Full wwPDB X-ray Structure Validation Report (i)

Jul 1, 2021 – 12:00 PM EDT

PDB ID	:	1ALD
Title	:	ACTIVITY AND SPECIFICITY OF HUMAN ALDOLASES
Authors	:	Watson, H.C.
Deposited on	:	1991-05-05
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/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:

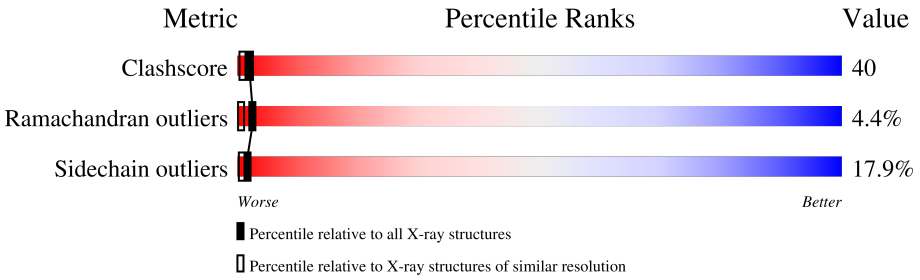
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	54% 32% 12% ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2763 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 ALDOLASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2763	1741	486	525	11	0	0	0

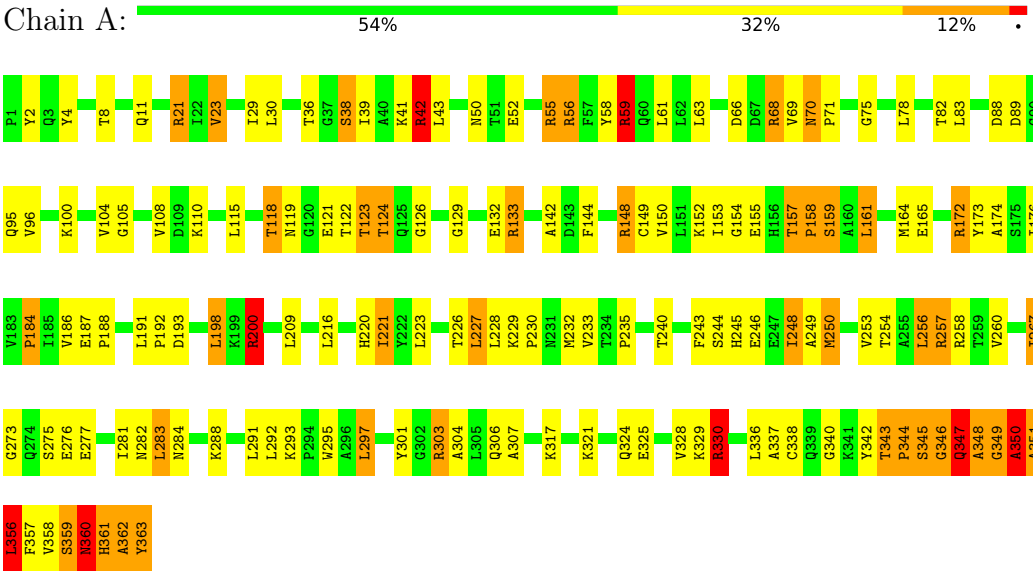
3 Residue-property plots (i)

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: ALDOLASE A

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.34Å 96.34Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	95.0 ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.93	1/2817 (0.0%)	1.23	22/3818 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ALA	C-N	6.90	1.50	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	A	21	ARG	CD-NE-CZ	-9.05	110.93	123.60
1	A	200	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	A	148	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	360	ASN	O-C-N	6.71	133.43	122.70
1	A	68	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	330	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	42	ARG	CD-NE-CZ	6.31	132.44	123.60
1	A	220	HIS	CB-CA-C	-6.18	98.04	110.40
1	A	164	MET	CG-SD-CE	6.09	109.94	100.20
1	A	250	MET	CG-SD-CE	6.09	109.94	100.20
1	A	232	MET	CG-SD-CE	6.06	109.89	100.20
1	A	91	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	172	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	21	ARG	NH1-CZ-NH2	-5.81	113.01	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	42	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	A	21	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	59	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	56	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	360	ASN	CA-C-N	-5.23	105.70	117.20
1	A	59	ARG	CD-NE-CZ	5.13	130.78	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ALA	Mainchain

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	2763	0	2782	224	1
All	All	2763	0	2782	224	1

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 40.

All (224) 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:152:LYS:HG3	1:A:157:THR:CG2	1.58	1.32
1:A:192:PRO:HD2	1:A:362:ALA:CB	1.62	1.29
1:A:42:ARG:HD3	1:A:303:ARG:NH1	1.51	1.25
1:A:342:TYR:CZ	1:A:344:PRO:HG2	1.76	1.19
1:A:148:ARG:HH22	1:A:361:HIS:CE1	1.60	1.19
1:A:275:SER:CB	1:A:355:SER:HB2	1.74	1.15
1:A:192:PRO:HG2	1:A:362:ALA:HB1	1.18	1.12
1:A:154:GLY:N	1:A:157:THR:OG1	1.83	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:CG	1:A:362:ALA:HB1	1.80	1.11
1:A:256:LEU:HD21	1:A:267:ILE:CD1	1.80	1.10
1:A:192:PRO:CD	1:A:362:ALA:CB	2.28	1.09
1:A:154:GLY:CA	1:A:157:THR:OG1	2.01	1.09
1:A:192:PRO:HD2	1:A:362:ALA:HB3	1.33	1.08
1:A:303:ARG:HE	1:A:303:ARG:HA	1.11	1.06
1:A:52:GLU:HA	1:A:55:ARG:HH21	1.21	1.05
1:A:275:SER:HB2	1:A:355:SER:CB	1.87	1.04
1:A:36:THR:HG23	1:A:55:ARG:HH11	1.22	1.03
1:A:192:PRO:HG2	1:A:362:ALA:CB	1.89	1.02
1:A:362:ALA:O	1:A:363:TYR:HB2	1.61	1.01
1:A:148:ARG:NH2	1:A:361:HIS:CE1	2.29	1.01
1:A:148:ARG:NH2	1:A:361:HIS:NE2	2.09	0.99
1:A:152:LYS:CG	1:A:157:THR:HG21	1.91	0.98
1:A:275:SER:HB2	1:A:355:SER:HB2	0.99	0.98
1:A:152:LYS:HG3	1:A:157:THR:HG21	0.99	0.97
1:A:192:PRO:CG	1:A:362:ALA:CB	2.43	0.96
1:A:157:THR:HB	1:A:158:PRO:HD3	1.47	0.96
1:A:36:THR:HG23	1:A:55:ARG:NH1	1.80	0.96
1:A:349:GLY:O	1:A:350:ALA:O	1.86	0.94
1:A:50:ASN:HD21	1:A:55:ARG:HD3	1.31	0.93
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.48	0.93
1:A:256:LEU:HD21	1:A:267:ILE:HD11	1.49	0.93
1:A:154:GLY:HA3	1:A:157:THR:OG1	1.67	0.93
1:A:148:ARG:HG3	1:A:187:GLU:CD	1.90	0.92
1:A:192:PRO:HD2	1:A:362:ALA:HB2	1.51	0.90
1:A:152:LYS:HE3	1:A:157:THR:HG23	1.50	0.90
1:A:152:LYS:CG	1:A:157:THR:CG2	2.47	0.90
1:A:347:GLN:O	1:A:349:GLY:N	2.03	0.90
1:A:123:THR:HG23	1:A:165:GLU:HG3	1.54	0.88
1:A:245:HIS:CD2	1:A:351:ALA:HA	2.09	0.88
1:A:235:PRO:HG3	1:A:243:PHE:CD1	2.09	0.88
1:A:42:ARG:CD	1:A:303:ARG:NH1	2.37	0.88
1:A:277:GLU:HA	1:A:330:ARG:NH2	1.89	0.88
1:A:42:ARG:HD3	1:A:303:ARG:HH11	1.32	0.86
1:A:275:SER:HB3	1:A:356:LEU:H	1.41	0.84
1:A:56:ARG:NH2	1:A:88:ASP:OD1	2.11	0.84
1:A:118:THR:HG21	1:A:121:GLU:HB2	1.60	0.84
1:A:123:THR:CG2	1:A:165:GLU:HG3	2.07	0.84
1:A:344:PRO:O	1:A:345:SER:O	1.95	0.83
1:A:52:GLU:CA	1:A:55:ARG:HH21	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:O	1:A:257:ARG:HG3	1.79	0.81
1:A:246:GLU:HG3	1:A:348:ALA:C	1.99	0.81
1:A:152:LYS:HG3	1:A:157:THR:HG22	1.62	0.81
1:A:342:TYR:OH	1:A:344:PRO:HG2	1.80	0.80
1:A:157:THR:HB	1:A:158:PRO:CD	2.12	0.79
1:A:303:ARG:HA	1:A:303:ARG:NE	1.95	0.79
1:A:50:ASN:ND2	1:A:55:ARG:HD3	1.97	0.79
1:A:303:ARG:HE	1:A:303:ARG:CA	1.92	0.78
1:A:192:PRO:CD	1:A:362:ALA:HB3	2.06	0.78
1:A:157:THR:O	1:A:159:SER:N	2.17	0.78
1:A:256:LEU:CD2	1:A:267:ILE:CD1	2.62	0.77
1:A:307:ALA:HB2	1:A:357:PHE:CE2	2.20	0.77
1:A:66:ASP:OD1	1:A:68:ARG:HD3	1.85	0.77
1:A:354:GLU:O	1:A:355:SER:OG	2.02	0.77
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.15	0.76
1:A:121:GLU:OE1	1:A:157:THR:O	2.02	0.76
1:A:281:ILE:HG12	1:A:345:SER:HB3	1.68	0.76
1:A:193:ASP:OD1	1:A:361:HIS:O	2.05	0.74
1:A:154:GLY:HA3	1:A:157:THR:HG1	1.50	0.73
1:A:246:GLU:HB2	1:A:349:GLY:HA2	1.69	0.73
1:A:104:VAL:HG13	1:A:142:ALA:HA	1.71	0.73
1:A:342:TYR:CZ	1:A:344:PRO:CG	2.65	0.71
1:A:267:ILE:HD11	1:A:269:PHE:CZ	2.26	0.71
1:A:152:LYS:HE3	1:A:157:THR:CG2	2.20	0.70
1:A:118:THR:CG2	1:A:121:GLU:H	2.06	0.69
1:A:273:GLY:HA2	1:A:357:PHE:O	1.91	0.69
1:A:359:SER:O	1:A:361:HIS:N	2.25	0.69
1:A:303:ARG:NH2	1:A:306:GLN:CD	2.45	0.69
1:A:161:LEU:O	1:A:161:LEU:HD22	1.94	0.68
1:A:235:PRO:HG3	1:A:243:PHE:HD1	1.57	0.68
1:A:118:THR:HG23	1:A:121:GLU:H	1.59	0.68
1:A:152:LYS:O	1:A:157:THR:HB	1.94	0.68
1:A:342:TYR:CE1	1:A:344:PRO:HD2	2.28	0.68
1:A:303:ARG:HH21	1:A:306:GLN:CD	1.97	0.67
1:A:245:HIS:CD2	1:A:351:ALA:CA	2.77	0.67
1:A:352:ALA:O	1:A:353:SER:OG	2.07	0.66
1:A:325:GLU:O	1:A:329:LYS:HG2	1.96	0.66
1:A:42:ARG:HD3	1:A:303:ARG:HH12	1.57	0.65
1:A:284:ASN:OD1	1:A:340:GLY:HA2	1.96	0.65
1:A:303:ARG:NH2	1:A:306:GLN:OE1	2.30	0.65
1:A:342:TYR:CD1	1:A:344:PRO:HD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:CG2	1:A:55:ARG:NH1	2.59	0.65
1:A:148:ARG:HH21	1:A:150:VAL:HG21	1.61	0.65
1:A:59:ARG:HG2	1:A:59:ARG:HH11	1.63	0.64
1:A:108:VAL:O	1:A:133:ARG:NH2	2.31	0.64
1:A:221:ILE:HD12	1:A:226:THR:HG21	1.81	0.63
1:A:250:MET:CE	1:A:291:LEU:HD11	2.29	0.62
1:A:270:LEU:HB2	1:A:363:TYR:HE1	1.65	0.61
1:A:246:GLU:HG3	1:A:349:GLY:N	2.15	0.61
1:A:52:GLU:HA	1:A:55:ARG:NH2	2.05	0.61
1:A:277:GLU:HA	1:A:330:ARG:HH21	1.66	0.60
1:A:343:THR:O	1:A:344:PRO:O	2.19	0.60
1:A:244:SER:O	1:A:248:ILE:HG23	2.02	0.59
1:A:254:THR:CG2	1:A:258:ARG:HH21	2.16	0.59
1:A:152:LYS:O	1:A:158:PRO:HD3	2.03	0.58
1:A:121:GLU:OE2	1:A:159:SER:HB2	2.02	0.58
1:A:123:THR:HG21	1:A:165:GLU:OE2	2.03	0.58
1:A:43:LEU:HD12	1:A:50:ASN:HD22	1.68	0.57
1:A:172:ARG:HH21	1:A:176:ILE:HD11	1.69	0.57
1:A:277:GLU:CA	1:A:330:ARG:HH21	2.17	0.57
1:A:277:GLU:CA	1:A:330:ARG:NH2	2.67	0.56
1:A:124:THR:HG21	1:A:148:ARG:O	2.06	0.56
1:A:256:LEU:CD2	1:A:267:ILE:HD13	2.34	0.56
1:A:277:GLU:HA	1:A:330:ARG:HH22	1.67	0.56
1:A:68:ARG:NH2	1:A:328:VAL:HG11	2.21	0.56
1:A:256:LEU:CD2	1:A:267:ILE:HD11	2.32	0.56
1:A:124:THR:HG21	1:A:149:CYS:HA	1.89	0.55
1:A:246:GLU:CG	1:A:349:GLY:N	2.70	0.55
1:A:342:TYR:CE1	1:A:344:PRO:CD	2.89	0.55
1:A:353:SER:O	1:A:354:GLU:HB2	2.06	0.55
1:A:153:ILE:HA	1:A:158:PRO:HD3	1.89	0.55
1:A:336:LEU:HB3	1:A:342:TYR:HA	1.89	0.54
1:A:257:ARG:HD2	1:A:292:LEU:O	2.07	0.54
1:A:254:THR:HG21	1:A:258:ARG:HH21	1.73	0.53
1:A:68:ARG:CZ	1:A:328:VAL:HG11	2.39	0.53
1:A:288:LYS:HD3	1:A:347:GLN:HG3	1.91	0.52
1:A:273:GLY:N	1:A:363:TYR:HA	2.24	0.52
1:A:356:LEU:HD23	1:A:357:PHE:N	2.25	0.52
1:A:345:SER:O	1:A:346:GLY:O	2.28	0.52
1:A:342:TYR:CE1	1:A:344:PRO:HG2	2.40	0.51
1:A:192:PRO:CD	1:A:362:ALA:HB2	2.23	0.51
1:A:59:ARG:HH11	1:A:59:ARG:CG	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HA	1:A:96:VAL:HG13	1.92	0.51
1:A:281:ILE:CG1	1:A:345:SER:HB3	2.40	0.51
1:A:123:THR:HG21	1:A:165:GLU:HG3	1.91	0.50
1:A:198:LEU:HD22	1:A:233:VAL:HG12	1.94	0.49
1:A:123:THR:CG2	1:A:165:GLU:CG	2.88	0.49
1:A:245:HIS:NE2	1:A:352:ALA:N	2.60	0.49
1:A:89:ASP:OD2	1:A:91:ARG:HB2	2.13	0.49
1:A:148:ARG:HH21	1:A:150:VAL:CG2	2.24	0.49
1:A:93:PHE:N	1:A:94:PRO:HD2	2.27	0.48
1:A:281:ILE:HD13	1:A:352:ALA:HB3	1.95	0.48
1:A:182:ILE:O	1:A:184:PRO:HD3	2.13	0.48
1:A:8:THR:HG23	1:A:11:GLN:OE1	2.14	0.48
1:A:337:ALA:HA	1:A:342:TYR:HB2	1.96	0.48
1:A:39:ILE:HA	1:A:42:ARG:HG3	1.95	0.47
1:A:83:LEU:HG	1:A:83:LEU:O	2.14	0.47
1:A:221:ILE:CD1	1:A:226:THR:HG21	2.42	0.47
1:A:342:TYR:CE1	1:A:344:PRO:CG	2.97	0.47
1:A:275:SER:CB	1:A:356:LEU:H	2.21	0.47
1:A:276:GLU:HB3	1:A:330:ARG:HE	1.79	0.47
1:A:307:ALA:HB2	1:A:357:PHE:HE2	1.73	0.47
1:A:228:LEU:C	1:A:230:PRO:HD3	2.35	0.47
1:A:275:SER:HB3	1:A:356:LEU:N	2.20	0.47
1:A:293:LYS:HD2	1:A:297:LEU:HD23	1.96	0.47
1:A:68:ARG:NH2	1:A:328:VAL:CG1	2.78	0.46
1:A:254:THR:CG2	1:A:258:ARG:NH2	2.78	0.46
1:A:124:THR:CG2	1:A:149:CYS:HA	2.45	0.46
1:A:229:LYS:HG3	1:A:268:THR:O	2.16	0.46
1:A:254:THR:HG21	1:A:258:ARG:NH2	2.30	0.46
1:A:304:ALA:HA	1:A:357:PHE:HZ	1.81	0.46
1:A:55:ARG:HE	1:A:55:ARG:HB2	1.32	0.46
1:A:23:VAL:O	1:A:23:VAL:HG13	2.15	0.46
1:A:93:PHE:N	1:A:94:PRO:CD	2.79	0.46
1:A:245:HIS:HD2	1:A:351:ALA:N	2.13	0.46
1:A:254:THR:O	1:A:258:ARG:HG3	2.16	0.46
1:A:257:ARG:HE	1:A:257:ARG:HB3	1.48	0.46
1:A:68:ARG:HH21	1:A:328:VAL:CG1	2.29	0.46
1:A:155:GLU:OE2	1:A:155:GLU:HA	2.16	0.46
1:A:186:VAL:HG12	1:A:188:PRO:HD3	1.97	0.46
1:A:246:GLU:HA	1:A:249:ALA:HB3	1.98	0.45
1:A:58:TYR:O	1:A:61:LEU:HB3	2.17	0.45
1:A:70:ASN:HD21	1:A:100:LYS:NZ	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASN:HD21	1:A:100:LYS:HZ1	1.65	0.45
1:A:344:PRO:C	1:A:345:SER:O	2.54	0.45
1:A:245:HIS:ND1	1:A:282:ASN:OD1	2.49	0.45
1:A:59:ARG:NH1	1:A:82:THR:OG1	2.49	0.45
1:A:248:ILE:HG13	1:A:249:ALA:N	2.32	0.44
1:A:105:GLY:HA2	1:A:144:PHE:O	2.17	0.44
1:A:353:SER:O	1:A:354:GLU:CB	2.65	0.44
1:A:355:SER:O	1:A:356:LEU:CB	2.65	0.44
1:A:245:HIS:CD2	1:A:351:ALA:N	2.85	0.44
1:A:152:LYS:O	1:A:157:THR:CB	2.65	0.44
1:A:153:ILE:CG2	1:A:200:ARG:HE	2.30	0.44
1:A:193:ASP:CG	1:A:361:HIS:O	2.56	0.44
1:A:250:MET:HE1	1:A:291:LEU:HD11	2.00	0.44
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.88	0.43
1:A:123:THR:HG21	1:A:165:GLU:CG	2.47	0.43
1:A:110:LYS:HG3	1:A:126:GLY:HA2	2.01	0.43
1:A:275:SER:HB3	1:A:355:SER:HB2	1.84	0.43
1:A:154:GLY:N	1:A:157:THR:CB	2.78	0.43
1:A:283:LEU:HB3	1:A:337:ALA:HB1	2.01	0.43
1:A:307:ALA:CB	1:A:357:PHE:HE2	2.31	0.43
1:A:118:THR:CG2	1:A:121:GLU:CB	2.94	0.43
1:A:70:ASN:HB2	1:A:71:PRO:HD3	2.00	0.43
1:A:118:THR:HG23	1:A:121:GLU:HB2	1.99	0.42
1:A:246:GLU:HB2	1:A:349:GLY:CA	2.42	0.42
1:A:284:ASN:OD1	1:A:340:GLY:CA	2.65	0.42
1:A:349:GLY:C	1:A:350:ALA:O	2.56	0.42
1:A:254:THR:HG22	1:A:258:ARG:NE	2.35	0.42
1:A:152:LYS:CG	1:A:157:THR:HG22	2.34	0.42
1:A:284:ASN:CG	1:A:342:TYR:HB3	2.40	0.42
1:A:38:SER:O	1:A:41:LYS:HG2	2.20	0.42
1:A:174:ALA:O	1:A:178:GLN:HG3	2.20	0.42
1:A:229:LYS:O	1:A:229:LYS:HG2	2.20	0.41
1:A:270:LEU:H	1:A:270:LEU:HG	1.80	0.41
1:A:293:LYS:HD2	1:A:297:LEU:CD2	2.50	0.41
1:A:41:LYS:HG3	1:A:42:ARG:NH1	2.36	0.41
1:A:52:GLU:CA	1:A:55:ARG:NH2	2.73	0.41
1:A:152:LYS:O	1:A:157:THR:CG2	2.69	0.41
1:A:172:ARG:HE	1:A:172:ARG:HB3	1.64	0.41
1:A:198:LEU:CD2	1:A:233:VAL:HG12	2.51	0.41
1:A:301:TYR:HB3	1:A:304:ALA:HB3	2.01	0.41
1:A:330:ARG:HD2	1:A:330:ARG:HA	1.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLY:HA2	1:A:132:GLU:OE2	2.21	0.41
1:A:254:THR:HG22	1:A:258:ARG:HE	1.85	0.41
1:A:361:HIS:O	1:A:362:ALA:HB2	2.19	0.41
1:A:324:GLN:O	1:A:328:VAL:HG23	2.21	0.41
1:A:161:LEU:HD22	1:A:161:LEU:C	2.41	0.41
1:A:221:ILE:O	1:A:221:ILE:HG13	2.16	0.41
1:A:281:ILE:CD1	1:A:345:SER:HB3	2.51	0.40
1:A:29:ILE:HA	1:A:75:GLY:O	2.21	0.40
1:A:277:GLU:N	1:A:330:ARG:HH21	2.18	0.40
1:A:346:GLY:O	1:A:347:GLN:OE1	2.39	0.40
1:A:148:ARG:CZ	1:A:361:HIS:CE1	3.03	0.40

All (1) 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)
1:A:4:TYR:CE2	1:A:119:ASN:CB[9_555]	1.92	0.28

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	361/363 (99%)	327 (91%)	18 (5%)	16 (4%)	2 0

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	A	345	SER
1	A	348	ALA
1	A	350	ALA
1	A	353	SER

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Mol	Chain	Res	Type
1	A	355	SER
1	A	360	ASN
1	A	361	HIS
1	A	346	GLY
1	A	347	GLN
1	A	351	ALA
1	A	362	ALA
1	A	354	GLU
1	A	356	LEU
1	A	158	PRO
1	A	349	GLY

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	291/291 (100%)	239 (82%)	52 (18%)	2 1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	21	ARG
1	A	23	VAL
1	A	30	LEU
1	A	38	SER
1	A	42	ARG
1	A	55	ARG
1	A	59	ARG
1	A	63	LEU
1	A	69	VAL
1	A	70	ASN
1	A	78	LEU
1	A	95	GLN
1	A	115	LEU
1	A	118	THR

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Mol	Chain	Res	Type
1	A	122	THR
1	A	123	THR
1	A	124	THR
1	A	157	THR
1	A	159	SER
1	A	161	LEU
1	A	173	TYR
1	A	184	PRO
1	A	191	LEU
1	A	198	LEU
1	A	200	ARG
1	A	209	LEU
1	A	216	LEU
1	A	221	ILE
1	A	223	LEU
1	A	227	LEU
1	A	240	THR
1	A	248	ILE
1	A	256	LEU
1	A	257	ARG
1	A	260	VAL
1	A	267	ILE
1	A	283	LEU
1	A	295	TRP
1	A	297	LEU
1	A	303	ARG
1	A	317	LYS
1	A	321	LYS
1	A	330	ARG
1	A	338	CYS
1	A	343	THR
1	A	347	GLN
1	A	356	LEU
1	A	358	VAL
1	A	359	SER
1	A	360	ASN
1	A	363	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN

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Mol	Chain	Res	Type
1	A	70	ASN
1	A	80	HIS
1	A	179	GLN
1	A	196	HIS
1	A	202	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 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.