W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:46 pm GMT

|		
PDB ID	:	1LLQ
Title	:	Crystal Structure of Malic Enzyme from Ascaris suum Complexed with Nicotinamide Adenine Dinucleotide
Authors	:	Coleman, D.E.; Jagannatha, G.S.; Goldsmith, E.J.; Cook, P.F.; Harris, B.G.
Deposited on	:	2002-04-29
Resolution	:	2.30 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
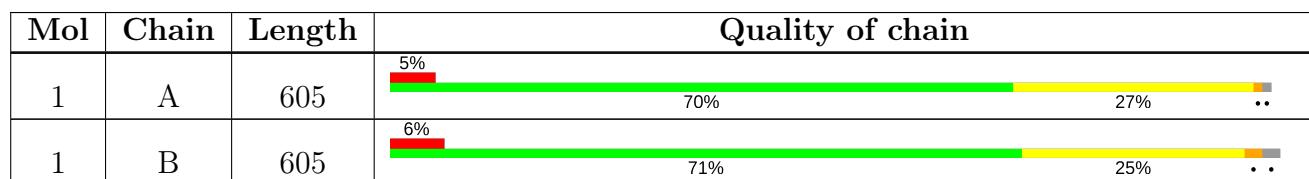
The reported resolution of this entry is 2.30 Å.

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 >=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 <=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	605	
1	B	605	

2 Entry composition ⓘ
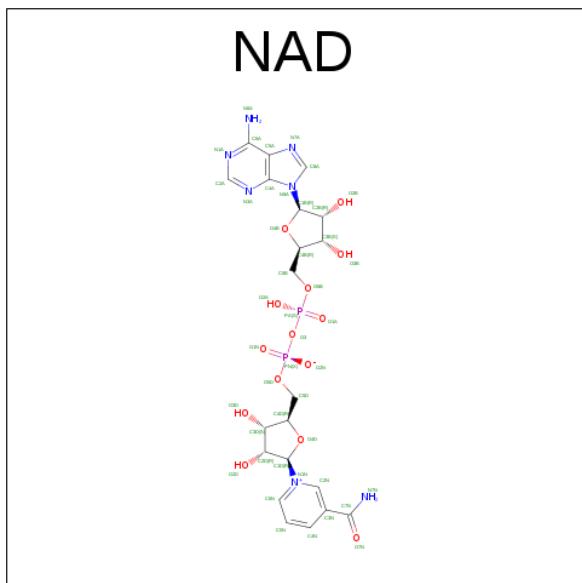
There are 3 unique types of molecules in this entry. The entry contains 9656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	109	0	0
			4775	3048	819	883	25			
1	B	592	Total	C	N	O	S	145	0	0
			4719	3011	807	876	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
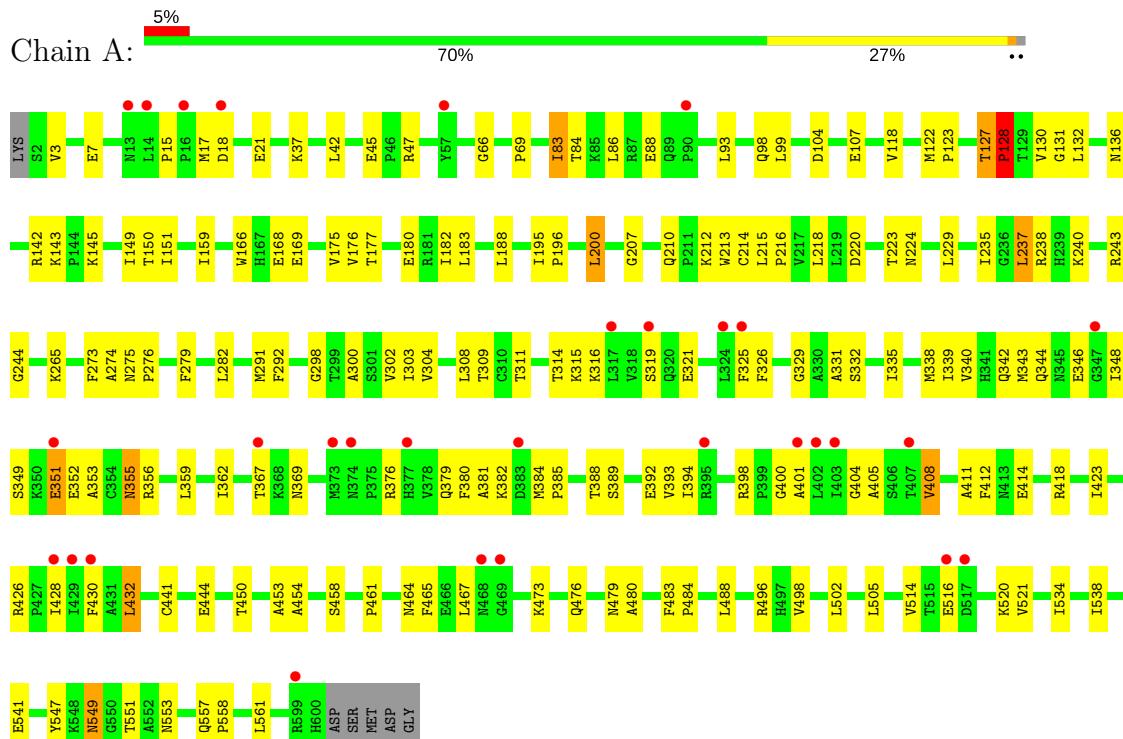
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	35	Total 35	O 35	0	0
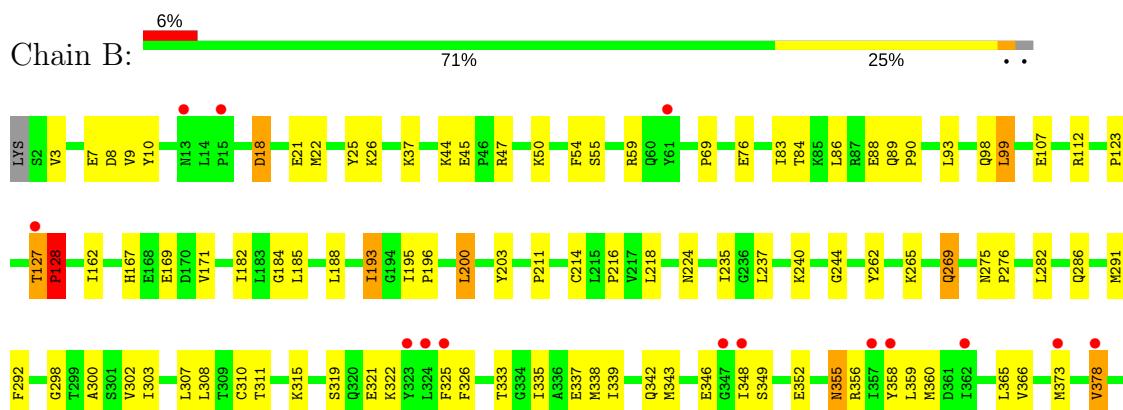
3 Residue-property plots ⓘ
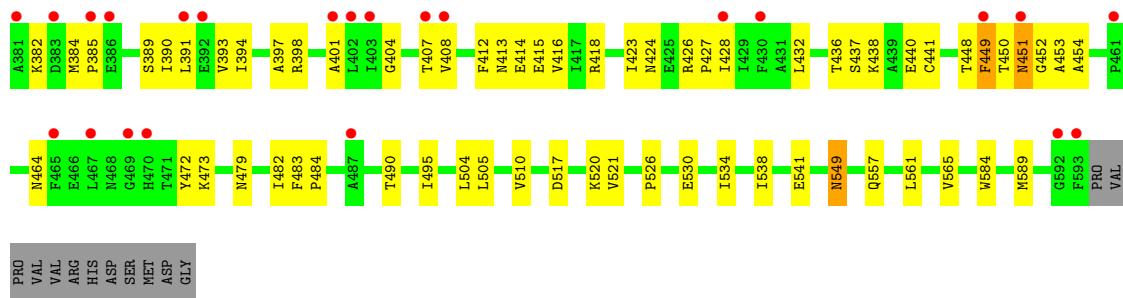
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NAD-dependent malic enzyme

Chain A:

- Molecule 1: NAD-dependent malic enzyme

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.62Å 130.62Å 149.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.51 – 2.30 24.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (24.51-2.30) 94.6 (24.57-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.28Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.247 , 0.280 0.247 , 0.280	Depositor DCC
R_{free} test set	3171 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9656	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/4880	0.59	0/6610
1	B	0.35	0/4821	0.61	0/6527
All	All	0.35	0/9701	0.60	0/13137

There are no bond length outliers.

There are no bond angle outliers.

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	4775	0	4771	149	0
1	B	4719	0	4710	129	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
3	A	39	0	0	1	0
3	B	35	0	0	2	0
All	All	9656	0	9533	274	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 15.

All (274) 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:B:384:MET:HB2	1:B:385:PRO:HD2	1.47	0.95
1:A:300:ALA:HB1	1:A:338:MET:HG3	1.47	0.94
1:B:200:LEU:HG	1:B:214:CYS:HB3	1.48	0.92
1:A:182:ILE:HD12	1:A:188:LEU:HB2	1.47	0.92
1:B:300:ALA:HB1	1:B:338:MET:HG3	1.53	0.91
1:A:384:MET:HB2	1:A:385:PRO:HD2	1.51	0.89
1:B:319:SER:HB2	1:B:348:ILE:HD12	1.56	0.88
1:B:302:VAL:HG21	1:B:479:ASN:HA	1.57	0.87
1:A:298:GLY:O	1:A:302:VAL:HG23	1.76	0.85
1:A:319:SER:HB2	1:A:348:ILE:HD12	1.57	0.85
1:A:127:THR:HB	1:A:128:PRO:CD	2.06	0.85
1:B:182:ILE:HD12	1:B:188:LEU:HD12	1.59	0.85
1:B:127:THR:HB	1:B:128:PRO:CD	2.07	0.84
1:B:22:MET:HE2	1:B:26:LYS:HE3	1.60	0.83
1:A:3:VAL:HG13	1:A:7:GLU:HB2	1.62	0.82
1:A:398:ARG:HB2	1:A:423:ILE:HG21	1.61	0.81
1:B:3:VAL:CG1	1:B:7:GLU:HB2	2.12	0.80
1:A:127:THR:HB	1:A:128:PRO:HD3	1.63	0.80
1:A:200:LEU:HG	1:A:214:CYS:HB3	1.62	0.80
1:B:3:VAL:HG13	1:B:7:GLU:HB2	1.65	0.79
1:B:348:ILE:HG22	1:B:349:SER:N	1.99	0.77
1:A:331:ALA:O	1:A:335:ILE:HG13	1.84	0.77
1:B:517:ASP:O	1:B:520:LYS:HG2	1.83	0.77
1:A:275:ASN:HB2	1:A:276:PRO:HD3	1.66	0.77
1:B:195:ILE:HB	1:B:196:PRO:HD3	1.65	0.76
1:B:412:PHE:HB2	1:B:441:CYS:HB3	1.69	0.74
1:B:348:ILE:HG22	1:B:349:SER:H	1.52	0.74
1:A:195:ILE:HB	1:A:196:PRO:HD3	1.70	0.74
1:B:47:ARG:HG2	1:B:107:GLU:OE2	1.88	0.73
1:B:413:ASN:OD1	1:B:416:VAL:HG23	1.89	0.73
1:A:321:GLU:OE2	1:A:400:GLY:HA3	1.89	0.72
1:B:355:ASN:HA	1:B:382:LYS:NZ	2.04	0.72
1:A:123:PRO:O	1:A:128:PRO:HD2	1.90	0.71
1:B:86:LEU:HD11	1:B:99:LEU:HD13	1.73	0.71
1:A:343:MET:HE3	1:A:353:ALA:HB1	1.72	0.70
1:B:300:ALA:CB	1:B:338:MET:HG3	2.22	0.70
1:B:184:GLY:O	1:B:185:LEU:HD23	1.90	0.70
1:B:123:PRO:HA	1:B:127:THR:HB	1.74	0.69
1:A:450:THR:HG21	1:A:454:ALA:HB2	1.73	0.69
1:A:348:ILE:HG22	1:A:349:SER:N	2.08	0.68
1:A:302:VAL:HG21	1:A:479:ASN:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HA	1:A:127:THR:HB	1.76	0.68
1:A:93:LEU:HD11	1:A:132:LEU:HD23	1.75	0.67
1:B:298:GLY:O	1:B:302:VAL:HG23	1.93	0.67
1:B:127:THR:HB	1:B:128:PRO:HD3	1.76	0.67
1:B:342:GLN:O	1:B:346:GLU:HG3	1.95	0.67
1:B:127:THR:CG2	1:B:128:PRO:HD3	2.25	0.67
1:B:333:THR:O	1:B:337:GLU:HG3	1.95	0.66
1:B:398:ARG:HB3	1:B:423:ILE:HG21	1.76	0.66
1:B:182:ILE:CD1	1:B:188:LEU:HD12	2.25	0.66
1:A:335:ILE:O	1:A:339:ILE:HG13	1.96	0.66
1:B:84:THR:O	1:B:88:GLU:HG3	1.95	0.65
1:B:450:THR:HG21	1:B:454:ALA:HB2	1.76	0.65
1:A:319:SER:HB2	1:A:348:ILE:CD1	2.27	0.65
1:A:127:THR:CB	1:A:128:PRO:HD3	2.27	0.64
1:A:182:ILE:HD12	1:A:188:LEU:CB	2.26	0.64
1:A:355:ASN:HA	1:A:382:LYS:HE3	1.79	0.64
1:A:401:ALA:CB	1:A:428:ILE:HB	2.27	0.64
1:B:127:THR:CB	1:B:128:PRO:CD	2.75	0.64
1:B:22:MET:HE3	1:B:25:TYR:HD2	1.62	0.64
1:B:404:GLY:HA3	1:B:440:GLU:HG2	1.80	0.63
1:B:365:LEU:HG	1:B:366:VAL:H	1.61	0.63
1:A:180:GLU:HG2	1:A:274:ALA:HB2	1.81	0.63
1:A:182:ILE:HD12	1:A:188:LEU:HD12	1.81	0.62
1:B:127:THR:CB	1:B:128:PRO:HD3	2.29	0.62
1:A:300:ALA:CB	1:A:338:MET:HG3	2.27	0.61
1:B:22:MET:CE	1:B:26:LYS:HE3	2.28	0.61
1:B:365:LEU:HG	1:B:366:VAL:N	2.16	0.61
1:A:558:PRO:HG2	1:A:561:LEU:HD23	1.83	0.61
1:B:348:ILE:CG2	1:B:349:SER:H	2.13	0.61
1:B:561:LEU:O	1:B:565:VAL:HG23	2.00	0.60
1:A:182:ILE:CD1	1:A:188:LEU:HB2	2.26	0.60
1:A:498:VAL:HA	1:A:502:LEU:HD12	1.83	0.60
1:A:104:ASP:OD1	1:A:145:LYS:HE3	2.01	0.60
1:B:127:THR:HG22	1:B:128:PRO:HD3	1.83	0.60
1:B:549:ASN:C	1:B:549:ASN:HD22	2.05	0.59
1:A:321:GLU:O	1:A:356:ARG:HD3	2.02	0.59
1:A:3:VAL:CG1	1:A:7:GLU:HB2	2.30	0.59
1:B:282:LEU:HA	1:B:291:MET:CE	2.33	0.59
1:B:530:GLU:O	1:B:534:ILE:HG13	2.03	0.59
1:B:521:VAL:O	1:B:521:VAL:HG12	2.02	0.58
1:A:412:PHE:HB2	1:A:441:CYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PRO:HB3	1:B:235:ILE:HD13	1.86	0.58
1:B:355:ASN:HA	1:B:382:LYS:HZ1	1.66	0.58
1:B:55:SER:O	1:B:59:ARG:HG3	2.04	0.58
1:A:84:THR:O	1:A:88:GLU:HG3	2.03	0.58
1:B:321:GLU:HG3	1:B:322:LYS:H	1.69	0.58
1:A:340:VAL:HG12	1:A:344:GLN:HE21	1.68	0.57
1:A:127:THR:CB	1:A:128:PRO:CD	2.79	0.57
1:A:339:ILE:O	1:A:343:MET:HG3	2.05	0.57
1:B:473:LYS:HD2	1:B:521:VAL:HG11	1.86	0.57
1:B:391:LEU:HD21	1:B:415:GLU:O	2.04	0.57
1:A:348:ILE:CG2	1:A:349:SER:N	2.67	0.57
1:B:584:TRP:HB2	1:B:589:MET:HG2	1.87	0.57
1:B:22:MET:CE	1:B:25:TYR:HD2	2.18	0.56
1:A:414:GLU:O	1:A:418:ARG:HG2	2.05	0.56
1:A:458:SER:O	1:A:476:GLN:HA	2.04	0.56
1:A:210:GLN:HB2	1:A:213:TRP:CD2	2.40	0.56
1:B:549:ASN:C	1:B:549:ASN:ND2	2.57	0.56
1:A:549:ASN:C	1:A:549:ASN:HD22	2.08	0.56
1:A:547:TYR:CE1	1:A:557:GLN:HG3	2.41	0.56
1:A:505:LEU:C	1:A:505:LEU:HD23	2.26	0.55
1:A:389:SER:HB3	1:A:392:GLU:HB2	1.89	0.55
1:A:42:LEU:HD23	1:A:42:LEU:C	2.27	0.55
1:B:182:ILE:HD12	1:B:188:LEU:CD1	2.36	0.55
1:B:452:GLY:HA3	1:B:472:TYR:OH	2.07	0.55
1:B:326:PHE:HE2	1:B:408:VAL:HG21	1.72	0.55
1:B:282:LEU:O	1:B:286:GLN:HB2	2.07	0.55
1:A:309:THR:HG21	1:A:514:VAL:HG21	1.89	0.54
1:A:394:ILE:O	1:A:398:ARG:HA	2.08	0.54
1:A:93:LEU:CD1	1:A:132:LEU:HD23	2.37	0.54
1:A:122:MET:N	1:A:123:PRO:HD2	2.24	0.53
1:B:505:LEU:HD11	1:B:541:GLU:HG3	1.88	0.53
1:A:149:ILE:HD13	1:A:159:ILE:HG23	1.90	0.53
1:A:224:ASN:HD21	1:A:243:ARG:NH2	2.06	0.53
1:A:505:LEU:HD21	1:A:541:GLU:HB3	1.89	0.53
1:B:127:THR:HB	1:B:128:PRO:HD2	1.90	0.53
1:A:223:THR:O	1:A:240:LYS:HA	2.09	0.53
1:A:516:GLU:O	1:A:520:LYS:HG3	2.10	0.52
1:A:521:VAL:HG12	1:A:521:VAL:O	2.09	0.52
1:A:352:GLU:O	1:A:356:ARG:HG3	2.09	0.52
1:B:325:PHE:HB2	1:B:359:LEU:HD23	1.91	0.52
1:B:352:GLU:O	1:B:356:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ILE:O	1:B:538:ILE:HG13	2.09	0.52
1:A:342:GLN:O	1:A:346:GLU:HG3	2.10	0.51
1:A:18:ASP:HB3	1:A:21:GLU:CG	2.41	0.51
1:B:394:ILE:O	1:B:398:ARG:HA	2.10	0.51
1:B:448:THR:C	1:B:450:THR:H	2.12	0.51
1:A:348:ILE:CG2	1:A:349:SER:H	2.23	0.51
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.10	0.51
1:B:384:MET:HB2	1:B:385:PRO:CD	2.30	0.51
1:B:490:THR:HA	1:B:495:ILE:HD12	1.93	0.51
1:B:505:LEU:HD23	1:B:505:LEU:C	2.31	0.51
1:A:15:PRO:O	1:A:17:MET:HG3	2.11	0.51
1:A:332:SER:OG	1:A:405:ALA:HB3	2.11	0.51
1:B:22:MET:HE2	1:B:26:LYS:CE	2.34	0.51
1:A:127:THR:CG2	1:A:128:PRO:HD3	2.41	0.51
1:B:450:THR:HG21	1:B:454:ALA:N	2.26	0.51
1:A:302:VAL:CG2	1:A:479:ASN:HA	2.40	0.51
1:B:269:GLN:HG3	1:B:292:PHE:CZ	2.45	0.51
1:B:360:MET:HG2	1:B:365:LEU:HD12	1.94	0.50
1:A:549:ASN:ND2	1:A:549:ASN:C	2.65	0.50
1:A:182:ILE:CD1	1:A:188:LEU:HD12	2.42	0.50
1:B:348:ILE:CG2	1:B:349:SER:N	2.66	0.50
1:A:224:ASN:ND2	1:A:243:ARG:NH2	2.60	0.49
1:A:465:PHE:CE2	1:A:467:LEU:HB2	2.47	0.49
1:B:171:VAL:HB	1:B:262:TYR:CD2	2.47	0.49
1:A:384:MET:HB2	1:A:385:PRO:CD	2.29	0.49
1:A:130:VAL:HG13	1:A:131:GLY:N	2.27	0.49
1:A:547:TYR:CD1	1:A:557:GLN:HG3	2.47	0.49
1:B:224:ASN:OD1	1:B:240:LYS:HB3	2.13	0.49
1:A:557:GLN:NE2	3:A:2014:HOH:O	2.34	0.48
1:A:401:ALA:HB2	1:A:428:ILE:HB	1.95	0.48
1:A:380:PHE:O	1:A:382:LYS:NZ	2.43	0.48
1:B:193:ILE:O	1:B:196:PRO:HD2	2.14	0.48
1:A:308:LEU:O	1:A:311:THR:HB	2.14	0.48
1:A:398:ARG:HB2	1:A:423:ILE:CG2	2.40	0.48
1:B:319:SER:HB2	1:B:348:ILE:CD1	2.38	0.48
1:B:414:GLU:HB2	1:B:449:PHE:CE1	2.48	0.48
1:A:389:SER:O	1:A:393:VAL:HG23	2.14	0.48
1:A:388:THR:O	1:A:388:THR:HG22	2.14	0.48
1:A:496:ARG:HG3	1:A:551:THR:O	2.14	0.48
1:A:349:SER:OG	1:A:351:GLU:HG3	2.14	0.47
1:B:436:THR:C	1:B:438:LYS:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:NZ	1:B:45:GLU:OE2	2.47	0.47
1:B:76:GLU:HG3	1:B:112:ARG:HH22	1.79	0.47
1:A:176:VAL:HG22	1:A:177:THR:N	2.30	0.47
1:B:373:MET:SD	1:B:378:VAL:HG22	2.54	0.47
1:A:224:ASN:ND2	1:A:243:ARG:HH21	2.11	0.47
1:B:282:LEU:HA	1:B:291:MET:HE3	1.96	0.47
1:A:123:PRO:HA	1:A:127:THR:CB	2.44	0.47
1:A:348:ILE:HG22	1:A:349:SER:H	1.80	0.47
1:B:308:LEU:O	1:B:311:THR:HB	2.15	0.46
1:B:8:ASP:OD1	1:B:9:VAL:N	2.48	0.46
1:A:326:PHE:CE2	1:A:411:ALA:HB1	2.50	0.46
1:B:321:GLU:HG3	1:B:322:LYS:N	2.30	0.46
1:B:414:GLU:O	1:B:418:ARG:HG2	2.15	0.46
1:A:325:PHE:HB2	1:A:359:LEU:HD23	1.96	0.46
1:A:534:ILE:O	1:A:538:ILE:HG13	2.15	0.46
1:A:83:ILE:HG22	1:A:84:THR:N	2.30	0.46
1:B:123:PRO:O	1:B:128:PRO:HD2	2.16	0.46
1:A:47:ARG:HG2	1:A:107:GLU:OE2	2.15	0.46
1:B:182:ILE:HD12	1:B:188:LEU:HB2	1.97	0.46
1:B:200:LEU:O	1:B:203:TYR:HB2	2.16	0.46
1:A:430:PHE:HB3	1:A:432:LEU:HD13	1.97	0.46
1:A:243:ARG:HG2	1:A:243:ARG:HH11	1.81	0.46
1:A:367:THR:O	1:A:381:ALA:HB1	2.16	0.45
1:B:18:ASP:O	1:B:21:GLU:N	2.49	0.45
1:B:211:PRO:HD2	3:B:2054:HOH:O	2.17	0.45
1:B:339:ILE:HG22	1:B:343:MET:HE2	1.99	0.45
1:A:224:ASN:HD21	1:A:243:ARG:HH21	1.62	0.45
1:A:300:ALA:O	1:A:304:VAL:HG23	2.16	0.45
1:A:168:GLU:HG2	1:A:212:LYS:O	2.17	0.45
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.82	0.45
1:B:464:ASN:CG	1:B:473:LYS:HG2	2.36	0.45
1:A:200:LEU:HD23	1:A:216:PRO:HG3	1.99	0.45
1:A:177:THR:HA	1:A:273:PHE:CE1	2.52	0.45
1:A:355:ASN:HD22	1:A:382:LYS:HE3	1.82	0.45
1:B:426:ARG:HA	1:B:453:ALA:O	2.17	0.45
1:B:22:MET:CE	1:B:25:TYR:CD2	2.99	0.45
1:A:291:MET:HG2	1:A:292:PHE:N	2.33	0.44
1:A:104:ASP:HB3	1:A:143:LYS:HD2	2.00	0.44
1:A:218:LEU:HD23	1:A:218:LEU:C	2.37	0.44
1:A:314:THR:O	1:A:316:LYS:N	2.50	0.44
1:A:66:GLY:HA3	1:B:162:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HD21	1:B:541:GLU:HB3	1.99	0.44
1:A:340:VAL:HA	1:A:343:MET:CE	2.48	0.44
1:A:340:VAL:HA	1:A:343:MET:HE2	1.98	0.44
1:A:86:LEU:HD13	1:A:98:GLN:NE2	2.32	0.44
1:A:282:LEU:HA	1:A:291:MET:CE	2.47	0.44
1:B:282:LEU:HA	1:B:291:MET:HE1	1.99	0.44
1:A:321:GLU:N	1:A:356:ARG:NH1	2.65	0.44
1:A:483:PHE:CG	1:A:484:PRO:HD3	2.52	0.44
1:A:143:LYS:HD3	1:B:44:LYS:HE2	2.00	0.43
1:A:37:LYS:NZ	1:A:45:GLU:OE2	2.50	0.43
1:A:473:LYS:H	1:A:521:VAL:HG12	1.83	0.43
1:B:450:THR:HG21	1:B:454:ALA:CB	2.44	0.43
1:A:408:VAL:HB	1:A:411:ALA:HB2	1.99	0.43
1:A:235:ILE:HD13	1:B:69:PRO:HB3	1.99	0.43
1:A:150:THR:HG22	1:A:220:ASP:HB3	2.01	0.43
1:A:83:ILE:CG2	1:A:84:THR:N	2.82	0.43
1:A:379:GLN:HG3	1:A:380:PHE:CD1	2.54	0.43
1:B:414:GLU:HA	1:B:449:PHE:CD1	2.54	0.43
1:A:175:VAL:HB	1:A:200:LEU:HD22	2.01	0.43
1:B:358:TYR:CD2	1:B:382:LYS:HG3	2.54	0.43
1:A:122:MET:N	1:A:123:PRO:CD	2.82	0.42
1:B:348:ILE:HG21	1:B:352:GLU:HB2	1.99	0.42
1:B:389:SER:O	1:B:393:VAL:HG23	2.19	0.42
1:B:303:ILE:HG21	1:B:335:ILE:HD13	2.01	0.42
1:B:510:VAL:HG13	1:B:526:PRO:HG2	2.01	0.42
1:A:303:ILE:HG13	1:A:335:ILE:HD13	2.00	0.42
1:A:473:LYS:N	1:A:521:VAL:HG12	2.35	0.42
1:B:473:LYS:CD	1:B:521:VAL:HG11	2.50	0.42
1:A:130:VAL:CG1	1:A:131:GLY:N	2.83	0.42
1:A:329:GLY:HA3	2:A:1001:NAD:O5B	2.20	0.42
1:A:136:ASN:N	1:A:136:ASN:HD22	2.18	0.42
1:A:210:GLN:HB2	1:A:213:TRP:CE3	2.54	0.41
1:B:557:GLN:NE2	3:B:2050:HOH:O	2.53	0.41
1:A:166:TRP:CE2	1:A:215:LEU:HD13	2.55	0.41
1:B:307:LEU:O	1:B:310:CYS:HB2	2.20	0.41
1:B:86:LEU:HD13	1:B:98:GLN:NE2	2.34	0.41
1:B:193:ILE:O	1:B:193:ILE:HG13	2.20	0.41
1:B:200:LEU:HD23	1:B:216:PRO:HG3	2.03	0.41
1:A:182:ILE:HD12	1:A:188:LEU:CD1	2.50	0.41
1:A:229:LEU:O	1:A:238:ARG:NH2	2.53	0.41
1:A:118:VAL:O	1:A:122:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:CB	1:A:276:PRO:HD3	2.43	0.41
1:B:397:ALA:O	1:B:398:ARG:C	2.58	0.41
1:B:450:THR:HG22	1:B:453:ALA:H	1.85	0.41
1:A:18:ASP:HB3	1:A:21:GLU:HG3	2.03	0.41
1:A:401:ALA:HB2	1:A:428:ILE:HD12	2.03	0.41
1:A:42:LEU:O	1:A:42:LEU:HD23	2.20	0.41
1:A:426:ARG:HD2	1:A:453:ALA:HB1	2.03	0.41
1:B:218:LEU:HD23	1:B:218:LEU:C	2.41	0.41
1:B:275:ASN:HB2	1:B:276:PRO:HD3	2.02	0.41
1:B:83:ILE:HA	1:B:83:ILE:HD13	1.92	0.41
1:A:444:GLU:HG2	1:A:465:PHE:CD1	2.56	0.41
1:A:480:ALA:HA	1:A:483:PHE:CE2	2.55	0.41
1:B:401:ALA:CB	1:B:428:ILE:HB	2.51	0.41
1:B:483:PHE:N	1:B:484:PRO:CD	2.84	0.41
1:A:464:ASN:CG	1:A:473:LYS:HG2	2.42	0.41
1:B:302:VAL:HG22	1:B:482:ILE:HG12	2.02	0.41
1:B:89:GLN:HA	1:B:90:PRO:HD3	1.91	0.41
1:B:360:MET:HE3	1:B:390:ILE:HG12	2.02	0.41
1:B:391:LEU:HD21	1:B:415:GLU:C	2.41	0.40
1:B:50:LYS:HD2	1:B:54:PHE:CD2	2.56	0.40
1:A:461:PRO:HG3	1:A:476:GLN:OE1	2.21	0.40
1:A:207:GLY:O	1:A:488:LEU:HD22	2.20	0.40
1:B:448:THR:O	1:B:450:THR:N	2.54	0.40
1:A:151:ILE:O	1:A:151:ILE:HG13	2.21	0.40
1:A:404:GLY:O	1:A:432:LEU:HB2	2.22	0.40
1:B:483:PHE:CG	1:B:484:PRO:HD3	2.57	0.40
1:A:279:PHE:CE1	1:A:376:ARG:CZ	3.04	0.40
1:B:424:ASN:O	1:B:427:PRO:HD3	2.22	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	597/605 (99%)	553 (93%)	38 (6%)	6 (1%)	18	20
1	B	590/605 (98%)	543 (92%)	37 (6%)	10 (2%)	11	9
All	All	1187/1210 (98%)	1096 (92%)	75 (6%)	16 (1%)	14	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	THR
1	B	127	THR
1	B	407	THR
1	A	128	PRO
1	A	244	GLY
1	A	315	LYS
1	B	378	VAL
1	B	437	SER
1	B	449	PHE
1	A	369	ASN
1	B	128	PRO
1	A	183	LEU
1	B	244	GLY
1	B	10	TYR
1	B	315	LYS
1	B	451	ASN

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	512/517 (99%)	497 (97%)	15 (3%)	48	64
1	B	505/517 (98%)	489 (97%)	16 (3%)	44	60
All	All	1017/1034 (98%)	986 (97%)	31 (3%)	46	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ILE
1	A	99	LEU
1	A	128	PRO
1	A	142	ARG
1	A	169	GLU
1	A	200	LEU
1	A	237	LEU
1	A	265	LYS
1	A	351	GLU
1	A	355	ASN
1	A	362	ILE
1	A	408	VAL
1	A	432	LEU
1	A	549	ASN
1	A	553	ASN
1	B	18	ASP
1	B	93	LEU
1	B	99	LEU
1	B	128	PRO
1	B	167	HIS
1	B	169	GLU
1	B	193	ILE
1	B	200	LEU
1	B	237	LEU
1	B	265	LYS
1	B	269	GLN
1	B	355	ASN
1	B	432	LEU
1	B	451	ASN
1	B	504	LEU
1	B	549	ASN

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	13	ASN
1	A	135	GLN
1	A	136	ASN
1	A	224	ASN
1	A	286	GLN
1	A	320	GLN
1	A	341	HIS
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	468	ASN
1	A	549	ASN
1	B	136	ASN
1	B	286	GLN
1	B	341	HIS
1	B	344	GLN
1	B	355	ASN
1	B	549	ASN
1	B	557	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 ⓘ

2 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	1001	-	41,48,48	1.91	8 (19%)	43,73,73	1.50	6 (13%)
2	NAD	B	1002	-	41,48,48	1.94	8 (19%)	43,73,73	1.54	7 (16%)

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	1001	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1002	-	-	0/22/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAD	O4B-C1B	2.21	1.44	1.41
2	A	1001	NAD	O4D-C1D	2.29	1.44	1.41
2	B	1002	NAD	O4D-C1D	2.38	1.44	1.41
2	A	1001	NAD	PN-O1N	2.38	1.59	1.50
2	B	1002	NAD	C4N-C3N	2.50	1.43	1.39
2	B	1002	NAD	PA-O1A	2.53	1.60	1.50
2	B	1002	NAD	PN-O1N	2.55	1.60	1.50
2	A	1001	NAD	C4N-C3N	2.66	1.43	1.39
2	B	1002	NAD	O4B-C1B	2.68	1.45	1.41
2	A	1001	NAD	PA-O1A	2.69	1.61	1.50
2	A	1001	NAD	C5A-C4A	2.87	1.47	1.40
2	A	1001	NAD	C2N-C3N	2.93	1.43	1.39
2	B	1002	NAD	C5A-C4A	2.94	1.47	1.40
2	B	1002	NAD	C2N-C3N	3.45	1.44	1.39
2	B	1002	NAD	C4A-N3A	9.09	1.48	1.35
2	A	1001	NAD	C4A-N3A	9.19	1.49	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	NAD	O7N-C7N-N7N	-6.02	114.02	122.58
2	A	1001	NAD	O7N-C7N-N7N	-5.88	114.22	122.58
2	A	1001	NAD	N6A-C6A-N1A	-2.45	113.91	118.77
2	B	1002	NAD	N6A-C6A-N1A	-2.43	113.94	118.77
2	B	1002	NAD	C2N-C3N-C7N	2.06	125.32	119.34
2	B	1002	NAD	C3N-C2N-N1N	2.12	122.56	120.43
2	A	1001	NAD	C3N-C2N-N1N	2.16	122.61	120.43
2	B	1002	NAD	C5A-C6A-N6A	2.19	124.94	120.47
2	A	1001	NAD	C5A-C6A-N6A	2.21	124.98	120.47
2	B	1002	NAD	O7N-C7N-C3N	3.51	123.72	119.62
2	A	1001	NAD	O7N-C7N-C3N	3.60	123.83	119.62
2	A	1001	NAD	C3N-C7N-N7N	3.65	121.94	117.77
2	B	1002	NAD	C3N-C7N-N7N	3.92	122.25	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	595/605 (98%)	0.18	30 (5%)	30	36	27, 49, 86, 96	17 (2%)
1	B	588/605 (97%)	0.12	37 (6%)	21	27	23, 43, 88, 103	26 (4%)
All	All	1183/1210 (97%)	0.15	67 (5%)	24	31	23, 47, 87, 103	43 (3%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	LEU	5.2
1	B	385	PRO	4.4
1	A	599	ARG	4.1
1	A	373	MET	4.1
1	A	377	HIS	4.0
1	B	465	PHE	4.0
1	B	381	ALA	3.9
1	B	383	ASP	3.9
1	B	593	PHE	3.8
1	A	468	ASN	3.8
1	A	402	LEU	3.6
1	A	324	LEU	3.6
1	A	367	THR	3.6
1	B	467	LEU	3.4
1	A	347	GLY	3.3
1	A	383	ASP	3.2
1	B	348	ILE	3.2
1	B	401	ALA	3.2
1	B	324	LEU	3.2
1	B	403	ILE	3.2
1	B	451	ASN	3.2
1	A	401	ALA	3.2
1	A	395	ARG	3.1
1	B	428	ILE	3.1

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	A	13	ASN	3.0
1	A	317	LEU	2.9
1	A	351	GLU	2.9
1	A	403	ILE	2.9
1	B	378	VAL	2.9
1	B	386	GLU	2.8
1	B	373	MET	2.8
1	A	430	PHE	2.8
1	A	469	GLY	2.7
1	A	407	THR	2.7
1	A	517	ASP	2.7
1	A	428	ILE	2.7
1	A	319	SER	2.7
1	B	362	ILE	2.6
1	B	449	PHE	2.6
1	B	392	GLU	2.6
1	B	13	ASN	2.5
1	B	592	GLY	2.5
1	B	357	ILE	2.4
1	A	16	PRO	2.4
1	B	127	THR	2.4
1	B	408	VAL	2.4
1	B	430	PHE	2.4
1	A	374	ASN	2.4
1	A	429	ILE	2.3
1	B	15	PRO	2.3
1	B	61	TYR	2.3
1	A	14	LEU	2.2
1	A	57	TYR	2.2
1	A	516	GLU	2.2
1	A	325	PHE	2.2
1	B	470	HIS	2.2
1	B	347	GLY	2.2
1	B	469	GLY	2.1
1	B	325	PHE	2.1
1	B	407	THR	2.1
1	B	358	TYR	2.1
1	A	90	PRO	2.1
1	B	461	PRO	2.1
1	A	18	ASP	2.0
1	B	323	TYR	2.0
1	B	391	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	487	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAD	A	1001	44/44	0.92	0.14	-0.07	65,68,74,74	0
2	NAD	B	1002	44/44	0.92	0.13	-0.21	55,64,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.