



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

PDB ID : 3DHY  
Title : Crystal Structures of Mycobacterium tuberculosis S-Adenosyl-L-Homocysteine Hydrolase in Ternary Complex with Substrate and Inhibitors  
Authors : Shetty, N.D.; Ioerger, T.R.; Gokulan, K.; Reddy, M.C.M.; Owen, J.L.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2008-06-19  
Resolution : 2.00 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

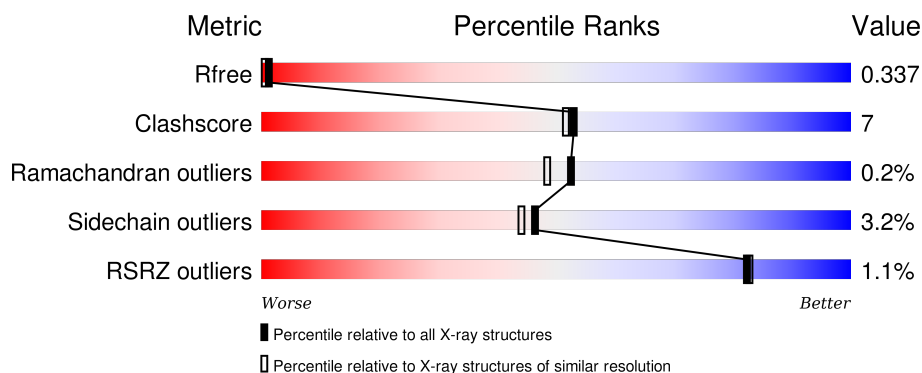
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 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	495	<div> <div>2%</div> <div>80%18%</div> <div>•</div> </div>
1	B	495	<div> <div>%</div> <div>86%12%</div> <div>•</div> </div>
1	C	495	<div> <div>%</div> <div>81%15%</div> <div>••</div> </div>
1	D	495	<div> <div>%</div> <div>80%17%</div> <div>••</div> </div>

## 2 Entry composition [i](#)

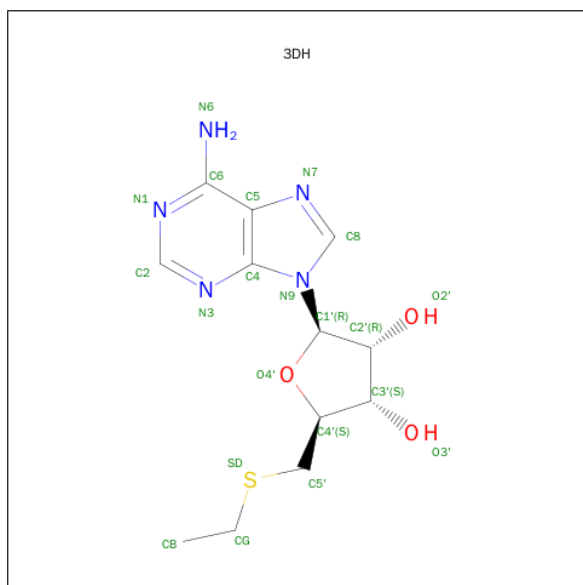
There are 4 unique types of molecules in this entry. The entry contains 15608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3754	2367	644	726	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			

- Molecule 2 is 5'-S-ETHYL-5'-THIOADENOSINE (three-letter code: 3DH) (formula:  $C_{12}H_{17}N_5O_3S$ ).



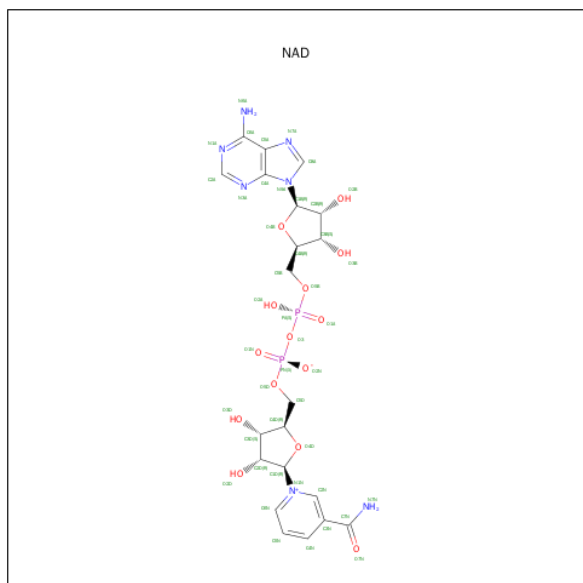
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	12	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	12	5	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			21	12	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	12	5	3	1		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	90	Total	O	0	0
			90	90		
4	C	91	Total	O	0	0
			91	91		

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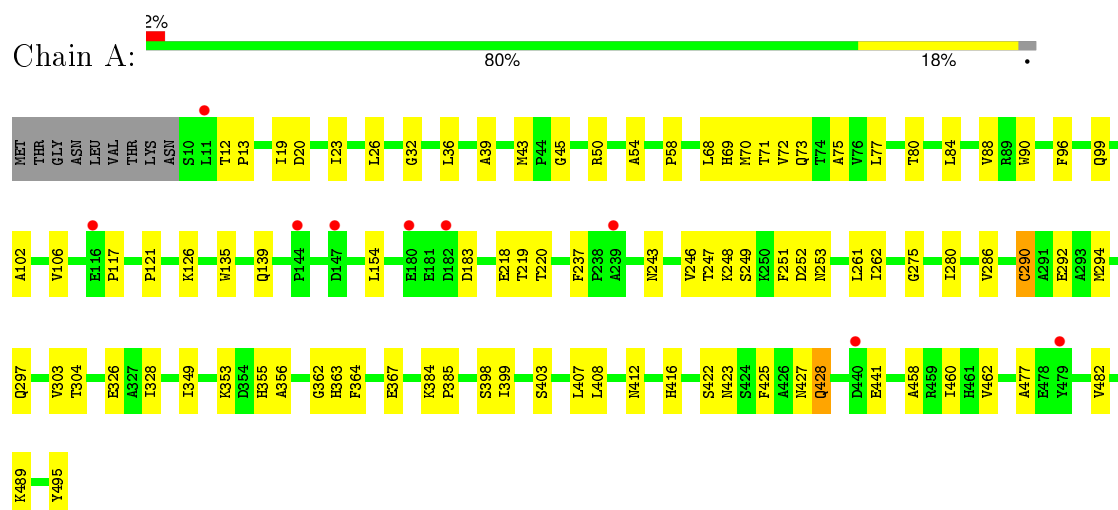
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	97	Total	O	0	0
			97	97		

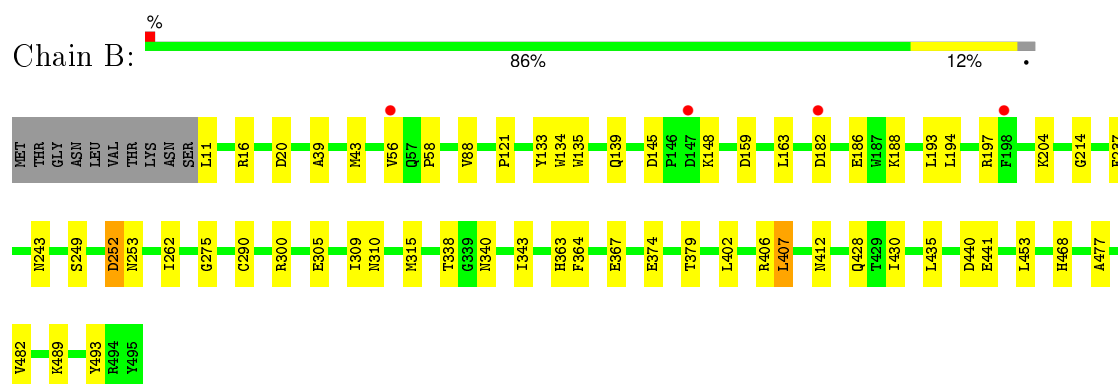
### 3 Residue-property plots [i](#)

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.

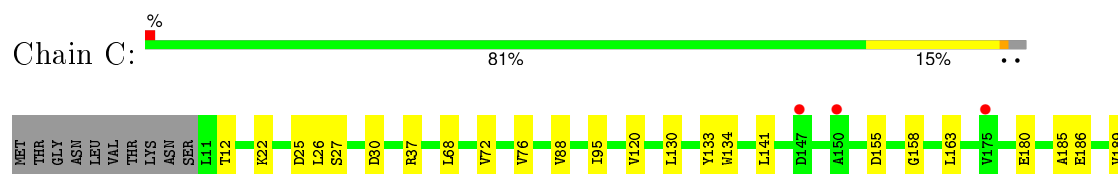
#### • Molecule 1: Adenosylhomocysteinase

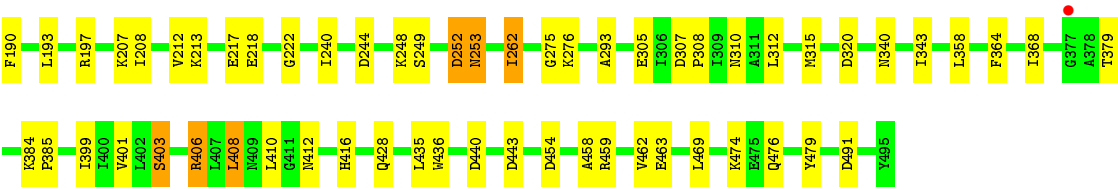


#### • Molecule 1: Adenosylhomocysteinase

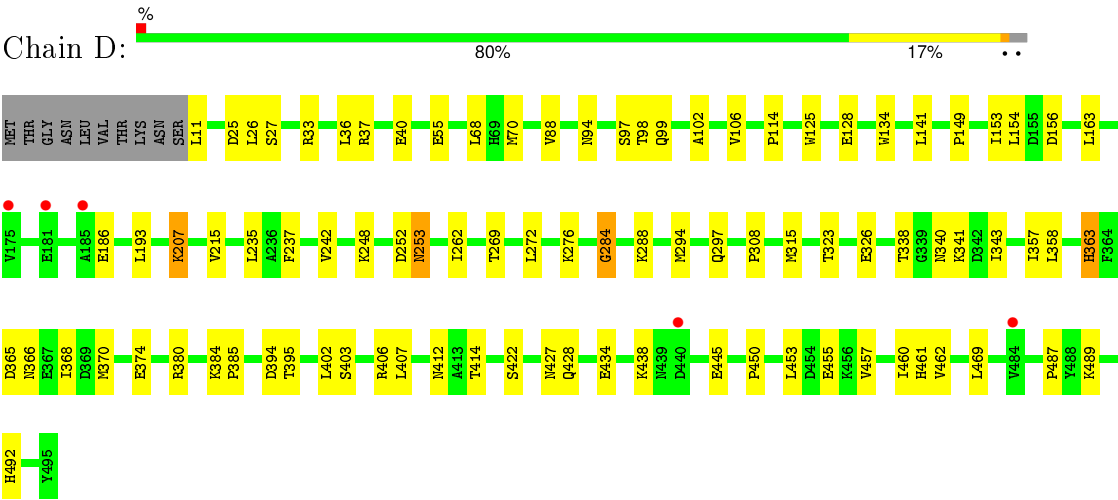


#### • Molecule 1: Adenosylhomocysteinase





● Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.20Å 111.69Å 100.13Å 90.00° 96.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 47.97 – 1.19	Depositor EDS
% Data completeness (in resolution range)	82.5 (30.00-2.00) 58.8 (47.97-1.19)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 1.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.260 , 0.340 0.260 , 0.337	Depositor DCC
$R_{free}$ test set	5714 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 384212 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.49% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DH, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	1/3830 (0.0%)	0.70	0/5194
1	B	0.67	2/3824 (0.1%)	0.75	0/5186
1	C	0.67	1/3824 (0.0%)	0.77	1/5186 (0.0%)
1	D	0.68	0/3824	0.76	1/5186 (0.0%)
All	All	0.67	4/15302 (0.0%)	0.75	2/20752 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	LYS	CD-CE	9.13	1.74	1.51
1	B	305	GLU	CG-CD	-6.25	1.42	1.51
1	A	290	CYS	CB-SG	-6.04	1.72	1.82
1	B	290	CYS	CB-SG	-5.15	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	GLY	N-CA-C	-5.71	98.83	113.10
1	C	26	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3754	0	3698	59	0
1	B	3748	0	3693	35	0
1	C	3748	0	3693	54	0
1	D	3748	0	3693	63	0
2	A	21	0	17	2	0
2	B	21	0	17	1	0
2	C	21	0	17	2	0
2	D	21	0	17	2	0
3	A	44	0	26	6	0
3	B	44	0	26	1	0
3	C	44	0	26	3	0
3	D	44	0	26	1	0
4	A	72	0	0	0	0
4	B	90	0	0	0	0
4	C	91	0	0	1	0
4	D	97	0	0	0	0
All	All	15608	0	14949	200	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 7.

All (200) 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:D:248:LYS:HZ3	1:D:253:ASN:HD21	1.23	0.86
1:D:248:LYS:NZ	1:D:253:ASN:HD21	1.73	0.86
1:C:218:GLU:HB2	1:C:428:GLN:HE21	1.42	0.85
1:C:248:LYS:NZ	1:C:253:ASN:HD21	1.74	0.84
1:C:248:LYS:HZ2	1:C:253:ASN:HD21	1.22	0.83
1:C:479:TYR:OH	1:D:363:HIS:HE1	1.60	0.82
1:B:338:THR:HG21	1:B:343:ILE:HD12	1.62	0.82
1:D:253:ASN:H	1:D:253:ASN:HD22	1.25	0.82
1:B:135:TRP:O	1:B:139:GLN:HG2	1.89	0.72
1:A:403:SER:OG	1:A:412:ASN:ND2	2.23	0.72
1:A:423:ASN:O	1:A:427:ASN:ND2	2.24	0.70
1:C:403:SER:OG	1:C:412:ASN:ND2	2.25	0.70
2:A:500:3DH:H3'	3:A:550:NAD:C4N	2.21	0.69
1:C:134:TRP:HE1	1:C:186:GLU:HG2	1.59	0.68
1:D:253:ASN:N	1:D:253:ASN:HD22	1.92	0.67
2:C:500:3DH:H3'	3:C:550:NAD:C4N	2.25	0.67
1:C:252:ASP:C	1:C:252:ASP:OD1	2.34	0.66
1:D:248:LYS:HZ3	1:D:253:ASN:ND2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:O	1:A:121:PRO:HB3	1.96	0.65
2:B:500:3DH:H3'	3:B:550:NAD:C4N	2.27	0.65
1:C:406:ARG:HG3	1:C:406:ARG:HH21	1.62	0.64
1:A:58:PRO:HD2	1:A:84:LEU:HB3	1.79	0.64
1:A:135:TRP:O	1:A:139:GLN:HG2	1.98	0.64
1:C:248:LYS:NZ	1:C:253:ASN:ND2	2.46	0.64
1:B:489:LYS:HD2	1:B:493:TYR:CD2	2.32	0.63
1:D:323:THR:OG1	1:D:326:GLU:HG2	1.98	0.63
1:A:19:ILE:HD12	1:A:117:PRO:HB2	1.81	0.62
1:D:134:TRP:HB3	1:D:193:LEU:HD13	1.80	0.62
1:A:70:MET:HE1	1:A:90:TRP:CD1	2.36	0.61
1:C:305:GLU:OE2	3:C:550:NAD:O2B	2.11	0.61
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.82	0.61
1:B:300:ARG:HD2	1:C:320:ASP:OD1	2.00	0.60
1:D:422:SER:HB3	1:D:461:HIS:NE2	2.16	0.60
1:A:262:ILE:HD13	1:A:294:MET:CE	2.31	0.60
1:A:77:LEU:HD13	1:A:425:PHE:HB3	1.83	0.60
1:B:249:SER:O	1:B:253:ASN:HB2	2.01	0.60
1:B:275:GLY:HA2	1:C:315:MET:O	2.02	0.59
1:B:440:ASP:OD2	1:B:441:GLU:HG3	2.01	0.59
1:A:247:THR:HA	1:A:251:PHE:HD2	1.68	0.59
1:B:197:ARG:HD2	1:B:204:LYS:HD2	1.83	0.58
1:C:310:ASN:HD21	1:D:489:LYS:HE2	1.68	0.58
1:B:363:HIS:CD2	1:B:364:PHE:CD2	2.92	0.58
1:C:406:ARG:HH21	1:C:406:ARG:CG	2.16	0.58
1:A:349:ILE:HG23	1:A:399:ILE:HD13	1.84	0.58
1:D:94:ASN:HB3	1:D:97:SER:OG	2.04	0.58
1:C:459:ARG:O	1:C:463:GLU:HG2	2.04	0.58
1:C:479:TYR:OH	1:D:363:HIS:CE1	2.49	0.58
1:D:402:LEU:HB3	1:D:412:ASN:ND2	2.19	0.58
1:A:353:LYS:HG3	1:A:356:ALA:HB2	1.85	0.57
1:A:23:ILE:HD11	1:A:26:LEU:HD13	1.86	0.57
1:C:253:ASN:H	1:C:253:ASN:HD22	1.52	0.57
1:D:235:LEU:HD23	1:D:445:GLU:HA	1.85	0.57
1:A:218:GLU:O	1:A:248:LYS:HE3	2.04	0.57
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.87	0.57
1:D:36:LEU:O	1:D:40:GLU:HG3	2.05	0.57
1:C:340:ASN:HB3	1:C:343:ILE:HD11	1.87	0.57
1:D:363:HIS:O	1:D:363:HIS:CD2	2.58	0.57
1:D:102:ALA:O	1:D:106:VAL:HG23	2.05	0.56
1:D:363:HIS:NE2	1:D:366:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD23	1:B:193:LEU:C	2.26	0.56
1:D:33:ARG:O	1:D:37:ARG:HG3	2.06	0.56
1:B:56:VAL:HG12	1:B:58:PRO:HD3	1.88	0.56
1:A:326:GLU:OE2	1:B:468:HIS:ND1	2.35	0.55
1:B:477:ALA:HB1	1:B:482:VAL:O	2.07	0.55
1:A:304:THR:OG1	3:A:550:NAD:H2A	2.07	0.55
1:D:262:ILE:CD1	1:D:294:MET:HE2	2.37	0.55
1:D:68:LEU:HD12	1:D:154:LEU:CD2	2.36	0.55
1:A:102:ALA:O	1:A:106:VAL:HG23	2.07	0.55
1:A:262:ILE:CD1	1:A:294:MET:HE2	2.37	0.55
1:A:477:ALA:HB1	1:A:482:VAL:O	2.07	0.55
1:C:217:GLU:CD	1:C:222:GLY:HA3	2.28	0.54
1:A:363:HIS:CD2	1:A:364:PHE:HD2	2.25	0.54
1:C:185:ALA:O	1:C:189:VAL:HG23	2.07	0.54
1:C:240:ILE:HG13	1:C:435:LEU:HD11	1.89	0.54
1:C:130:LEU:HD22	1:C:186:GLU:HG3	1.89	0.54
1:B:315:MET:O	1:C:275:GLY:HA2	2.08	0.54
1:C:155:ASP:OD2	1:C:158:GLY:HA2	2.07	0.54
1:A:262:ILE:HD13	1:A:294:MET:HE2	1.90	0.54
1:B:262:ILE:HD12	1:D:297:GLN:NE2	2.22	0.54
1:B:214:GLY:HA3	1:B:435:LEU:HD13	1.88	0.54
2:C:500:3DH:H3'	3:C:550:NAD:C3N	2.37	0.54
1:C:249:SER:O	1:C:253:ASN:HB2	2.08	0.53
1:B:489:LYS:HD2	1:B:493:TYR:CE2	2.43	0.53
1:A:243:ASN:HA	1:A:248:LYS:HG2	1.91	0.53
1:A:407:LEU:HD22	3:A:550:NAD:N7N	2.23	0.53
1:A:407:LEU:CD2	3:A:550:NAD:N7N	2.72	0.53
1:C:218:GLU:O	1:C:248:LYS:HE3	2.10	0.52
1:D:272:LEU:O	1:D:276:LYS:HG3	2.10	0.52
1:D:402:LEU:HB3	1:D:412:ASN:HD21	1.74	0.52
1:C:276:LYS:NZ	4:C:610:HOH:O	2.42	0.52
1:A:275:GLY:HA2	1:D:315:MET:O	2.10	0.52
1:D:134:TRP:HE1	1:D:186:GLU:HG2	1.75	0.51
1:A:384:LYS:HB2	1:A:385:PRO:HD2	1.92	0.51
1:C:308:PRO:HB3	1:D:469:LEU:HD11	1.92	0.51
1:D:262:ILE:HD13	1:D:294:MET:CE	2.41	0.51
1:C:358:LEU:HG	1:C:368:ILE:HD13	1.93	0.51
1:A:384:LYS:HB2	1:A:385:PRO:CD	2.41	0.50
1:B:20:ASP:O	1:B:121:PRO:HB3	2.11	0.50
1:D:26:LEU:HB3	1:D:114:PRO:HB3	1.93	0.50
1:A:458:ALA:O	1:A:462:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:36:LEU:HD13	2.12	0.50
1:D:338:THR:HG21	1:D:343:ILE:HD12	1.93	0.50
1:C:399:ILE:HD12	1:C:401:VAL:HG23	1.94	0.50
1:D:99:GLN:NE2	1:D:414:THR:HB	2.27	0.49
1:A:246:VAL:HG21	1:A:495:TYR:CE1	2.46	0.49
1:D:68:LEU:HG	1:D:156:ASP:HB2	1.95	0.49
2:D:500:3DH:H3'	3:D:550:NAD:C4N	2.42	0.49
1:B:338:THR:HG21	1:B:343:ILE:CD1	2.38	0.49
1:B:39:ALA:O	1:B:43:MET:HG3	2.13	0.49
1:C:25:ASP:OD1	1:C:27:SER:OG	2.29	0.49
1:C:458:ALA:O	1:C:462:VAL:HG23	2.12	0.49
1:C:262:ILE:HG13	1:C:293:ALA:HB1	1.94	0.49
1:C:252:ASP:OD1	1:C:416:HIS:CE1	2.67	0.48
1:C:248:LYS:HZ3	1:C:253:ASN:ND2	2.12	0.47
1:B:340:ASN:O	1:B:367:GLU:HG2	2.15	0.47
1:D:253:ASN:N	1:D:253:ASN:ND2	2.61	0.47
1:B:163:LEU:HD12	1:B:194:LEU:HD21	1.97	0.47
1:B:133:TYR:OH	1:B:159:ASP:OD2	2.20	0.47
1:D:450:PRO:HG2	1:D:453:LEU:HD12	1.97	0.46
1:C:72:VAL:O	1:C:76:VAL:HG23	2.15	0.46
1:D:284:GLY:O	1:D:288:LYS:HG3	2.15	0.46
1:B:363:HIS:HD2	1:B:364:PHE:CD2	2.34	0.46
1:C:406:ARG:NH2	1:C:406:ARG:CG	2.78	0.46
1:C:134:TRP:HB3	1:C:193:LEU:HD13	1.98	0.46
1:B:145:ASP:OD2	1:B:148:LYS:HE3	2.16	0.46
1:C:218:GLU:HB2	1:C:428:GLN:NE2	2.20	0.46
1:A:71:THR:HG22	1:A:99:GLN:NE2	2.31	0.46
1:D:253:ASN:H	1:D:253:ASN:ND2	2.03	0.45
1:A:303:VAL:HG12	1:A:304:THR:N	2.32	0.45
1:D:153:ILE:HB	1:D:215:VAL:HG23	1.98	0.45
1:D:358:LEU:HG	1:D:368:ILE:HD13	1.99	0.45
1:C:208:ILE:O	1:C:212:VAL:HG23	2.16	0.45
1:D:125:TRP:O	1:D:128:GLU:HG3	2.17	0.45
1:B:363:HIS:CD2	1:B:364:PHE:HD2	2.34	0.45
1:A:68:LEU:HD12	1:A:154:LEU:HD22	1.97	0.45
1:D:406:ARG:O	1:D:407:LEU:C	2.55	0.45
1:A:407:LEU:HD11	2:A:500:3DH:SD	2.56	0.45
1:D:156:ASP:OD1	2:D:500:3DH:H4'	2.17	0.45
1:A:45:GLY:H	1:A:422:SER:HG	1.64	0.45
1:C:408:LEU:C	1:C:408:LEU:HD12	2.37	0.45
1:A:355:HIS:N	1:A:398:SER:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:H	1:A:73:GLN:CD	2.20	0.44
1:A:262:ILE:HD12	1:A:297:GLN:HG3	1.99	0.44
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.82	0.44
1:A:407:LEU:HD22	3:A:550:NAD:H72N	1.82	0.44
1:D:242:VAL:HG13	1:D:427:ASN:HB3	1.99	0.44
1:D:149:PRO:HG2	1:D:207:LYS:HD2	1.99	0.44
1:A:247:THR:HA	1:A:251:PHE:CD2	2.50	0.44
1:A:280:ILE:HD12	1:A:290:CYS:HB3	2.00	0.44
1:A:68:LEU:HD12	1:A:154:LEU:CD2	2.48	0.44
1:D:384:LYS:HB2	1:D:385:PRO:HD2	1.99	0.44
1:D:70:MET:HB3	1:D:98:THR:HG23	1.99	0.43
1:C:163:LEU:HD12	1:C:190:PHE:CE1	2.53	0.43
1:D:363:HIS:C	1:D:363:HIS:CD2	2.91	0.43
1:D:365:ASP:HB3	1:D:406:ARG:HG2	2.01	0.43
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.46	0.43
1:C:312:LEU:HB2	1:D:462:VAL:HG23	2.01	0.43
1:D:370:MET:O	1:D:374:GLU:HG3	2.19	0.43
1:A:96:PHE:O	1:A:126:LYS:NZ	2.51	0.43
1:A:428:GLN:HE21	1:A:428:GLN:CA	2.32	0.43
1:C:358:LEU:HG	1:C:368:ILE:CD1	2.49	0.43
1:C:141:LEU:HD12	1:C:163:LEU:HD23	2.00	0.43
1:C:95:ILE:HG22	1:C:133:TYR:HB2	2.01	0.43
1:B:430:ILE:CG2	1:B:453:LEU:HD13	2.49	0.43
1:A:72:VAL:O	1:A:75:ALA:HB3	2.19	0.42
1:D:141:LEU:HD12	1:D:163:LEU:HD23	2.01	0.42
1:C:213:LYS:HD3	1:C:436:TRP:CZ3	2.54	0.42
1:D:457:VAL:HA	1:D:460:ILE:HD12	2.01	0.42
1:D:207:LYS:HD3	1:D:207:LYS:O	2.20	0.42
1:C:476:GLN:HG2	1:D:340:ASN:HD21	1.83	0.42
1:A:362:GLY:HA3	1:A:367:GLU:OE2	2.20	0.42
1:C:307:ASP:OD1	1:C:308:PRO:HD2	2.19	0.42
1:A:45:GLY:HA2	1:A:460:ILE:HG21	2.01	0.42
1:A:286:VAL:HG21	3:A:550:NAD:C6N	2.49	0.41
1:A:246:VAL:HG11	1:B:309:ILE:HG21	2.02	0.41
1:A:70:MET:CE	1:A:90:TRP:CD1	3.01	0.41
1:B:243:ASN:O	1:B:249:SER:HB3	2.21	0.41
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.73	0.41
1:A:39:ALA:O	1:A:43:MET:HG3	2.20	0.41
1:C:305:GLU:HG3	1:C:307:ASP:H	1.85	0.41
1:D:269:THR:HG21	1:D:357:ILE:HD11	2.01	0.41
1:D:455:GLU:OE1	1:D:487:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:THR:OG1	1:B:343:ILE:HD11	2.20	0.41
1:D:25:ASP:OD1	1:D:27:SER:OG	2.27	0.41
1:A:80:THR:O	1:A:84:LEU:HG	2.21	0.41
1:B:134:TRP:HE1	1:B:186:GLU:CG	2.34	0.41
1:D:434:GLU:OE1	1:D:438:LYS:HD2	2.20	0.41
1:D:394:ASP:OD1	1:D:395:THR:N	2.53	0.41
1:A:489:LYS:HE2	1:B:310:ASN:HD21	1.86	0.41
1:C:469:LEU:HD21	1:D:308:PRO:HA	2.03	0.41
1:D:163:LEU:HD11	1:D:193:LEU:HD22	2.02	0.41
1:A:50:ARG:O	1:A:54:ALA:HB2	2.20	0.41
1:A:261:LEU:HD12	1:A:408:LEU:HD11	2.02	0.41
1:B:252:ASP:OD1	1:B:252:ASP:C	2.60	0.41
1:B:402:LEU:HB3	1:B:412:ASN:ND2	2.36	0.41
1:D:450:PRO:CG	1:D:453:LEU:HD12	2.51	0.40
1:D:403:SER:OG	1:D:412:ASN:ND2	2.54	0.40
1:B:406:ARG:O	1:B:407:LEU:C	2.60	0.40
1:A:249:SER:O	1:A:253:ASN:HB2	2.22	0.40
1:A:12:THR:HA	1:A:13:PRO:HD3	1.95	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	484/495 (98%)	462 (96%)	21 (4%)	1 (0%)	52	48
1	B	483/495 (98%)	463 (96%)	20 (4%)	0	100	100
1	C	483/495 (98%)	463 (96%)	18 (4%)	2 (0%)	39	33
1	D	483/495 (98%)	460 (95%)	22 (5%)	1 (0%)	52	48
All	All	1933/1980 (98%)	1848 (96%)	81 (4%)	4 (0%)	52	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	D	252	ASP
1	C	364	PHE
1	C	403	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	396/404 (98%)	387 (98%)	9 (2%)	58	60
1	B	395/404 (98%)	384 (97%)	11 (3%)	51	50
1	C	395/404 (98%)	374 (95%)	21 (5%)	28	22
1	D	395/404 (98%)	385 (98%)	10 (2%)	55	55
All	All	1581/1616 (98%)	1530 (97%)	51 (3%)	46	44

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	183	ASP
1	A	219	THR
1	A	220	THR
1	A	237	PHE
1	A	292	GLU
1	A	328	ILE
1	A	428	GLN
1	A	441	GLU
1	B	11	LEU
1	B	16	ARG
1	B	88	VAL
1	B	182	ASP
1	B	188	LYS
1	B	237	PHE
1	B	252	ASP
1	B	374	GLU
1	B	379	THR

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Mol	Chain	Res	Type
1	B	407	LEU
1	B	428	GLN
1	C	12	THR
1	C	22	LYS
1	C	30	ASP
1	C	37	ARG
1	C	68	LEU
1	C	88	VAL
1	C	120	VAL
1	C	180	GLU
1	C	197	ARG
1	C	252	ASP
1	C	253	ASN
1	C	262	ILE
1	C	379	THR
1	C	406	ARG
1	C	408	LEU
1	C	410	LEU
1	C	440	ASP
1	C	443	ASP
1	C	454	ASP
1	C	474	LYS
1	C	491	ASP
1	D	11	LEU
1	D	55	GLU
1	D	88	VAL
1	D	207	LYS
1	D	237	PHE
1	D	253	ASN
1	D	341	LYS
1	D	363	HIS
1	D	380	ARG
1	D	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	99	GLN
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS

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Mol	Chain	Res	Type
1	A	439	ASN
1	B	57	GLN
1	B	310	ASN
1	B	382	ASN
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	427	ASN
1	B	428	GLN
1	C	57	GLN
1	C	253	ASN
1	C	259	HIS
1	C	310	ASN
1	C	382	ASN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	439	ASN
1	D	94	ASN
1	D	253	ASN
1	D	259	HIS
1	D	310	ASN
1	D	340	ASN
1	D	363	HIS
1	D	382	ASN
1	D	412	ASN
1	D	416	HIS
1	D	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 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	3DH	A	500	-	18,23,23	2.18	2 (11%)	18,33,33	3.25	3 (16%)
3	NAD	A	550	-	38,48,48	1.33	4 (10%)	47,73,73	2.01	9 (19%)
2	3DH	B	500	-	18,23,23	0.84	1 (5%)	18,33,33	2.76	5 (27%)
3	NAD	B	550	-	38,48,48	1.26	4 (10%)	47,73,73	1.84	8 (17%)
2	3DH	C	500	-	18,23,23	1.59	2 (11%)	18,33,33	2.71	4 (22%)
3	NAD	C	550	-	38,48,48	1.44	4 (10%)	47,73,73	2.33	11 (23%)
2	3DH	D	500	-	18,23,23	0.85	1 (5%)	18,33,33	2.76	5 (27%)
3	NAD	D	550	-	38,48,48	1.35	5 (13%)	47,73,73	2.08	13 (27%)

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	3DH	A	500	-	-	0/4/24/24	0/3/3/3
3	NAD	A	550	-	-	0/22/62/62	0/5/5/5
2	3DH	B	500	-	-	0/4/24/24	0/3/3/3
3	NAD	B	550	-	-	0/22/62/62	0/5/5/5
2	3DH	C	500	-	-	0/4/24/24	0/3/3/3
3	NAD	C	550	-	-	0/22/62/62	0/5/5/5
2	3DH	D	500	-	-	0/4/24/24	0/3/3/3
3	NAD	D	550	-	-	0/22/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	550	NAD	C7N-N7N	-3.95	1.25	1.33
3	A	550	NAD	C7N-N7N	-3.54	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	550	NAD	C7N-N7N	-3.10	1.26	1.33
3	B	550	NAD	C7N-N7N	-2.52	1.27	1.33
3	C	550	NAD	O4B-C4B	-2.31	1.39	1.45
2	A	500	3DH	C5-N7	-2.13	1.32	1.39
3	A	550	NAD	PN-O1N	-2.02	1.43	1.51
2	B	500	3DH	O4'-C1'	2.16	1.43	1.41
2	D	500	3DH	O4'-C1'	2.21	1.44	1.41
3	D	550	NAD	C2A-N3A	2.27	1.36	1.32
2	C	500	3DH	C5'-C4'	2.35	1.59	1.52
3	B	550	NAD	O4D-C1D	2.44	1.44	1.41
3	D	550	NAD	C5A-C4A	2.47	1.46	1.40
3	D	550	NAD	O4D-C1D	2.51	1.44	1.41
3	C	550	NAD	C5A-C4A	2.74	1.46	1.40
3	A	550	NAD	C5A-C4A	3.33	1.48	1.40
3	B	550	NAD	C5A-C4A	3.41	1.48	1.40
3	B	550	NAD	O7N-C7N	4.11	1.32	1.24
3	A	550	NAD	O7N-C7N	4.36	1.33	1.24
3	D	550	NAD	O7N-C7N	4.40	1.33	1.24
2	C	500	3DH	O4'-C1'	5.17	1.47	1.41
3	C	550	NAD	O7N-C7N	5.23	1.35	1.24
2	A	500	3DH	O4'-C1'	8.18	1.51	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	3DH	N3-C2-N1	-10.13	121.14	128.89
3	C	550	NAD	N3A-C2A-N1A	-9.77	121.42	128.89
2	B	500	3DH	N3-C2-N1	-9.33	121.75	128.89
2	D	500	3DH	N3-C2-N1	-9.31	121.77	128.89
3	B	550	NAD	N3A-C2A-N1A	-8.79	122.16	128.89
2	C	500	3DH	N3-C2-N1	-8.76	122.19	128.89
2	A	500	3DH	C4'-O4'-C1'	-7.86	101.09	109.72
3	A	550	NAD	N3A-C2A-N1A	-7.66	123.03	128.89
3	D	550	NAD	N3A-C2A-N1A	-7.18	123.40	128.89
3	D	550	NAD	C1B-N9A-C4A	-5.56	118.56	126.94
2	D	500	3DH	C4'-O4'-C1'	-5.16	104.05	109.72
2	B	500	3DH	C4'-O4'-C1'	-5.12	104.09	109.72
3	C	550	NAD	O4D-C1D-N1N	-4.61	103.07	108.13
3	D	550	NAD	C4B-O4B-C1B	-4.61	104.66	109.72
2	C	500	3DH	C4-C5-N7	-4.46	105.38	109.48
3	C	550	NAD	C1B-N9A-C4A	-4.43	120.25	126.94
2	C	500	3DH	C4'-O4'-C1'	-4.39	104.90	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	O7N-C7N-N7N	-4.02	116.94	122.59
3	A	550	NAD	C2B-C1B-N9A	-3.73	108.60	114.29
3	D	550	NAD	C4A-C5A-N7A	-3.64	106.13	109.48
3	C	550	NAD	O7N-C7N-N7N	-3.57	117.57	122.59
3	B	550	NAD	C4A-C5A-N7A	-3.20	106.53	109.48
3	C	550	NAD	C4A-C5A-N7A	-3.19	106.54	109.48
2	D	500	3DH	C2'-C1'-N9	-3.16	109.46	114.29
2	B	500	3DH	C2'-C1'-N9	-3.16	109.47	114.29
3	A	550	NAD	C4A-C5A-N7A	-3.14	106.59	109.48
3	B	550	NAD	C1B-N9A-C4A	-3.00	122.41	126.94
3	B	550	NAD	C5N-C4N-C3N	-2.54	117.14	120.33
3	D	550	NAD	O3D-C3D-C4D	-2.52	103.48	111.05
3	D	550	NAD	O3-PN-O5D	-2.51	96.29	102.94
3	B	550	NAD	O3-PN-O5D	-2.39	96.59	102.94
3	D	550	NAD	O4D-C1D-N1N	-2.34	105.56	108.13
3	C	550	NAD	O3-PN-O5D	-2.28	96.88	102.94
2	C	500	3DH	O4'-C4'-C3'	-2.24	100.63	105.15
3	A	550	NAD	C5N-C4N-C3N	-2.18	117.60	120.33
2	B	500	3DH	C4-C5-N7	-2.12	107.53	109.48
2	B	500	3DH	C5'-C4'-C3'	-2.12	109.49	114.98
2	D	500	3DH	C4-C5-N7	-2.10	107.54	109.48
2	D	500	3DH	C5'-C4'-C3'	-2.10	109.55	114.98
3	D	550	NAD	PN-O3-PA	-2.07	126.90	132.73
3	D	550	NAD	O3B-C3B-C4B	-2.06	104.88	111.05
3	D	550	NAD	O7N-C7N-N7N	-2.04	119.73	122.59
3	D	550	NAD	O2N-PN-O1N	2.07	123.77	112.53
3	B	550	NAD	C2A-N1A-C6A	2.08	122.49	118.77
3	B	550	NAD	C4D-O4D-C1D	2.11	112.03	109.72
3	C	550	NAD	C4D-O4D-C1D	2.21	112.15	109.72
3	B	550	NAD	O2N-PN-O3	2.22	115.16	105.09
3	C	550	NAD	O2A-PA-O3	2.39	115.93	105.09
3	A	550	NAD	O2N-PN-O1N	2.43	125.72	112.53
3	D	550	NAD	O2A-PA-O3	2.65	117.11	105.09
3	C	550	NAD	C2B-C3B-C4B	2.77	108.31	102.61
2	A	500	3DH	O4'-C1'-N9	2.88	114.12	108.10
3	A	550	NAD	C3N-C2N-N1N	3.09	123.92	120.36
3	C	550	NAD	C2A-N1A-C6A	3.20	124.48	118.77
3	D	550	NAD	C3N-C7N-N7N	3.54	121.69	117.82
3	A	550	NAD	O4D-C1D-N1N	3.71	112.20	108.13
3	A	550	NAD	O7N-C7N-C3N	3.92	123.87	119.59
3	C	550	NAD	O7N-C7N-C3N	4.95	124.99	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	3DH	2	0
3	A	550	NAD	6	0
2	B	500	3DH	1	0
3	B	550	NAD	1	0
2	C	500	3DH	2	0
3	C	550	NAD	3	0
2	D	500	3DH	2	0
3	D	550	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	486/495 (98%)	0.07	9 (1%) 70 70	19, 36, 57, 88	0
1	B	485/495 (97%)	0.01	4 (0%) 87 88	15, 33, 51, 82	0
1	C	485/495 (97%)	-0.02	4 (0%) 87 88	18, 32, 52, 66	0
1	D	485/495 (97%)	-0.04	5 (1%) 84 84	16, 32, 49, 67	0
All	All	1941/1980 (98%)	0.00	22 (1%) 82 83	15, 33, 53, 88	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	ASP	5.0
1	B	182	ASP	4.8
1	A	144	PRO	3.7
1	C	150	ALA	3.3
1	D	175	VAL	3.3
1	A	180	GLU	3.0
1	A	239	ALA	2.6
1	A	182	ASP	2.6
1	B	147	ASP	2.6
1	C	377	GLY	2.6
1	B	198	PHE	2.5
1	D	185	ALA	2.4
1	A	11	LEU	2.4
1	A	479	TYR	2.4
1	C	175	VAL	2.4
1	A	116	GLU	2.3
1	A	440	ASP	2.3
1	D	440	ASP	2.3
1	D	181	GLU	2.2
1	A	147	ASP	2.2
1	B	56	VAL	2.2
1	D	484	VAL	2.2

## 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( $\text{\AA}^2$ )	Q<0.9
2	3DH	C	500	21/21	0.88	0.17	1.80	7,28,38,46	0
2	3DH	D	500	21/21	0.82	0.16	1.01	18,26,43,61	0
3	NAD	B	550	44/44	0.91	0.14	0.86	18,30,39,44	0
3	NAD	A	550	44/44	0.92	0.12	0.43	15,32,41,47	0
2	3DH	B	500	21/21	0.90	0.15	0.35	12,28,53,65	0
3	NAD	D	550	44/44	0.92	0.11	-0.05	9,25,33,36	0
3	NAD	C	550	44/44	0.92	0.12	-0.23	16,26,35,38	0
2	3DH	A	500	21/21	0.87	0.13	-0.37	21,27,38,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.