



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:50 PM UTC

PDB ID : 8ADH / pdb_00008adh
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

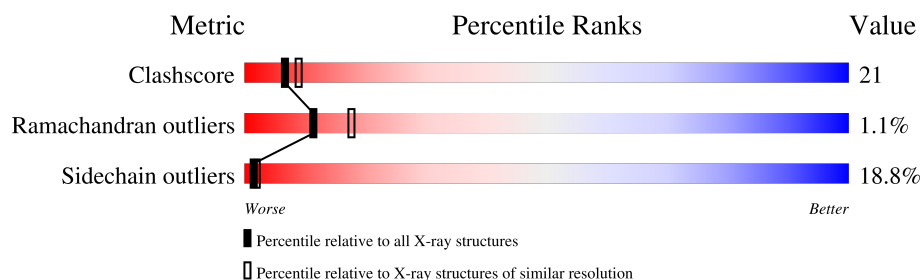
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

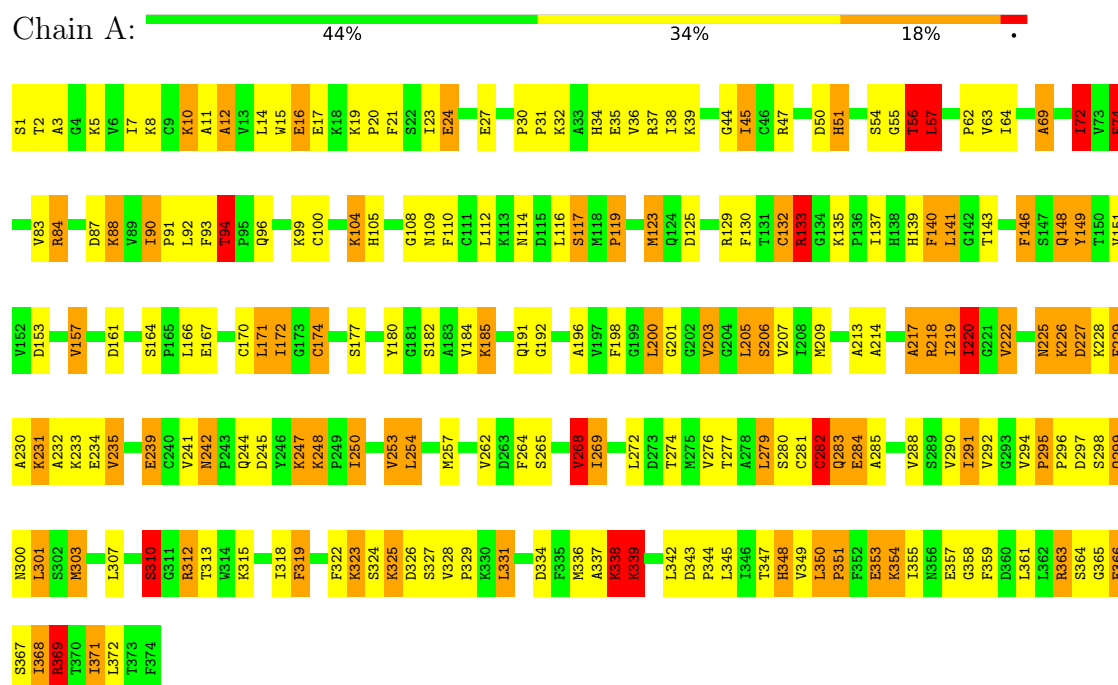
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.59	18/2837 (0.6%)	2.44	151/3834 (3.9%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	GLY	N-CA	-9.29	1.33	1.44
1	A	367	SER	N-CA	-7.19	1.37	1.46
1	A	45	ILE	CA-C	7.10	1.61	1.52
1	A	220	ILE	C-N	-6.56	1.27	1.33
1	A	184	VAL	C-O	6.52	1.32	1.24
1	A	201	GLY	C-O	5.52	1.29	1.23
1	A	325	LYS	C-O	5.49	1.30	1.24
1	A	319	PHE	CA-CB	5.44	1.61	1.53
1	A	133	ARG	CD-NE	5.35	1.53	1.46
1	A	201	GLY	C-N	-5.29	1.27	1.33
1	A	218	ARG	N-CA	5.24	1.52	1.46
1	A	349	VAL	CA-C	5.14	1.59	1.52
1	A	368	ILE	N-CA	5.14	1.52	1.46
1	A	291	ILE	N-CA	5.06	1.52	1.46
1	A	351	PRO	C-N	-5.04	1.27	1.33
1	A	366	GLU	CA-CB	-5.04	1.45	1.53
1	A	290	VAL	N-CA	5.01	1.52	1.46
1	A	38	ILE	CA-CB	5.01	1.61	1.54

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	25.32	147.57	110.60
1	A	366	GLU	CA-CB-CG	18.66	151.42	114.10
1	A	74	GLU	CB-CG-CD	14.12	136.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CA-CB-CG	12.72	125.32	112.60
1	A	366	GLU	CA-C-O	11.96	134.33	120.70
1	A	366	GLU	CA-C-N	11.54	139.49	121.72
1	A	366	GLU	C-N-CA	11.54	139.49	121.72
1	A	295	PRO	O-C-N	10.26	126.03	121.31
1	A	201	GLY	CA-C-N	10.15	131.16	120.00
1	A	201	GLY	C-N-CA	10.15	131.16	120.00
1	A	323	LYS	N-CA-C	-10.13	92.96	108.67
1	A	368	ILE	N-CA-C	-9.35	101.23	110.30
1	A	93	PHE	CA-CB-CG	9.21	123.01	113.80
1	A	133	ARG	CD-NE-CZ	-8.93	111.89	124.40
1	A	74	GLU	CA-CB-CG	8.92	131.95	114.10
1	A	268	VAL	CA-C-O	-8.59	111.55	120.14
1	A	94	THR	CB-CA-C	8.53	122.07	110.13
1	A	110	PHE	CA-CB-CG	8.05	121.86	113.80
1	A	303	MET	N-CA-CB	-7.78	98.67	111.66
1	A	44	GLY	CA-C-N	7.78	133.12	122.93
1	A	44	GLY	C-N-CA	7.78	133.12	122.93
1	A	327	SER	N-CA-C	7.75	123.23	112.45
1	A	222	VAL	CA-C-O	7.62	128.39	120.39
1	A	36	VAL	CA-C-O	-7.53	112.48	120.76
1	A	242	ASN	CB-CA-C	7.49	118.48	110.17
1	A	133	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	A	92	LEU	N-CA-C	7.46	120.95	108.20
1	A	280	SER	N-CA-C	7.30	119.31	111.36
1	A	94	THR	CA-C-O	7.28	126.46	119.62
1	A	353	GLU	CA-CB-CG	7.22	128.54	114.10
1	A	74	GLU	N-CA-CB	7.20	122.43	110.33
1	A	2	THR	N-CA-C	-7.18	103.73	114.64
1	A	225	ASN	CA-CB-CG	-7.15	105.45	112.60
1	A	177	SER	CA-CB-OG	-7.13	96.84	111.10
1	A	322	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	105	HIS	CA-C-N	7.10	126.78	119.82
1	A	105	HIS	C-N-CA	7.10	126.78	119.82
1	A	30	PRO	O-C-N	7.10	124.49	121.15
1	A	262	VAL	CB-CA-C	7.08	119.38	111.45
1	A	283	GLN	N-CA-CB	7.01	120.78	109.28
1	A	17	GLU	CB-CG-CD	6.94	124.40	112.60
1	A	114	ASN	O-C-N	6.94	130.71	122.94
1	A	164	SER	N-CA-C	6.93	119.68	109.50
1	A	350	LEU	O-C-N	6.90	128.26	121.57
1	A	133	ARG	CB-CG-CD	6.82	126.99	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	O-C-N	6.69	130.28	123.26
1	A	331	LEU	CB-CA-C	6.64	122.13	110.85
1	A	146	PHE	CA-CB-CG	6.60	120.40	113.80
1	A	310	SER	CA-C-O	-6.52	113.64	120.55
1	A	227	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	10	LYS	CA-C-N	6.43	132.89	122.29
1	A	10	LYS	C-N-CA	6.43	132.89	122.29
1	A	132	CYS	O-C-N	6.40	133.16	122.93
1	A	225	ASN	OD1-CG-ND2	6.38	128.98	122.60
1	A	363	ARG	N-CA-C	6.31	118.16	111.28
1	A	203	VAL	N-CA-C	-6.20	104.46	110.72
1	A	148	GLN	OE1-CD-NE2	6.19	128.79	122.60
1	A	114	ASN	CA-C-O	-6.17	114.44	121.72
1	A	326	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	35	GLU	N-CA-C	-6.14	100.62	110.14
1	A	90	ILE	O-C-N	6.13	128.08	121.10
1	A	269	ILE	CB-CA-C	-6.12	104.51	111.55
1	A	119	PRO	CA-C-O	6.12	127.99	121.32
1	A	182	SER	CA-C-N	6.12	130.79	120.88
1	A	182	SER	C-N-CA	6.12	130.79	120.88
1	A	367	SER	O-C-N	6.08	130.26	123.40
1	A	219	ILE	CB-CA-C	6.06	117.32	110.41
1	A	34	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	84	ARG	O-C-N	6.01	126.15	121.88
1	A	218	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	47	ARG	NE-CZ-NH2	-5.96	113.83	119.20
1	A	222	VAL	CB-CA-C	5.92	119.39	110.63
1	A	2	THR	O-C-N	5.92	128.20	121.93
1	A	180	TYR	CA-C-N	5.92	127.54	120.14
1	A	180	TYR	C-N-CA	5.92	127.54	120.14
1	A	312	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	56	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	361	LEU	CA-C-N	5.87	128.62	120.63
1	A	361	LEU	C-N-CA	5.87	128.62	120.63
1	A	348	HIS	CA-CB-CG	5.87	119.67	113.80
1	A	324	SER	N-CA-C	5.79	118.09	111.02
1	A	84	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	365	GLY	CA-C-O	5.78	126.96	121.30
1	A	225	ASN	CA-C-N	5.78	128.29	120.38
1	A	225	ASN	C-N-CA	5.78	128.29	120.38
1	A	140	PHE	O-C-N	5.74	131.72	122.99
1	A	51	HIS	N-CA-CB	5.73	118.54	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	O-C-N	5.70	127.70	121.83
1	A	245	ASP	CA-C-O	-5.69	112.61	119.27
1	A	369	ARG	CD-NE-CZ	-5.69	116.44	124.40
1	A	172	ILE	CB-CG1-CD1	5.68	125.73	113.80
1	A	184	VAL	CA-C-O	-5.65	114.37	120.47
1	A	12	ALA	CA-C-O	-5.63	115.06	120.92
1	A	229	PHE	N-CA-C	5.63	118.18	111.71
1	A	99	LYS	CB-CA-C	-5.62	101.00	110.44
1	A	358	GLY	O-C-N	5.59	127.62	122.19
1	A	280	SER	CB-CA-C	-5.56	101.40	110.85
1	A	234	GLU	CA-CB-CG	5.51	125.13	114.10
1	A	130	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	282	CYS	N-CA-CB	-5.49	101.34	110.23
1	A	23	ILE	N-CA-C	-5.47	101.62	108.84
1	A	363	ARG	CB-CG-CD	5.46	123.86	111.30
1	A	109	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	55	GLY	N-CA-C	-5.42	107.62	115.27
1	A	203	VAL	CA-C-N	5.42	126.11	119.99
1	A	203	VAL	C-N-CA	5.42	126.11	119.99
1	A	31	PRO	N-CA-C	5.35	119.27	111.03
1	A	57	LEU	CB-CA-C	5.35	119.34	110.78
1	A	262	VAL	N-CA-CB	-5.34	100.90	111.15
1	A	24	GLU	CG-CD-OE1	5.33	130.66	118.40
1	A	133	ARG	CA-C-O	-5.32	115.07	121.40
1	A	182	SER	CA-CB-OG	-5.32	100.46	111.10
1	A	123	MET	CA-C-O	-5.31	114.97	121.88
1	A	319	PHE	CA-C-N	5.31	131.07	120.77
1	A	319	PHE	C-N-CA	5.31	131.07	120.77
1	A	44	GLY	N-CA-C	-5.31	104.58	113.02
1	A	276	VAL	CB-CA-C	5.28	118.94	112.02
1	A	213	ALA	CA-C-N	5.27	128.32	120.31
1	A	213	ALA	C-N-CA	5.27	128.32	120.31
1	A	281	CYS	CA-C-N	5.27	129.89	122.09
1	A	281	CYS	C-N-CA	5.27	129.89	122.09
1	A	207	VAL	N-CA-C	-5.25	105.59	110.53
1	A	299	GLN	CA-CB-CG	-5.25	103.60	114.10
1	A	301	LEU	CB-CA-C	5.24	118.45	109.80
1	A	292	VAL	CB-CA-C	5.24	119.04	111.65
1	A	354	LYS	CA-C-N	5.24	127.64	120.77
1	A	354	LYS	C-N-CA	5.24	127.64	120.77
1	A	298	SER	CA-C-O	5.22	127.26	121.56
1	A	174	CYS	CA-C-N	5.22	131.64	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	CYS	C-N-CA	5.22	131.64	121.41
1	A	83	VAL	O-C-N	5.22	128.83	123.04
1	A	277	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	207	VAL	O-C-N	5.19	127.30	121.90
1	A	239	GLU	CB-CA-C	-5.18	99.32	110.45
1	A	24	GLU	CB-CG-CD	5.17	121.40	112.60
1	A	217	ALA	N-CA-C	-5.17	107.14	113.50
1	A	368	ILE	CB-CA-C	5.16	118.26	111.81
1	A	239	GLU	O-C-N	5.15	129.12	123.25
1	A	72	ILE	CB-CG1-CD1	5.14	124.60	113.80
1	A	149	TYR	O-C-N	5.14	129.54	123.33
1	A	214	ALA	O-C-N	5.12	128.57	122.27
1	A	230	ALA	CA-C-N	5.11	127.12	120.28
1	A	230	ALA	C-N-CA	5.11	127.12	120.28
1	A	313	THR	CA-CB-CG2	5.10	119.17	110.50
1	A	56	THR	CA-CB-CG2	5.10	119.17	110.50
1	A	319	PHE	CA-CB-CG	-5.09	108.70	113.80
1	A	200	LEU	CB-CA-C	5.09	118.22	111.14
1	A	218	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	A	201	GLY	CA-C-O	-5.07	116.20	122.03
1	A	63	VAL	N-CA-CB	-5.05	104.83	112.35
1	A	247	LYS	N-CA-C	-5.02	106.75	112.92

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	2785	0	2848	121	0
2	A	2	0	0	0	0
3	A	168	0	0	11	2
All	All	2955	0	2848	121	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 (121) 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
1:A:123:MET:HE3	1:A:139:HIS:CE1	2.13	0.84
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:HD13	1:A:250:ILE:N	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:123:MET:HE1	1:A:151:VAL:O	1.89	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:218:ARG:C	1:A:219:ILE:HG13	2.20	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:303:MET:HA	3:A:471:HOH:O	1.95	0.64
1:A:157:VAL:O	1:A:325:LYS:HE3	1.99	0.62
1:A:250:ILE:O	1:A:254:LEU:HB2	2.00	0.62
1:A:250:ILE:N	1:A:250:ILE:CD1	2.61	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: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:108:GLY:O	1:A:323:LYS:NZ	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:O	1:A:235:VAL:HB	2.03	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:91:PRO:HB2	1:A:143:THR:HG22	1.86	0.57
1:A:123:MET:CE	1:A:151:VAL:O	2.53	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
1:A:15:TRP:HA	1:A:62:PRO:HB3	1.86	0.56
1:A:72:ILE:HD12	1:A:166:LEU:HD11	1.86	0.56
1:A:132:CYS:O	1:A:133:ARG:HB2	2.04	0.56
1:A:50:ASP:OD1	1:A:363:ARG:HD3	2.05	0.56
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.88	0.56
1:A:64:ILE:HG13	1:A:137:ILE:CG2	2.36	0.55
1:A:296:PRO:HB3	3:A:542:HOH:O	2.05	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:206:SER:HA	1:A:209:MET:HE3	1.89	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:284:GLU:O	1:A:310:SER:HB2	2.09	0.52
1:A:364:SER:HB3	3:A:446:HOH:O	2.10	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:209:MET:HE1	1:A:345:LEU:HD11	1.93	0.50
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:39:LYS:NZ	3:A:518:HOH:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:N	1:A:344:PRO:CD	2.78	0.46
1:A:32:LYS:HD2	1:A:129:ARG:CZ	2.46	0.46
1:A:192:GLY:HA2	1:A:217:ALA:HB2	1.98	0.46
1:A:220:ILE:HD12	1:A:220:ILE:H	1.80	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:123:MET:HE3	1:A:139:HIS:ND1	2.30	0.45
1:A:161:ASP:OD2	1:A:336:MET:HE2	2.17	0.45
1:A:185:LYS:O	1:A:185:LYS:HG3	2.16	0.45
1:A:7:ILE:HG22	1:A:8:LYS:N	2.31	0.45
1:A:353:GLU:CG	3:A:445:HOH:O	2.54	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:200:LEU:HD13	1:A:232:ALA:HB2	2.00	0.44
1:A:319:PHE:O	1:A:319:PHE:CG	2.69	0.44
1:A:354:LYS:O	1:A:357:GLU:HB2	2.17	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:HE2	1:A:247:LYS:HB3	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:282:CYS:O	1:A:312:ARG:NH2	2.50	0.42
1:A:100:CYS:O	1:A:104:LYS:CG	2.68	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: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:117:SER:C	1:A:119:PRO:HD3	2.46	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:10:LYS:HZ2	1:A:353:GLU:CD	2.30	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 [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	372/374 (100%)	338 (91%)	30 (8%)	4 (1%)	11 18

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 [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	308/308 (100%)	250 (81%)	58 (19%)	1 2

All (58) 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	16	GLU
1	A	54	SER
1	A	56	THR
1	A	57	LEU
1	A	72	ILE
1	A	74	GLU
1	A	84	ARG
1	A	88	LYS
1	A	90	ILE
1	A	94	THR
1	A	96	GLN
1	A	104	LYS
1	A	116	LEU
1	A	117	SER
1	A	133	ARG
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	172	ILE
1	A	185	LYS
1	A	191	GLN
1	A	205	LEU
1	A	206	SER
1	A	220	ILE
1	A	222	VAL
1	A	226	LYS
1	A	231	LYS
1	A	235	VAL
1	A	239	GLU
1	A	241	VAL
1	A	244	GLN
1	A	248	LYS
1	A	250	ILE
1	A	253	VAL
1	A	254	LEU
1	A	268	VAL
1	A	279	LEU

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Mol	Chain	Res	Type
1	A	282	CYS
1	A	284	GLU
1	A	291	ILE
1	A	294	VAL
1	A	299	GLN
1	A	310	SER
1	A	315	LYS
1	A	331	LEU
1	A	338	LYS
1	A	339	LYS
1	A	350	LEU
1	A	366	GLU
1	A	369	ARG
1	A	371	ILE
1	A	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
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 oligosaccharides 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 [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.