



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:54 AM GMT

PDB ID : 3GGP  
Title : Crystal structure of prephenate dehydrogenase from *A. aeolicus* in complex with hydroxyphenyl propionate and NAD<sup>+</sup>  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

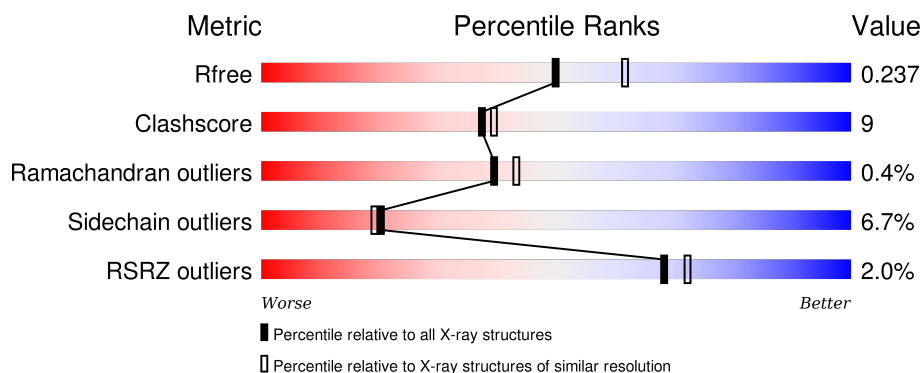
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>69% 18% • 9%</div> </div>
1	B	314	<div> <div>2%</div> <div>70% 17% • 10%</div> </div>
1	C	314	<div> <div>•</div> <div>75% 14% • 9%</div> </div>
1	D	314	<div> <div>3%</div> <div>72% 16% • 9%</div> </div>

## 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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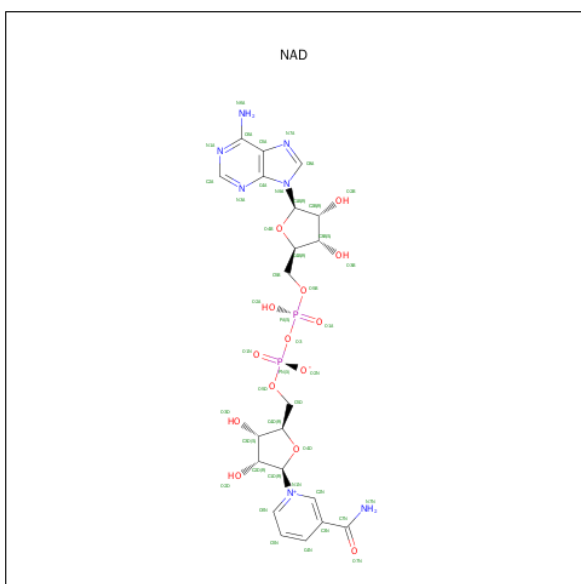
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP O67636
B	-1	GLY	-	EXPRESSION TAG	UNP O67636
B	0	SER	-	EXPRESSION TAG	UNP O67636
B	1	SER	-	EXPRESSION TAG	UNP O67636
B	2	HIS	-	EXPRESSION TAG	UNP O67636
B	3	HIS	-	EXPRESSION TAG	UNP O67636
B	4	HIS	-	EXPRESSION TAG	UNP O67636
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 (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).

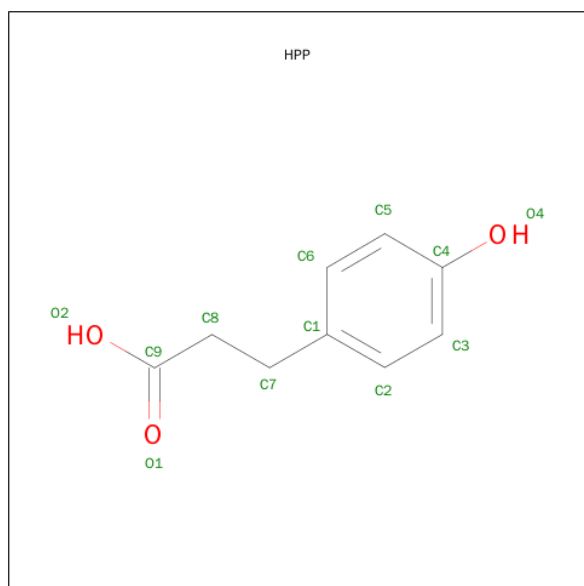


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is HYDROXYPHENYL PROPIONIC ACID (three-letter code: HPP) (formula: C<sub>9</sub>H<sub>10</sub>O<sub>3</sub>).



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		

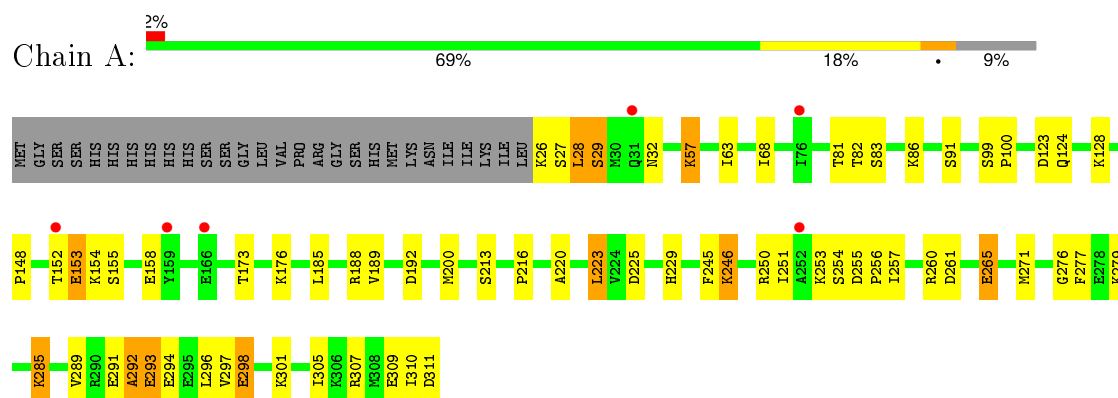
- Molecule 5 is water.

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

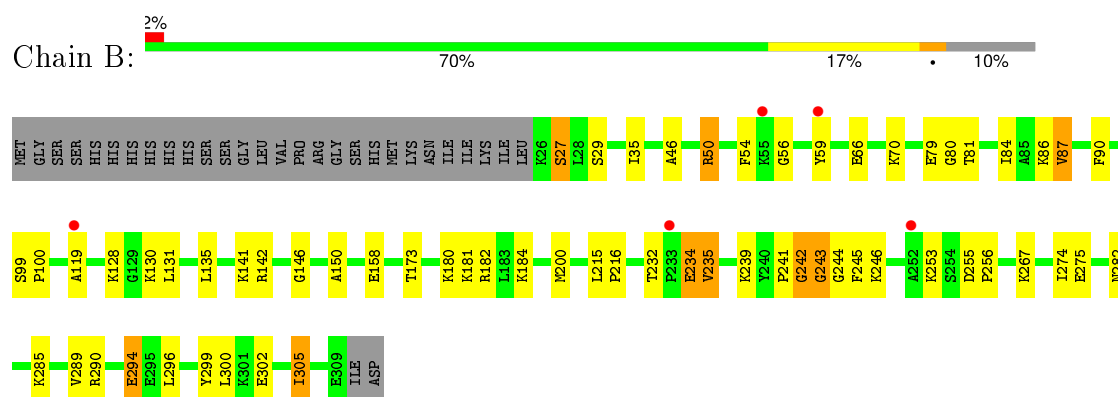
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

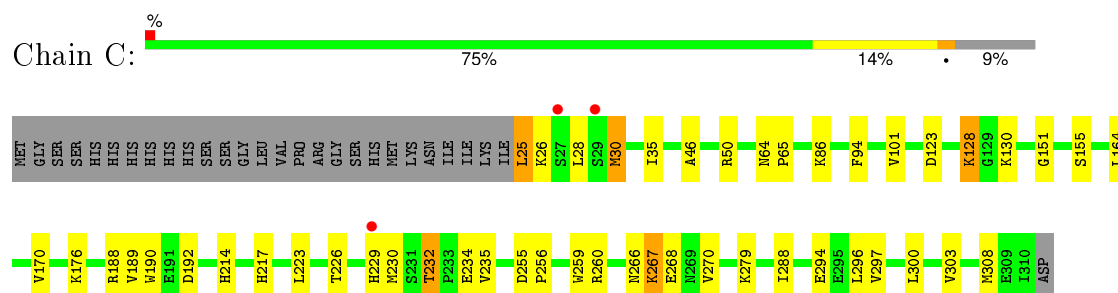
- Molecule 1: Prephenate dehydrogenase



- Molecule 1: Prephenate dehydrogenase

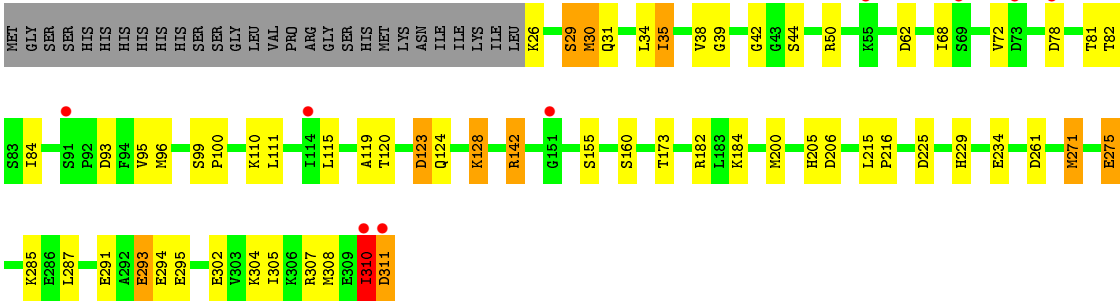


- Molecule 1: Prephenate dehydrogenase



- Molecule 1: Prephenate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.06 Å 92.36 Å 163.83 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.24 Å)	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 (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58166 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HPP, NAD, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.96	1/2303 (0.0%)	0.88	2/3098 (0.1%)
1	B	0.97	1/2287 (0.0%)	0.89	1/3076 (0.0%)
1	C	1.03	1/2303 (0.0%)	0.88	0/3098
1	D	0.91	1/2303 (0.0%)	0.86	4/3098 (0.1%)
All	All	0.97	4/9196 (0.0%)	0.88	7/12370 (0.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLU	CB-CG	5.69	1.62	1.52
1	B	275	GLU	CG-CD	5.68	1.60	1.51
1	C	268	GLU	CG-CD	5.58	1.60	1.51
1	D	311	ASP	N-CA	5.44	1.57	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	290	ARG	NE-CZ-NH2	-5.67	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	30	MET	N-CA-C	5.47	125.76	111.00
1	A	192	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	261	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	261	ASP	CB-CG-OD2	-5.04	113.76	118.30

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	46	0
1	B	2244	0	2296	41	0
1	C	2260	0	2318	48	0
1	D	2260	0	2311	53	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	173	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 9.

All (173) 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:D:96:MET:HE2	1:D:124:GLN:HG3	1.26	1.14
1:B:50:ARG:HH11	1:B:50:ARG:HG3	1.06	1.14
1:C:232:THR:HG23	1:C:234:GLU:H	1.23	1.03
1:A:276:GLY:HA3	1:C:230:MET:HE3	1.40	1.00
1:A:276:GLY:HA3	1:C:230:MET:HE2	1.50	0.91
1:B:50:ARG:NH1	1:B:50:ARG:HG3	1.77	0.90
1:D:307:ARG:HH12	1:D:311:ASP:C	1.74	0.90
1:D:96:MET:CE	1:D:124:GLN:HG3	2.02	0.89
1:B:294:GLU:CD	1:B:294:GLU:H	1.75	0.89
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
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:96:MET:HE2	1:D:124:GLN:CG	2.13	0.77
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:C:35:ILE:CD1	1:C:46:ALA:HB2	2.15	0.76
1:C:214:HIS:HD2	1:C:266:ASN:HD22	1.35	0.73
1:A:276:GLY:CA	1:C:230:MET:CE	2.60	0.72
1:D:307:ARG:NH1	1:D:311:ASP:C	2.43	0.71
1:D:99:SER:HB2	1:D:100:PRO:CD	2.22	0.70
1:B:35:ILE:HD13	1:B:46:ALA:HB2	1.74	0.69
1:D:96:MET:CE	1:D:123:ASP:C	2.61	0.69
1:D:96:MET:CE	1:D:124:GLN:CG	2.68	0.69
1:C:294:GLU:H	1:C:294:GLU:CD	1.96	0.68
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:D:96:MET:HE3	1:D:123:ASP:CA	2.25	0.66
1:B:84:ILE:O	1:B:87:VAL:HG13	1.96	0.66
1:D:96:MET:HE3	1:D:123:ASP:C	2.16	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:C:35:ILE:HD13	1:C:46:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:CA	1:C:230:MET:HE2	2.28	0.63
1:A:271:MET:HE3	1:C:288:ILE:CG2	2.28	0.63
1:D:35:ILE:CD1	1:D:42:GLY:CA	2.78	0.61
1:D:96:MET:HE3	1:D:123:ASP:HA	1.83	0.60
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:A:246:LYS:HD3	1:A:246:LYS:C	2.23	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
1:D:304:LYS:O	1:D:308:MET:HG3	2.04	0.56
1:D:35:ILE:CD1	1:D:42:GLY:HA3	2.33	0.56
1:A:292:ALA:O	1:A:293:GLU:CB	2.53	0.56
1:A:153:GLU:HG2	1:A:153:GLU:O	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:305:ILE:O	1:A:309:GLU:HG3	2.06	0.56
1:A:27:SER:O	1:A:28:LEU:HD13	2.06	0.56
1:C:234:GLU:O	1:C:234:GLU:HG2	2.06	0.55
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: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:A:271:MET:HE3	1:C:288:ILE:HG22	1.91	0.52
1:D:35:ILE:HD13	1:D:42:GLY:CA	2.40	0.52
1:B:294:GLU:CD	1:B:294:GLU:N	2.52	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:D:96:MET:HE1	1:D:123:ASP:C	2.30	0.51
1:B:235:VAL:O	1:B:235:VAL:CG2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD13	1:A:245:PHE:CE1	2.46	0.51
1:D:38:VAL:O	1:D:38:VAL:HG23	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: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:D:96:MET:HE1	1:D:124:GLN:CG	2.41	0.49
1:B:79:GLU:CG	1:B:80:GLY:N	2.76	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:C:267:LYS:HB3	1:C:267:LYS:HE3	1.52	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:D:291:GLU:O	1:D:293:GLU:N	2.47	0.47
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:287:LEU:HD22	1:D:295:GLU:HB2	1.95	0.47
1:D:111:LEU:HB3	1:D:115:LEU:HD12	1.97	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:A:152:THR:OG1	1:A:154:LYS:HE3	2.14	0.47
1:D:123:ASP:OD2	1:D:128:LYS:NZ	2.41	0.47
1:C:128:LYS:HA	1:C:128:LYS:HE3	1.97	0.47
1:B:158:GLU:H	1:B:158:GLU:CD	2.18	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:D:96:MET:HE1	1:D:124:GLN:HG2	1.97	0.46
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:D:35:ILE:HD13	1:D:42:GLY:HA2	1.97	0.46
1:D:50:ARG:HA	1:D:50:ARG:HD3	1.73	0.46
1:D:142:ARG:HA	1:D:182:ARG:NE	2.31	0.46
1:C:30:MET:HE2	1:C:94:PHE:CG	2.51	0.46
1:B:119:ALA:O	1:B:142:ARG:HG2	2.16	0.46
1:A:152:THR:O	1:A:154:LYS:HG3	2.16	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:C:123:ASP:OD2	1:C:128:LYS:NZ	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:H	1:D:310:ILE:HD12	1.82	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: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:B:239:LYS:C	1:B:241:PRO:HD3	2.38	0.44
1:C:255:ASP:HA	1:C:256:PRO:HD3	1.80	0.44
1:D:120:THR:OG1	1:D:182:ARG:HG2	2.19	0.43
1:B:274:ILE:HG21	1:D:285:LYS:HD2	2.00	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:C:294:GLU:N	1:C:294:GLU:CD	2.69	0.43
1:B:241:PRO:O	1:B:242:GLY:C	2.57	0.43
1:B:54:PHE:CZ	1:B:56:GLY:HA3	2.54	0.43
1:D:128:LYS:HG3	1:D:205:HIS:CG	2.53	0.43
1:A:176:LYS:HG2	5:A:1417:HOH:O	2.18	0.43
1:C:30:MET:HE1	1:C:189:VAL:HG21	2.01	0.43
1:B:246:LYS:HE3	1:B:246:LYS:HB3	1.72	0.43
1:D:310:ILE:N	1:D:310:ILE:HD12	2.34	0.43
1:C:214:HIS:CE1	5:C:1005:HOH:O	2.68	0.43
1:D:96:MET:CE	1:D:124:GLN:N	2.83	0.42
1:C:217:HIS:CD2	1:C:259:TRP:CZ2	3.07	0.42
1:D:128:LYS:HA	1:D:128:LYS:HE3	2.01	0.42
1:D:39:GLY:HA3	2:D:312:NAD:O5B	2.19	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:A:152:THR:O	1:A:154:LYS:N	2.52	0.42
1:D:310:ILE:O	1:D:310:ILE:CG2	2.56	0.42
1:C:30:MET:CE	1:C:189:VAL:HG21	2.50	0.41
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:C:234:GLU:O	1:C:235:VAL:HB	2.20	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: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:170:VAL:HG11	1:C:190:TRP:CG	2.56	0.41
1:A:185:LEU:O	1:A:189:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:C	1:B:29:SER:H	2.23	0.41
1:B:66:GLU:O	1:B:70:LYS:HG3	2.21	0.41
1:C:266:ASN:O	1:C:270:VAL:HG23	2.21	0.41
1:A:28:LEU:HB3	1:A:29:SER:H	1.76	0.41
1:B:150:ALA:O	2:B:312:NAD:H4N	2.21	0.40
1:B:244:GLY:O	1:B:245:PHE:C	2.59	0.40
1:D:302:GLU:HA	1:D:305:ILE:HG12	2.04	0.40
1:D:30:MET:HA	1:D:93:ASP:OD2	2.22	0.40
1:B:296:LEU:O	1:B:300:LEU:HG	2.22	0.40
1:A:213:SER:C	1:A:216:PRO:HD2	2.41	0.40
1:C:155:SER:OG	1:C:255:ASP:HB2	2.20	0.40
1:C:50:ARG:HA	1:C:50:ARG:HD3	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/314 (90%)	272 (96%)	10 (4%)	2 (1%)	26	26
1	B	282/314 (90%)	265 (94%)	16 (6%)	1 (0%)	39	43
1	C	284/314 (90%)	270 (95%)	14 (5%)	0	100	100
1	D	284/314 (90%)	269 (95%)	14 (5%)	1 (0%)	39	43
All	All	1134/1256 (90%)	1076 (95%)	54 (5%)	4 (0%)	39	43

All (4) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	225 (90%)	25 (10%)	9	7
1	B	248/275 (90%)	235 (95%)	13 (5%)	29	31
1	C	250/275 (91%)	237 (95%)	13 (5%)	29	31
1	D	250/275 (91%)	234 (94%)	16 (6%)	22	21
All	All	998/1100 (91%)	931 (93%)	67 (7%)	20	19

All (67) 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	123	ASP
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	246	LYS
1	A	250	ARG
1	A	254	SER
1	A	257	ILE
1	A	265	GLU

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Mol	Chain	Res	Type
1	A	285	LYS
1	A	297	VAL
1	A	298	GLU
1	A	301	LYS
1	A	310	ILE
1	B	27	SER
1	B	50	ARG
1	B	87	VAL
1	B	130	LYS
1	B	141	LYS
1	B	181	LYS
1	B	234	GLU
1	B	235	VAL
1	B	267	LYS
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	223	LEU
1	C	229	HIS
1	C	232	THR
1	C	267	LYS
1	C	279	LYS
1	C	296	LEU
1	D	26	LYS
1	D	29	SER
1	D	31	GLN
1	D	35	ILE
1	D	72	VAL
1	D	78	ASP
1	D	123	ASP
1	D	128	LYS
1	D	155	SER
1	D	184	LYS
1	D	234	GLU

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Mol	Chain	Res	Type
1	D	271	MET
1	D	275	GLU
1	D	293	GLU
1	D	294	GLU
1	D	310	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
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 carbohydrates 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	$\# Z  > 2$
2	NAD	A	312	-	38,48,48	1.89	5 (13%)	47,73,73	2.46	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	312	-	38,48,48	1.69	5 (13%)	47,73,73	2.34	11 (23%)
4	HPP	B	313	-	9,12,12	1.17	0	12,15,15	1.57	3 (25%)
2	NAD	C	312	-	38,48,48	1.85	4 (10%)	47,73,73	2.82	12 (25%)
4	HPP	C	313	-	9,12,12	1.79	1 (11%)	12,15,15	0.76	0
2	NAD	D	312	-	38,48,48	1.79	3 (7%)	47,73,73	2.33	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	312	-	-	0/22/62/62	0/5/5/5
2	NAD	B	312	-	-	0/22/62/62	0/5/5/5
4	HPP	B	313	-	-	0/3/5/5	0/1/1/1
2	NAD	C	312	-	-	0/22/62/62	0/5/5/5
4	HPP	C	313	-	-	0/3/5/5	0/1/1/1
2	NAD	D	312	-	-	0/22/62/62	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	312	NAD	PA-O2A	-2.31	1.45	1.54
2	B	312	NAD	PA-O2A	-2.18	1.45	1.54
2	C	312	NAD	O4B-C4B	-2.02	1.40	1.45
2	B	312	NAD	C7N-N7N	-2.01	1.28	1.33
2	A	312	NAD	O4B-C1B	2.17	1.44	1.41
2	A	312	NAD	C2A-N1A	2.45	1.38	1.33
2	C	312	NAD	C2A-N3A	2.50	1.36	1.32
2	D	312	NAD	C2A-N1A	2.64	1.38	1.33
2	B	312	NAD	C2A-N1A	2.86	1.39	1.33
4	C	313	HPP	C3-C2	3.61	1.45	1.38
2	A	312	NAD	C2N-C3N	3.70	1.44	1.39
2	D	312	NAD	C2A-N3A	3.76	1.38	1.32
2	A	312	NAD	C2A-N3A	3.98	1.39	1.32
2	B	312	NAD	C2A-N3A	5.00	1.41	1.32
2	B	312	NAD	O7N-C7N	5.95	1.36	1.24
2	A	312	NAD	O7N-C7N	8.07	1.41	1.24
2	D	312	NAD	O7N-C7N	8.34	1.42	1.24
2	C	312	NAD	O7N-C7N	8.75	1.42	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	312	NAD	N3A-C2A-N1A	-14.41	117.86	128.89
2	A	312	NAD	N3A-C2A-N1A	-13.93	118.23	128.89
2	D	312	NAD	N3A-C2A-N1A	-12.36	119.43	128.89
2	B	312	NAD	N3A-C2A-N1A	-11.61	120.00	128.89
2	C	312	NAD	PN-O3-PA	-5.75	116.58	132.73
2	B	312	NAD	C1B-N9A-C4A	-5.15	119.18	126.94
2	D	312	NAD	PN-O3-PA	-4.12	121.17	132.73
2	B	312	NAD	PN-O3-PA	-3.70	122.33	132.73
2	A	312	NAD	O5B-C5B-C4B	-3.60	95.86	109.12
2	C	312	NAD	O7N-C7N-N7N	-3.51	117.65	122.59
2	C	312	NAD	C1B-N9A-C4A	-3.51	121.65	126.94
2	B	312	NAD	O7N-C7N-N7N	-3.41	117.80	122.59
2	B	312	NAD	O4D-C1D-N1N	-3.39	104.41	108.13
4	B	313	HPP	C7-C8-C9	-3.37	106.56	112.75
2	D	312	NAD	C1B-N9A-C4A	-3.24	122.06	126.94
2	D	312	NAD	O5D-PN-O1N	-2.67	99.26	109.62
2	A	312	NAD	O2A-PA-O5B	-2.53	95.71	108.46
2	B	312	NAD	C3N-C2N-N1N	-2.49	117.49	120.36
4	B	313	HPP	C6-C5-C4	-2.43	117.06	119.87
2	B	312	NAD	C4B-O4B-C1B	-2.39	107.09	109.72
2	B	312	NAD	O3-PN-O5D	-2.33	96.76	102.94
2	C	312	NAD	O3-PN-O5D	-2.20	97.10	102.94
2	A	312	NAD	O7N-C7N-C3N	-2.00	117.40	119.59
2	B	312	NAD	O2A-PA-O3	2.02	114.27	105.09
2	B	312	NAD	C2N-C3N-C4N	2.03	120.55	118.29
2	C	312	NAD	C2D-C3D-C4D	2.05	106.83	102.61
2	A	312	NAD	C2N-C3N-C4N	2.13	120.66	118.29
2	A	312	NAD	O4D-C1D-N1N	2.19	110.54	108.13
4	B	313	HPP	C2-C3-C4	2.23	122.44	119.87
2	C	312	NAD	O2N-PN-O1N	2.30	124.98	112.53
2	C	312	NAD	C6N-C5N-C4N	2.33	122.96	119.44
2	B	312	NAD	O7N-C7N-C3N	2.37	122.17	119.59
2	A	312	NAD	O4B-C1B-N9A	2.41	113.14	108.10
2	A	312	NAD	O2N-PN-O1N	2.68	127.05	112.53
2	C	312	NAD	C2A-N1A-C6A	2.90	123.95	118.77
2	C	312	NAD	O3-PA-O5B	3.06	111.06	102.94
2	C	312	NAD	O2A-PA-O3	3.18	119.53	105.09
2	D	312	NAD	O4D-C1D-N1N	3.32	111.78	108.13
2	D	312	NAD	O3-PA-O5B	3.38	111.91	102.94
2	A	312	NAD	O2A-PA-O3	4.00	123.25	105.09
2	C	312	NAD	O7N-C7N-C3N	4.78	124.80	119.59

There are no chirality outliers.

There are no torsion outliers.

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	286/314 (91%)	0.01	6 (2%) 67 71	43, 58, 73, 86	0
1	B	284/314 (90%)	0.07	5 (1%) 71 75	43, 55, 67, 87	0
1	C	286/314 (91%)	-0.05	3 (1%) 84 85	47, 54, 74, 111	0
1	D	286/314 (91%)	0.12	9 (3%) 52 57	47, 61, 80, 91	0
All	All	1142/1256 (90%)	0.04	23 (2%) 68 72	43, 57, 76, 111	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	LYS	4.4
1	D	151	GLY	3.6
1	D	311	ASP	3.4
1	D	55	LYS	3.3
1	B	233	PRO	3.2
1	C	27	SER	3.1
1	A	159	TYR	2.9
1	A	152	THR	2.8
1	C	29	SER	2.6
1	D	91	SER	2.5
1	D	114	ILE	2.5
1	A	166	GLU	2.4
1	D	73	ASP	2.4
1	C	229	HIS	2.3
1	D	310	ILE	2.3
1	B	252	ALA	2.2
1	A	31	GLN	2.2
1	A	252	ALA	2.2
1	B	59	TYR	2.0
1	D	69	SER	2.0
1	A	76	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	78	ASP	2.0
1	B	119	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	313	1/1	0.99	0.17	1.25	42,42,42,42	0
2	NAD	D	312	44/44	0.94	0.15	0.21	51,62,70,71	0
2	NAD	A	312	44/44	0.95	0.15	-0.02	38,48,57,59	0
3	CL	B	314	1/1	0.99	0.10	-0.65	43,43,43,43	0
4	HPP	B	313	12/12	0.98	0.11	-1.44	28,30,33,35	0
2	NAD	C	312	44/44	0.98	0.08	-2.03	28,36,42,47	0
4	HPP	C	313	12/12	0.97	0.10	-2.42	29,33,36,37	0
2	NAD	B	312	44/44	0.98	0.07	-2.47	28,37,46,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.