Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:54 PM GMT

PDB ID	:	1D1T
Title	:	MUTANT OF HUMAN SIGMA ALCOHOL DEHYDROGENASE WITH LEUCINE AT POSITION 141
Authors	:	Xie, P.T.; Hurley, T.D.
Deposited on	:	1999-09-21
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

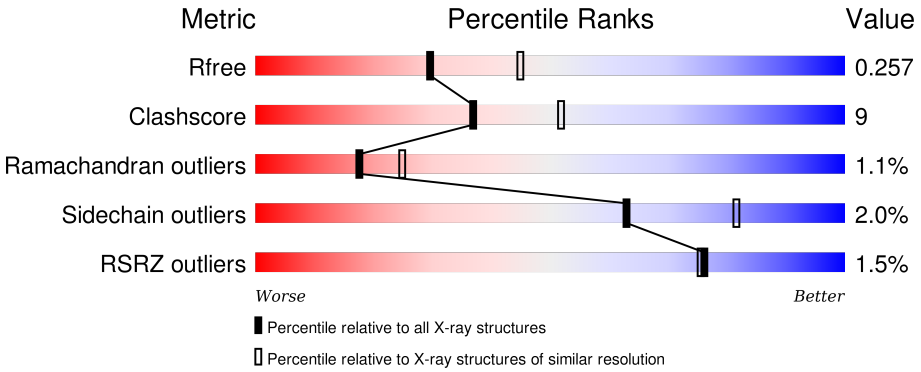
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	373	2% 80% 19%
1	B	373	77% 21%
1	C	373	3% 76% 23%
1	D	373	% 80% 19%

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	C	505	-	-	-	X
3	ACT	D	509	-	-	X	-
4	CAC	A	994	-	-	-	X
4	CAC	B	995	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11799 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	1773	468	526	22			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			

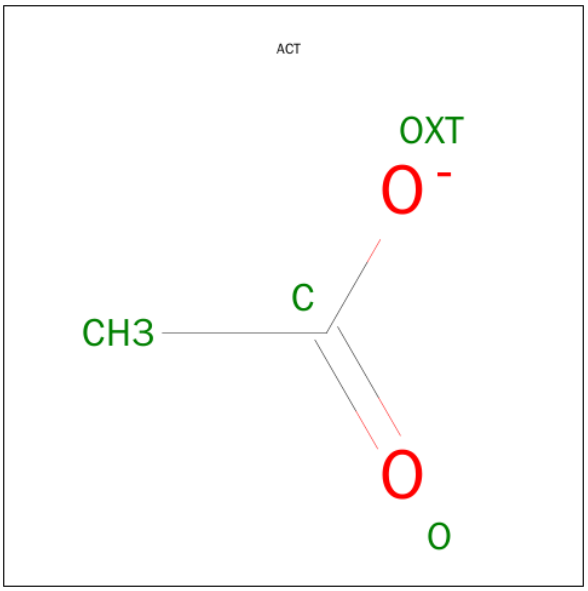
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	MET	ENGINEERED	UNP P40394
B	141	LEU	MET	ENGINEERED	UNP P40394
C	141	LEU	MET	ENGINEERED	UNP P40394
D	141	LEU	MET	ENGINEERED	UNP P40394

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

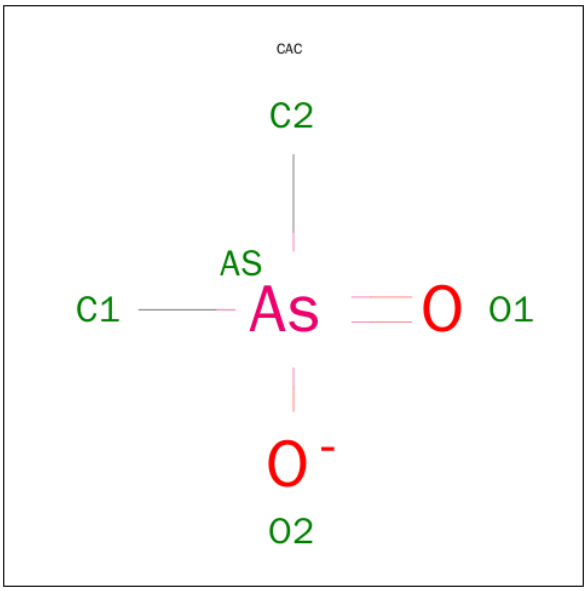
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	6	Total	Zn	0	0
			6	6		
2	D	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



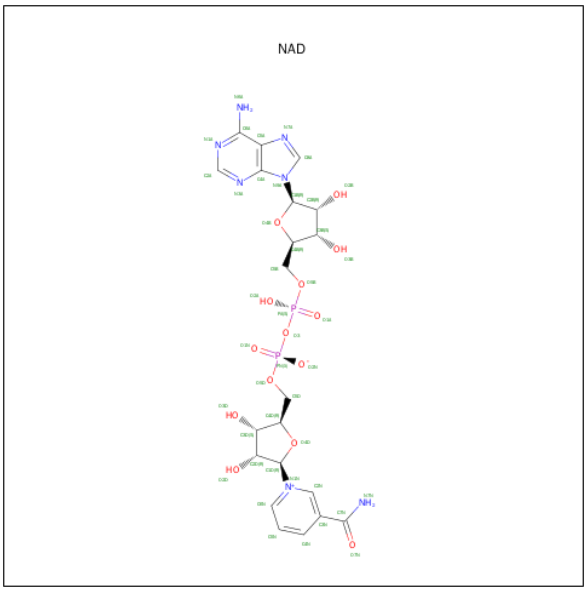
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0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

- 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: $C_{21}H_{27}N_7O_{14}P_2$).



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.

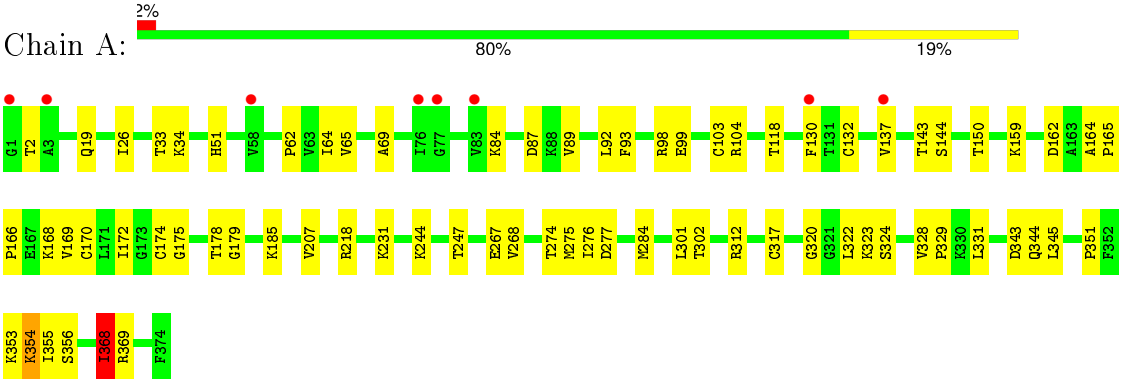
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	126	Total	O	0	0
			126	126		
6	C	45	Total	O	0	0
			45	45		
6	D	121	Total	O	0	0
			121	121		

3 Residue-property plots (i)

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

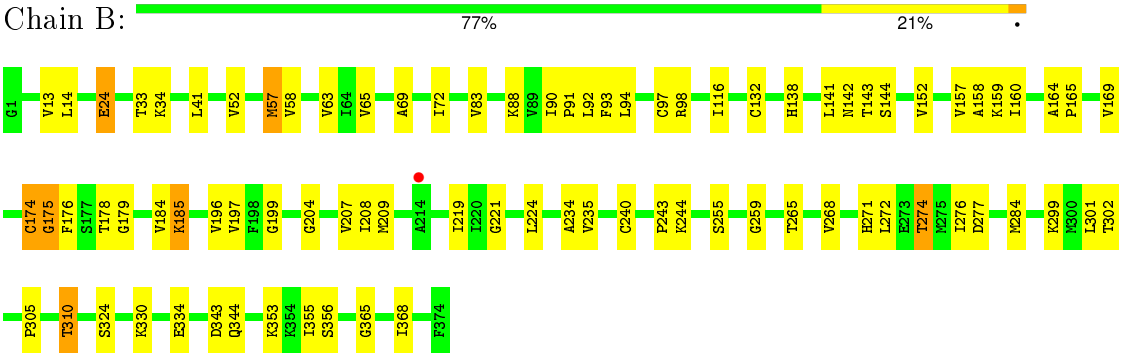
- Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain A:



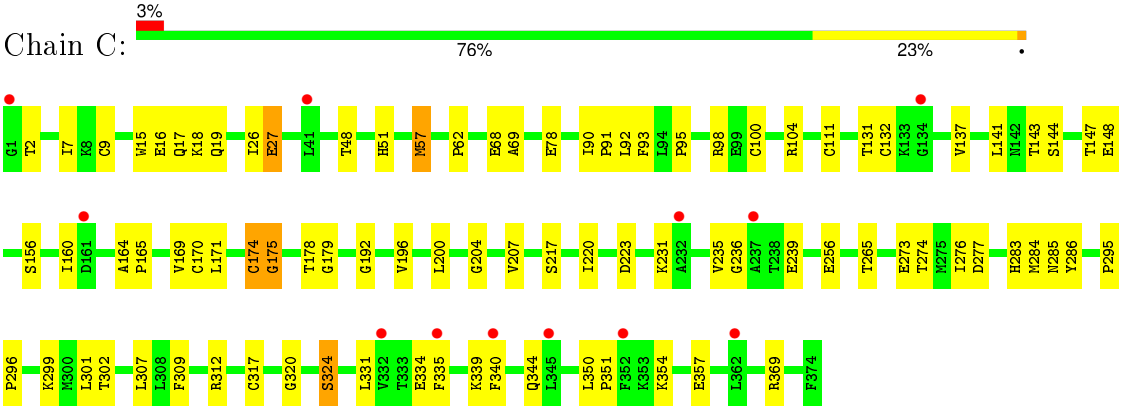
- Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain B:



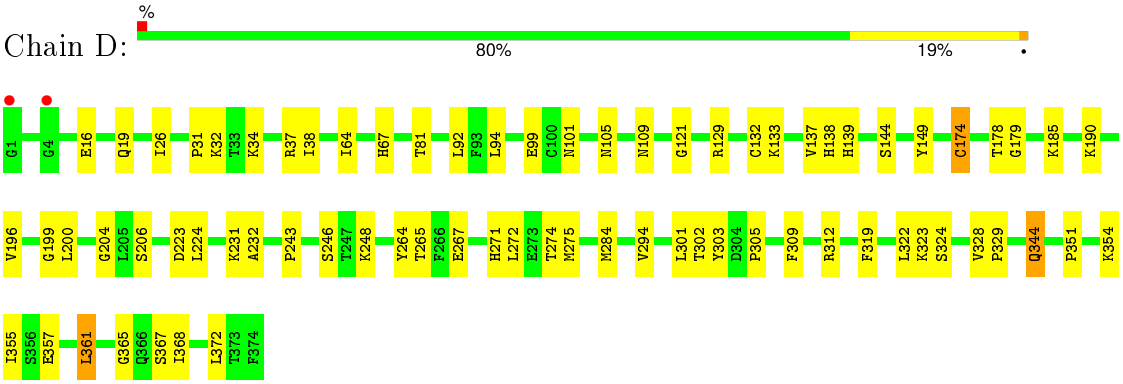
- Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain C:



• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.90Å 90.50Å 119.80Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 45.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.0 (50.00-2.40) 90.8 (45.50-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.274 0.205 , 0.257	Depositor DCC
R_{free} test set	4522 reflections (7.58%)	DCC
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 64216 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11799	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.69	1/3840 (0.0%)
1	B	0.50	0/2840	0.72	1/3840 (0.0%)
1	C	0.42	0/2840	0.66	0/3840
1	D	0.48	0/2840	0.71	1/3840 (0.0%)
All	All	0.46	0/11360	0.69	3/15360 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	368	ILE	N-CA-C	-6.16	94.36	111.00
1	D	323	LYS	N-CA-C	-5.16	97.08	111.00
1	A	368	ILE	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2789	0	2860	48	0
1	B	2789	0	2860	64	0
1	C	2789	0	2860	59	0
1	D	2789	0	2860	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
3	B	8	0	6	1	0
3	C	8	0	6	1	0
3	D	20	0	15	3	0
4	A	5	0	0	0	0
4	B	20	0	0	1	0
5	A	44	0	26	2	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	4	0
6	A	79	0	0	5	0
6	B	126	0	0	4	0
6	C	45	0	0	2	0
6	D	121	0	0	9	0
All	All	11799	0	11583	216	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 9.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:HD13	1:D:324:SER:HB2	1.64	0.78
1:C:307:LEU:O	1:C:312:ARG:HD2	1.82	0.78
1:D:351:PRO:HD2	1:D:354:LYS:HD2	1.64	0.77
1:D:344:GLN:HB2	6:D:882:HOH:O	1.85	0.77
1:C:204:GLY:O	1:C:207:VAL:HG12	1.84	0.76
1:A:276:ILE:HD11	1:A:301:LEU:HD11	1.65	0.76
1:C:301:LEU:HB2	1:D:305:PRO:HG3	1.70	0.74
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.68	0.74
1:B:179:GLY:O	1:B:207:VAL:HA	1.90	0.71
1:C:26:ILE:HG22	1:C:132:CYS:HB2	1.73	0.70
1:B:24:GLU:HG2	1:B:132:CYS:SG	2.32	0.70
1:C:295:PRO:HG3	6:D:716:HOH:O	1.92	0.68
1:B:184:VAL:HG12	1:B:185:LYS:HE2	1.75	0.68
1:B:58:VAL:HA	6:B:928:HOH:O	1.93	0.68
1:D:231:LYS:HE2	1:D:344:GLN:NE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:ACT:H1	6:A:912:HOH:O	1.96	0.66
1:D:231:LYS:HE2	1:D:344:GLN:HE21	1.59	0.66
1:B:92:LEU:HD13	1:B:324:SER:HB3	1.76	0.66
1:B:24:GLU:HG3	6:B:896:HOH:O	1.95	0.65
1:B:353:LYS:HD2	1:B:353:LYS:H	1.61	0.65
1:A:345:LEU:O	1:A:369:ARG:HB2	1.96	0.65
1:C:301:LEU:HD12	1:C:302:THR:H	1.62	0.64
1:C:178:THR:HG21	5:C:3377:NAD:C4N	2.27	0.64
1:B:69:ALA:O	1:B:91:PRO:HD2	1.97	0.64
1:B:41:LEU:HD11	1:B:72:ILE:HG12	1.78	0.64
1:B:208:ILE:HG23	1:B:219:ILE:HG21	1.78	0.63
1:B:276:ILE:HD11	1:B:301:LEU:HD11	1.81	0.62
1:B:224:LEU:HD23	1:B:243:PRO:HD2	1.81	0.62
1:D:92:LEU:HA	6:D:778:HOH:O	1.98	0.62
1:C:92:LEU:HD13	1:C:324:SER:HB2	1.82	0.61
1:C:301:LEU:HD12	1:C:302:THR:N	2.16	0.61
1:A:62:PRO:HG2	1:A:137:VAL:HA	1.82	0.61
1:B:164:ALA:HB1	1:B:169:VAL:HG11	1.81	0.61
1:C:27:GLU:HG2	1:C:131:THR:HB	1.82	0.60
1:D:185:LYS:HD2	1:D:322:LEU:HD23	1.83	0.60
1:D:309:PHE:HB2	6:D:716:HOH:O	2.00	0.60
1:D:271:HIS:HB2	1:D:274:THR:OG1	2.02	0.60
1:B:33:THR:HG22	1:B:34:LYS:HG3	1.82	0.60
1:B:143:THR:O	1:B:144:SER:HB2	2.02	0.59
1:D:361:LEU:HB3	1:D:367:SER:HB2	1.83	0.59
1:B:92:LEU:HD11	1:B:158:ALA:HB2	1.84	0.59
1:D:64:ILE:HA	6:D:688:HOH:O	2.02	0.59
1:D:272:LEU:HB3	1:D:301:LEU:HD13	1.84	0.59
1:D:174:CYS:SG	5:D:4377:NAD:H5N	2.44	0.58
1:D:196:VAL:HB	1:D:265:THR:HG22	1.84	0.58
1:C:231:LYS:O	1:C:235:VAL:HG23	2.02	0.58
1:C:95:PRO:HG2	1:C:111:CYS:HB3	1.86	0.57
1:B:271:HIS:HB2	1:B:274:THR:OG1	2.03	0.57
1:A:172:ILE:O	1:A:172:ILE:HG22	2.02	0.57
1:D:272:LEU:HG	6:D:824:HOH:O	2.04	0.57
1:C:301:LEU:O	1:D:302:THR:HA	2.05	0.57
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.86	0.57
1:D:64:ILE:HG13	1:D:137:VAL:HG11	1.86	0.57
1:C:17:GLN:HG2	1:C:18:LYS:HG3	1.87	0.57
1:B:365:GLY:HA2	6:B:755:HOH:O	2.06	0.56
1:C:164:ALA:HB1	1:C:169:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:HD23	1:D:243:PRO:HD2	1.87	0.56
1:A:143:THR:O	1:A:144:SER:HB2	2.06	0.56
1:B:176:PHE:HE2	1:B:209:MET:HE2	1.71	0.56
1:B:152:VAL:HG21	1:B:157:VAL:HG22	1.87	0.56
1:C:91:PRO:HB2	1:C:143:THR:HG22	1.88	0.55
1:B:234:ALA:HA	1:D:81:THR:HG21	1.87	0.55
1:C:143:THR:O	1:C:144:SER:HB2	2.07	0.55
1:B:93:PHE:HB2	1:B:141:LEU:HB3	1.89	0.55
1:C:283:HIS:HD2	1:C:286:TYR:H	1.55	0.55
1:B:152:VAL:CG2	1:B:157:VAL:HG22	2.37	0.54
1:B:209:MET:HG3	1:B:235:VAL:HG13	1.89	0.54
1:A:317:CYS:SG	1:A:320:GLY:HA2	2.47	0.54
1:B:178:THR:HG21	5:B:2377:NAD:C4N	2.39	0.53
1:C:174:CYS:SG	1:C:175:GLY:N	2.82	0.53
1:C:283:HIS:CD2	1:C:285:ASN:H	2.27	0.53
1:D:16:GLU:HB3	1:D:19:GLN:OE1	2.09	0.53
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.23	0.53
1:A:164:ALA:HB1	1:A:169:VAL:HG11	1.91	0.52
1:C:192:GLY:HA2	1:C:217:SER:OG	2.10	0.52
1:A:178:THR:HG21	5:A:1377:NAD:C4N	2.40	0.52
1:D:185:LYS:HD2	1:D:322:LEU:CD2	2.39	0.52
1:A:33:THR:HG22	1:A:34:LYS:HG3	1.90	0.52
1:A:93:PHE:CE2	3:A:501:ACT:H3	2.44	0.52
1:A:284:MET:HE1	1:B:116:ILE:HD13	1.91	0.51
1:D:31:PRO:HD3	1:D:37:ARG:HB2	1.93	0.51
1:D:303:TYR:O	1:D:305:PRO:HD3	2.11	0.51
1:C:15:TRP:O	1:C:16:GLU:HG2	2.11	0.51
1:C:92:LEU:HA	6:C:950:HOH:O	2.11	0.50
1:B:199:GLY:O	1:B:204:GLY:HA3	2.11	0.50
1:B:276:ILE:HD11	1:B:301:LEU:CD1	2.42	0.50
1:D:267:GLU:HG3	1:D:275:MET:HA	1.93	0.50
1:B:63:VAL:HG23	1:B:138:HIS:O	2.11	0.50
1:C:174:CYS:SG	5:C:3377:NAD:H5N	2.51	0.50
1:D:34:LYS:NZ	3:D:509:ACT:H3	2.27	0.49
1:A:164:ALA:O	1:A:166:PRO:HD3	2.12	0.49
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.94	0.49
1:C:231:LYS:HZ3	1:C:344:GLN:HE21	1.60	0.49
4:B:992:CAC:AS	4:B:993:CAC:O2	2.91	0.49
1:B:72:ILE:HD13	1:B:88:LYS:HA	1.94	0.49
1:B:209:MET:HG3	1:B:235:VAL:CG1	2.43	0.49
1:D:34:LYS:HD3	3:D:509:ACT:H1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MET:CE	1:B:310:THR:HG21	2.43	0.48
1:B:52:VAL:HG22	1:B:57:MET:HG2	1.94	0.48
1:C:296:PRO:HG2	1:C:299:LYS:HG3	1.94	0.48
1:A:301:LEU:HD12	1:A:302:THR:N	2.29	0.48
1:B:301:LEU:HD12	1:B:302:THR:N	2.29	0.48
1:C:231:LYS:NZ	1:C:344:GLN:HE21	2.11	0.48
1:A:351:PRO:HG2	1:A:354:LYS:HD2	1.95	0.48
1:A:284:MET:HE1	1:B:116:ILE:CD1	2.43	0.48
1:C:354:LYS:HE2	1:C:357:GLU:HB2	1.95	0.48
1:D:26:ILE:HG22	1:D:132:CYS:HB2	1.95	0.48
1:A:132:CYS:HA	6:A:741:HOH:O	2.14	0.48
1:B:93:PHE:CE2	3:B:506:ACT:H2	2.49	0.47
1:D:199:GLY:O	1:D:204:GLY:HA3	2.14	0.47
1:A:276:ILE:CD1	1:A:301:LEU:HD11	2.41	0.47
1:C:98:ARG:HH21	1:C:98:ARG:HG2	1.79	0.47
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.95	0.47
1:B:94:LEU:HB3	1:B:324:SER:HG	1.79	0.47
1:B:197:VAL:HG21	1:B:208:ILE:HG12	1.94	0.47
1:D:357:GLU:O	1:D:361:LEU:HD22	2.13	0.47
1:B:330:LYS:O	1:B:334:GLU:HG3	2.14	0.47
1:C:276:ILE:HD11	1:C:301:LEU:HD11	1.96	0.47
1:B:274:THR:HA	1:B:277:ASP:HB2	1.97	0.47
1:D:178:THR:HG21	5:D:4377:NAD:C4N	2.44	0.47
1:A:179:GLY:O	1:A:207:VAL:HA	2.14	0.47
1:C:51:HIS:HB3	1:C:57:MET:HB2	1.97	0.47
1:C:331:LEU:O	1:C:340:PHE:HZ	1.98	0.47
1:A:69:ALA:HA	1:A:170:CYS:HB2	1.97	0.47
1:C:93:PHE:CZ	3:C:505:ACT:H3	2.50	0.47
1:B:343:ASP:HB3	1:D:99:GLU:HG2	1.97	0.47
1:B:272:LEU:HD11	1:B:299:LYS:HB3	1.97	0.46
1:B:174:CYS:SG	5:B:2377:NAD:H5N	2.55	0.46
1:D:101:ASN:O	1:D:105:ASN:HB2	2.16	0.46
1:D:38:ILE:O	1:D:149:TYR:HA	2.15	0.46
1:C:2:THR:HB	1:C:7:ILE:HD11	1.98	0.46
1:C:68:GLU:OE1	1:C:171:LEU:HD23	2.15	0.46
1:C:171:LEU:HD22	1:C:369:ARG:HG3	1.97	0.46
1:A:162:ASP:N	6:A:887:HOH:O	2.49	0.46
1:D:94:LEU:HD22	1:D:319:PHE:HB3	1.98	0.46
1:A:231:LYS:HD2	1:A:344:GLN:HG3	1.98	0.45
1:C:100:CYS:HB2	6:C:849:HOH:O	2.16	0.45
1:B:255:SER:O	1:B:259:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HB2	1:B:305:PRO:HG3	1.98	0.45
1:A:62:PRO:CG	1:A:137:VAL:HG12	2.47	0.45
1:D:272:LEU:HB3	1:D:301:LEU:CD1	2.46	0.45
1:B:174:CYS:SG	1:B:175:GLY:N	2.89	0.45
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.98	0.45
1:B:90:ILE:CG1	1:B:160:ILE:HD13	2.43	0.44
1:A:84:LYS:O	1:A:87:ASP:HB2	2.18	0.44
1:C:274:THR:HA	1:C:277:ASP:HB2	1.98	0.44
1:D:190:LYS:HG3	1:D:264:TYR:OH	2.16	0.44
1:B:221:GLY:O	1:B:240:CYS:HA	2.17	0.44
1:C:334:GLU:O	1:C:339:LYS:HB2	2.16	0.44
1:D:223:ASP:OD1	5:D:4377:NAD:H1B	2.17	0.44
1:C:69:ALA:HA	1:C:170:CYS:HB2	1.99	0.44
1:C:301:LEU:CB	1:D:305:PRO:HG3	2.42	0.44
1:B:209:MET:CG	1:B:235:VAL:HG13	2.48	0.44
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.98	0.44
1:D:138:HIS:CE1	6:D:867:HOH:O	2.71	0.44
1:A:164:ALA:HA	1:A:165:PRO:HD3	1.79	0.44
1:A:323:LYS:HG2	6:A:914:HOH:O	2.17	0.43
1:A:64:ILE:HA	6:A:884:HOH:O	2.17	0.43
1:A:98:ARG:HA	1:A:103:CYS:HB3	1.99	0.43
1:A:26:ILE:HG22	1:A:132:CYS:HB2	2.00	0.43
1:B:353:LYS:N	1:B:353:LYS:HD2	2.31	0.43
1:A:301:LEU:HD12	1:A:302:THR:H	1.84	0.43
1:D:365:GLY:HA2	6:D:860:HOH:O	2.18	0.43
1:C:90:ILE:HG13	1:C:160:ILE:HD13	2.00	0.43
1:A:99:GLU:O	1:A:104:ARG:NH2	2.51	0.43
1:D:34:LYS:HZ1	3:D:509:ACT:H3	1.84	0.43
1:C:48:THR:O	1:C:51:HIS:HB2	2.18	0.43
1:D:246:SER:OG	1:D:248:LYS:HG2	2.18	0.43
1:A:276:ILE:HD11	1:A:301:LEU:CD1	2.40	0.43
1:B:93:PHE:HA	1:B:141:LEU:O	2.18	0.43
1:A:51:HIS:HE1	5:A:1377:NAD:O2D	2.01	0.43
1:B:355:ILE:HG23	1:B:356:SER:N	2.34	0.43
1:C:95:PRO:HB3	1:C:156:SER:OG	2.19	0.42
1:B:196:VAL:HB	1:B:265:THR:HG22	2.01	0.42
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.88	0.42
1:C:309:PHE:CZ	1:D:294:VAL:HG22	2.54	0.42
1:B:284:MET:HE2	1:B:310:THR:HG21	2.01	0.42
1:C:171:LEU:CD2	1:C:369:ARG:HG3	2.49	0.42
1:A:185:LYS:HD2	1:A:322:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ALA:HA	1:B:165:PRO:HD2	1.95	0.42
1:C:196:VAL:HB	1:C:265:THR:HG22	2.01	0.42
1:C:220:ILE:HG12	1:C:239:GLU:HG3	2.01	0.42
1:B:97:CYS:O	1:B:98:ARG:HB2	2.19	0.42
1:B:13:VAL:HG12	1:B:14:LEU:N	2.34	0.42
1:B:276:ILE:CG1	1:B:301:LEU:HD11	2.50	0.42
1:A:274:THR:HA	1:A:277:ASP:HB2	2.02	0.42
1:A:284:MET:CE	1:B:116:ILE:CD1	2.98	0.42
1:C:273:GLU:H	1:C:273:GLU:CD	2.23	0.41
1:C:317:CYS:SG	1:C:320:GLY:HA2	2.59	0.41
1:A:267:GLU:HG3	1:A:275:MET:HA	2.01	0.41
1:A:168:LYS:HE2	1:A:343:ASP:OD2	2.21	0.41
1:C:9:CYS:HB2	1:C:148:GLU:HB2	2.03	0.41
1:B:141:LEU:O	1:B:142:ASN:HB2	2.21	0.41
1:A:284:MET:HA	1:A:312:ARG:CZ	2.50	0.41
1:D:200:LEU:HD13	1:D:232:ALA:HB2	2.03	0.41
1:A:92:LEU:HD22	1:A:324:SER:HB2	2.03	0.41
1:C:16:GLU:HB2	1:C:19:GLN:OE1	2.21	0.41
1:A:130:PHE:HZ	1:A:150:THR:OG1	2.03	0.41
1:D:284:MET:HG2	6:D:714:HOH:O	2.20	0.41
1:C:179:GLY:O	1:C:207:VAL:HA	2.20	0.41
1:B:41:LEU:HD11	1:B:72:ILE:CG1	2.48	0.41
1:C:164:ALA:HA	1:C:165:PRO:HD2	1.88	0.41
1:B:142:ASN:ND2	6:B:933:HOH:O	2.49	0.41
1:C:93:PHE:HA	1:C:141:LEU:O	2.21	0.41
1:C:335:PHE:HB2	1:C:340:PHE:CE2	2.56	0.41
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.70	0.41
1:A:355:ILE:HG23	1:A:356:SER:N	2.36	0.41
1:D:284:MET:HA	1:D:312:ARG:CZ	2.52	0.40
1:A:172:ILE:O	1:A:172:ILE:CG2	2.67	0.40
1:C:350:LEU:HB3	1:C:351:PRO:HD2	2.04	0.40
1:C:62:PRO:HG2	1:C:137:VAL:HA	2.03	0.40
1:D:121:GLY:HA2	1:D:139:HIS:O	2.22	0.40
1:A:368:ILE:HG22	1:A:369:ARG:N	2.36	0.40
1:D:294:VAL:HG23	5:D:4377:NAD:H1D	2.03	0.40
1:D:179:GLY:HA3	1:D:206:SER:HB2	2.02	0.40
1:D:355:ILE:HG13	1:D:372:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/373 (100%)	340 (92%)	27 (7%)	4 (1%)	17	25
1	B	371/373 (100%)	343 (92%)	25 (7%)	3 (1%)	24	35
1	C	371/373 (100%)	335 (90%)	31 (8%)	5 (1%)	15	21
1	D	371/373 (100%)	344 (93%)	22 (6%)	5 (1%)	15	21
All	All	1484/1492 (100%)	1362 (92%)	105 (7%)	17 (1%)	17	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	175	GLY
1	C	174	CYS
1	C	324	SER
1	D	109	ASN
1	D	174	CYS
1	A	174	CYS
1	A	65	VAL
1	A	175	GLY
1	C	284	MET
1	D	144	SER
1	A	368	ILE
1	B	65	VAL
1	C	175	GLY
1	D	67	HIS
1	D	368	ILE
1	C	236	GLY

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%)	304 (97%)	8 (3%)	54 74
1	B	312/312 (100%)	304 (97%)	8 (3%)	54 74
1	C	312/312 (100%)	306 (98%)	6 (2%)	65 83
1	D	312/312 (100%)	309 (99%)	3 (1%)	82 93
All	All	1248/1248 (100%)	1223 (98%)	25 (2%)	63 81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	19	GLN
1	A	118	THR
1	A	218	ARG
1	A	244	LYS
1	A	247	THR
1	A	268	VAL
1	A	354	LYS
1	B	24	GLU
1	B	57	MET
1	B	185	LYS
1	B	244	LYS
1	B	268	VAL
1	B	274	THR
1	B	310	THR
1	B	344	GLN
1	C	27	GLU
1	C	57	MET
1	C	78	GLU
1	C	104	ARG
1	C	147	THR
1	C	256	GLU
1	D	133	LYS
1	D	344	GLN
1	D	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	142	ASN
1	A	225	ASN
1	A	261	ASN
1	B	344	GLN
1	C	225	ASN
1	C	283	HIS
1	C	344	GLN
1	D	17	GLN
1	D	344	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.86	7 (18%)	47,73,73	2.62	13 (27%)
3	ACT	A	501	2	1,3,3	1.50	0	0,3,3	0.00	-
3	ACT	A	502	2	1,3,3	0.71	0	0,3,3	0.00	-
3	ACT	A	504	2	1,3,3	1.66	0	0,3,3	0.00	-
3	ACT	A	513	2	1,3,3	1.48	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAC	A	994	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	B	2377	2	38,48,48	2.06	6 (15%)	47,73,73	2.36	14 (29%)
3	ACT	B	506	2	1,3,3	1.09	0	0,3,3	0.00	-
3	ACT	B	507	2	1,3,3	1.77	0	0,3,3	0.00	-
4	CAC	B	991	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	992	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	993	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	995	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	C	3377	2	38,48,48	1.90	7 (18%)	47,73,73	2.27	12 (25%)
3	ACT	C	505	2	1,3,3	0.84	0	0,3,3	0.00	-
3	ACT	C	510	2	1,3,3	2.59	1 (100%)	0,3,3	0.00	-
5	NAD	D	4377	2	38,48,48	2.29	9 (23%)	47,73,73	2.36	11 (23%)
3	ACT	D	508	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
3	ACT	D	509	2	1,3,3	1.03	0	0,3,3	0.00	-
3	ACT	D	511	2	1,3,3	1.99	0	0,3,3	0.00	-
3	ACT	D	512	-	1,3,3	0.26	0	0,3,3	0.00	-
3	ACT	D	514	2	1,3,3	2.45	1 (100%)	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	994	-	-	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	991	2	-	0/0/0/0	0/0/0/0
4	CAC	B	992	2	-	0/0/0/0	0/0/0/0
4	CAC	B	993	2	-	0/0/0/0	0/0/0/0
4	CAC	B	995	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	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	-9.66	1.35	1.50
5	C	3377	NAD	C3N-C7N	-7.81	1.38	1.50
5	B	2377	NAD	C3N-C7N	-7.24	1.39	1.50
5	A	1377	NAD	C3N-C7N	-7.10	1.39	1.50
5	D	4377	NAD	C2N-C3N	-3.63	1.33	1.39
5	B	2377	NAD	C2N-C3N	-3.41	1.33	1.39
5	A	1377	NAD	C2N-C3N	-2.80	1.34	1.39
5	C	3377	NAD	C2N-C3N	-2.63	1.34	1.39
5	D	4377	NAD	C4N-C3N	-2.23	1.35	1.39
3	D	508	ACT	CH3-C	2.01	1.51	1.48
5	C	3377	NAD	O4D-C1D	2.07	1.43	1.41
5	D	4377	NAD	C4A-N3A	2.15	1.38	1.35
5	A	1377	NAD	C4A-N3A	2.21	1.38	1.35
3	D	514	ACT	CH3-C	2.45	1.52	1.48
5	C	3377	NAD	C4A-N3A	2.52	1.39	1.35
3	C	510	ACT	CH3-C	2.59	1.52	1.48
5	A	1377	NAD	O5D-C5D	2.64	1.55	1.44
5	D	4377	NAD	C8A-N7A	2.67	1.39	1.34
5	B	2377	NAD	C8A-N7A	2.75	1.39	1.34
5	C	3377	NAD	C8A-N7A	2.82	1.40	1.34
5	D	4377	NAD	O4B-C1B	2.97	1.45	1.41
5	A	1377	NAD	C8A-N7A	3.00	1.40	1.34
5	B	2377	NAD	C4A-N3A	3.23	1.40	1.35
5	C	3377	NAD	C2A-N1A	3.44	1.40	1.33
5	A	1377	NAD	C2A-N1A	3.44	1.40	1.33
5	D	4377	NAD	C2A-N3A	3.49	1.38	1.32
5	D	4377	NAD	C2A-N1A	3.51	1.40	1.33
5	C	3377	NAD	C2A-N3A	4.35	1.39	1.32
5	A	1377	NAD	C2A-N3A	4.35	1.39	1.32
5	D	4377	NAD	O4D-C1D	4.44	1.46	1.41
5	B	2377	NAD	C2A-N1A	4.76	1.42	1.33
5	B	2377	NAD	C2A-N3A	6.13	1.43	1.32

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1377	NAD	N3A-C2A-N1A	-10.20	121.08	128.89
5	D	4377	NAD	N3A-C2A-N1A	-9.26	121.80	128.89
5	D	4377	NAD	O7N-C7N-N7N	-8.60	110.49	122.59
5	B	2377	NAD	O7N-C7N-N7N	-8.58	110.51	122.59
5	A	1377	NAD	O7N-C7N-N7N	-7.71	111.75	122.59
5	C	3377	NAD	N3A-C2A-N1A	-7.70	123.00	128.89
5	C	3377	NAD	O7N-C7N-N7N	-7.46	112.10	122.59
5	B	2377	NAD	N3A-C2A-N1A	-6.82	123.67	128.89
5	A	1377	NAD	C4B-O4B-C1B	-4.46	104.82	109.72
5	C	3377	NAD	C4B-O4B-C1B	-4.04	105.28	109.72
5	A	1377	NAD	O4D-C1D-N1N	-4.01	103.73	108.13
5	B	2377	NAD	O4D-C1D-N1N	-3.95	103.79	108.13
5	B	2377	NAD	C4B-O4B-C1B	-3.42	105.96	109.72
5	C	3377	NAD	O4D-C1D-N1N	-3.41	104.39	108.13
5	C	3377	NAD	C2B-C3B-C4B	-3.08	96.29	102.61
5	A	1377	NAD	C3N-C7N-N7N	-3.07	114.46	117.82
5	B	2377	NAD	O5B-C5B-C4B	-2.93	98.30	109.12
5	C	3377	NAD	O5B-C5B-C4B	-2.73	99.06	109.12
5	B	2377	NAD	C2B-C3B-C4B	-2.63	97.20	102.61
5	D	4377	NAD	C4B-O4B-C1B	-2.59	106.87	109.72
5	A	1377	NAD	O5B-C5B-C4B	-2.53	99.79	109.12
5	D	4377	NAD	O5B-C5B-C4B	-2.41	100.23	109.12
5	B	2377	NAD	C2B-C1B-N9A	-2.27	110.82	114.29
5	A	1377	NAD	C2B-C1B-N9A	-2.26	110.85	114.29
5	D	4377	NAD	O4D-C1D-N1N	-2.25	105.66	108.13
5	C	3377	NAD	PN-O3-PA	-2.21	126.53	132.73
5	A	1377	NAD	C2B-C3B-C4B	-2.20	98.08	102.61
5	B	2377	NAD	O2A-PA-O3	2.11	114.66	105.09
5	D	4377	NAD	O5D-C5D-C4D	2.28	117.51	109.12
5	B	2377	NAD	C1B-N9A-C4A	2.35	130.49	126.94
5	B	2377	NAD	O7N-C7N-C3N	2.37	122.18	119.59
5	C	3377	NAD	O2A-PA-O3	2.39	115.92	105.09
5	D	4377	NAD	O5B-PA-O1A	2.41	118.98	109.62
5	C	3377	NAD	C3N-C7N-N7N	2.50	120.55	117.82
5	C	3377	NAD	O3-PA-O5B	2.51	109.60	102.94
5	D	4377	NAD	O2A-PA-O3	2.65	117.14	105.09
5	A	1377	NAD	C3N-C2N-N1N	2.68	123.45	120.36
5	B	2377	NAD	O4B-C4B-C3B	2.75	110.68	105.15
5	B	2377	NAD	O2N-PN-O3	2.79	117.76	105.09
5	D	4377	NAD	O4B-C4B-C3B	2.87	110.93	105.15
5	A	1377	NAD	O2N-PN-O3	2.89	118.18	105.09
5	D	4377	NAD	O2N-PN-O3	3.20	119.62	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1377	NAD	O3-PA-O5B	3.29	111.67	102.94
5	B	2377	NAD	N6A-C6A-N1A	3.35	126.39	119.20
5	C	3377	NAD	O4B-C4B-C3B	3.37	111.93	105.15
5	A	1377	NAD	O4B-C4B-C3B	3.43	112.07	105.15
5	D	4377	NAD	C3N-C7N-N7N	3.72	121.89	117.82
5	C	3377	NAD	O7N-C7N-C3N	3.99	123.94	119.59
5	B	2377	NAD	C4A-C5A-N7A	4.72	113.82	109.48
5	A	1377	NAD	O7N-C7N-C3N	5.26	125.33	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1377	NAD	2	0
3	A	501	ACT	2	0
5	B	2377	NAD	2	0
3	B	506	ACT	1	0
4	B	992	CAC	1	0
4	B	993	CAC	1	0
5	C	3377	NAD	2	0
3	C	505	ACT	1	0
5	D	4377	NAD	4	0
3	D	509	ACT	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.07	8 (2%)	67	66	16, 40, 58, 65	0
1	B	373/373 (100%)	-0.15	1 (0%)	94	94	12, 33, 49, 62	0
1	C	373/373 (100%)	0.34	12 (3%)	51	51	22, 52, 67, 74	0
1	D	373/373 (100%)	-0.16	2 (0%)	91	91	16, 30, 46, 57	0
All	All	1492/1492 (100%)	0.02	23 (1%)	76	75	12, 38, 62, 74	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	4.3
1	C	332	VAL	3.2
1	C	232	ALA	3.0
1	A	83	VAL	3.0
1	A	77	GLY	3.0
1	C	134	GLY	2.8
1	A	76	ILE	2.8
1	C	340	PHE	2.6
1	C	362	LEU	2.6
1	C	1	GLY	2.5
1	B	214	ALA	2.5
1	D	1	GLY	2.5
1	C	237	ALA	2.4
1	C	352	PHE	2.3
1	C	161	ASP	2.3
1	A	58	VAL	2.3
1	C	345	LEU	2.2
1	C	335	PHE	2.2
1	D	4	GLY	2.2
1	A	3	ALA	2.1
1	C	41	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	2.1
1	A	130	PHE	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^{th} 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	B	506	4/4	0.93	0.21	10.76	12,26,27,37	0
4	CAC	A	994	5/5	0.97	0.17	4.88	69,70,71,73	0
4	CAC	B	995	5/5	0.96	0.22	3.27	74,74,76,77	0
3	ACT	C	505	4/4	0.98	0.18	2.10	33,34,35,41	0
3	ACT	A	502	4/4	0.95	0.27	1.09	50,51,51,51	4
3	ACT	A	501	4/4	0.97	0.17	1.01	37,39,40,41	0
3	ACT	D	511	4/4	0.98	0.14	0.06	26,29,32,32	0
5	NAD	D	4377	44/44	0.98	0.14	-0.14	21,29,35,37	0
3	ACT	D	509	4/4	0.97	0.14	-0.26	16,18,20,20	0
5	NAD	B	2377	44/44	0.98	0.13	-0.37	14,25,35,39	0
5	NAD	A	1377	44/44	0.97	0.12	-0.57	23,30,35,38	0
2	ZN	B	375	1/1	0.98	0.12	-1.00	28,28,28,28	0
2	ZN	B	404	1/1	0.98	0.12	-1.05	31,31,31,31	0
2	ZN	C	375	1/1	1.00	0.10	-1.22	43,43,43,43	0
5	NAD	C	3377	44/44	0.95	0.12	-1.23	19,49,55,60	0
2	ZN	B	376	1/1	0.99	0.11	-1.25	28,28,28,28	0
2	ZN	C	376	1/1	0.98	0.10	-1.48	46,46,46,46	0
2	ZN	D	375	1/1	1.00	0.11	-1.74	30,30,30,30	0
2	ZN	D	376	1/1	0.99	0.12	-1.93	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	408	1/1	0.98	0.10	-2.05	47,47,47,47	0
2	ZN	A	376	1/1	0.99	0.08	-2.68	35,35,35,35	0
4	CAC	B	991	5/5	0.99	0.09	-3.12	17,32,35,38	0
2	ZN	A	375	1/1	0.98	0.07	-3.17	49,49,49,49	0
3	ACT	B	507	4/4	0.97	0.14	-	23,24,25,29	0
4	CAC	B	993	5/5	0.97	0.15	-	47,49,51,55	0
2	ZN	B	406	1/1	0.98	0.05	-	42,42,42,42	0
2	ZN	A	401	1/1	0.97	0.10	-	48,48,48,48	0
2	ZN	B	405	1/1	0.98	0.09	-	51,51,51,51	0
2	ZN	D	409	1/1	0.97	0.12	-	48,48,48,48	0
3	ACT	A	513	4/4	0.95	0.33	-	52,52,53,54	4
3	ACT	D	508	4/4	0.98	0.14	-	23,25,26,31	0
2	ZN	A	402	1/1	0.91	0.17	-	50,50,50,50	1
2	ZN	C	407	1/1	0.93	0.06	-	63,63,63,63	0
2	ZN	D	411	1/1	0.98	0.08	-	48,48,48,48	0
4	CAC	B	992	5/5	0.98	0.10	-	49,52,55,57	0
3	ACT	D	512	4/4	0.94	0.20	-	32,35,38,39	0
2	ZN	D	410	1/1	0.84	0.23	-	47,47,47,47	1
3	ACT	C	510	4/4	0.97	0.09	-	33,33,34,34	0
3	ACT	D	514	4/4	0.90	0.51	-	49,52,53,54	4
3	ACT	A	504	4/4	0.97	0.14	-	15,18,19,19	0
2	ZN	A	403	1/1	0.98	0.12	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.