Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 AM GMT

PDB ID : 2EIH
Title : Crystal Structure of NAD-dependent alcohol dehydrogenase
Authors : Kamiya, N.; Hikima, T.; Matsu, T.; Maoka, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-13
Resolution : 2.30 Å(reported)

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

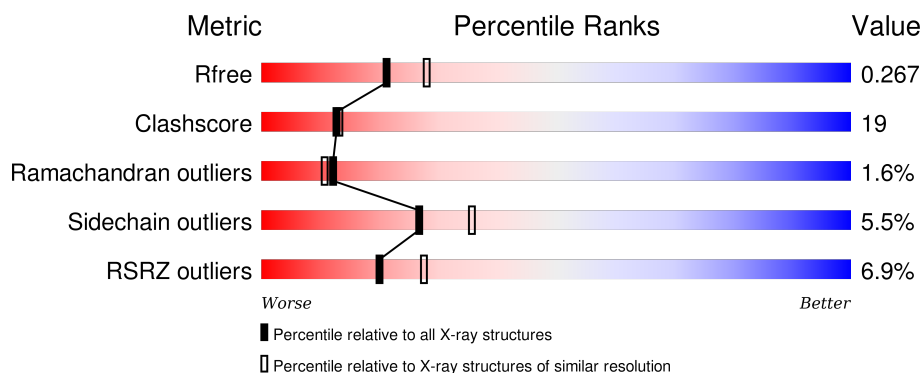|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		19
Ramachandran outliers		1.6%
Sidechain outliers		5.5%
RSRZ outliers		6.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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	343	8% 63% 34% •
1	B	343	6% 63% 34% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5385 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total 2566	C 1631	N 462	O 464	S 9	0	0	0
1	B	343	Total 2566	C 1631	N 462	O 464	S 9	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	141	Total 141	O 141	0	0

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

Chain A:

- Molecule 1: Alcohol dehydrogenase

Chain B:
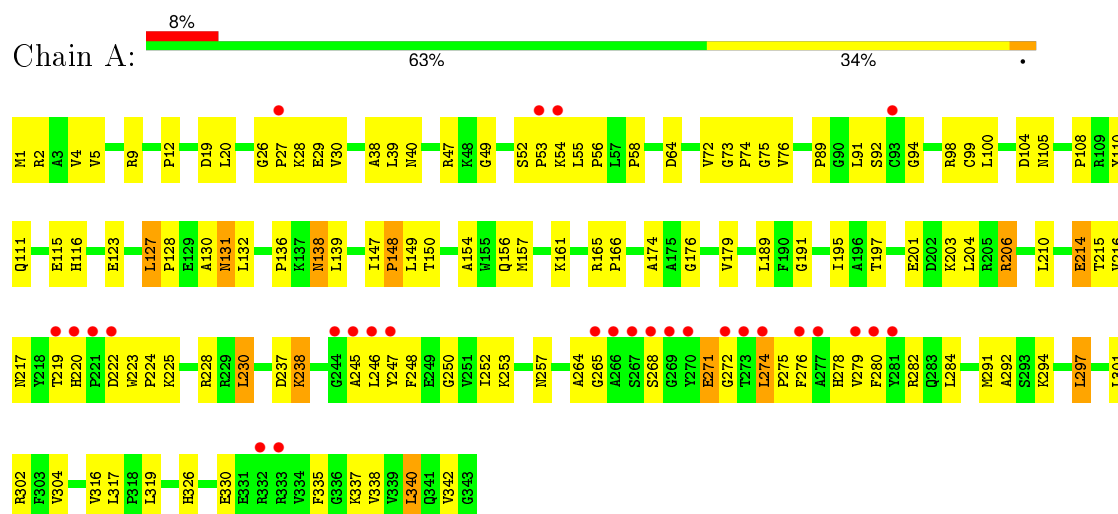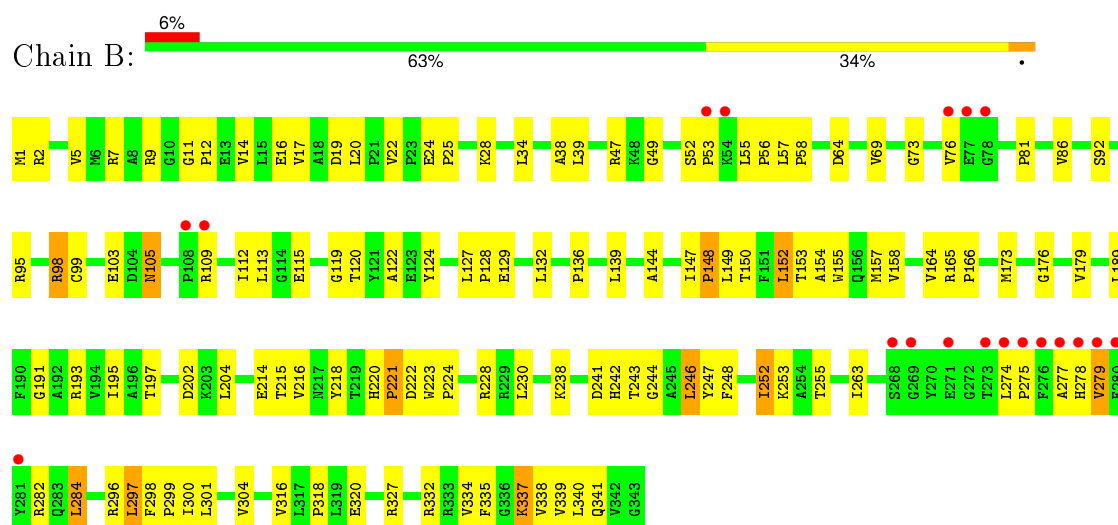
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	75.58Å 133.89Å 75.67Å 90.00° 107.29° 90.00°	Depositor
Resolution (Å)	19.69 – 2.30 19.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.4 (19.69-2.30) 81.5 (19.68-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	0.87 (at 2.21Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.267 0.209 , 0.267	Depositor DCC
R_{free} test set	2819 reflections (10.02%)	DCC
Wilson B-factor (Å²)	29.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 44.3	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 31848 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0.375 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: ZN

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	0.37	0/2619	0.62	0/3553
1	B	0.38	0/2619	0.63	0/3553
All	All	0.37	0/5238	0.62	0/7106

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 ⓘ

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	2566	0	2625	104	0
1	B	2566	0	2625	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	110	0	0	7	0
3	B	141	0	0	5	0
All	All	5385	0	5250	200	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 19.

All (200) 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:127:LEU:HD11	1:B:132:LEU:HD13	1.32	1.07
1:B:274:LEU:HD22	1:B:275:PRO:HD2	1.38	1.02
1:A:245:ALA:HB3	1:A:268:SER:HB3	1.43	0.99
1:A:72:VAL:HB	1:A:76:VAL:HG11	1.55	0.87
1:A:138:ASN:HD22	1:A:138:ASN:H	1.24	0.82
1:A:257:ASN:ND2	1:A:282:ARG:HD2	2.00	0.77
1:B:195:ILE:HG12	3:B:518:HOH:O	1.86	0.76
1:A:30:VAL:HG11	1:A:132:LEU:HD22	1.66	0.76
1:B:105:ASN:HD22	1:B:105:ASN:H	1.32	0.74
1:B:274:LEU:HD22	1:B:275:PRO:CD	2.16	0.73
1:B:275:PRO:HG2	1:B:279:VAL:HG21	1.69	0.73
1:A:257:ASN:HD21	1:A:282:ARG:HD2	1.53	0.72
1:B:55:LEU:HD12	1:B:56:PRO:HD2	1.72	0.71
1:B:136:PRO:HG2	1:B:139:LEU:HD12	1.73	0.71
1:B:105:ASN:HD22	1:B:105:ASN:N	1.84	0.70
1:B:5:VAL:HG21	1:B:58:PRO:HB2	1.73	0.70
1:A:9:ARG:HH11	1:A:55:LEU:HB3	1.58	0.68
1:A:131:ASN:N	1:A:131:ASN:HD22	1.91	0.68
1:A:214:GLU:HG2	1:A:230:LEU:HG	1.74	0.68
1:A:127:LEU:HD12	1:A:131:ASN:HB2	1.75	0.67
1:A:130:ALA:C	1:A:131:ASN:HD22	1.99	0.65
1:A:157:MET:HE1	1:A:179:VAL:HG21	1.79	0.64
1:A:166:PRO:HA	1:A:191:GLY:O	1.97	0.64
1:B:5:VAL:CG2	1:B:58:PRO:HB2	2.28	0.63
1:B:224:PRO:O	1:B:228:ARG:HG2	1.99	0.63
1:A:222:ASP:HB3	1:A:225:LYS:HD2	1.81	0.63
1:B:202:ASP:HB3	3:B:538:HOH:O	1.97	0.63
1:A:111:GLN:HG2	1:A:116:HIS:HD2	1.64	0.63
1:A:276:PHE:HB2	1:A:280:PHE:CE2	2.34	0.62
1:B:11:GLY:O	1:B:14:VAL:HG22	1.99	0.62
1:A:9:ARG:HD3	1:A:49:GLY:HA2	1.83	0.61
1:B:105:ASN:H	1:B:105:ASN:ND2	1.99	0.61
1:B:246:LEU:HD22	1:B:247:TYR:CD2	2.35	0.61
1:B:204:LEU:HD22	1:B:215:THR:HB	1.81	0.60
1:A:147:ILE:HB	1:A:148:PRO:HD3	1.84	0.59
1:A:197:THR:HG22	1:A:216:VAL:HB	1.84	0.59
1:A:276:PHE:C	1:A:278:HIS:H	2.05	0.59
1:A:127:LEU:HB2	1:A:128:PRO:HD2	1.85	0.59
1:A:279:VAL:HG13	1:A:284:LEU:HB2	1.84	0.59
1:A:91:LEU:HB2	1:A:111:GLN:O	2.03	0.58
1:B:139:LEU:HD11	1:B:304:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:O	1:B:252:ILE:HG23	2.04	0.57
1:B:223:TRP:CD1	1:B:224:PRO:HD3	2.39	0.57
1:B:214:GLU:HG2	1:B:230:LEU:HG	1.87	0.57
1:A:27:PRO:HA	1:A:74:PRO:HD2	1.87	0.56
1:B:9:ARG:HH22	1:B:57:LEU:HD11	1.70	0.56
1:A:92:SER:HB2	1:A:99:CYS:SG	2.45	0.56
1:B:34:LEU:HD12	1:B:122:ALA:O	2.05	0.56
1:B:153:THR:O	1:B:157:MET:HG3	2.05	0.56
1:B:52:SER:N	1:B:53:PRO:HD3	2.21	0.55
1:B:113:LEU:HD22	1:B:119:GLY:HA2	1.89	0.55
1:B:220:HIS:HD2	1:B:221:PRO:HD2	1.71	0.55
1:A:176:GLY:HA3	1:A:335:PHE:CD1	2.41	0.55
1:B:255:THR:O	1:B:282:ARG:NH2	2.39	0.55
1:A:131:ASN:ND2	1:A:131:ASN:N	2.54	0.55
1:B:341:GLN:HG3	1:B:341:GLN:O	2.07	0.55
1:A:157:MET:CE	1:A:179:VAL:HG21	2.37	0.54
1:B:223:TRP:CG	1:B:224:PRO:HD3	2.41	0.54
1:B:11:GLY:HA2	1:B:47:ARG:HH11	1.72	0.54
1:A:12:PRO:HA	1:A:47:ARG:HD2	1.90	0.54
1:B:320:GLU:H	1:B:320:GLU:CD	2.10	0.54
1:A:54:LYS:HD2	1:A:54:LYS:N	2.22	0.54
1:A:9:ARG:HD3	1:A:49:GLY:CA	2.38	0.54
1:A:150:THR:HG23	1:A:337:LYS:NZ	2.22	0.54
1:A:39:LEU:CD1	1:A:340:LEU:HD13	2.37	0.54
1:A:271:GLU:O	1:A:274:LEU:HD13	2.07	0.54
1:B:95:ARG:HH22	1:B:109:ARG:NH2	2.05	0.53
1:B:38:ALA:HB3	1:B:64:ASP:CB	2.38	0.53
1:A:214:GLU:CG	1:A:230:LEU:HG	2.38	0.53
1:B:19:ASP:O	1:B:20:LEU:HD23	2.08	0.53
1:A:111:GLN:HG2	1:A:116:HIS:CD2	2.44	0.52
1:A:223:TRP:N	1:A:224:PRO:CD	2.72	0.52
1:A:55:LEU:HD12	1:A:56:PRO:HD2	1.90	0.52
1:A:265:GLY:HA2	3:A:526:HOH:O	2.08	0.52
1:A:220:HIS:CE1	1:A:222:ASP:HB2	2.44	0.52
1:B:193:ARG:NH1	3:B:544:HOH:O	2.43	0.52
1:B:92:SER:HB2	1:B:99:CYS:SG	2.50	0.52
1:B:318:PRO:HA	1:B:341:GLN:HG3	1.92	0.52
1:A:52:SER:N	1:A:53:PRO:HD3	2.24	0.52
1:B:297:LEU:HD22	1:B:301:LEU:HG	1.92	0.51
1:B:9:ARG:HD3	1:B:49:GLY:HA2	1.93	0.51
1:A:9:ARG:NH1	1:A:55:LEU:HB3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:OD2	1:A:294:LYS:HG3	2.12	0.50
1:B:9:ARG:HH21	1:B:9:ARG:HG3	1.75	0.50
1:A:30:VAL:CG1	1:A:132:LEU:HD22	2.38	0.50
1:A:64:ASP:OD2	1:A:148:PRO:HB2	2.12	0.50
1:A:39:LEU:HD11	1:A:340:LEU:HD13	1.94	0.49
1:B:69:VAL:O	1:B:81:PRO:HA	2.12	0.49
1:B:2:ARG:HD2	1:B:17:VAL:CG1	2.42	0.49
1:A:279:VAL:HG13	1:A:284:LEU:CB	2.41	0.49
1:A:5:VAL:HB	1:A:58:PRO:HB2	1.95	0.49
1:A:98:ARG:HG2	3:A:511:HOH:O	2.13	0.49
1:A:123:GLU:HA	1:A:342:VAL:HG11	1.94	0.49
1:A:74:PRO:HG2	1:A:75:GLY:H	1.78	0.49
1:A:206:ARG:HG2	1:A:335:PHE:CE2	2.48	0.49
1:B:334:VAL:HG11	1:B:338:VAL:CG2	2.43	0.49
1:B:55:LEU:CD1	1:B:56:PRO:HD2	2.42	0.49
1:B:38:ALA:HB3	1:B:64:ASP:HB2	1.94	0.48
1:B:155:TRP:CD1	1:B:296:ARG:HG3	2.48	0.48
1:B:9:ARG:HD3	1:B:49:GLY:CA	2.44	0.48
1:B:246:LEU:HD22	1:B:247:TYR:CE2	2.48	0.48
1:B:98:ARG:NH1	1:B:103:GLU:OE2	2.45	0.48
1:B:241:ASP:O	1:B:263:ILE:HA	2.14	0.48
1:A:156:GLN:NE2	1:A:292:ALA:HA	2.29	0.48
1:A:223:TRP:CG	1:A:224:PRO:HD3	2.49	0.48
1:B:165:ARG:HB2	1:B:166:PRO:HD2	1.96	0.48
1:A:138:ASN:H	1:A:138:ASN:ND2	2.03	0.48
1:A:38:ALA:HB3	1:A:64:ASP:HB3	1.95	0.48
1:A:245:ALA:CB	1:A:268:SER:HB3	2.29	0.47
1:A:165:ARG:HB2	1:A:166:PRO:HD2	1.96	0.47
1:A:91:LEU:HD12	1:A:91:LEU:N	2.30	0.47
1:A:138:ASN:HD22	1:A:138:ASN:N	1.97	0.47
1:B:278:HIS:CE1	1:B:282:ARG:HD2	2.50	0.47
1:B:28:LYS:O	1:B:129:GLU:HG2	2.15	0.47
1:B:52:SER:O	1:B:55:LEU:HB2	2.15	0.46
1:B:252:ILE:HG13	1:B:253:LYS:N	2.29	0.46
1:B:1:MET:SD	1:B:124:TYR:HB2	2.54	0.46
1:A:108:PRO:HD3	3:A:557:HOH:O	2.15	0.46
1:A:223:TRP:CD1	1:A:224:PRO:HD3	2.51	0.46
1:A:326:HIS:O	1:A:330:GLU:HG3	2.16	0.46
1:A:4:VAL:HG23	1:A:319:LEU:CD1	2.46	0.46
1:A:195:ILE:HD12	1:A:195:ILE:N	2.31	0.46
1:A:302:ARG:HD3	3:A:547:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HB	1:A:76:VAL:CG1	2.36	0.45
1:A:276:PHE:C	1:A:278:HIS:N	2.70	0.45
1:A:26:GLY:O	1:A:73:GLY:HA3	2.16	0.45
1:B:7:ARG:HG3	1:B:16:GLU:OE1	2.16	0.45
1:A:38:ALA:HB3	1:A:64:ASP:CB	2.46	0.45
1:A:204:LEU:HD22	1:A:215:THR:HB	1.97	0.45
1:B:12:PRO:HG3	1:B:327:ARG:HG3	1.97	0.45
1:B:57:LEU:N	1:B:57:LEU:HD12	2.32	0.45
1:B:150:THR:HG21	1:B:337:LYS:HE3	1.98	0.45
1:A:297:LEU:HD22	1:A:301:LEU:HG	1.98	0.45
1:B:148:PRO:O	1:B:152:LEU:HD22	2.16	0.45
1:B:274:LEU:C	1:B:274:LEU:HD13	2.38	0.45
1:A:40:ASN:HD21	1:A:337:LYS:NZ	2.14	0.45
1:B:154:ALA:O	1:B:158:VAL:HG23	2.17	0.45
1:B:73:GLY:O	1:B:76:VAL:HG23	2.17	0.45
1:A:39:LEU:HD22	1:A:338:VAL:CG1	2.47	0.44
1:B:153:THR:HG22	1:B:157:MET:CE	2.48	0.44
1:B:127:LEU:HB2	1:B:128:PRO:HD2	1.97	0.44
1:B:275:PRO:HG2	1:B:279:VAL:CG2	2.45	0.44
1:A:279:VAL:HA	1:A:284:LEU:HD22	2.00	0.44
1:A:224:PRO:O	1:A:228:ARG:HG2	2.18	0.44
1:B:147:ILE:HB	1:B:148:PRO:HD3	1.98	0.44
1:A:316:VAL:C	1:A:317:LEU:HD22	2.37	0.44
1:B:24:GLU:HG3	1:B:25:PRO:HD2	1.99	0.44
1:A:237:ASP:C	1:A:238:LYS:HD2	2.38	0.44
1:B:298:PHE:N	1:B:299:PRO:HD2	2.33	0.44
1:B:193:ARG:NH2	1:B:230:LEU:O	2.51	0.44
1:A:30:VAL:HG23	1:A:72:VAL:HG12	1.99	0.44
1:A:150:THR:HG23	1:A:337:LYS:HZ2	1.83	0.44
1:B:173:MET:HA	1:B:197:THR:OG1	2.18	0.44
1:B:86:VAL:CG1	1:B:144:ALA:HB1	2.48	0.43
1:B:166:PRO:HA	1:B:191:GLY:O	2.18	0.43
1:A:105:ASN:HA	1:A:110:TYR:CE2	2.53	0.43
1:B:112:ILE:O	1:B:115:GLU:HB3	2.19	0.43
1:A:154:ALA:HA	1:A:157:MET:HE2	1.99	0.43
1:A:176:GLY:HA3	1:A:335:PHE:CE1	2.54	0.43
1:A:89:PRO:HG2	1:A:291:MET:CE	2.48	0.43
1:B:34:LEU:HD13	1:B:120:THR:O	2.17	0.43
1:B:279:VAL:O	1:B:284:LEU:HB2	2.19	0.43
1:B:316:VAL:HA	1:B:339:VAL:O	2.17	0.43
1:B:300:ILE:O	1:B:304:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PRO:O	1:B:279:VAL:HB	2.19	0.43
1:A:27:PRO:HG2	1:A:28:LYS:H	1.83	0.42
1:B:318:PRO:HA	1:B:341:GLN:CG	2.48	0.42
1:B:158:VAL:HG13	1:B:164:VAL:HG21	2.01	0.42
1:B:220:HIS:C	1:B:222:ASP:H	2.22	0.42
1:A:217:ASN:OD1	1:A:219:THR:HG22	2.19	0.42
1:B:39:LEU:HD13	1:B:340:LEU:HD13	2.00	0.42
1:B:55:LEU:O	1:B:57:LEU:HD12	2.19	0.42
1:B:242:HIS:HE1	3:B:542:HOH:O	2.03	0.42
1:A:1:MET:O	1:A:19:ASP:HA	2.20	0.42
1:A:150:THR:HG22	3:A:553:HOH:O	2.20	0.41
1:A:1:MET:HG2	1:A:20:LEU:O	2.20	0.41
1:A:247:TYR:O	1:A:250:GLY:N	2.52	0.41
1:B:176:GLY:HA2	1:B:335:PHE:CD1	2.55	0.41
1:B:221:PRO:HA	3:B:613:HOH:O	2.18	0.41
1:A:52:SER:HG	1:A:115:GLU:HG2	1.86	0.41
1:B:1:MET:HB3	1:B:22:VAL:HG22	2.02	0.41
1:A:26:GLY:N	1:A:29:GLU:HB2	2.35	0.41
1:B:243:THR:HG23	1:B:244:GLY:H	1.86	0.41
1:A:157:MET:HA	1:A:161:LYS:HB2	2.03	0.41
1:B:153:THR:HG22	1:B:157:MET:HE2	2.02	0.41
1:A:40:ASN:ND2	1:A:337:LYS:HZ1	2.19	0.41
1:A:2:ARG:HD3	3:A:508:HOH:O	2.19	0.41
1:B:157:MET:CE	1:B:179:VAL:HG11	2.51	0.41
1:A:139:LEU:HD11	1:A:304:VAL:HG11	2.03	0.41
1:A:136:PRO:HB2	1:A:138:ASN:ND2	2.35	0.41
1:A:39:LEU:HD13	1:A:340:LEU:HD13	2.01	0.41
1:A:248:PHE:CE2	1:A:252:ILE:HD11	2.56	0.41
1:A:94:GLY:HA2	1:A:99:CYS:HB3	2.01	0.41
1:A:150:THR:CG2	1:A:337:LYS:HZ2	2.34	0.41
1:B:95:ARG:HH22	1:B:109:ARG:HH21	1.69	0.40
1:B:9:ARG:NH2	1:B:57:LEU:HD21	2.35	0.40
1:A:89:PRO:HG2	1:A:291:MET:HE1	2.03	0.40
1:B:197:THR:HA	1:B:216:VAL:O	2.22	0.40
1:A:203:LYS:HG2	1:A:335:PHE:HD1	1.87	0.40
1:A:2:ARG:NE	3:A:508:HOH:O	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/343 (99%)	308 (90%)	26 (8%)	7 (2%)	9	7
1	B	341/343 (99%)	322 (94%)	15 (4%)	4 (1%)	16	16
All	All	682/686 (99%)	630 (92%)	41 (6%)	11 (2%)	12	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	PRO
1	A	272	GLY
1	B	277	ALA
1	A	264	ALA
1	B	148	PRO
1	A	174	ALA
1	A	246	LEU
1	A	275	PRO
1	B	279	VAL
1	A	274	LEU
1	B	221	PRO

5.3.2 Protein sidechains (i)

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	263/263 (100%)	247 (94%)	16 (6%)	23	30
1	B	263/263 (100%)	250 (95%)	13 (5%)	31	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	526/526 (100%)	497 (94%)	29 (6%)	27 36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	127	LEU
1	A	131	ASN
1	A	138	ASN
1	A	149	LEU
1	A	189	LEU
1	A	201	GLU
1	A	206	ARG
1	A	210	LEU
1	A	214	GLU
1	A	230	LEU
1	A	238	LYS
1	A	253	LYS
1	A	271	GLU
1	A	297	LEU
1	A	340	LEU
1	B	98	ARG
1	B	105	ASN
1	B	149	LEU
1	B	152	LEU
1	B	189	LEU
1	B	218	TYR
1	B	238	LYS
1	B	246	LEU
1	B	252	ILE
1	B	284	LEU
1	B	297	LEU
1	B	332	ARG
1	B	337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	116	HIS
1	A	131	ASN

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	156	GLN
1	A	257	ASN
1	A	315	GLN
1	B	40	ASN
1	B	105	ASN
1	B	131	ASN
1	B	156	GLN
1	B	220	HIS
1	B	278	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	343/343 (100%)	0.36	28 (8%)	14	20	16, 36, 80, 120	0
1	B	343/343 (100%)	0.12	19 (5%)	29	37	17, 35, 67, 85	0
All	All	686/686 (100%)	0.24	47 (6%)	20	27	16, 36, 72, 120	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLY	15.0
1	A	270	TYR	11.9
1	B	275	PRO	8.5
1	A	268	SER	6.7
1	A	266	ALA	6.2
1	A	245	ALA	5.8
1	A	220	HIS	5.2
1	A	267	SER	5.1
1	A	272	GLY	4.8
1	A	273	THR	4.7
1	A	280	PHE	4.6
1	A	221	PRO	4.5
1	B	54	LYS	4.4
1	B	278	HIS	4.3
1	A	277	ALA	4.3
1	A	276	PHE	4.2
1	A	219	THR	3.7
1	A	246	LEU	3.7
1	B	279	VAL	3.2
1	A	247	TYR	3.2
1	A	281	TYR	3.1
1	B	280	PHE	3.0
1	A	274	LEU	3.0
1	B	281	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	2.8
1	A	27	PRO	2.8
1	B	77	GLU	2.8
1	B	273	THR	2.7
1	B	268	SER	2.7
1	B	109	ARG	2.6
1	A	54	LYS	2.6
1	B	274	LEU	2.5
1	B	78	GLY	2.5
1	B	271	GLU	2.4
1	A	279	VAL	2.4
1	A	333	ARG	2.3
1	A	244	GLY	2.2
1	A	53	PRO	2.2
1	B	53	PRO	2.2
1	A	93	CYS	2.2
1	A	222	ASP	2.2
1	A	332	ARG	2.2
1	B	276	PHE	2.2
1	B	108	PRO	2.1
1	B	269	GLY	2.0
1	B	277	ALA	2.0
1	B	76	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	ZN	B	501	1/1	0.98	0.03	-1.78	43,43,43,43	0
2	ZN	A	500	1/1	0.99	0.04	-3.51	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.