Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2016 – 12:00 AM GMT

PDB ID	:	8ADH
Title	:	INTERDOMAIN MOTION IN LIVER ALCOHOL DEHYDROGENASE. STRUCTURAL AND ENERGETIC ANALYSIS OF THE HINGE BENDING MODE
Authors	:	Jones, T.A.; Eklund, H.
Deposited on	:	1989-04-20
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 (i)) were used in the production of this report:

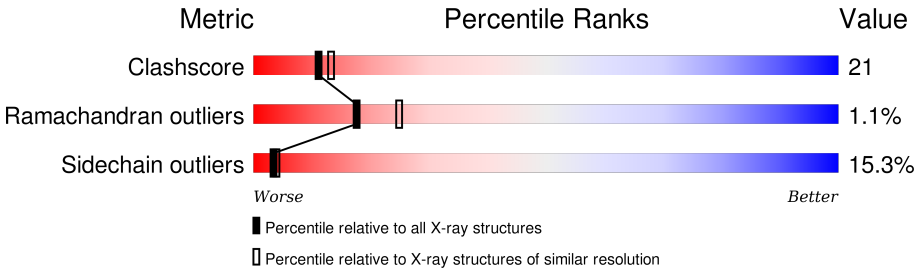
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	56% 30% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2955 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 APO-LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		

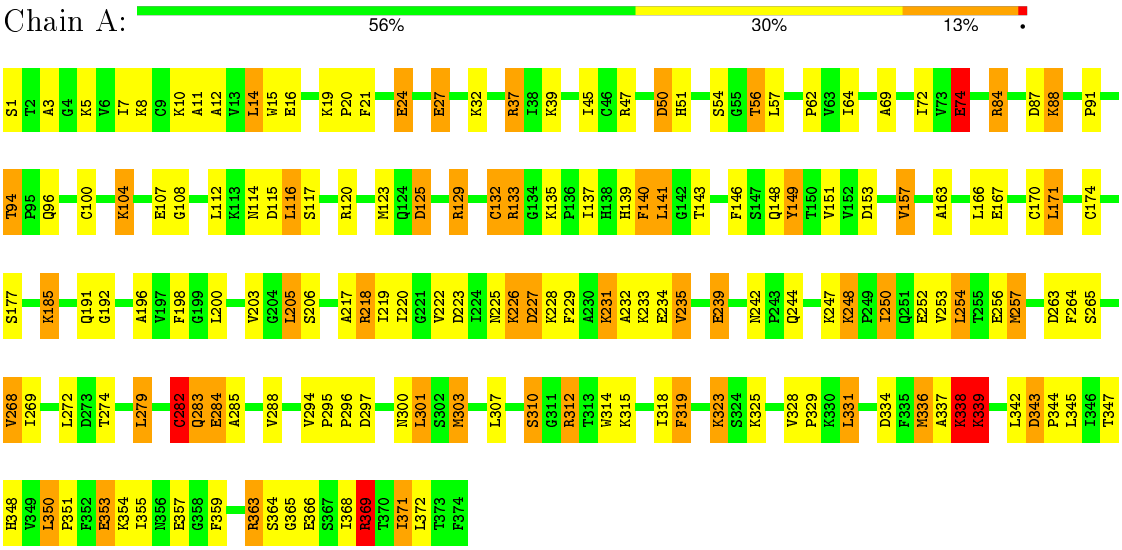
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: APO-LIVER ALCOHOL DEHYDROGENASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	56.00Å 75.20Å 181.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2955	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

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	1.24	5/2837 (0.2%)	1.91	69/3834 (1.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	GLY	N-CA	-8.17	1.33	1.46
1	A	252	GLU	CD-OE1	-5.42	1.19	1.25
1	A	282	CYS	CB-SG	-5.28	1.73	1.81
1	A	365	GLY	CA-C	-5.12	1.43	1.51
1	A	239	GLU	CD-OE1	-5.03	1.20	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	366	GLU	CA-CB-CG	17.28	151.42	113.40
1	A	84	ARG	NE-CZ-NH1	13.97	127.29	120.30
1	A	365	GLY	N-CA-C	13.79	147.57	113.10
1	A	47	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	A	133	ARG	NE-CZ-NH1	-12.56	114.02	120.30
1	A	50	ASP	CB-CG-OD1	10.98	128.18	118.30
1	A	37	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	A	87	ASP	CB-CG-OD1	9.93	127.24	118.30
1	A	218	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	A	47	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	363	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	149	TYR	CB-CG-CD2	-8.49	115.91	121.00
1	A	312	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	A	74	GLU	CA-CB-CG	8.43	131.95	113.40
1	A	133	ARG	CD-NE-CZ	-8.36	111.89	123.60
1	A	74	GLU	CB-CG-CD	8.30	136.60	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	115	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	115	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	366	GLU	C-N-CA	7.12	139.49	121.70
1	A	353	GLU	CA-CB-CG	6.88	128.54	113.40
1	A	227	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	366	GLU	CA-C-O	6.78	134.33	120.10
1	A	323	LYS	N-CA-C	-6.68	92.96	111.00
1	A	303	MET	N-CA-CB	-6.63	98.67	110.60
1	A	312	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	A	74	GLU	N-CA-CB	6.57	122.43	110.60
1	A	132	CYS	O-C-N	6.54	133.16	122.70
1	A	319	PHE	CB-CG-CD1	-6.52	116.23	120.80
1	A	343	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	129	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	331	LEU	CB-CA-C	6.28	122.13	110.20
1	A	24	GLU	CG-CD-OE1	6.18	130.66	118.30
1	A	350	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	336	MET	CG-SD-CE	6.05	109.87	100.20
1	A	263	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	A	120	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	133	ARG	CB-CG-CD	5.92	126.99	111.60
1	A	107	GLU	OE1-CD-OE2	5.91	130.39	123.30
1	A	218	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	A	331	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	257	MET	CG-SD-CE	5.75	109.41	100.20
1	A	283	GLN	N-CA-CB	5.66	120.78	110.60
1	A	140	PHE	O-C-N	5.64	131.72	122.70
1	A	107	GLU	CG-CD-OE2	-5.55	107.20	118.30
1	A	239	GLU	CB-CA-C	-5.54	99.32	110.40
1	A	87	ASP	CA-CB-CG	5.42	125.32	113.40
1	A	125	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	149	TYR	CB-CG-CD1	5.36	124.21	121.00
1	A	27	GLU	CG-CD-OE2	-5.35	107.60	118.30
1	A	234	GLU	CA-CB-CG	5.33	125.13	113.40
1	A	177	SER	CA-CB-OG	-5.32	96.84	111.20
1	A	223	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	256	GLU	CG-CD-OE1	5.30	128.90	118.30
1	A	14	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	84	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	256	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	A	129	ARG	NH1-CZ-NH2	-5.25	113.62	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	133	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	366	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	A	116	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	282	CYS	N-CA-CB	-5.14	101.34	110.60
1	A	315	LYS	CD-CE-NZ	-5.14	99.89	111.70
1	A	369	ARG	CD-NE-CZ	-5.11	116.44	123.60
1	A	252	GLU	CG-CD-OE1	5.11	128.52	118.30
1	A	27	GLU	CG-CD-OE1	5.08	128.47	118.30
1	A	263	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	114	ASN	O-C-N	5.00	130.71	122.70

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	2785	0	2848	117	0
2	A	2	0	0	0	0
3	A	168	0	0	11	2
All	All	2955	0	2848	117	2

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 21.

All (117) 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:A:272:LEU:HD22	1:A:301:LEU:HB3	1.43	0.98
1:A:347:THR:HG21	1:A:368:ILE:H	1.29	0.97
1:A:337:ALA:O	1:A:338:LYS:HB2	1.65	0.94
1:A:226:LYS:HD3	1:A:242:ASN:HD22	1.31	0.92
1:A:347:THR:HG21	1:A:368:ILE:N	1.88	0.88
1:A:10:LYS:O	1:A:148:GLN:HG3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:H	1:A:250:ILE:HD13	1.43	0.84
1:A:334:ASP:O	1:A:339:LYS:HB2	1.79	0.82
1:A:250:ILE:N	1:A:250:ILE:HD13	1.95	0.82
1:A:250:ILE:HA	1:A:253:VAL:HG13	1.60	0.81
1:A:268:VAL:HG23	1:A:268:VAL:O	1.84	0.77
1:A:250:ILE:H	1:A:250:ILE:CD1	1.98	0.76
1:A:353:GLU:HG2	3:A:445:HOH:O	1.87	0.74
1:A:205:LEU:HD23	1:A:345:LEU:HD23	1.69	0.73
1:A:56:THR:CG2	1:A:296:PRO:HG2	2.18	0.72
1:A:170:CYS:SG	1:A:371:ILE:HD13	2.31	0.71
1:A:171:LEU:HD23	1:A:342:LEU:HD22	1.72	0.71
1:A:283:GLN:OE1	1:A:285:ALA:HB3	1.92	0.70
1:A:64:ILE:HG13	1:A:137:ILE:HG21	1.75	0.67
1:A:269:ILE:HD12	1:A:274:THR:HG21	1.76	0.66
1:A:347:THR:HG23	1:A:348:HIS:ND1	2.10	0.66
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.79	0.65
1:A:123:MET:HE3	1:A:151:VAL:O	1.97	0.65
1:A:303:MET:HA	3:A:471:HOH:O	1.95	0.64
1:A:250:ILE:O	1:A:254:LEU:HB2	2.00	0.62
1:A:157:VAL:O	1:A:325:LYS:HE3	1.99	0.62
1:A:250:ILE:CD1	1:A:250:ILE:N	2.61	0.62
1:A:218:ARG:C	1:A:219:ILE:HG13	2.20	0.62
1:A:56:THR:HG22	1:A:296:PRO:HG2	1.80	0.62
1:A:226:LYS:HD3	1:A:242:ASN:ND2	2.10	0.61
1:A:337:ALA:O	1:A:338:LYS:CB	2.43	0.61
1:A:51:HIS:HB3	1:A:56:THR:HG22	1.83	0.61
1:A:203:VAL:HG23	3:A:420:HOH:O	2.00	0.61
1:A:347:THR:HG22	1:A:369:ARG:H	1.67	0.60
1:A:37:ARG:HD2	1:A:74:GLU:OE1	2.01	0.59
1:A:39:LYS:NZ	3:A:518:HOH:O	2.33	0.59
1:A:56:THR:HG23	1:A:296:PRO:HG2	1.84	0.59
1:A:140:PHE:CE1	1:A:141:LEU:HD22	2.38	0.59
1:A:334:ASP:O	1:A:339:LYS:CB	2.50	0.59
1:A:231:LYS:O	1:A:235:VAL:HB	2.03	0.58
1:A:108:GLY:O	1:A:323:LYS:NZ	2.33	0.58
1:A:171:LEU:HD11	1:A:369:ARG:HG3	1.86	0.57
1:A:300:ASN:O	3:A:474:HOH:O	2.17	0.57
1:A:123:MET:CE	1:A:151:VAL:O	2.53	0.57
1:A:91:PRO:HB2	1:A:143:THR:HG22	1.86	0.57
1:A:72:ILE:HD11	1:A:88:LYS:CD	2.35	0.56
1:A:16:GLU:OE1	1:A:19:LYS:HE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HD12	1:A:166:LEU:HD11	1.86	0.56
1:A:15:TRP:HA	1:A:62:PRO:HB3	1.86	0.56
1:A:132:CYS:O	1:A:133:ARG:HB2	2.04	0.56
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.88	0.56
1:A:50:ASP:OD1	1:A:363:ARG:HD3	2.05	0.56
1:A:296:PRO:HB3	3:A:542:HOH:O	2.05	0.55
1:A:64:ILE:HG13	1:A:137:ILE:CG2	2.36	0.55
1:A:69:ALA:O	1:A:91:PRO:HD2	2.05	0.55
1:A:37:ARG:NH1	1:A:74:GLU:OE1	2.36	0.54
1:A:88:LYS:HE3	1:A:166:LEU:HG	1.89	0.53
1:A:354:LYS:NZ	3:A:451:HOH:O	2.42	0.52
1:A:225:ASN:ND2	1:A:227:ASP:HB2	2.25	0.52
1:A:10:LYS:HA	1:A:24:GLU:O	2.10	0.52
1:A:364:SER:HB3	3:A:446:HOH:O	2.10	0.52
1:A:284:GLU:O	1:A:310:SER:HB2	2.09	0.52
1:A:334:ASP:HB3	1:A:339:LYS:HD2	1.94	0.50
1:A:100:CYS:O	1:A:104:LYS:HG3	2.12	0.50
1:A:123:MET:HE3	1:A:139:HIS:CE1	2.47	0.49
1:A:7:ILE:O	1:A:27:GLU:HA	2.13	0.49
1:A:328:VAL:N	1:A:329:PRO:CD	2.75	0.49
1:A:196:ALA:O	1:A:265:SER:HA	2.13	0.48
1:A:248:LYS:HG3	1:A:253:VAL:HG12	1.96	0.48
1:A:229:PHE:O	1:A:233:LYS:HG3	2.14	0.48
1:A:72:ILE:HD11	1:A:88:LYS:HD3	1.96	0.47
1:A:307:LEU:O	1:A:312:ARG:HD2	2.15	0.47
1:A:284:GLU:HB3	3:A:469:HOH:O	2.14	0.47
1:A:220:ILE:N	1:A:220:ILE:HD12	2.31	0.47
1:A:72:ILE:HD12	1:A:166:LEU:CD1	2.44	0.46
1:A:225:ASN:HB3	1:A:228:LYS:HG3	1.98	0.46
1:A:295:PRO:HB2	1:A:297:ASP:OD2	2.15	0.46
1:A:171:LEU:HD13	1:A:371:ILE:HD11	1.97	0.46
1:A:279:LEU:O	1:A:282:CYS:HB2	2.15	0.46
1:A:343:ASP:N	1:A:344:PRO:CD	2.78	0.46
1:A:220:ILE:H	1:A:220:ILE:HD12	1.80	0.46
1:A:192:GLY:HA2	1:A:217:ALA:HB2	1.98	0.46
1:A:32:LYS:HD2	1:A:129:ARG:CZ	2.46	0.46
1:A:10:LYS:NZ	1:A:353:GLU:OE2	2.47	0.45
1:A:264:PHE:HA	1:A:288:VAL:O	2.16	0.45
1:A:125:ASP:OD2	1:A:129:ARG:NH2	2.48	0.45
1:A:319:PHE:O	1:A:319:PHE:CG	2.69	0.45
1:A:185:LYS:HG3	1:A:185:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:CG	3:A:445:HOH:O	2.54	0.45
1:A:7:ILE:HG22	1:A:8:LYS:N	2.31	0.45
1:A:7:ILE:HD12	1:A:149:TYR:CD1	2.52	0.45
1:A:45:ILE:HD13	1:A:359:PHE:CD1	2.52	0.44
1:A:225:ASN:HB3	1:A:228:LYS:CG	2.47	0.44
1:A:146:PHE:CD1	1:A:355:ILE:HD11	2.52	0.44
1:A:226:LYS:CD	1:A:242:ASN:HD22	2.17	0.44
1:A:354:LYS:O	1:A:357:GLU:HB2	2.17	0.44
1:A:200:LEU:HD13	1:A:232:ALA:HB2	2.00	0.44
1:A:12:ALA:HB1	1:A:21:PHE:HB3	2.00	0.44
1:A:72:ILE:HD11	1:A:88:LYS:HD2	1.99	0.44
1:A:359:PHE:O	1:A:363:ARG:HG3	2.18	0.43
1:A:253:VAL:O	1:A:257:MET:HG3	2.18	0.43
1:A:20:PRO:HA	3:A:416:HOH:O	2.18	0.43
1:A:247:LYS:HB3	1:A:247:LYS:HE2	1.63	0.43
1:A:64:ILE:CG1	1:A:137:ILE:HG21	2.47	0.42
1:A:11:ALA:HB1	1:A:64:ILE:HD13	2.01	0.42
1:A:123:MET:CE	1:A:139:HIS:CE1	3.02	0.42
1:A:282:CYS:O	1:A:312:ARG:NH2	2.50	0.42
1:A:198:PHE:O	1:A:268:VAL:HG22	2.20	0.42
1:A:205:LEU:HD23	1:A:345:LEU:CD2	2.46	0.42
1:A:100:CYS:O	1:A:104:LYS:CG	2.68	0.42
1:A:351:PRO:HG2	1:A:354:LYS:HD2	2.02	0.42
1:A:57:LEU:HB2	1:A:296:PRO:HG3	2.02	0.41
1:A:94:THR:HG21	1:A:318:ILE:HG22	2.03	0.41
1:A:32:LYS:HD3	1:A:129:ARG:NH2	2.36	0.41
1:A:170:CYS:SG	1:A:371:ILE:CD1	3.07	0.41
1:A:328:VAL:N	1:A:329:PRO:HD2	2.36	0.41
1:A:163:ALA:HB3	1:A:336:MET:HE2	2.03	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:HOH:O	3:A:435:HOH:O[3_655]	1.52	0.68
3:A:520:HOH:O	3:A:521:HOH:O[4_555]	1.83	0.37

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	372/374 (100%)	338 (91%)	30 (8%)	4 (1%)	17 25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	A	339	LYS
1	A	3	ALA
1	A	338	LYS

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	308/308 (100%)	261 (85%)	47 (15%)	3 4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	14	LEU
1	A	54	SER
1	A	56	THR
1	A	74	GLU
1	A	84	ARG

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Mol	Chain	Res	Type
1	A	88	LYS
1	A	94	THR
1	A	96	GLN
1	A	104	LYS
1	A	116	LEU
1	A	117	SER
1	A	135	LYS
1	A	141	LEU
1	A	153	ASP
1	A	157	VAL
1	A	167	GLU
1	A	171	LEU
1	A	185	LYS
1	A	191	GLN
1	A	205	LEU
1	A	206	SER
1	A	222	VAL
1	A	226	LYS
1	A	231	LYS
1	A	235	VAL
1	A	239	GLU
1	A	244	GLN
1	A	248	LYS
1	A	250	ILE
1	A	254	LEU
1	A	268	VAL
1	A	279	LEU
1	A	282	CYS
1	A	284	GLU
1	A	294	VAL
1	A	301	LEU
1	A	310	SER
1	A	314	TRP
1	A	331	LEU
1	A	338	LYS
1	A	339	LYS
1	A	350	LEU
1	A	369	ARG
1	A	371	ILE
1	A	372	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	225	ASN
1	A	259	ASN
1	A	299	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 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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.