



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 AM GMT

PDB ID : 2ZJ1  
Title : Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and 3'-keto-aristeromycin  
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.  
Deposited on : 2008-02-29  
Resolution : 2.01 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

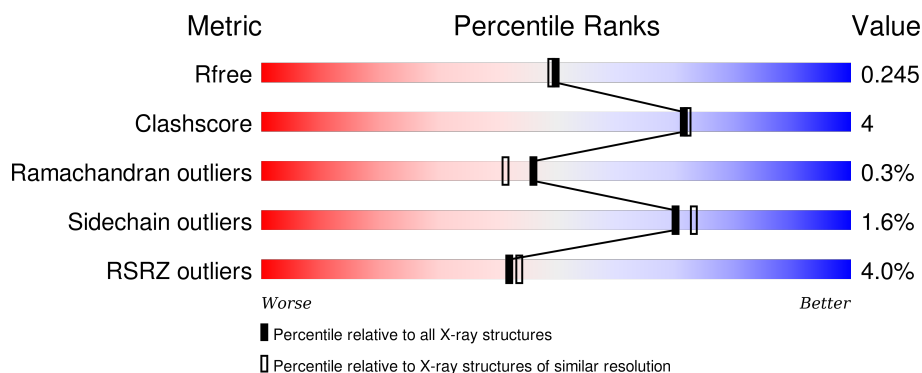
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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>3%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	495	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	495	<div> <div>8%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	D	495	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ARJ	A	500	X	-	-	-
2	ARJ	B	500	X	-	-	-
2	ARJ	C	500	X	-	-	-
2	ARJ	D	500	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16088 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.

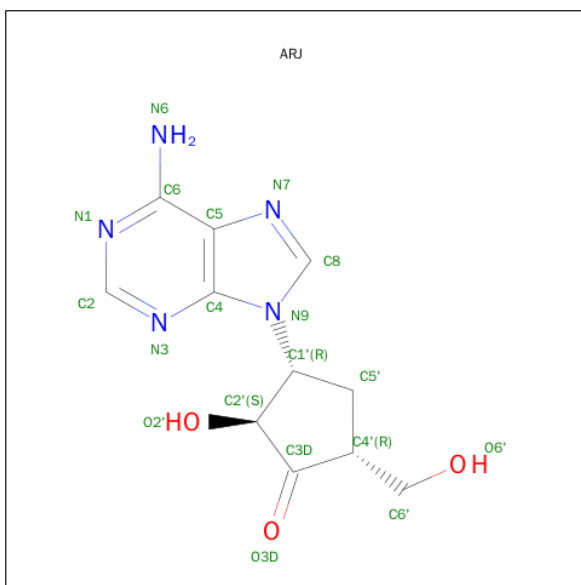
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	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			

There are 4 discrepancies between the modelled and reference sequences:

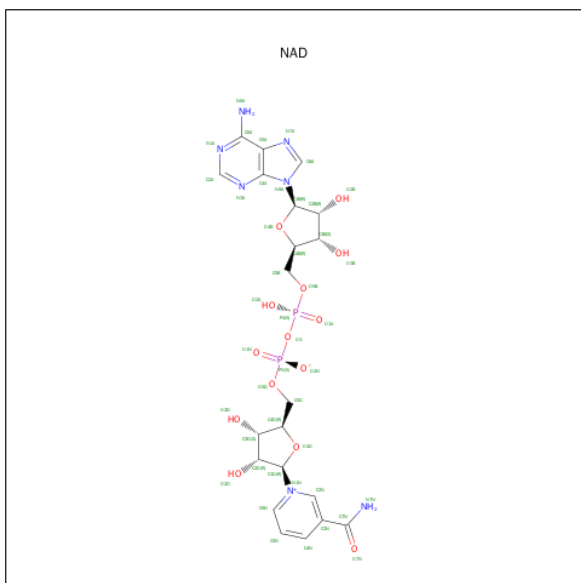
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P60176
B	1	MET	-	EXPRESSION TAG	UNP P60176
C	1	MET	-	EXPRESSION TAG	UNP P60176
D	1	MET	-	EXPRESSION TAG	UNP P60176

- Molecule 2 is (2S,3R,5R)-3-(6-AMINO-9H-PURIN-9-YL)-2-HYDROXY-5-(HYDROXYMETHYL)CYCLOPENTANONE (three-letter code: ARJ) (formula: C<sub>11</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 19	C 11	N 5	O 3	0	0
2	B	1	Total 19	C 11	N 5	O 3	0	0
2	C	1	Total 19	C 11	N 5	O 3	0	0
2	D	1	Total 19	C 11	N 5	O 3	0	0

- 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		

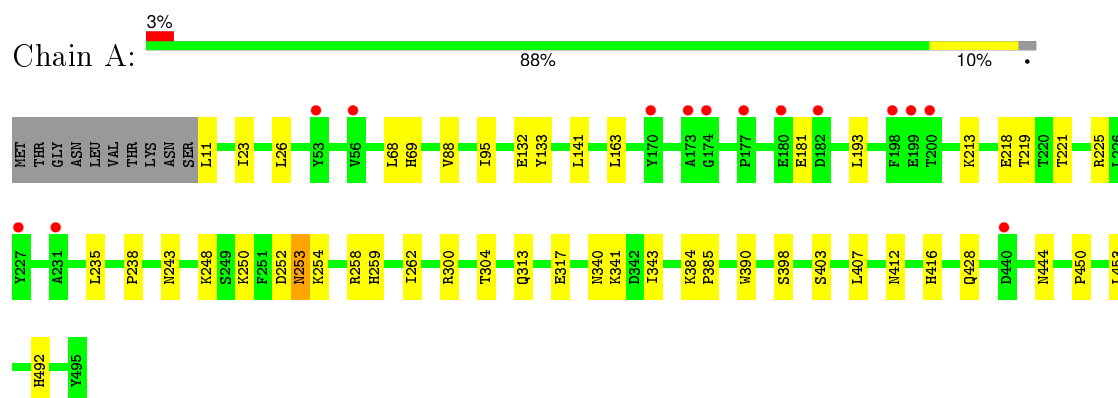
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	236	Total	O	0	0
			236	236		
4	C	193	Total	O	0	0
			193	193		
4	D	220	Total	O	0	0
			220	220		

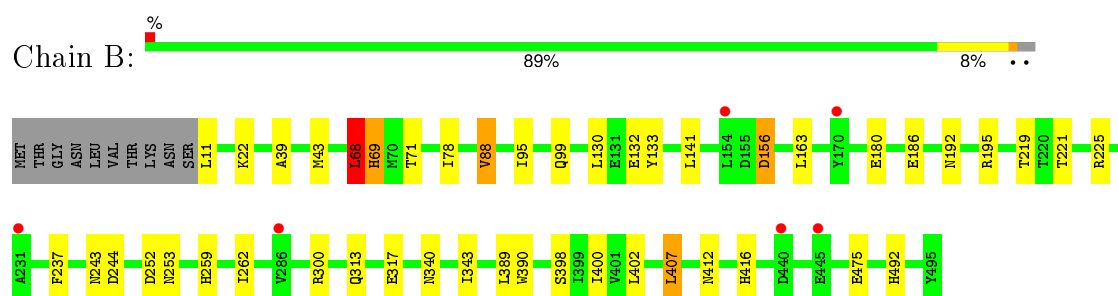
### 3 Residue-property plots [i](#)

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.

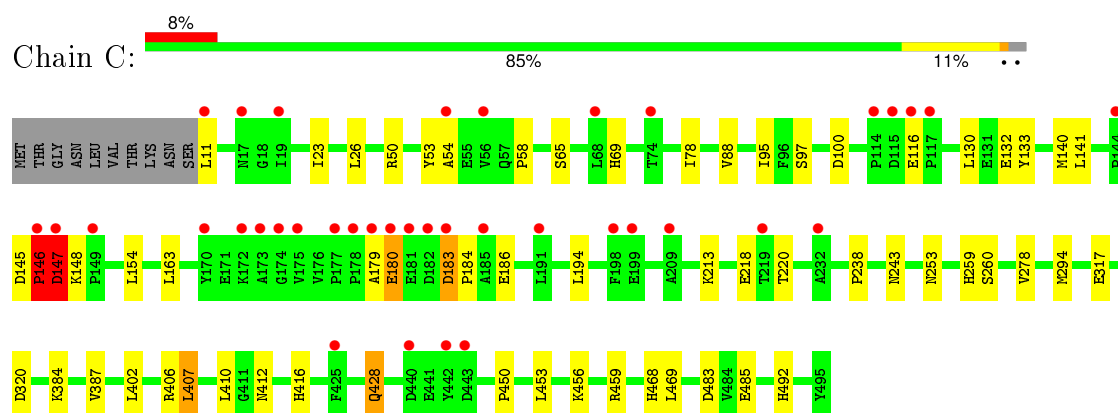
#### • Molecule 1: Adenosylhomocysteinase



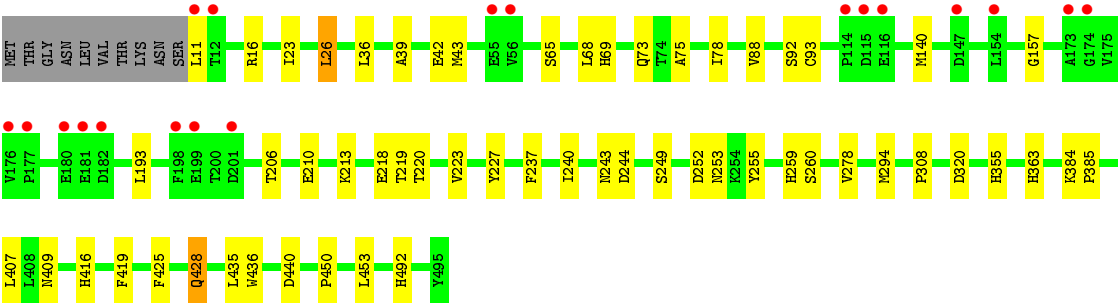
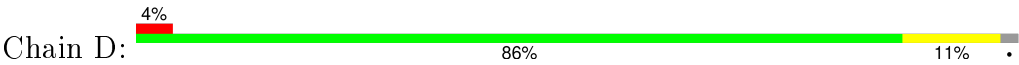
#### • Molecule 1: Adenosylhomocysteinase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	94.85Å 111.85Å 100.40Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	34.59 – 2.01 34.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.59-2.01) 98.9 (34.59-2.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.247 0.189 , 0.245	Depositor DCC
$R_{free}$ test set	6853 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136366 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: ARJ, 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	0.73	0/3824	0.73	1/5186 (0.0%)
1	B	0.77	0/3824	0.73	3/5186 (0.1%)
1	C	0.70	0/3824	0.71	4/5186 (0.1%)
1	D	0.74	0/3824	0.70	1/5186 (0.0%)
All	All	0.73	0/15296	0.72	9/20744 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	68	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	407	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	258	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	146	PRO	N-CA-C	5.34	126.00	112.10
1	B	156	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	146	PRO	C-N-CA	5.28	134.89	121.70
1	C	100	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	407	LEU	CA-CB-CG	5.11	127.05	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	3748	0	3693	24	0
1	B	3748	0	3693	30	0
1	C	3748	0	3693	48	0
1	D	3748	0	3693	36	0
2	A	19	0	10	0	0
2	B	19	0	10	2	0
2	C	19	0	10	0	0
2	D	19	0	10	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	195	0	0	2	0
4	B	236	0	0	3	0
4	C	193	0	0	8	0
4	D	220	0	0	3	0
All	All	16088	0	14916	131	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 4.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:ASP:HB3	1:C:485:GLU:OE2	1.49	1.10
1:C:145:ASP:OD2	1:C:147:ASP:HB3	1.54	1.06
1:B:130:LEU:HD22	1:B:186:GLU:HG3	1.61	0.81
1:C:146:PRO:HB2	1:C:147:ASP:HB2	1.63	0.81
1:B:68:LEU:HD22	1:B:156:ASP:HB2	1.69	0.74
1:C:146:PRO:CB	1:C:147:ASP:HB2	2.18	0.73
1:A:262:ILE:HD11	4:A:663:HOH:O	1.89	0.71
1:D:39:ALA:HB1	1:D:43:MET:CE	2.21	0.70
1:B:262:ILE:HD11	4:B:713:HOH:O	1.91	0.69
1:D:39:ALA:HB1	1:D:43:MET:HE3	1.71	0.69
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.42	0.66
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.43	0.65
1:C:146:PRO:CA	1:C:147:ASP:HB2	2.27	0.64
4:A:587:HOH:O	1:C:259:HIS:HE1	1.80	0.64
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.82	0.63
1:A:11:LEU:HD11	1:A:132:GLU:HG2	1.81	0.63
1:D:43:MET:HE2	1:D:73:GLN:HG3	1.81	0.63
1:C:260:SER:OG	1:C:416:HIS:HD2	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:SER:HB3	1:D:140:MET:SD	2.42	0.60
1:B:313:GLN:O	1:B:317:GLU:HG2	2.03	0.59
1:C:145:ASP:OD2	1:C:147:ASP:CB	2.43	0.57
1:B:11:LEU:HD11	1:B:132:GLU:HG2	1.85	0.57
1:A:259:HIS:HE1	4:C:727:HOH:O	1.86	0.57
1:B:141:LEU:HD12	1:B:163:LEU:HD23	1.86	0.56
4:B:718:HOH:O	1:D:259:HIS:HE1	1.88	0.56
1:D:243:ASN:HD21	1:D:253:ASN:HD21	1.52	0.56
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.59	0.56
1:A:252:ASP:OD1	1:A:416:HIS:HE1	1.89	0.55
1:B:11:LEU:HD22	1:B:22:LYS:HE2	1.89	0.55
1:C:450:PRO:HD2	1:C:453:LEU:HD12	1.88	0.55
1:C:78:ILE:HG23	1:C:88:VAL:HG21	1.88	0.54
1:B:141:LEU:CD1	1:B:163:LEU:HD23	2.37	0.54
1:B:95:ILE:HG22	1:B:133:TYR:HB2	1.89	0.54
1:C:468:HIS:HB3	4:C:744:HOH:O	2.07	0.54
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.90	0.54
1:C:492:HIS:HD2	4:C:783:HOH:O	1.91	0.54
1:D:492:HIS:HD2	4:D:948:HOH:O	1.91	0.54
1:A:218:GLU:O	1:A:248:LYS:HE3	2.08	0.53
1:C:218:GLU:HG2	1:C:428:GLN:HE22	1.74	0.53
1:C:213:LYS:O	1:C:238:PRO:HD2	2.08	0.53
1:B:390:TRP:O	1:B:398:SER:HA	2.09	0.53
1:C:278:VAL:HG11	1:C:294:MET:HG3	1.90	0.53
1:C:163:LEU:HD12	1:C:194:LEU:HD21	1.92	0.52
1:C:145:ASP:HB3	1:C:148:LYS:HB2	1.93	0.51
1:D:213:LYS:HG3	1:D:436:TRP:HZ3	1.75	0.51
1:A:492:HIS:HE1	1:B:244:ASP:OD2	1.94	0.50
1:A:141:LEU:HD12	1:A:163:LEU:HD23	1.92	0.50
1:D:355:HIS:HE1	4:D:892:HOH:O	1.95	0.50
1:C:183:ASP:HB2	1:C:184:PRO:CD	2.43	0.49
1:B:389:LEU:HD13	1:B:400:ILE:HG13	1.95	0.49
1:B:69:HIS:CD2	2:B:500:ARJ:H5A'	2.48	0.48
1:C:459:ARG:NH2	4:C:748:HOH:O	2.45	0.48
1:D:213:LYS:HG3	1:D:436:TRP:CZ3	2.47	0.48
1:B:252:ASP:OD1	1:B:416:HIS:HE1	1.97	0.48
1:D:78:ILE:HG23	1:D:88:VAL:HG21	1.95	0.48
1:C:163:LEU:CD1	1:C:194:LEU:HD21	2.43	0.48
1:D:260:SER:OG	1:D:416:HIS:HD2	1.97	0.48
1:B:402:LEU:HB3	1:B:412:ASN:HD21	1.79	0.48
1:C:218:GLU:CG	1:C:428:GLN:HE22	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:SER:HB3	1:C:140:MET:SD	2.54	0.47
1:C:53:TYR:CD1	1:C:58:PRO:HG3	2.49	0.47
1:B:300:ARG:HD2	1:C:320:ASP:OD1	2.14	0.47
1:C:95:ILE:HG22	1:C:133:TYR:HB2	1.96	0.47
1:D:260:SER:HB2	1:D:409:ASN:HB2	1.96	0.47
1:B:259:HIS:HE1	4:B:712:HOH:O	1.98	0.47
1:A:300:ARG:HD2	1:D:320:ASP:OD1	2.14	0.47
1:C:146:PRO:N	1:C:147:ASP:HB2	2.30	0.47
1:A:313:GLN:O	1:A:317:GLU:HG2	2.14	0.47
1:A:340:ASN:HB3	1:A:343:ILE:HD11	1.97	0.47
1:D:193:LEU:HD23	1:D:193:LEU:C	2.36	0.47
1:B:402:LEU:HB3	1:B:412:ASN:ND2	2.30	0.46
1:D:39:ALA:HB1	1:D:43:MET:HE1	1.96	0.46
1:A:221:THR:O	1:A:225:ARG:HG3	2.16	0.46
1:D:219:THR:O	1:D:223:VAL:HG23	2.16	0.46
1:B:252:ASP:OD1	1:B:416:HIS:CE1	2.69	0.46
1:C:485:GLU:CD	1:C:485:GLU:H	2.19	0.46
1:D:23:ILE:HD11	1:D:26:LEU:HD13	1.98	0.46
1:B:39:ALA:O	1:B:43:MET:HG3	2.15	0.46
1:B:492:HIS:CD2	1:B:492:HIS:H	2.35	0.45
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.63	0.45
1:C:317:GLU:OE2	1:D:255:TYR:OH	2.30	0.45
1:C:384:LYS:HE3	1:C:387:VAL:HG21	1.98	0.45
1:C:492:HIS:CD2	4:C:783:HOH:O	2.67	0.45
1:B:71:THR:HG22	1:B:99:GLN:NE2	2.31	0.45
1:A:23:ILE:HD11	1:A:26:LEU:HD13	1.98	0.45
1:A:68:LEU:O	1:A:69:HIS:C	2.55	0.45
1:C:141:LEU:HD12	1:C:163:LEU:HD23	1.99	0.45
1:C:406:ARG:NE	4:C:732:HOH:O	2.46	0.44
1:D:206:THR:O	1:D:210:GLU:HG3	2.17	0.44
1:B:313:GLN:O	1:B:317:GLU:CG	2.65	0.44
1:D:218:GLU:HG3	1:D:428:GLN:NE2	2.31	0.44
1:A:213:LYS:O	1:A:238:PRO:HD2	2.17	0.44
1:D:384:LYS:HB2	1:D:385:PRO:CD	2.47	0.44
1:C:130:LEU:HD22	1:C:186:GLU:HG3	1.99	0.44
1:A:95:ILE:HG22	1:A:133:TYR:HB2	2.00	0.44
1:C:469:LEU:HD11	1:D:308:PRO:HB3	2.00	0.44
1:B:192:ASN:OD1	1:B:195:ARG:NH1	2.51	0.44
1:D:69:HIS:CE1	1:D:93:CYS:SG	3.10	0.44
1:A:403:SER:OG	1:A:412:ASN:ND2	2.50	0.44
1:B:78:ILE:HG23	1:B:88:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:O	1:B:225:ARG:HG3	2.18	0.43
1:A:341:LYS:HE3	1:B:475:GLU:HG2	2.00	0.43
1:D:157:GLY:HA3	1:D:363:HIS:NE2	2.33	0.43
1:C:179:ALA:O	1:C:180:GLU:CB	2.66	0.43
1:B:252:ASP:OD2	2:B:500:ARJ:O2'	2.36	0.43
1:D:450:PRO:HD2	1:D:453:LEU:HD12	2.00	0.43
1:D:42:GLU:O	1:D:419:PHE:HA	2.20	0.42
1:C:456:LYS:NZ	4:C:776:HOH:O	2.48	0.42
1:A:235:LEU:O	1:A:444:ASN:HB3	2.19	0.42
1:A:450:PRO:HD2	1:A:453:LEU:HD12	2.01	0.42
1:B:340:ASN:HB3	1:B:343:ILE:HD11	2.01	0.42
1:C:50:ARG:O	1:C:54:ALA:HB2	2.20	0.42
1:A:390:TRP:O	1:A:398:SER:HA	2.20	0.42
1:D:278:VAL:HG11	1:D:294:MET:HG3	2.02	0.42
1:C:146:PRO:HB2	1:C:147:ASP:CB	2.44	0.41
1:C:218:GLU:CG	1:C:428:GLN:NE2	2.83	0.41
1:A:250:LYS:NZ	1:A:254:LYS:NZ	2.68	0.41
1:C:154:LEU:HD11	1:C:428:GLN:HG2	2.02	0.41
1:A:384:LYS:HB2	1:A:385:PRO:HD2	2.03	0.41
1:D:240:ILE:HD12	1:D:435:LEU:HG	2.02	0.41
1:C:406:ARG:NH2	4:C:732:HOH:O	2.51	0.41
1:C:97:SER:HB2	1:C:410:LEU:HB3	2.02	0.41
1:C:402:LEU:HB3	1:C:412:ASN:ND2	2.36	0.41
1:D:227:TYR:HD2	4:D:941:HOH:O	2.03	0.41
1:C:11:LEU:HD11	1:C:132:GLU:HG2	2.03	0.41
1:D:243:ASN:O	1:D:249:SER:HB3	2.21	0.41
1:D:69:HIS:HA	1:D:92:SER:OG	2.21	0.41
1:D:68:LEU:HD21	1:D:425:PHE:CE1	2.56	0.41
1:C:116:GLU:HG3	1:C:116:GLU:O	2.21	0.41
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.86	0.40
1:D:36:LEU:HD21	1:D:75:ALA:HB1	2.03	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	483/495 (98%)	473 (98%)	10 (2%)	0	100	100
1	B	483/495 (98%)	472 (98%)	10 (2%)	1 (0%)	52	48
1	C	483/495 (98%)	465 (96%)	13 (3%)	5 (1%)	19	11
1	D	483/495 (98%)	471 (98%)	12 (2%)	0	100	100
All	All	1932/1980 (98%)	1881 (97%)	45 (2%)	6 (0%)	46	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	ASP
1	B	69	HIS
1	C	180	GLU
1	C	69	HIS
1	C	183	ASP
1	C	146	PRO

### 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	395/404 (98%)	387 (98%)	8 (2%)	63	65
1	B	395/404 (98%)	389 (98%)	6 (2%)	72	75
1	C	395/404 (98%)	391 (99%)	4 (1%)	82	85
1	D	395/404 (98%)	387 (98%)	8 (2%)	63	65
All	All	1580/1616 (98%)	1554 (98%)	26 (2%)	70	73

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	181	GLU

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	219	THR
1	A	253	ASN
1	A	304	THR
1	A	407	LEU
1	A	428	GLN
1	B	68	LEU
1	B	88	VAL
1	B	180	GLU
1	B	219	THR
1	B	237	PHE
1	B	407	LEU
1	C	147	ASP
1	C	220	THR
1	C	407	LEU
1	C	428	GLN
1	D	11	LEU
1	D	16	ARG
1	D	26	LEU
1	D	220	THR
1	D	237	PHE
1	D	407	LEU
1	D	428	GLN
1	D	440	ASP

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	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	492	HIS
1	B	57	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	355	HIS
1	B	412	ASN
1	B	416	HIS

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Mol	Chain	Res	Type
1	B	492	HIS
1	C	57	GLN
1	C	243	ASN
1	C	259	HIS
1	C	310	ASN
1	C	355	HIS
1	C	412	ASN
1	C	416	HIS
1	C	428	GLN
1	C	492	HIS
1	D	57	GLN
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN
1	D	492	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](#)

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	ARJ	A	500	-	16,21,21	3.45	3 (18%)	7,31,31	4.62	3 (42%)
3	NAD	A	550	-	38,48,48	1.45	5 (13%)	47,73,73	2.50	12 (25%)
2	ARJ	B	500	-	16,21,21	3.36	3 (18%)	7,31,31	4.49	3 (42%)
3	NAD	B	550	-	38,48,48	1.64	6 (15%)	47,73,73	1.84	9 (19%)
2	ARJ	C	500	-	16,21,21	3.38	3 (18%)	7,31,31	3.80	4 (57%)
3	NAD	C	550	-	38,48,48	1.49	3 (7%)	47,73,73	1.69	7 (14%)
2	ARJ	D	500	-	16,21,21	3.38	4 (25%)	7,31,31	4.16	2 (28%)
3	NAD	D	550	-	38,48,48	1.60	5 (13%)	47,73,73	2.20	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARJ	A	500	-	2/2/4/4	0/2/22/22	0/3/3/3
3	NAD	A	550	-	-	0/22/62/62	0/5/5/5
2	ARJ	B	500	-	2/2/4/4	0/2/22/22	0/3/3/3
3	NAD	B	550	-	-	0/22/62/62	0/5/5/5
2	ARJ	C	500	-	2/2/4/4	0/2/22/22	0/3/3/3
3	NAD	C	550	-	-	0/22/62/62	0/5/5/5
2	ARJ	D	500	-	2/2/4/4	0/2/22/22	0/3/3/3
3	NAD	D	550	-	-	0/22/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ARJ	C4'-C3D	-9.85	1.34	1.51
2	B	500	ARJ	C4'-C3D	-9.46	1.34	1.51
2	D	500	ARJ	C4'-C3D	-9.10	1.35	1.51
2	C	500	ARJ	C4'-C3D	-8.99	1.35	1.51
2	A	500	ARJ	C2'-C3D	-7.80	1.32	1.52
2	C	500	ARJ	C2'-C3D	-7.63	1.33	1.52
2	D	500	ARJ	C2'-C3D	-7.57	1.33	1.52
2	B	500	ARJ	C2'-C3D	-7.32	1.34	1.52
2	D	500	ARJ	O2'-C2'	-5.39	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	ARJ	O2'-C2'	-5.35	1.31	1.42
2	B	500	ARJ	O2'-C2'	-4.84	1.32	1.42
2	A	500	ARJ	O2'-C2'	-4.83	1.32	1.42
3	B	550	NAD	C7N-N7N	-3.75	1.25	1.33
3	A	550	NAD	C7N-N7N	-3.14	1.26	1.33
2	D	500	ARJ	O3D-C3D	2.05	1.25	1.21
3	A	550	NAD	O2B-C2B	2.13	1.48	1.43
3	B	550	NAD	O2B-C2B	2.35	1.48	1.43
3	D	550	NAD	O3D-C3D	2.57	1.49	1.43
3	B	550	NAD	O3B-C3B	2.71	1.49	1.43
3	D	550	NAD	C5A-C4A	3.16	1.47	1.40
3	D	550	NAD	C3N-C7N	3.20	1.55	1.50
3	B	550	NAD	C5A-C4A	3.28	1.47	1.40
3	A	550	NAD	C5A-C4A	3.61	1.48	1.40
3	C	550	NAD	O4D-C1D	3.65	1.45	1.41
3	B	550	NAD	O7N-C7N	3.74	1.32	1.24
3	A	550	NAD	O4D-C1D	3.77	1.46	1.41
3	A	550	NAD	O7N-C7N	4.05	1.32	1.24
3	C	550	NAD	C5A-C4A	4.09	1.49	1.40
3	D	550	NAD	O7N-C7N	4.21	1.33	1.24
3	D	550	NAD	O4D-C1D	5.26	1.47	1.41
3	B	550	NAD	O4D-C1D	5.32	1.47	1.41
3	C	550	NAD	O7N-C7N	5.37	1.35	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	N3A-C2A-N1A	-12.74	119.14	128.89
2	A	500	ARJ	N3-C2-N1	-11.23	120.29	128.89
2	B	500	ARJ	N3-C2-N1	-10.55	120.81	128.89
2	D	500	ARJ	N3-C2-N1	-9.78	121.41	128.89
3	D	550	NAD	N3A-C2A-N1A	-9.17	121.87	128.89
2	C	500	ARJ	N3-C2-N1	-8.62	122.29	128.89
3	C	550	NAD	N3A-C2A-N1A	-7.14	123.42	128.89
3	B	550	NAD	N3A-C2A-N1A	-6.83	123.66	128.89
3	A	550	NAD	C4B-O4B-C1B	-4.95	104.28	109.72
3	D	550	NAD	O7N-C7N-N7N	-4.44	116.35	122.59
3	D	550	NAD	C4B-O4B-C1B	-3.61	105.76	109.72
3	A	550	NAD	C1B-N9A-C4A	-3.59	121.52	126.94
3	B	550	NAD	O4D-C1D-N1N	-3.56	104.22	108.13
3	B	550	NAD	O3D-C3D-C4D	-3.44	100.72	111.05
3	A	550	NAD	C5N-C4N-C3N	-3.30	116.19	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	550	NAD	C4A-C5A-N7A	-3.05	106.67	109.48
3	A	550	NAD	O4D-C1D-N1N	-3.00	104.83	108.13
3	A	550	NAD	PN-O3-PA	-2.86	124.70	132.73
3	B	550	NAD	C1B-N9A-C4A	-2.82	122.68	126.94
3	C	550	NAD	PN-O3-PA	-2.75	125.00	132.73
3	B	550	NAD	O7N-C7N-N7N	-2.48	119.10	122.59
3	B	550	NAD	C4A-C5A-N7A	-2.34	107.33	109.48
2	C	500	ARJ	C4-C5-N7	-2.31	107.36	109.48
3	C	550	NAD	O3D-C3D-C4D	-2.22	104.38	111.05
3	A	550	NAD	O7N-C7N-N7N	-2.22	119.47	122.59
3	C	550	NAD	O7N-C7N-N7N	-2.19	119.51	122.59
3	A	550	NAD	C4A-C5A-N7A	-2.17	107.49	109.48
2	C	500	ARJ	C2-N1-C6	2.12	122.55	118.77
2	A	500	ARJ	N6-C6-N1	2.19	123.91	119.20
3	C	550	NAD	C3N-C7N-N7N	2.20	120.23	117.82
3	D	550	NAD	C3N-C2N-N1N	2.36	123.08	120.36
3	A	550	NAD	C4D-O4D-C1D	2.38	112.33	109.72
3	D	550	NAD	C2A-N1A-C6A	2.49	123.22	118.77
3	A	550	NAD	C3N-C2N-N1N	2.52	123.27	120.36
3	B	550	NAD	C4D-O4D-C1D	2.72	112.71	109.72
2	B	500	ARJ	C2-N1-C6	2.73	123.64	118.77
3	C	550	NAD	C3N-C2N-N1N	2.74	123.52	120.36
3	C	550	NAD	C2A-N1A-C6A	2.77	123.71	118.77
3	A	550	NAD	C2A-N1A-C6A	3.04	124.20	118.77
3	B	550	NAD	C2A-N1A-C6A	3.12	124.34	118.77
3	A	550	NAD	C3N-C7N-N7N	3.15	121.27	117.82
3	B	550	NAD	C3N-C7N-N7N	3.63	121.79	117.82
2	A	500	ARJ	C1'-C2'-C3D	3.86	110.23	103.73
2	C	500	ARJ	C1'-C2'-C3D	4.00	110.48	103.73
2	B	500	ARJ	C1'-C2'-C3D	4.18	110.78	103.73
2	D	500	ARJ	C1'-C2'-C3D	4.42	111.18	103.73
3	D	550	NAD	C3N-C7N-N7N	7.21	125.70	117.82

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	500	ARJ	C2'
2	C	500	ARJ	C4'
2	A	500	ARJ	C2'
2	A	500	ARJ	C4'
2	B	500	ARJ	C2'
2	B	500	ARJ	C4'

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Mol	Chain	Res	Type	Atom
2	D	500	ARJ	C2'
2	D	500	ARJ	C4'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	ARJ	2	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	485/495 (97%)	-0.00	14 (2%) 55 56	14, 25, 44, 72	0
1	B	485/495 (97%)	-0.05	6 (1%) 81 81	12, 22, 41, 64	0
1	C	485/495 (97%)	0.32	38 (7%) 16 17	12, 28, 56, 101	0
1	D	485/495 (97%)	0.05	19 (3%) 43 45	12, 24, 47, 81	0
All	All	1940/1980 (97%)	0.08	77 (3%) 42 44	12, 24, 49, 101	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	GLU	7.6
1	D	182	ASP	5.8
1	A	440	ASP	5.3
1	C	180	GLU	5.0
1	C	179	ALA	5.0
1	D	181	GLU	4.5
1	C	56	VAL	4.5
1	C	177	PRO	4.5
1	C	144	PRO	4.3
1	C	440	ASP	4.1
1	D	56	VAL	3.9
1	C	175	VAL	3.8
1	C	174	GLY	3.8
1	C	68	LEU	3.7
1	C	114	PRO	3.7
1	C	198	PHE	3.6
1	C	182	ASP	3.5
1	C	172	LYS	3.4
1	D	198	PHE	3.3
1	C	425	PHE	3.2
1	D	114	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	ASP	3.1
1	A	199	GLU	3.1
1	D	177	PRO	3.1
1	A	231	ALA	3.1
1	C	219	THR	3.1
1	C	170	TYR	3.0
1	A	200	THR	3.0
1	A	177	PRO	3.0
1	C	442	TYR	2.9
1	D	55	GLU	2.9
1	D	115	ASP	2.9
1	C	74	THR	2.9
1	C	191	LEU	2.8
1	C	147	ASP	2.8
1	C	117	PRO	2.7
1	A	227	TYR	2.7
1	C	19	ILE	2.6
1	C	232	ALA	2.6
1	C	11	LEU	2.6
1	A	173	ALA	2.6
1	C	173	ALA	2.6
1	D	180	GLU	2.6
1	C	199	GLU	2.5
1	A	198	PHE	2.5
1	D	173	ALA	2.5
1	B	154	LEU	2.5
1	D	154	LEU	2.5
1	A	180	GLU	2.4
1	C	178	PRO	2.4
1	D	116	GLU	2.4
1	C	183	ASP	2.4
1	B	231	ALA	2.3
1	D	201	ASP	2.3
1	B	445	GLU	2.3
1	C	149	PRO	2.3
1	B	440	ASP	2.3
1	D	199	GLU	2.3
1	C	115	ASP	2.3
1	A	53	TYR	2.2
1	D	174	GLY	2.2
1	A	174	GLY	2.2
1	C	185	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	170	TYR	2.2
1	D	11	LEU	2.1
1	D	176	VAL	2.1
1	C	146	PRO	2.1
1	C	54	ALA	2.1
1	A	56	VAL	2.1
1	C	17	ASN	2.1
1	C	443	ASP	2.1
1	A	182	ASP	2.1
1	C	209	ALA	2.1
1	C	116	GLU	2.0
1	D	12	THR	2.0
1	B	170	TYR	2.0
1	B	286	VAL	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
2	ARJ	B	500	19/19	0.94	0.17	0.47	11,17,27,31	0
2	ARJ	D	500	19/19	0.95	0.16	0.40	14,19,29,32	0
2	ARJ	C	500	19/19	0.95	0.19	0.22	14,21,33,34	0
2	ARJ	A	500	19/19	0.95	0.15	0.13	13,20,31,31	0
3	NAD	C	550	44/44	0.95	0.11	-0.31	12,19,23,24	0
3	NAD	D	550	44/44	0.96	0.10	-0.54	12,17,21,23	0
3	NAD	A	550	44/44	0.96	0.10	-0.59	15,20,23,26	0
3	NAD	B	550	44/44	0.96	0.09	-1.02	9,17,19,23	0

## 6.5 Other polymers

There are no such residues in this entry.