



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:54 PM GMT

PDB ID : 1D1S
Title : WILD-TYPE HUMAN SIGMA (CLASS IV) ALCOHOL DEHYDROGE-
NASE
Authors : Xie, P.T.; Hurley, T.D.
Deposited on : 1999-09-21
Resolution : 2.50 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
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

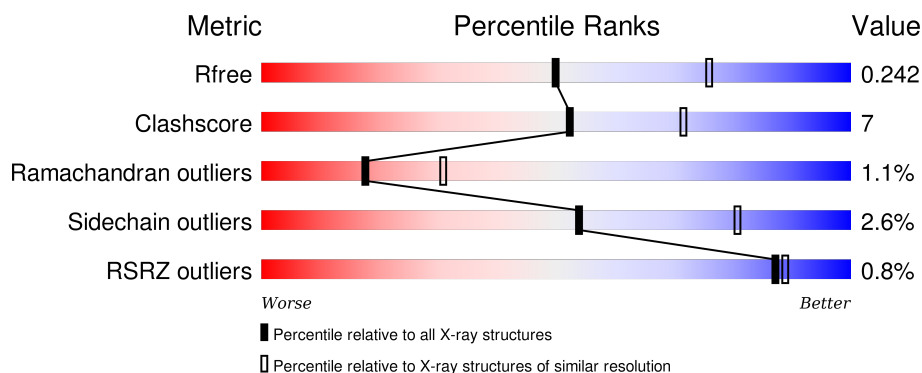
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	373	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	373	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	373	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	D	373	<div> <div>87%</div> <div>12%</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	ACT	A	501	-	-	-	X
3	ACT	B	506	-	-	X	-
3	ACT	D	511	-	-	-	X
4	CAC	B	555	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11836 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.

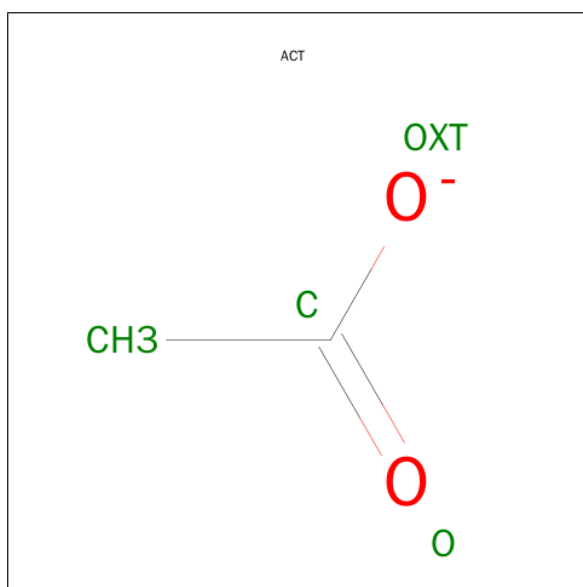
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

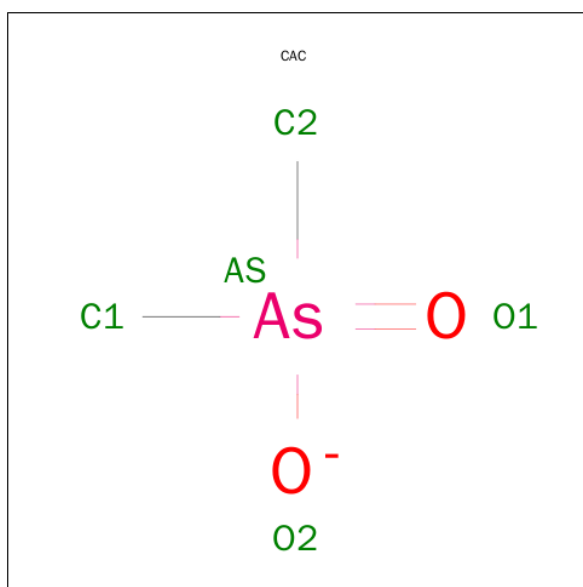
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	6	Total	Zn	0	0
			6	6		
2	D	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



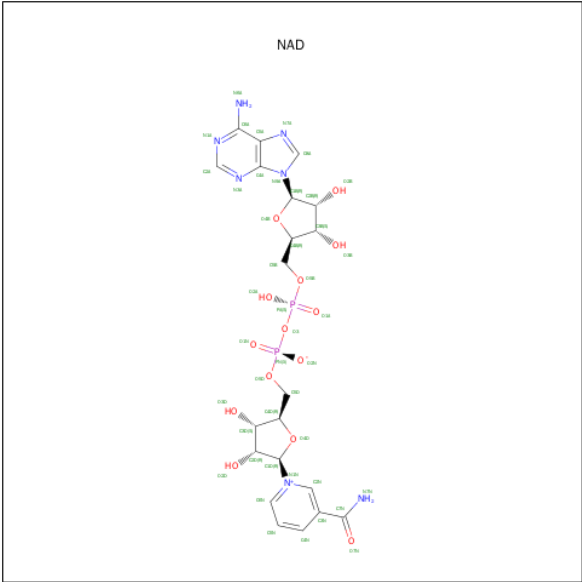
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

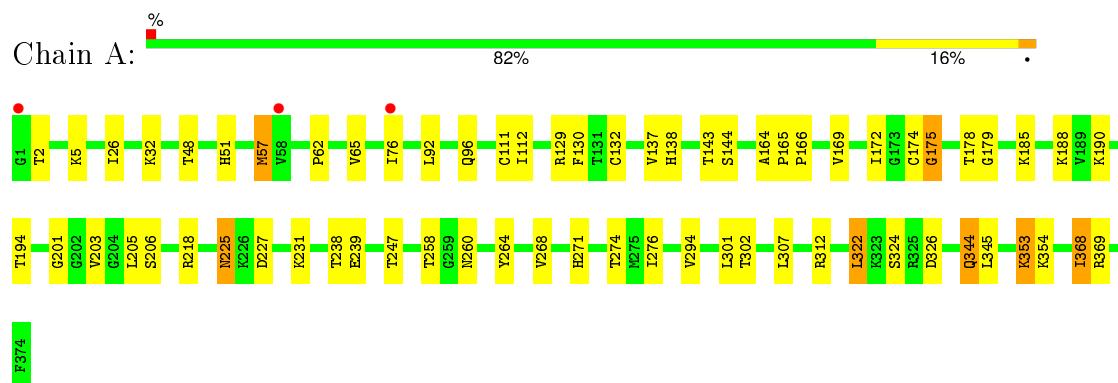
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	124	Total	O	0	0
			124	124		
6	C	58	Total	O	0	0
			58	58		
6	D	135	Total	O	0	0
			135	135		

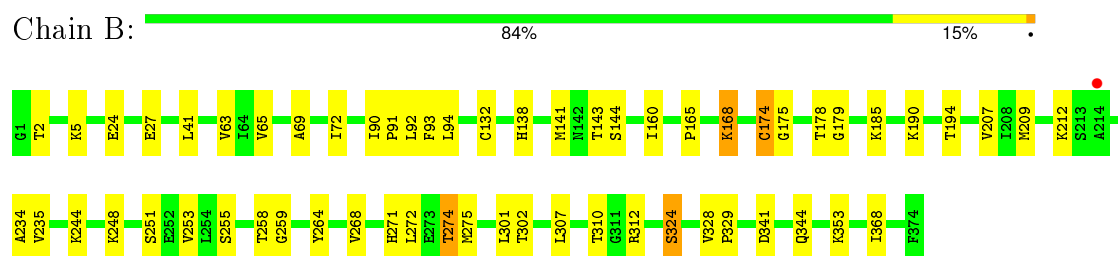
3 Residue-property plots

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.

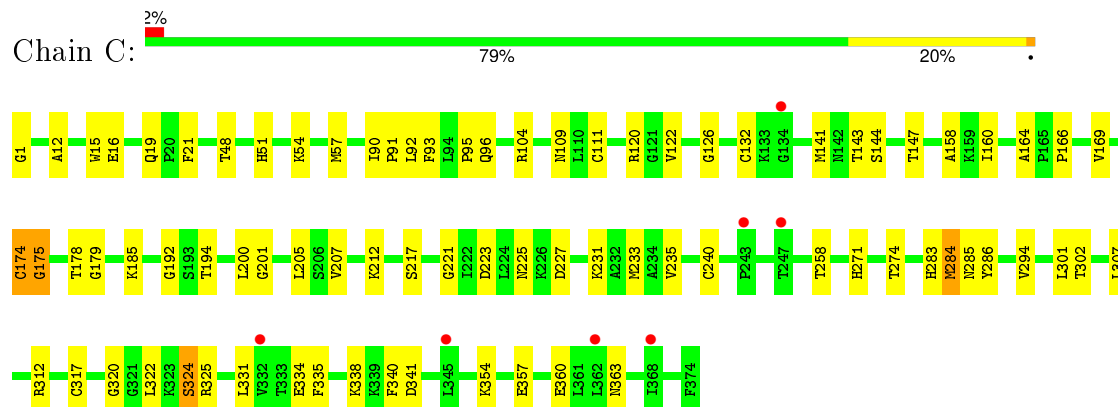
• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN



• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN



• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

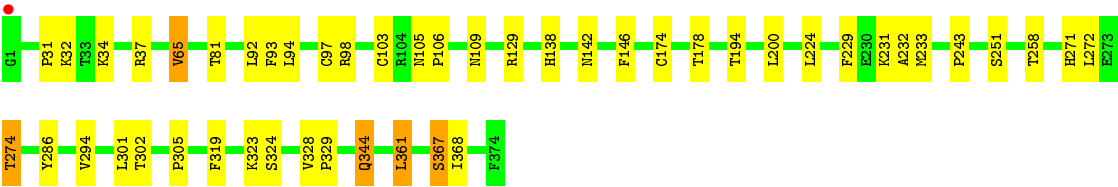


• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain D:

87%

12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40 Å 90.90 Å 121.10 Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.50) 87.9 (49.90-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.51 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.217 , 0.268 0.198 , 0.242	Depositor DCC
R_{free} test set	4166 reflections (7.95%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 58662 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11836	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CAC, ZN, NAD, ACT

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	0.46	0/2840	0.71	2/3839 (0.1%)
1	B	0.50	0/2840	0.73	1/3839 (0.0%)
1	C	0.41	0/2840	0.66	0/3839
1	D	0.49	0/2840	0.73	1/3839 (0.0%)
All	All	0.47	0/11360	0.71	4/15356 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	368	ILE	N-CA-C	-5.57	95.97	111.00
1	D	323	LYS	N-CA-C	-5.22	96.89	111.00
1	A	368	ILE	N-CA-C	-5.20	96.95	111.00

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	2789	0	2858	41	0
1	B	2789	0	2858	32	0
1	C	2789	0	2858	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2789	0	2858	32	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
3	A	16	0	12	1	0
3	B	8	0	6	2	0
3	C	8	0	6	0	0
3	D	20	0	15	2	0
4	A	5	0	0	0	0
4	B	20	0	0	1	0
5	A	44	0	26	3	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	2	0
6	A	91	0	0	3	0
6	B	124	0	0	2	0
6	C	58	0	0	4	0
6	D	135	0	0	5	0
All	All	11836	0	11575	154	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 (154) 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:341:ASP:HB3	1:B:344:GLN:NE2	1.92	0.85
1:A:130:PHE:HB2	1:A:137:VAL:HG23	1.64	0.79
1:C:301:LEU:HB2	1:D:305:PRO:HG3	1.65	0.78
1:B:271:HIS:HB2	1:B:274:THR:OG1	1.84	0.77
1:B:41:LEU:HD11	1:B:72:ILE:HG12	1.69	0.74
1:C:307:LEU:O	1:C:312:ARG:HD2	1.89	0.72
1:D:231:LYS:HE2	1:D:344:GLN:NE2	2.04	0.72
1:C:178:THR:HG21	5:C:3377:NAD:C4N	2.21	0.71
1:B:24:GLU:HG2	1:B:132:CYS:SG	2.32	0.70
1:C:283:HIS:HD2	1:C:286:TYR:H	1.41	0.68
1:D:92:LEU:HD13	1:D:324:SER:HB2	1.77	0.66
1:C:192:GLY:HA2	1:C:217:SER:OG	1.97	0.64
1:D:344:GLN:HB2	6:D:882:HOH:O	1.98	0.63
1:B:92:LEU:HD13	1:B:324:SER:HB3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CB	1:A:137:VAL:HG23	2.30	0.61
1:C:301:LEU:HD12	1:C:302:THR:N	2.16	0.60
1:D:142:ASN:ND2	6:D:982:HOH:O	2.36	0.59
1:C:109:ASN:HA	6:C:959:HOH:O	2.03	0.58
1:C:301:LEU:HD12	1:C:302:THR:H	1.68	0.58
1:C:301:LEU:CB	1:D:305:PRO:HG3	2.34	0.57
1:C:120:ARG:HG3	6:C:960:HOH:O	2.05	0.57
1:C:164:ALA:O	1:C:166:PRO:HD3	2.05	0.56
1:A:271:HIS:HB2	1:A:274:THR:OG1	2.06	0.56
1:D:286:TYR:O	1:D:286:TYR:HD1	1.89	0.55
1:B:212:LYS:HD2	6:B:797:HOH:O	2.04	0.55
1:C:231:LYS:O	1:C:235:VAL:HG23	2.06	0.55
1:A:172:ILE:O	1:A:172:ILE:HG22	2.07	0.55
1:A:276:ILE:HD11	1:A:301:LEU:HD11	1.88	0.55
1:B:63:VAL:HG23	1:B:138:HIS:O	2.06	0.55
1:B:41:LEU:HD11	1:B:72:ILE:CG1	2.35	0.55
1:B:174:CYS:SG	5:B:2377:NAD:H5N	2.47	0.54
1:D:105:ASN:OD1	1:D:106:PRO:HD2	2.08	0.54
1:C:283:HIS:CD2	1:C:285:ASN:H	2.25	0.54
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.90	0.54
1:B:301:LEU:HD12	1:B:302:THR:N	2.23	0.54
1:C:174:CYS:SG	1:C:175:GLY:N	2.80	0.54
1:B:178:THR:HG21	5:B:2377:NAD:C4N	2.38	0.53
1:B:194:THR:HG21	1:B:258:THR:HG21	1.89	0.53
1:C:15:TRP:HZ2	1:C:132:CYS:HG	1.55	0.53
1:A:48:THR:O	1:A:51:HIS:HB2	2.08	0.53
1:C:317:CYS:SG	1:C:320:GLY:HA2	2.49	0.52
1:C:91:PRO:HB2	1:C:143:THR:HG22	1.90	0.52
1:D:231:LYS:HE2	1:D:344:GLN:HE21	1.71	0.52
1:C:194:THR:HG21	1:C:258:THR:HG21	1.90	0.52
1:C:354:LYS:HZ1	1:C:357:GLU:HB2	1.75	0.52
1:D:272:LEU:HB3	1:D:301:LEU:HD13	1.92	0.52
1:C:51:HIS:HB3	1:C:57:MET:HB2	1.92	0.52
1:A:92:LEU:HD13	1:A:324:SER:HB2	1.92	0.51
1:C:95:PRO:HG2	1:C:111:CYS:HB3	1.92	0.51
1:A:225:ASN:ND2	1:A:227:ASP:H	2.07	0.51
1:C:335:PHE:HB2	1:C:340:PHE:CE2	2.46	0.51
1:A:26:ILE:HG22	1:A:132:CYS:HB2	1.91	0.51
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.93	0.51
1:C:271:HIS:HB2	1:C:274:THR:OG1	2.10	0.51
1:D:92:LEU:HA	6:D:778:HOH:O	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:HA3	1:A:206:SER:HB2	1.93	0.50
1:C:54:LYS:NZ	1:C:363:ASN:OD1	2.43	0.50
1:D:229:PHE:O	1:D:233:MET:HG2	2.12	0.50
1:A:194:THR:HG21	1:A:258:THR:HG21	1.94	0.50
1:A:201:GLY:O	1:A:205:LEU:HG	2.12	0.50
1:A:5:LYS:HD2	1:A:5:LYS:N	2.27	0.50
1:C:354:LYS:HE2	1:C:354:LYS:HA	1.94	0.49
1:A:76:ILE:HG13	1:A:76:ILE:O	2.13	0.49
1:B:209:MET:HG2	1:B:235:VAL:HG22	1.93	0.49
1:C:179:GLY:O	1:C:207:VAL:HA	2.11	0.49
1:C:120:ARG:O	1:C:122:VAL:HG13	2.12	0.49
1:A:294:VAL:HG23	5:A:1377:NAD:H2N	1.94	0.49
1:C:357:GLU:O	1:C:360:GLU:HB3	2.12	0.49
1:A:178:THR:HG21	5:A:1377:NAD:C4N	2.43	0.49
1:B:143:THR:O	1:B:144:SER:HB2	2.13	0.49
1:D:361:LEU:HB3	1:D:367:SER:HB2	1.95	0.49
1:B:190:LYS:HG2	1:B:264:TYR:OH	2.13	0.49
1:A:301:LEU:HA	6:A:720:HOH:O	2.13	0.48
1:D:178:THR:HG21	5:D:4377:NAD:C4N	2.43	0.48
1:C:16:GLU:HB2	1:C:19:GLN:OE1	2.13	0.48
1:C:1:GLY:N	6:C:677:HOH:O	2.43	0.48
1:D:286:TYR:CD1	1:D:286:TYR:O	2.66	0.48
1:B:93:PHE:CZ	3:B:506:ACT:H2	2.49	0.48
1:D:200:LEU:HD13	1:D:232:ALA:HB2	1.95	0.48
1:A:62:PRO:CG	1:A:137:VAL:HG12	2.44	0.47
1:A:185:LYS:HD2	1:A:322:LEU:HD23	1.96	0.47
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.96	0.47
1:B:248:LYS:HG3	1:B:253:VAL:HG23	1.97	0.47
1:B:94:LEU:HB3	1:B:324:SER:HG	1.80	0.47
1:D:31:PRO:HD3	1:D:37:ARG:HB2	1.97	0.47
1:C:334:GLU:HB3	1:C:340:PHE:HE1	1.80	0.46
1:B:24:GLU:HG3	6:B:896:HOH:O	2.14	0.46
1:B:93:PHE:CE2	3:B:506:ACT:H2	2.50	0.46
1:B:307:LEU:O	1:B:312:ARG:HD2	2.16	0.46
1:B:69:ALA:O	1:B:91:PRO:HD2	2.15	0.46
1:C:331:LEU:O	1:C:340:PHE:HZ	1.98	0.46
1:D:34:LYS:HD3	3:D:509:ACT:H1	1.98	0.46
1:A:231:LYS:HE2	1:A:344:GLN:HG3	1.97	0.46
1:C:201:GLY:O	1:C:205:LEU:HG	2.15	0.46
1:A:260:ASN:HB3	4:B:555:CAC:C2	2.46	0.46
1:C:96:GLN:HB3	1:C:325:ARG:HD3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HD2	1:A:129:ARG:NH2	2.30	0.46
1:C:354:LYS:NZ	1:C:357:GLU:HB2	2.31	0.46
1:D:271:HIS:HB2	1:D:274:THR:OG1	2.17	0.45
1:D:224:LEU:HD23	1:D:243:PRO:HD2	1.98	0.45
1:A:51:HIS:HB3	1:A:57:MET:HB2	1.97	0.45
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.84	0.45
1:D:65:VAL:HG22	6:D:688:HOH:O	2.17	0.44
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.98	0.44
1:C:334:GLU:HB3	1:C:340:PHE:CE1	2.52	0.44
1:D:65:VAL:HG23	1:D:146:PHE:CD1	2.53	0.44
1:A:132:CYS:HA	6:A:741:HOH:O	2.18	0.44
1:B:93:PHE:HB2	1:B:141:MET:HB3	2.00	0.44
1:A:294:VAL:HG23	5:A:1377:NAD:H1D	1.99	0.43
1:C:185:LYS:HD2	1:C:322:LEU:HD23	1.99	0.43
1:C:12:ALA:HB1	1:C:21:PHE:CD2	2.52	0.43
1:C:96:GLN:HB3	1:C:325:ARG:CD	2.48	0.43
1:A:164:ALA:HA	1:A:165:PRO:HD3	1.92	0.43
1:A:188:LYS:NZ	6:A:1006:HOH:O	2.52	0.43
1:B:301:LEU:HD12	1:B:302:THR:H	1.82	0.43
1:A:165:PRO:O	1:A:169:VAL:HG22	2.18	0.43
1:A:111:CYS:SG	1:A:112:ILE:N	2.92	0.43
1:C:225:ASN:OD1	1:C:227:ASP:HB2	2.19	0.43
1:B:165:PRO:HB2	1:B:168:LYS:HG3	2.01	0.43
1:C:164:ALA:HB1	1:C:169:VAL:HG11	2.01	0.42
1:D:138:HIS:CE1	6:D:867:HOH:O	2.71	0.42
1:D:294:VAL:HG23	5:D:4377:NAD:H1D	2.00	0.42
1:C:48:THR:HG21	1:C:141:MET:CE	2.49	0.42
1:A:143:THR:O	1:A:144:SER:HB2	2.19	0.42
1:A:238:THR:O	1:A:239:GLU:HB3	2.19	0.42
1:A:345:LEU:O	1:A:369:ARG:HB2	2.20	0.42
1:C:284:MET:HG2	6:C:970:HOH:O	2.20	0.42
1:D:93:PHE:CZ	3:D:511:ACT:CH3	3.02	0.42
1:B:179:GLY:O	1:B:207:VAL:HA	2.19	0.42
1:C:122:VAL:HG21	1:C:126:GLY:HA2	2.02	0.42
1:D:194:THR:HG21	1:D:258:THR:HG21	2.02	0.42
1:D:98:ARG:HA	1:D:103:CYS:HB3	2.01	0.42
1:B:234:ALA:HA	1:D:81:THR:HG21	2.02	0.41
1:A:302:THR:HA	1:B:301:LEU:O	2.20	0.41
1:C:221:GLY:O	1:C:240:CYS:HA	2.20	0.41
1:A:164:ALA:O	1:A:166:PRO:HD3	2.21	0.41
1:A:138:HIS:HE1	3:A:513:ACT:OXT	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HG3	1:A:264:TYR:OH	2.20	0.41
1:B:255:SER:O	1:B:259:GLY:N	2.54	0.41
1:A:62:PRO:HG2	1:A:137:VAL:HG12	2.01	0.41
1:A:307:LEU:O	1:A:312:ARG:HD2	2.20	0.41
1:C:92:LEU:HD13	1:C:324:SER:HB2	2.03	0.41
1:C:143:THR:O	1:C:144:SER:HB2	2.21	0.41
1:C:301:LEU:O	1:D:302:THR:HA	2.21	0.40
1:B:328:VAL:HB	1:B:329:PRO:HD3	2.03	0.40
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.36	0.40
1:D:94:LEU:HD22	1:D:319:PHE:HB3	2.03	0.40
1:C:294:VAL:HG23	5:C:3377:NAD:H1D	2.03	0.40
1:C:48:THR:HG21	1:C:141:MET:HE1	2.03	0.40
1:A:96:GLN:NE2	1:A:326:ASP:OD1	2.54	0.40
1:C:93:PHE:HB2	1:C:141:MET:HB3	2.04	0.40
1:B:272:LEU:O	1:B:275:MET:HB2	2.21	0.40
1:C:92:LEU:HD21	1:C:158:ALA:HB2	2.02	0.40
1:C:90:ILE:HG13	1:C:160:ILE:HD13	2.02	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	371/373 (100%)	340 (92%)	27 (7%)	4 (1%)	17	31
1	B	371/373 (100%)	341 (92%)	26 (7%)	4 (1%)	17	31
1	C	371/373 (100%)	331 (89%)	36 (10%)	4 (1%)	17	31
1	D	371/373 (100%)	345 (93%)	22 (6%)	4 (1%)	17	31
All	All	1484/1492 (100%)	1357 (91%)	111 (8%)	16 (1%)	17	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
1	A	174	CYS
1	A	175	GLY
1	B	174	CYS
1	B	324	SER
1	C	174	CYS
1	C	175	GLY
1	C	324	SER
1	D	174	CYS
1	D	109	ASN
1	B	65	VAL
1	B	175	GLY
1	A	368	ILE
1	A	65	VAL
1	D	368	ILE
1	D	65	VAL

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	312/312 (100%)	303 (97%)	9 (3%)	50	77
1	B	312/312 (100%)	301 (96%)	11 (4%)	43	70
1	C	312/312 (100%)	306 (98%)	6 (2%)	65	87
1	D	312/312 (100%)	306 (98%)	6 (2%)	65	87
All	All	1248/1248 (100%)	1216 (97%)	32 (3%)	54	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	57	MET
1	A	218	ARG
1	A	225	ASN
1	A	247	THR
1	A	268	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	GLN
1	A	353	LYS
1	A	354	LYS
1	B	2	THR
1	B	5	LYS
1	B	27	GLU
1	B	168	LYS
1	B	185	LYS
1	B	244	LYS
1	B	251	SER
1	B	268	VAL
1	B	274	THR
1	B	310	THR
1	B	353	LYS
1	C	104	ARG
1	C	147	THR
1	C	212	LYS
1	C	233	MET
1	C	284	MET
1	C	341	ASP
1	D	97	CYS
1	D	251	SER
1	D	274	THR
1	D	344	GLN
1	D	361	LEU
1	D	367	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	225	ASN
1	A	261	ASN
1	A	344	GLN
1	B	17	GLN
1	B	344	GLN
1	C	51	HIS
1	C	260	ASN
1	C	283	HIS
1	C	344	GLN
1	D	17	GLN
1	D	19	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	138	HIS
1	D	344	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 ⓘ

Of 41 ligands modelled in this entry, 19 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAD	A	1377	2	38,48,48	1.95	5 (13%)	47,73,73	2.22	12 (25%)
3	ACT	A	501	2	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
3	ACT	A	502	2	1,3,3	5.14	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	2	1,3,3	1.82	0	0,3,3	0.00	-
3	ACT	A	513	2	1,3,3	5.45	1 (100%)	0,3,3	0.00	-
4	CAC	A	554	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	B	2377	2	38,48,48	1.93	6 (15%)	47,73,73	2.51	11 (23%)
3	ACT	B	506	2	1,3,3	0.02	0	0,3,3	0.00	-
3	ACT	B	507	2	1,3,3	1.85	0	0,3,3	0.00	-
4	CAC	B	551	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	552	2	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAC	B	553	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	555	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	C	3377	2	38,48,48	2.00	8 (21%)	47,73,73	2.27	12 (25%)
3	ACT	C	505	2	1,3,3	1.77	0	0,3,3	0.00	-
3	ACT	C	510	2	1,3,3	2.47	1 (100%)	0,3,3	0.00	-
5	NAD	D	4377	2	38,48,48	2.14	8 (21%)	47,73,73	2.74	13 (27%)
3	ACT	D	508	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
3	ACT	D	509	2	1,3,3	0.76	0	0,3,3	0.00	-
3	ACT	D	511	2	1,3,3	0.71	0	0,3,3	0.00	-
3	ACT	D	512	2	1,3,3	1.03	0	0,3,3	0.00	-
3	ACT	D	514	2	1,3,3	0.77	0	0,3,3	0.00	-

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
5	NAD	A	1377	2	-	0/22/62/62	0/5/5/5
3	ACT	A	501	2	-	0/0/0/0	0/0/0/0
3	ACT	A	502	2	-	0/0/0/0	0/0/0/0
3	ACT	A	504	2	-	0/0/0/0	0/0/0/0
3	ACT	A	513	2	-	0/0/0/0	0/0/0/0
4	CAC	A	554	-	-	0/0/0/0	0/0/0/0
5	NAD	B	2377	2	-	0/22/62/62	0/5/5/5
3	ACT	B	506	2	-	0/0/0/0	0/0/0/0
3	ACT	B	507	2	-	0/0/0/0	0/0/0/0
4	CAC	B	551	2	-	0/0/0/0	0/0/0/0
4	CAC	B	552	2	-	0/0/0/0	0/0/0/0
4	CAC	B	553	2	-	0/0/0/0	0/0/0/0
4	CAC	B	555	-	-	0/0/0/0	0/0/0/0
5	NAD	C	3377	2	-	0/22/62/62	0/5/5/5
3	ACT	C	505	2	-	0/0/0/0	0/0/0/0
3	ACT	C	510	2	-	0/0/0/0	0/0/0/0
5	NAD	D	4377	2	-	0/22/62/62	0/5/5/5
3	ACT	D	508	-	-	0/0/0/0	0/0/0/0
3	ACT	D	509	2	-	0/0/0/0	0/0/0/0
3	ACT	D	511	2	-	0/0/0/0	0/0/0/0
3	ACT	D	512	2	-	0/0/0/0	0/0/0/0
3	ACT	D	514	2	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4377	NAD	C3N-C7N	-9.48	1.35	1.50
5	A	1377	NAD	C3N-C7N	-8.53	1.37	1.50
5	C	3377	NAD	C3N-C7N	-7.39	1.38	1.50
5	B	2377	NAD	C3N-C7N	-7.35	1.38	1.50
5	D	4377	NAD	C2N-C3N	-3.40	1.33	1.39
5	C	3377	NAD	C2N-C3N	-3.32	1.33	1.39
5	B	2377	NAD	C2N-C3N	-3.12	1.34	1.39
5	D	4377	NAD	O4B-C4B	-2.61	1.39	1.45
5	D	4377	NAD	C4N-C3N	-2.55	1.34	1.39
5	C	3377	NAD	C4N-C3N	-2.18	1.35	1.39
3	A	501	ACT	CH3-C	2.04	1.51	1.48
5	C	3377	NAD	C8A-N7A	2.23	1.38	1.34
3	D	508	ACT	CH3-C	2.26	1.52	1.48
5	D	4377	NAD	C2A-N1A	2.34	1.38	1.33
3	C	510	ACT	CH3-C	2.47	1.52	1.48
5	A	1377	NAD	C4A-N3A	2.53	1.39	1.35
5	B	2377	NAD	C8A-N7A	2.80	1.40	1.34
5	C	3377	NAD	C4A-N3A	2.84	1.39	1.35
5	D	4377	NAD	O4D-C1D	3.11	1.45	1.41
5	D	4377	NAD	C2A-N3A	3.24	1.37	1.32
5	A	1377	NAD	C2A-N1A	3.32	1.40	1.33
5	D	4377	NAD	C8A-N7A	3.34	1.41	1.34
5	C	3377	NAD	O4D-C1D	3.47	1.45	1.41
5	B	2377	NAD	C2A-N1A	3.48	1.40	1.33
5	A	1377	NAD	C8A-N7A	3.79	1.41	1.34
5	B	2377	NAD	C4A-N3A	3.86	1.41	1.35
5	C	3377	NAD	C2A-N1A	3.90	1.41	1.33
5	A	1377	NAD	C2A-N3A	4.00	1.39	1.32
5	B	2377	NAD	C2A-N3A	4.49	1.40	1.32
5	C	3377	NAD	C2A-N3A	4.58	1.40	1.32
3	A	502	ACT	CH3-C	5.14	1.55	1.48
3	A	513	ACT	CH3-C	5.45	1.56	1.48

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4377	NAD	N3A-C2A-N1A	-12.01	119.70	128.89
5	B	2377	NAD	N3A-C2A-N1A	-10.99	120.48	128.89
5	C	3377	NAD	N3A-C2A-N1A	-9.59	121.55	128.89
5	A	1377	NAD	N3A-C2A-N1A	-8.90	122.08	128.89
5	D	4377	NAD	O7N-C7N-N7N	-8.73	110.31	122.59
5	B	2377	NAD	O7N-C7N-N7N	-6.13	113.97	122.59
5	A	1377	NAD	O7N-C7N-N7N	-6.12	113.97	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1377	NAD	O4D-C1D-N1N	-5.62	101.95	108.13
5	C	3377	NAD	C4B-O4B-C1B	-5.56	103.61	109.72
5	C	3377	NAD	O7N-C7N-N7N	-5.07	115.46	122.59
5	D	4377	NAD	C2B-C1B-N9A	-4.19	107.89	114.29
5	B	2377	NAD	C4B-O4B-C1B	-3.99	105.33	109.72
5	D	4377	NAD	C4B-O4B-C1B	-3.60	105.76	109.72
5	B	2377	NAD	C2B-C3B-C4B	-2.95	96.56	102.61
5	A	1377	NAD	C4B-O4B-C1B	-2.68	106.78	109.72
5	A	1377	NAD	C2B-C3B-C4B	-2.56	97.35	102.61
5	D	4377	NAD	O4D-C1D-N1N	-2.33	105.57	108.13
5	A	1377	NAD	O5B-C5B-C4B	-2.30	100.65	109.12
5	A	1377	NAD	O3-PN-O5D	-2.26	96.93	102.94
5	B	2377	NAD	O5D-PN-O1N	-2.24	100.92	109.62
5	C	3377	NAD	O5B-PA-O1A	-2.11	101.43	109.62
5	A	1377	NAD	C2B-C1B-N9A	-2.10	111.08	114.29
5	D	4377	NAD	C1B-N9A-C4A	-2.01	123.91	126.94
5	C	3377	NAD	C4A-C5A-N7A	2.03	111.35	109.48
5	C	3377	NAD	O4B-C4B-C3B	2.10	109.38	105.15
5	C	3377	NAD	O2A-PA-O3	2.13	114.74	105.09
5	C	3377	NAD	O7N-C7N-C3N	2.14	121.92	119.59
5	A	1377	NAD	O2A-PA-O3	2.16	114.88	105.09
5	C	3377	NAD	C3N-C2N-N1N	2.21	122.90	120.36
5	D	4377	NAD	O2N-PN-O3	2.37	115.83	105.09
5	D	4377	NAD	O7N-C7N-C3N	2.47	122.29	119.59
5	B	2377	NAD	C3N-C2N-N1N	2.51	123.25	120.36
5	B	2377	NAD	O2N-PN-O3	2.54	116.62	105.09
5	B	2377	NAD	O4B-C4B-C3B	2.56	110.30	105.15
5	D	4377	NAD	O5D-C5D-C4D	2.58	118.63	109.12
5	A	1377	NAD	O4B-C4B-C3B	2.65	110.48	105.15
5	D	4377	NAD	C2A-N1A-C6A	2.73	123.64	118.77
5	C	3377	NAD	O2N-PN-O3	2.88	118.15	105.09
5	A	1377	NAD	O3-PA-O5B	2.90	110.63	102.94
5	C	3377	NAD	O3-PA-O5B	2.97	110.82	102.94
5	D	4377	NAD	O4B-C4B-C3B	2.99	111.17	105.15
5	D	4377	NAD	C4A-C5A-N7A	3.00	112.24	109.48
5	B	2377	NAD	N6A-C6A-N1A	3.09	125.84	119.20
5	D	4377	NAD	O2A-PA-O3	3.26	119.88	105.09
5	C	3377	NAD	O5D-C5D-C4D	3.44	121.81	109.12
5	A	1377	NAD	O2N-PN-O3	3.55	121.18	105.09
5	B	2377	NAD	O3-PA-O5B	3.94	113.39	102.94
5	B	2377	NAD	C4A-C5A-N7A	5.53	114.57	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1377	NAD	3	0
3	A	513	ACT	1	0
5	B	2377	NAD	2	0
3	B	506	ACT	2	0
4	B	555	CAC	1	0
5	C	3377	NAD	2	0
5	D	4377	NAD	2	0
3	D	509	ACT	1	0
3	D	511	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	373/373 (100%)	-0.10	3 (0%) 87 89	11, 35, 57, 66	0
1	B	373/373 (100%)	-0.30	1 (0%) 94 95	14, 31, 47, 61	0
1	C	373/373 (100%)	0.24	7 (1%) 70 73	23, 51, 67, 77	0
1	D	373/373 (100%)	-0.36	1 (0%) 94 95	9, 27, 45, 55	0
All	All	1492/1492 (100%)	-0.13	12 (0%) 87 89	9, 34, 61, 77	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	LEU	4.2
1	C	134	GLY	2.8
1	D	1	GLY	2.6
1	A	58	VAL	2.6
1	A	76	ILE	2.6
1	C	243	PRO	2.5
1	C	247	THR	2.4
1	A	1	GLY	2.4
1	C	332	VAL	2.3
1	C	345	LEU	2.2
1	B	214	ALA	2.0
1	C	368	ILE	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 ⓘ

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
3	ACT	A	501	4/4	0.94	0.25	4.33	42,45,45,46	0
3	ACT	D	511	4/4	0.97	0.17	4.00	34,34,34,36	0
4	CAC	B	555	5/5	0.95	0.23	2.48	76,78,80,80	0
3	ACT	B	506	4/4	0.97	0.16	1.84	17,27,29,32	0
4	CAC	A	554	5/5	0.96	0.14	0.65	76,77,78,81	0
3	ACT	D	509	4/4	0.96	0.15	0.13	13,13,14,16	0
5	NAD	B	2377	44/44	0.98	0.13	-0.46	11,25,31,36	0
5	NAD	A	1377	44/44	0.97	0.12	-0.47	19,25,30,33	0
3	ACT	C	505	4/4	0.96	0.15	-0.65	39,41,42,43	0
5	NAD	C	3377	44/44	0.95	0.14	-0.73	20,48,53,55	0
5	NAD	D	4377	44/44	0.97	0.11	-0.84	18,24,29,32	0
2	ZN	B	375	1/1	0.99	0.10	-1.11	24,24,24,24	0
2	ZN	D	376	1/1	0.99	0.10	-1.20	28,28,28,28	0
2	ZN	B	404	1/1	0.99	0.09	-1.47	27,27,27,27	0
2	ZN	B	376	1/1	0.99	0.10	-1.57	24,24,24,24	0
2	ZN	D	375	1/1	0.99	0.08	-1.61	25,25,25,25	0
4	CAC	B	551	5/5	0.99	0.10	-1.82	16,31,35,38	0
2	ZN	C	375	1/1	0.99	0.09	-1.98	35,35,35,35	0
2	ZN	C	376	1/1	0.93	0.08	-2.18	50,50,50,50	0
2	ZN	A	376	1/1	0.98	0.07	-2.28	33,33,33,33	0
2	ZN	A	375	1/1	0.99	0.06	-2.71	42,42,42,42	0
2	ZN	A	408	1/1	0.99	0.06	-3.10	37,37,37,37	0
3	ACT	A	504	4/4	0.98	0.14	-	20,20,21,23	0
4	CAC	B	553	5/5	0.99	0.09	-	45,46,50,55	0
2	ZN	C	407	1/1	0.96	0.06	-	61,61,61,61	0
3	ACT	D	512	4/4	0.91	0.22	-	25,26,28,31	0
2	ZN	A	401	1/1	0.97	0.08	-	40,40,40,40	0
4	CAC	B	552	5/5	0.98	0.12	-	47,49,52,52	0
3	ACT	D	508	4/4	0.96	0.18	-	18,21,22,23	0
2	ZN	B	405	1/1	0.97	0.07	-	48,48,48,48	0
2	ZN	D	410	1/1	0.89	0.15	-	41,41,41,41	1
2	ZN	A	402	1/1	0.94	0.13	-	40,40,40,40	1
2	ZN	B	406	1/1	0.98	0.05	-	43,43,43,43	0
3	ACT	D	514	4/4	0.90	0.36	-	52,52,52,53	4
3	ACT	C	510	4/4	0.98	0.09	-	29,32,33,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACT	A	502	4/4	0.93	0.27	-	46,47,47,47	4
3	ACT	B	507	4/4	0.96	0.18	-	20,28,30,31	0
2	ZN	D	411	1/1	0.98	0.04	-	53,53,53,53	0
2	ZN	D	409	1/1	0.97	0.10	-	42,42,42,42	0
2	ZN	A	403	1/1	0.98	0.12	-	48,48,48,48	0
3	ACT	A	513	4/4	0.90	0.32	-	52,53,53,54	4

6.5 Other polymers [i](#)

There are no such residues in this entry.