYR	2.1
1	C	32	ASN	2.1
1	D	162	ASP	2.1
1	D	91	SER	2.0
1	B	89	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

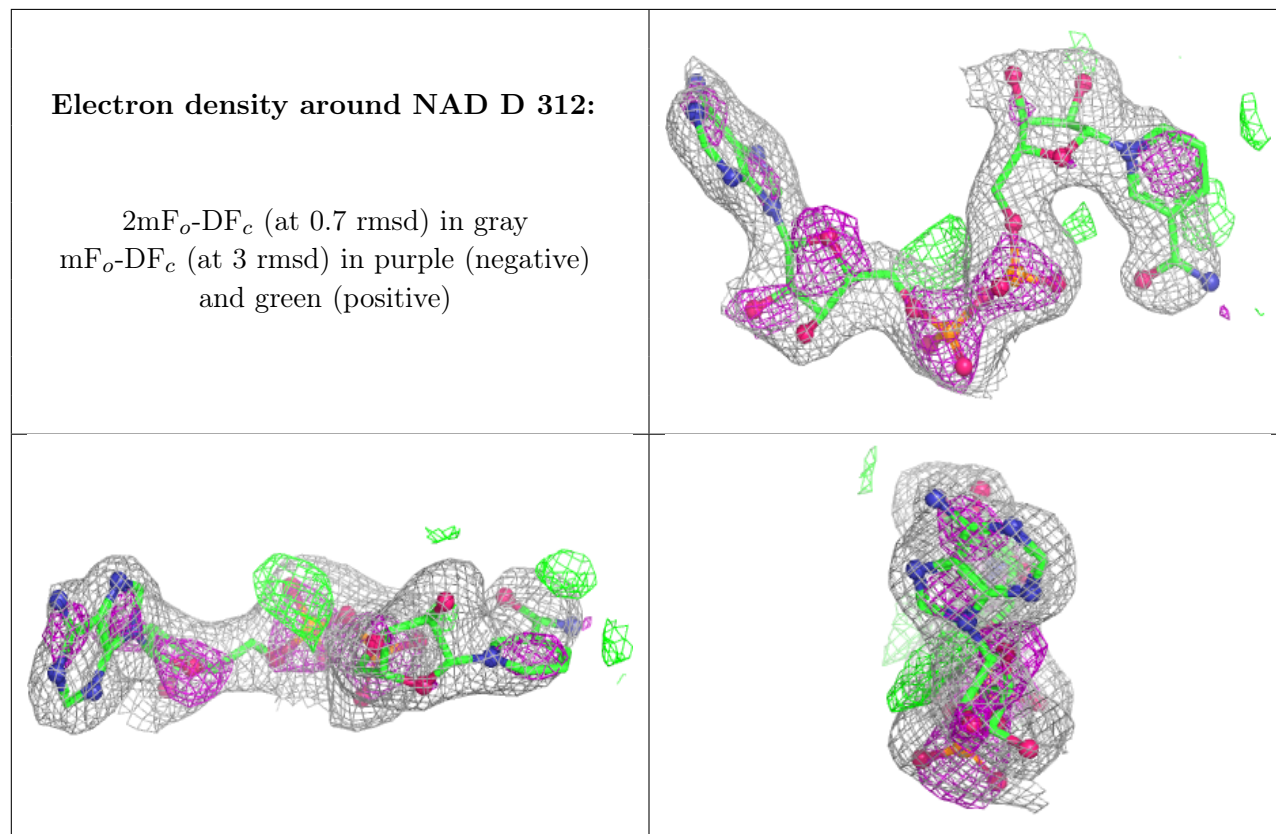
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	D	312	44/44	0.87	0.15	51,62,70,71	0
2	NAD	A	312	44/44	0.89	0.13	38,48,57,59	0
4	HPP	B	313	12/12	0.92	0.11	28,30,33,35	0
2	NAD	B	312	44/44	0.93	0.12	28,37,46,49	0
2	NAD	C	312	44/44	0.94	0.11	28,36,42,47	0
4	HPP	C	313	12/12	0.94	0.10	29,33,36,37	0
3	CL	A	313	1/1	0.97	0.24	42,42,42,42	0
3	CL	B	314	1/1	0.98	0.15	43,43,43,43	0

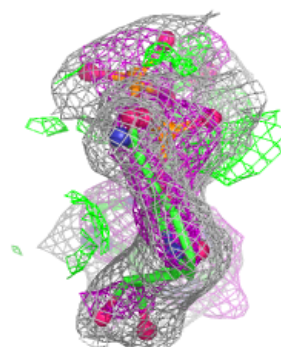
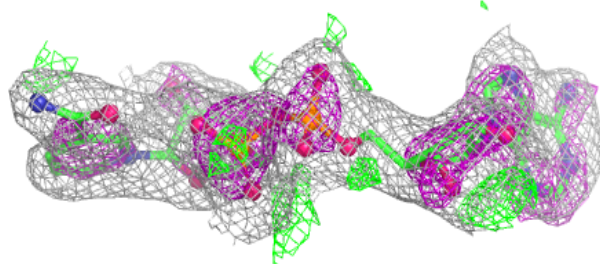
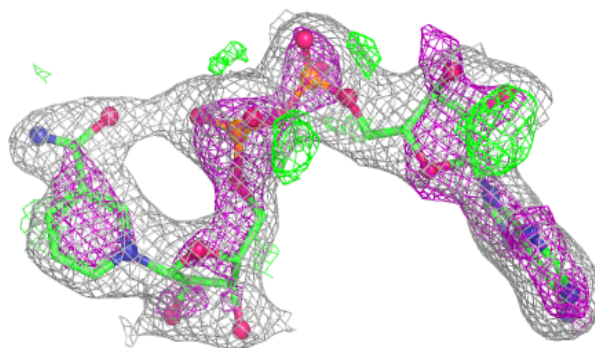
The following is a graphical depiction of the model fit to experimental electron density of all

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

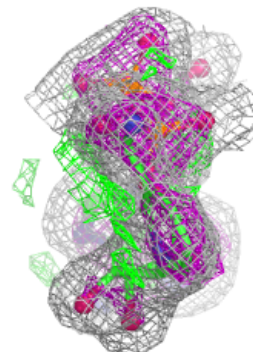
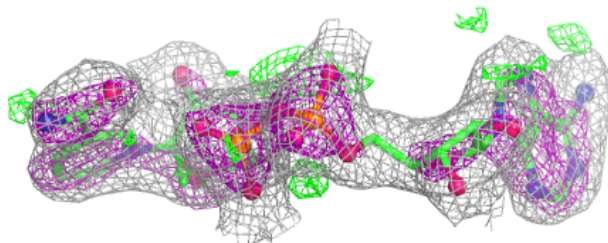
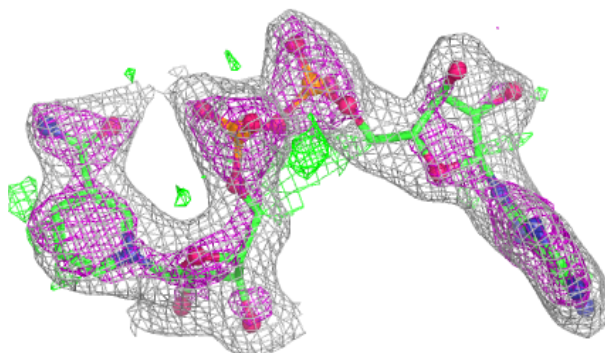


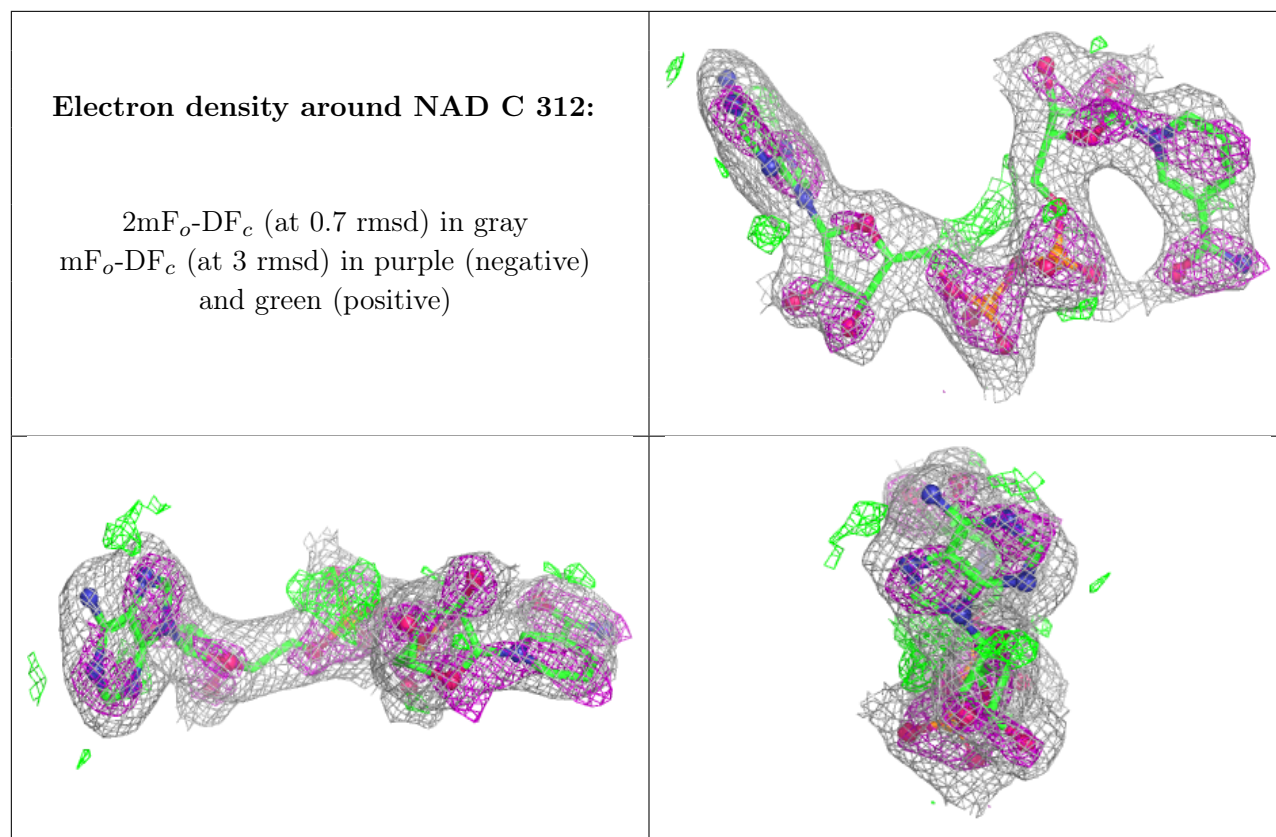
Electron density around NAD A 312:

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

**Electron density around NAD B 312:**

$2mF_o-DF_c$ (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.