



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:40 AM GMT

PDB ID : 2DVM  
Title : NAD complex structure of PH1275 protein from *Pyrococcus horikoshii*  
Authors : Lokanath, N.K.; Mizutani, H.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-07-31  
Resolution : 1.60 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.

---

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

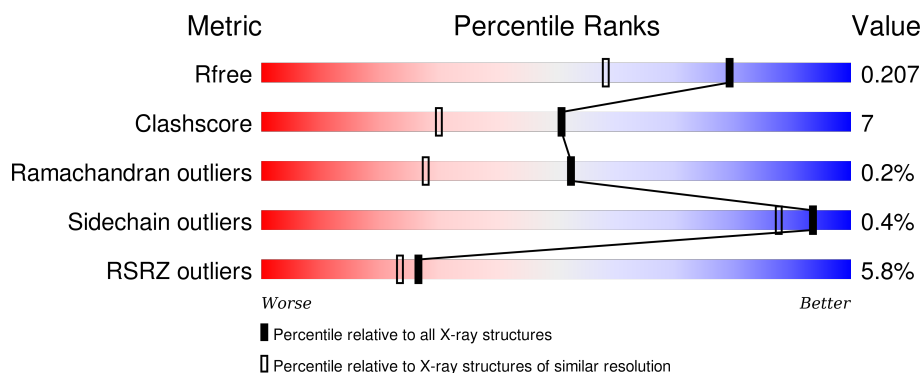
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	439	<div> <div>11%</div> <div>84%</div> <div>16%</div> </div>
1	B	439	<div> <div>5%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
1	C	439	<div> <div>4%</div> <div>86%</div> <div>13%</div> </div>
1	D	439	<div> <div>3%</div> <div>84%</div> <div>15%</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
3	MES	A	2759	-	-	-	X
3	MES	A	2760	-	-	-	X
3	MES	C	2758	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15499 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 439aa long hypotheticalal malate oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3377	2166	579	625	7			
1	B	434	Total	C	N	O	S	0	0	0
			3345	2147	572	619	7			
1	C	438	Total	C	N	O	S	0	0	0
			3377	2166	579	625	7			
1	D	436	Total	C	N	O	S	0	0	0
			3358	2156	574	621	7			

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



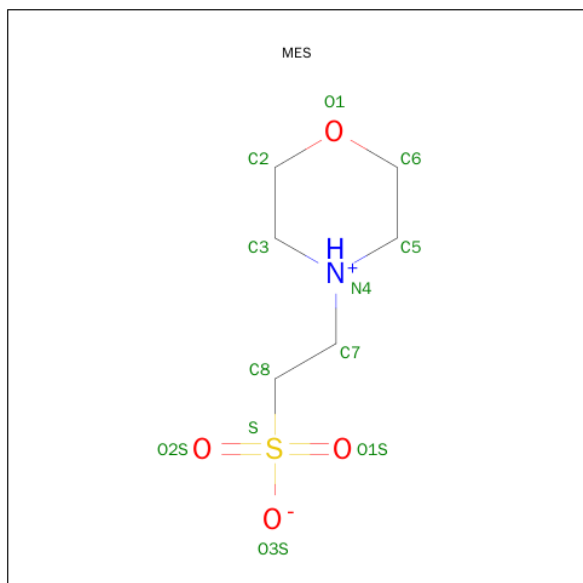
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

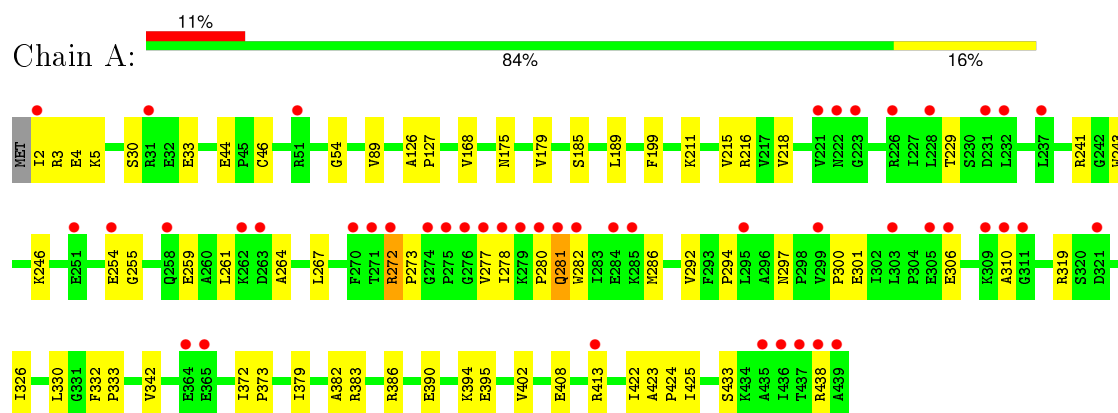
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	383	Total	O	0	0
			383	383		
4	B	454	Total	O	0	0
			454	454		
4	C	483	Total	O	0	0
			483	483		
4	D	510	Total	O	0	0
			510	510		

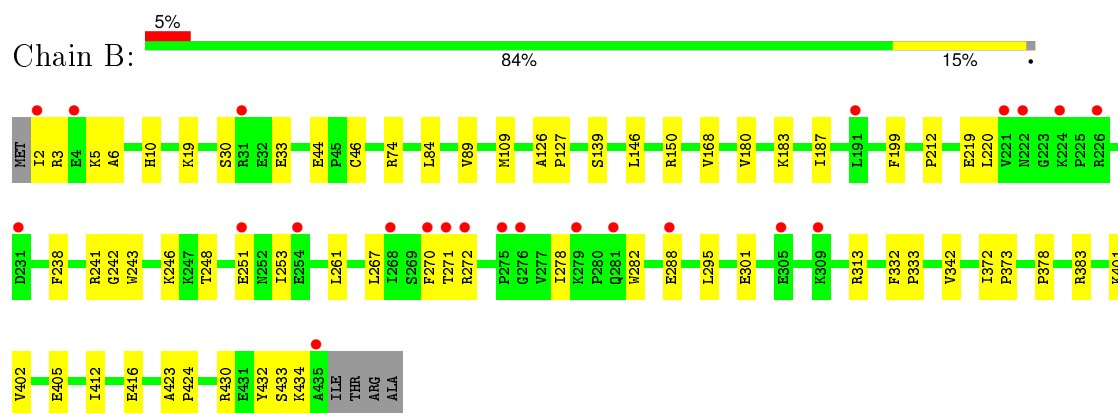
### 3 Residue-property plots

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.

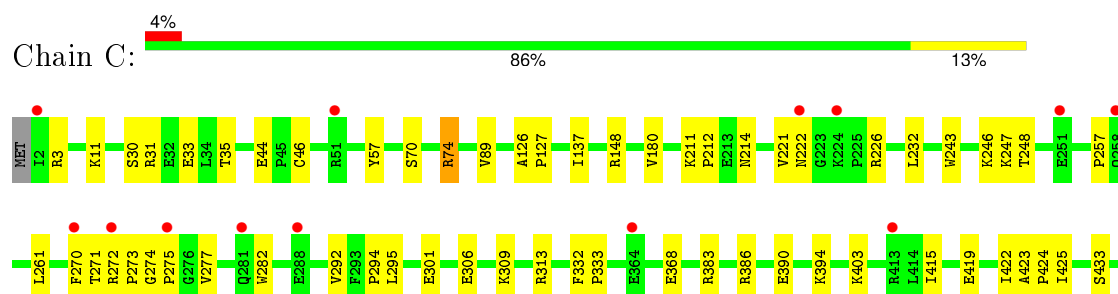
- Molecule 1: 439aa long hypothetical malate oxidoreductase



- Molecule 1: 439aa long hypothetical malate oxidoreductase

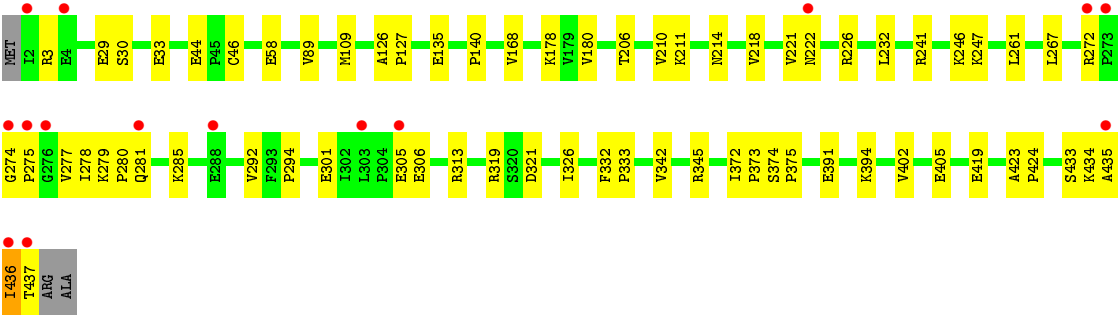
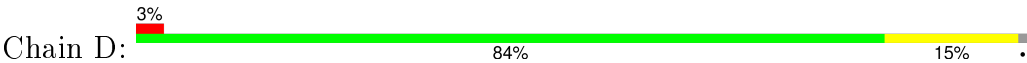


- Molecule 1: 439aa long hypothetical malate oxidoreductase





● Molecule 1: 439aa long hypothetical malate oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.86Å 74.29Å 141.16Å 90.00° 100.37° 90.00°	Depositor
Resolution (Å)	29.84 – 1.60 29.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.84-1.60) 99.6 (29.84-1.60)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.191 , 0.207 0.190 , 0.207	Depositor DCC
$R_{free}$ test set	13525 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 273210 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: MES, 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	0.34	0/3441	0.59	0/4660
1	B	0.32	0/3409	0.61	1/4618 (0.0%)
1	C	0.34	0/3441	0.65	0/4660
1	D	0.36	0/3422	0.66	0/4636
All	All	0.34	0/13713	0.63	1/18574 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	PRO	N-CD-CG	5.06	110.79	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	LEU	Mainchain

## 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	3377	0	3490	55	0
1	B	3345	0	3454	45	0
1	C	3377	0	3490	49	0
1	D	3358	0	3467	52	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	24	0	26	4	0
3	C	12	0	13	3	0
4	A	383	0	0	2	0
4	B	454	0	0	6	0
4	C	483	0	0	13	0
4	D	510	0	0	11	0
All	All	15499	0	14044	190	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 (190) 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:57:TYR:HE2	3:C:2758:MES:H21	1.28	0.96
1:C:226:ARG:NH1	1:C:232:LEU:HD11	1.85	0.92
1:A:273:PRO:HG3	1:A:297:ASN:O	1.72	0.90
1:B:243:TRP:HA	1:B:246:LYS:HE3	1.57	0.85
1:D:372:ILE:HG13	1:D:373:PRO:HD2	1.63	0.80
1:A:2:ILE:HG12	1:A:5:LYS:HD3	1.66	0.78
1:A:267:LEU:HD12	1:A:292:VAL:HG13	1.65	0.77
1:C:31:ARG:HD3	4:C:2891:HOH:O	1.84	0.77
1:D:394:LYS:HE3	4:D:2667:HOH:O	1.85	0.77
1:C:57:TYR:CE2	3:C:2758:MES:H21	2.17	0.75
3:C:2758:MES:H52	4:C:3090:HOH:O	1.88	0.72
1:D:436:ILE:O	1:D:436:ILE:HG22	1.91	0.70
1:C:180:VAL:HG12	1:C:313:ARG:HD3	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2759:MES:O2S	1:B:84:LEU:HD21	1.94	0.68
1:B:372:ILE:HG13	1:B:373:PRO:HD2	1.75	0.68
1:C:292:VAL:HG12	1:C:294:PRO:HD3	1.77	0.67
1:B:261:LEU:HD12	1:B:282:TRP:HB3	1.77	0.65
1:D:274:GLY:HA2	1:D:277:VAL:HG23	1.79	0.64
1:A:127:PRO:HA	3:A:2759:MES:O2S	1.99	0.62
1:C:368:GLU:HG2	4:C:3204:HOH:O	2.00	0.60
1:C:419:GLU:HG2	4:D:2760:HOH:O	1.99	0.60
1:B:219:GLU:HG2	1:B:238:PHE:CE1	2.36	0.60
1:B:261:LEU:HD21	1:B:267:LEU:HD13	1.83	0.60
1:B:342:VAL:HG12	1:B:402:VAL:HG22	1.81	0.60
1:B:6:ALA:O	1:B:10:HIS:HD2	1.85	0.60
1:C:403:LYS:HA	1:C:403:LYS:HE2	1.84	0.59
1:D:292:VAL:HG12	1:D:294:PRO:HD3	1.85	0.59
1:C:46:CYS:SG	1:D:89:VAL:HG23	2.42	0.58
1:C:261:LEU:HD12	1:C:282:TRP:HB3	1.86	0.58
1:D:342:VAL:HG12	1:D:402:VAL:HG22	1.84	0.58
1:C:415:ILE:HD11	4:C:3211:HOH:O	2.04	0.57
1:D:405:GLU:HG3	4:D:2631:HOH:O	2.03	0.57
1:C:3:ARG:HA	1:D:44:GLU:HG3	1.85	0.57
1:A:46:CYS:SG	1:B:89:VAL:HG23	2.45	0.57
3:A:2759:MES:H82	1:B:84:LEU:HD11	1.87	0.57
1:D:211:LYS:HB2	1:D:214:ASN:ND2	2.20	0.57
1:B:30:SER:OG	1:B:33:GLU:HG3	2.04	0.57
1:D:30:SER:OG	1:D:33:GLU:HG3	2.06	0.56
1:C:30:SER:OG	1:C:33:GLU:HG3	2.06	0.56
1:C:44:GLU:HG3	1:D:3:ARG:HA	1.87	0.55
1:A:44:GLU:HG3	1:B:3:ARG:HA	1.88	0.55
1:A:30:SER:OG	1:A:33:GLU:HG3	2.07	0.54
1:B:270:PHE:CZ	1:B:295:LEU:HD12	2.43	0.54
1:C:394:LYS:HE3	4:C:3201:HOH:O	2.07	0.54
1:C:74:ARG:HD3	4:C:3232:HOH:O	2.08	0.54
1:C:423:ALA:HB3	1:C:424:PRO:HD3	1.90	0.54
1:A:168:VAL:HG12	1:A:326:ILE:HG23	1.90	0.54
1:B:288:GLU:HG3	4:B:2646:HOH:O	2.08	0.53
1:A:372:ILE:HD12	1:A:373:PRO:HD2	1.89	0.53
1:B:423:ALA:HB3	1:B:424:PRO:HD3	1.90	0.53
1:D:261:LEU:HD21	1:D:267:LEU:HD22	1.90	0.53
1:C:226:ARG:HH12	1:C:232:LEU:HD11	1.68	0.53
1:A:394:LYS:HE3	1:A:395:GLU:OE2	2.09	0.52
1:A:423:ALA:HB3	1:A:424:PRO:HD3	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:N	1:A:272:ARG:HD3	2.25	0.52
1:D:436:ILE:O	1:D:436:ILE:CG2	2.56	0.52
1:C:211:LYS:HB2	1:C:214:ASN:ND2	2.25	0.52
1:B:251:GLU:HG3	4:B:2753:HOH:O	2.10	0.51
1:D:345:ARG:HG2	1:D:345:ARG:O	2.10	0.51
1:B:242:GLY:O	1:B:246:LYS:HG2	2.10	0.51
1:A:394:LYS:NZ	4:A:2886:HOH:O	2.44	0.51
1:A:127:PRO:HB2	1:B:109:MET:HB2	1.92	0.51
1:C:422:ILE:O	1:C:425:ILE:HG13	2.10	0.51
1:A:126:ALA:N	1:A:127:PRO:CD	2.74	0.51
1:A:280:PRO:HG3	1:A:306:GLU:HB3	1.93	0.51
1:C:127:PRO:HB2	1:D:109:MET:HB2	1.93	0.51
1:D:180:VAL:HG12	1:D:313:ARG:HD3	1.92	0.51
1:A:300:PRO:HD3	1:A:319:ARG:HD2	1.93	0.51
1:A:272:ARG:HE	1:A:277:VAL:HG13	1.74	0.51
1:C:221:VAL:O	1:C:222:ASN:HB2	2.11	0.51
1:C:243:TRP:HA	1:C:246:LYS:HE2	1.92	0.51
1:B:126:ALA:N	1:B:127:PRO:CD	2.75	0.50
1:B:146:LEU:O	1:B:150:ARG:HG3	2.10	0.50
1:D:267:LEU:HD21	1:D:278:ILE:HD13	1.92	0.50
1:A:89:VAL:HG23	1:B:46:CYS:SG	2.51	0.50
1:B:405:GLU:HG3	4:B:2587:HOH:O	2.11	0.50
1:D:211:LYS:HB2	1:D:214:ASN:HD22	1.75	0.50
1:C:270:PHE:CZ	1:C:295:LEU:HD12	2.47	0.50
1:B:219:GLU:HG2	1:B:238:PHE:CZ	2.46	0.50
1:D:178:LYS:HE2	4:D:2803:HOH:O	2.12	0.50
1:D:135:GLU:OE2	4:D:2943:HOH:O	2.19	0.50
1:B:10:HIS:HE1	1:B:19:LYS:NZ	2.10	0.49
1:A:278:ILE:HA	1:A:282:TRP:HZ3	1.76	0.49
1:C:70:SER:HA	1:C:137:ILE:HD11	1.95	0.49
1:A:261:LEU:HD21	1:A:267:LEU:HD23	1.94	0.49
1:A:272:ARG:H	1:A:272:ARG:HD3	1.77	0.49
1:B:2:ILE:HG23	1:B:5:LYS:H	1.78	0.49
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.78	0.48
1:B:74:ARG:CZ	1:B:139:SER:H	2.26	0.48
1:A:3:ARG:HA	1:B:44:GLU:HG3	1.94	0.48
1:B:401:LYS:HD3	4:B:2762:HOH:O	2.13	0.48
1:A:281:GLN:N	1:A:281:GLN:OE1	2.46	0.48
1:C:247:LYS:HE3	4:C:2989:HOH:O	2.13	0.48
1:A:379:ILE:HG22	1:A:383:ARG:HG3	1.96	0.48
1:D:226:ARG:NH1	1:D:232:LEU:HD11	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLU:CG	4:D:2665:HOH:O	2.61	0.47
1:A:438:ARG:HH11	1:A:438:ARG:HG2	1.78	0.47
1:C:212:PRO:O	1:C:248:THR:HA	2.13	0.47
1:D:423:ALA:HB3	1:D:424:PRO:HD3	1.96	0.47
1:C:257:PRO:HD2	4:C:3234:HOH:O	2.14	0.47
1:D:435:ALA:C	1:D:437:THR:H	2.18	0.47
1:A:218:VAL:O	2:A:2503:NAD:H2A	2.15	0.47
1:D:434:LYS:HA	1:D:434:LYS:HD3	1.72	0.47
1:A:4:GLU:CD	1:A:4:GLU:H	2.19	0.47
1:D:285:LYS:HB2	4:D:2794:HOH:O	2.15	0.47
1:C:271:THR:OG1	1:C:272:ARG:N	2.48	0.46
1:C:309:LYS:NZ	1:C:309:LYS:HB2	2.31	0.46
1:A:332:PHE:CG	1:A:333:PRO:HD3	2.50	0.46
1:D:126:ALA:N	1:D:127:PRO:CD	2.78	0.46
1:A:292:VAL:HG12	1:A:294:PRO:HD3	1.98	0.46
1:D:261:LEU:HD21	1:D:267:LEU:HD13	1.97	0.46
1:B:2:ILE:N	4:B:2872:HOH:O	2.48	0.46
1:D:285:LYS:HD3	1:D:285:LYS:HA	1.70	0.46
1:C:274:GLY:HA2	1:C:277:VAL:HG23	1.98	0.46
1:A:280:PRO:HB3	1:A:310:ALA:HB2	1.97	0.45
1:D:247:LYS:NZ	4:D:2966:HOH:O	2.27	0.45
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.81	0.45
1:A:261:LEU:HD12	1:A:282:TRP:HB3	1.98	0.45
1:A:54:GLY:HA2	3:A:2759:MES:H22	1.98	0.45
1:B:412:ILE:O	1:B:416:GLU:HG3	2.16	0.45
1:A:294:PRO:HB2	1:A:300:PRO:HB3	1.99	0.45
1:C:89:VAL:HG23	1:D:46:CYS:SG	2.57	0.45
1:B:271:THR:OG1	1:B:272:ARG:N	2.49	0.45
1:A:267:LEU:HD12	1:A:292:VAL:CG1	2.41	0.45
1:C:332:PHE:CG	1:C:333:PRO:HD3	2.51	0.45
1:A:278:ILE:HA	1:A:282:TRP:CZ3	2.51	0.44
1:C:126:ALA:N	1:C:127:PRO:CD	2.80	0.44
1:C:148:ARG:HD3	1:C:148:ARG:HH11	1.60	0.44
1:B:332:PHE:CG	1:B:333:PRO:HD3	2.53	0.44
1:A:413:ARG:HH21	1:B:432:TYR:HA	1.81	0.44
1:A:229:THR:HG21	1:A:254:GLU:OE1	2.18	0.44
1:A:386:ARG:O	1:A:390:GLU:HG3	2.17	0.44
1:C:247:LYS:NZ	4:C:3001:HOH:O	2.50	0.44
1:A:199:PHE:CG	1:A:241:ARG:HG2	2.53	0.44
1:A:2:ILE:HG12	1:A:5:LYS:CD	2.41	0.44
1:C:403:LYS:CE	1:C:403:LYS:HA	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:VAL:HG12	1:D:326:ILE:HG23	2.00	0.44
1:B:212:PRO:O	1:B:248:THR:HA	2.17	0.44
1:D:278:ILE:HG13	1:D:301:GLU:HB3	1.98	0.43
1:C:211:LYS:HB2	1:C:214:ASN:HD22	1.83	0.43
1:C:277:VAL:HB	1:C:301:GLU:HB3	2.00	0.43
1:D:218:VAL:O	2:D:2504:NAD:H2A	2.18	0.43
1:D:274:GLY:HA3	1:D:275:PRO:HA	1.74	0.43
1:A:259:GLU:H	1:A:259:GLU:CD	2.21	0.43
1:B:219:GLU:HG3	1:B:220:LEU:N	2.34	0.43
1:D:267:LEU:HD23	1:D:292:VAL:HG13	2.01	0.43
1:C:11:LYS:NZ	1:D:58:GLU:OE2	2.35	0.43
1:D:332:PHE:CG	1:D:333:PRO:HD3	2.54	0.43
4:C:3220:HOH:O	1:D:29:GLU:HG2	2.17	0.43
1:B:74:ARG:HH12	1:B:139:SER:HB3	1.83	0.43
1:C:31:ARG:O	1:C:35:THR:HG23	2.19	0.43
1:D:140:PRO:HB3	1:D:241:ARG:NH2	2.33	0.43
1:C:438:ARG:HD2	1:C:438:ARG:HH11	1.64	0.42
1:D:419:GLU:CG	4:D:2763:HOH:O	2.65	0.42
1:B:278:ILE:HG13	1:B:301:GLU:HB3	2.01	0.42
1:B:383:ARG:HD3	4:B:2754:HOH:O	2.19	0.42
1:A:422:ILE:O	1:A:425:ILE:HG13	2.18	0.42
1:A:264:ALA:O	1:A:286:MET:HB3	2.19	0.42
1:A:199:PHE:CD2	1:A:241:ARG:HG2	2.54	0.42
1:B:251:GLU:HB2	1:B:253:ILE:HG13	2.01	0.42
1:A:372:ILE:CD1	1:A:373:PRO:HD2	2.49	0.42
1:C:275:PRO:HB3	4:C:3194:HOH:O	2.18	0.42
1:B:168:VAL:HG13	1:B:372:ILE:HD11	2.00	0.42
1:D:246:LYS:HE2	4:D:2900:HOH:O	2.18	0.42
1:C:306:GLU:OE1	4:C:3194:HOH:O	2.22	0.42
1:C:386:ARG:O	1:C:390:GLU:HG3	2.20	0.42
1:A:189:LEU:HB3	1:A:215:VAL:HG22	2.01	0.42
1:D:206:THR:HA	1:D:210:VAL:O	2.20	0.41
1:D:305:GLU:HG2	1:D:306:GLU:N	2.35	0.41
1:D:272:ARG:HD2	4:D:2903:HOH:O	2.20	0.41
1:D:221:VAL:O	1:D:222:ASN:HB2	2.19	0.41
1:A:342:VAL:HG12	1:A:402:VAL:HG22	2.02	0.41
1:B:199:PHE:CG	1:B:241:ARG:HG2	2.55	0.41
4:A:3082:HOH:O	1:B:430:ARG:HD2	2.20	0.41
1:A:255:GLY:HA3	1:A:259:GLU:HG2	2.01	0.41
1:D:279:LYS:HA	1:D:280:PRO:HD3	1.95	0.41
1:B:180:VAL:HG12	1:B:313:ARG:HD3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:O	1:B:187:ILE:HG23	2.21	0.41
1:D:319:ARG:HB3	1:D:321:ASP:OD1	2.21	0.41
1:D:391:GLU:OE1	1:D:394:LYS:HE2	2.21	0.41
1:C:272:ARG:HB2	1:C:273:PRO:HD2	2.03	0.40
1:B:434:LYS:HE3	1:B:434:LYS:HA	2.02	0.40
1:A:185:SER:O	1:A:211:LYS:HE2	2.21	0.40
1:D:281:GLN:H	1:D:281:GLN:CD	2.23	0.40
1:A:277:VAL:HB	1:A:301:GLU:HB3	2.02	0.40
1:A:243:TRP:HA	1:A:246:LYS:HE2	2.04	0.40
1:A:175:ASN:O	1:A:179:VAL:HG23	2.22	0.40
1:C:415:ILE:CD1	4:C:3211:HOH:O	2.68	0.40
1:D:374:SER:HA	1:D:375:PRO:HD3	1.94	0.40
1:A:382:ALA:HB1	1:A:408:GLU:HG3	2.04	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	436/439 (99%)	420 (96%)	15 (3%)	1 (0%)	52	28
1	B	432/439 (98%)	419 (97%)	12 (3%)	1 (0%)	52	28
1	C	436/439 (99%)	424 (97%)	11 (2%)	1 (0%)	52	28
1	D	434/439 (99%)	422 (97%)	11 (2%)	1 (0%)	52	28
All	All	1738/1756 (99%)	1685 (97%)	49 (3%)	4 (0%)	52	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	SER
1	B	433	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	433	SER
1	D	433	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	357/358 (100%)	354 (99%)	3 (1%)	86	75
1	B	354/358 (99%)	354 (100%)	0	100	100
1	C	357/358 (100%)	355 (99%)	2 (1%)	90	82
1	D	355/358 (99%)	354 (100%)	1 (0%)	94	90
All	All	1423/1432 (99%)	1417 (100%)	6 (0%)	93	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	272	ARG
1	A	281	GLN
1	C	74	ARG
1	C	438	ARG
1	D	436	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	214	ASN
1	A	222	ASN
1	A	252	ASN
1	A	297	ASN
1	B	10	HIS
1	B	162	GLN
1	B	214	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	252	ASN
1	B	281	GLN
1	B	297	ASN
1	C	116	ASN
1	C	162	GLN
1	C	214	ASN
1	C	297	ASN
1	D	214	ASN
1	D	222	ASN
1	D	252	ASN

### 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 ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	A	2503	-	38,48,48	1.56	3 (7%)	47,73,73	2.10	7 (14%)
3	MES	A	2759	-	11,12,12	2.19	5 (45%)	14,16,16	4.77	6 (42%)
3	MES	A	2760	-	11,12,12	2.24	5 (45%)	14,16,16	4.52	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	2502	-	38,48,48	1.55	3 (7%)	47,73,73	2.12	7 (14%)
2	NAD	C	2501	-	38,48,48	1.55	3 (7%)	47,73,73	2.06	7 (14%)
3	MES	C	2758	-	11,12,12	2.32	5 (45%)	14,16,16	4.38	7 (50%)
2	NAD	D	2504	-	38,48,48	1.55	3 (7%)	47,73,73	2.10	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	2503	-	-	0/22/62/62	0/5/5/5
3	MES	A	2759	-	-	0/6/14/14	0/1/1/1
3	MES	A	2760	-	-	0/6/14/14	0/1/1/1
2	NAD	B	2502	-	-	0/22/62/62	0/5/5/5
2	NAD	C	2501	-	-	0/22/62/62	0/5/5/5
3	MES	C	2758	-	-	0/6/14/14	0/1/1/1
2	NAD	D	2504	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2759	MES	O3S-S	-3.57	1.37	1.46
3	A	2760	MES	O3S-S	-3.57	1.37	1.46
3	C	2758	MES	O3S-S	-3.46	1.37	1.46
3	A	2760	MES	C5-N4	2.06	1.52	1.46
3	A	2759	MES	C5-N4	2.11	1.52	1.46
3	C	2758	MES	C5-N4	2.20	1.52	1.46
3	A	2760	MES	C7-N4	2.67	1.53	1.47
3	A	2760	MES	C3-N4	2.69	1.54	1.46
3	A	2759	MES	C7-N4	2.70	1.53	1.47
3	A	2759	MES	C3-N4	2.78	1.54	1.46
3	C	2758	MES	C3-N4	2.85	1.54	1.46
2	A	2503	NAD	C2A-N1A	3.22	1.40	1.33
2	D	2504	NAD	C2A-N1A	3.24	1.40	1.33
2	C	2501	NAD	C2A-N1A	3.29	1.40	1.33
2	B	2502	NAD	C2A-N1A	3.33	1.40	1.33
3	C	2758	MES	C7-N4	3.40	1.55	1.47
2	A	2503	NAD	C2A-N3A	3.74	1.38	1.32
2	D	2504	NAD	C2A-N3A	3.77	1.38	1.32
3	A	2759	MES	O2S-S	3.80	1.57	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2502	NAD	C2A-N3A	3.86	1.39	1.32
2	C	2501	NAD	C2A-N3A	3.88	1.39	1.32
3	C	2758	MES	O2S-S	4.01	1.57	1.45
3	A	2760	MES	O2S-S	4.16	1.58	1.45
2	B	2502	NAD	O7N-C7N	6.31	1.37	1.24
2	D	2504	NAD	O7N-C7N	6.31	1.37	1.24
2	C	2501	NAD	O7N-C7N	6.31	1.37	1.24
2	A	2503	NAD	O7N-C7N	6.43	1.37	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2759	MES	O1S-S-C8	-12.79	95.99	106.91
3	A	2760	MES	O1S-S-C8	-11.97	96.69	106.91
2	B	2502	NAD	N3A-C2A-N1A	-10.90	120.55	128.89
2	C	2501	NAD	N3A-C2A-N1A	-10.85	120.59	128.89
2	D	2504	NAD	N3A-C2A-N1A	-10.80	120.62	128.89
2	A	2503	NAD	N3A-C2A-N1A	-10.68	120.72	128.89
3	C	2758	MES	O1S-S-C8	-10.31	98.11	106.91
3	C	2758	MES	O2S-S-C8	-7.81	100.24	106.91
3	A	2759	MES	O2S-S-C8	-6.64	101.24	106.91
3	A	2760	MES	O2S-S-C8	-5.86	101.91	106.91
2	B	2502	NAD	C4B-O4B-C1B	-4.52	104.76	109.72
2	A	2503	NAD	C4B-O4B-C1B	-4.31	104.98	109.72
2	D	2504	NAD	C4B-O4B-C1B	-4.09	105.22	109.72
3	A	2759	MES	C2-C3-N4	-3.85	104.29	110.12
3	A	2760	MES	C2-C3-N4	-3.74	104.46	110.12
2	C	2501	NAD	C4B-O4B-C1B	-3.65	105.70	109.72
2	A	2503	NAD	C1B-N9A-C4A	-3.16	122.18	126.94
2	B	2502	NAD	C1B-N9A-C4A	-3.14	122.20	126.94
3	C	2758	MES	C2-C3-N4	-3.14	105.36	110.12
2	D	2504	NAD	C1B-N9A-C4A	-3.09	122.28	126.94
2	A	2503	NAD	O7N-C7N-N7N	-2.78	118.69	122.59
2	B	2502	NAD	O7N-C7N-N7N	-2.75	118.72	122.59
2	C	2501	NAD	C1B-N9A-C4A	-2.75	122.80	126.94
2	D	2504	NAD	O7N-C7N-N7N	-2.73	118.75	122.59
3	A	2759	MES	O3S-S-O2S	-2.69	105.34	111.61
2	C	2501	NAD	O7N-C7N-N7N	-2.68	118.82	122.59
3	A	2760	MES	O3S-S-O2S	-2.62	105.51	111.61
3	C	2758	MES	O3S-S-O2S	-2.42	105.97	111.61
2	A	2503	NAD	C4A-C5A-N7A	-2.33	107.33	109.48
2	B	2502	NAD	C4A-C5A-N7A	-2.32	107.34	109.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2501	NAD	C4A-C5A-N7A	-2.30	107.36	109.48
2	D	2504	NAD	C4A-C5A-N7A	-2.26	107.40	109.48
3	C	2758	MES	C7-N4-C3	-2.11	105.86	111.27
3	A	2760	MES	C6-C5-N4	2.61	114.08	110.12
3	A	2759	MES	C6-C5-N4	2.70	114.22	110.12
3	C	2758	MES	C6-C5-N4	2.71	114.23	110.12
2	B	2502	NAD	C2B-C1B-N9A	2.99	118.86	114.29
2	A	2503	NAD	C2B-C1B-N9A	3.06	118.96	114.29
2	D	2504	NAD	C2B-C1B-N9A	3.18	119.15	114.29
2	C	2501	NAD	C2B-C1B-N9A	3.23	119.23	114.29
2	C	2501	NAD	C3N-C7N-N7N	4.81	123.08	117.82
2	B	2502	NAD	C3N-C7N-N7N	5.07	123.36	117.82
2	D	2504	NAD	C3N-C7N-N7N	5.12	123.42	117.82
2	A	2503	NAD	C3N-C7N-N7N	5.18	123.49	117.82
3	C	2758	MES	O3S-S-O1S	8.28	130.87	111.61
3	A	2760	MES	O3S-S-O1S	8.44	131.24	111.61
3	A	2759	MES	O3S-S-O1S	8.52	131.44	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2503	NAD	1	0
3	A	2759	MES	4	0
3	C	2758	MES	3	0
2	D	2504	NAD	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	438/439 (99%)	0.40	47 (10%) <b>8</b> <b>7</b>	14, 24, 54, 59	0
1	B	434/439 (98%)	0.17	23 (5%) <b>30</b> <b>27</b>	13, 21, 44, 53	0
1	C	438/439 (99%)	0.14	17 (3%) <b>43</b> <b>40</b>	11, 20, 41, 48	0
1	D	436/439 (99%)	0.12	15 (3%) <b>49</b> <b>45</b>	10, 19, 38, 54	0
All	All	1746/1756 (99%)	0.21	102 (5%) <b>26</b> <b>23</b>	10, 21, 46, 59	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	436	ILE	10.3
1	D	437	THR	10.2
1	A	437	THR	6.5
1	A	282	TRP	5.9
1	A	439	ALA	5.9
1	A	2	ILE	5.8
1	B	2	ILE	5.3
1	C	2	ILE	5.3
1	A	436	ILE	5.1
1	B	275	PRO	5.1
1	A	438	ARG	5.0
1	D	272	ARG	5.0
1	A	309	LYS	5.0
1	A	281	GLN	4.9
1	B	221	VAL	4.8
1	C	439	ALA	4.7
1	A	272	ARG	4.7
1	D	275	PRO	4.6
1	B	435	ALA	4.5
1	A	251	GLU	4.4
1	A	275	PRO	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	273	PRO	4.3
1	B	222	ASN	4.1
1	D	222	ASN	4.0
1	C	436	ILE	4.0
1	A	285	LYS	3.9
1	A	280	PRO	3.8
1	A	221	VAL	3.7
1	A	222	ASN	3.7
1	A	284	GLU	3.6
1	A	262	LYS	3.6
1	C	438	ARG	3.6
1	D	276	GLY	3.5
1	D	435	ALA	3.5
1	B	276	GLY	3.5
1	C	437	THR	3.4
1	A	278	ILE	3.4
1	D	2	ILE	3.3
1	A	435	ALA	3.3
1	A	263	ASP	3.2
1	A	274	GLY	3.2
1	D	274	GLY	3.1
1	A	276	GLY	3.0
1	C	364	GLU	3.0
1	C	275	PRO	3.0
1	B	268	ILE	3.0
1	A	232	LEU	2.9
1	B	281	GLN	2.9
1	B	251	GLU	2.9
1	A	231	ASP	2.8
1	B	309	LYS	2.8
1	D	288	GLU	2.8
1	B	271	THR	2.8
1	D	305	GLU	2.8
1	D	303	LEU	2.8
1	A	306	GLU	2.7
1	A	254	GLU	2.7
1	B	224	LYS	2.7
1	A	271	THR	2.7
1	A	305	GLU	2.7
1	C	224	LYS	2.7
1	C	222	ASN	2.7
1	C	272	ARG	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	277	VAL	2.6
1	A	321	ASP	2.6
1	C	281	GLN	2.6
1	C	270	PHE	2.6
1	B	272	ARG	2.6
1	A	303	LEU	2.5
1	A	310	ALA	2.5
1	A	258	GLN	2.5
1	B	254	GLU	2.5
1	B	270	PHE	2.5
1	A	364	GLU	2.4
1	B	31	ARG	2.4
1	B	305	GLU	2.4
1	B	231	ASP	2.4
1	B	279	LYS	2.4
1	B	226	ARG	2.4
1	A	295	LEU	2.3
1	C	258	GLN	2.3
1	C	413	ARG	2.3
1	A	223	GLY	2.3
1	A	228	LEU	2.3
1	B	191	LEU	2.3
1	A	413	ARG	2.3
1	A	311	GLY	2.3
1	C	251	GLU	2.2
1	D	4	GLU	2.2
1	A	31	ARG	2.2
1	A	279	LYS	2.2
1	B	4	GLU	2.2
1	A	299	VAL	2.2
1	A	270	PHE	2.1
1	A	237	LEU	2.1
1	C	51	ARG	2.1
1	D	281	GLN	2.1
1	A	51	ARG	2.1
1	B	288	GLU	2.1
1	A	226	ARG	2.0
1	A	365	GLU	2.0
1	C	288	GLU	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( $\text{\AA}^2$ )	Q<0.9
3	MES	A	2760	12/12	0.81	0.25	10.92	48,48,49,49	0
3	MES	A	2759	12/12	0.71	0.30	8.70	45,46,50,51	0
3	MES	C	2758	12/12	0.90	0.20	4.18	26,34,36,37	0
2	NAD	B	2502	44/44	0.83	0.20	1.76	34,36,41,43	0
2	NAD	D	2504	44/44	0.81	0.23	1.43	32,36,41,43	0
2	NAD	A	2503	44/44	0.86	0.18	0.70	41,45,48,49	0
2	NAD	C	2501	44/44	0.92	0.11	-0.10	23,27,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.