



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:50 PM UTC

PDB ID : 9ATC / pdb_00009atc
Title : ATCASE Y165F MUTANT
Authors : Ha, Y.; Allewell, N.M.
Deposited on : 1998-06-26
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

<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

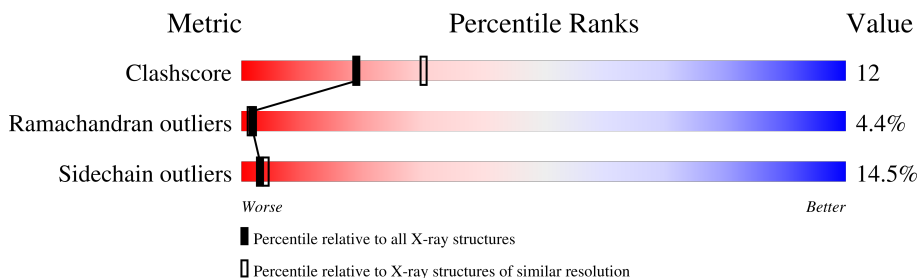
1 Overall quality at a glance

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	310	
2	B	146	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3409 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 ASPARTATE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2378	1509	415	445	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	PHE	TYR	engineered mutation	UNP P0A786

- Molecule 2 is a protein called ASPARTATE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1030	647	182	197	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

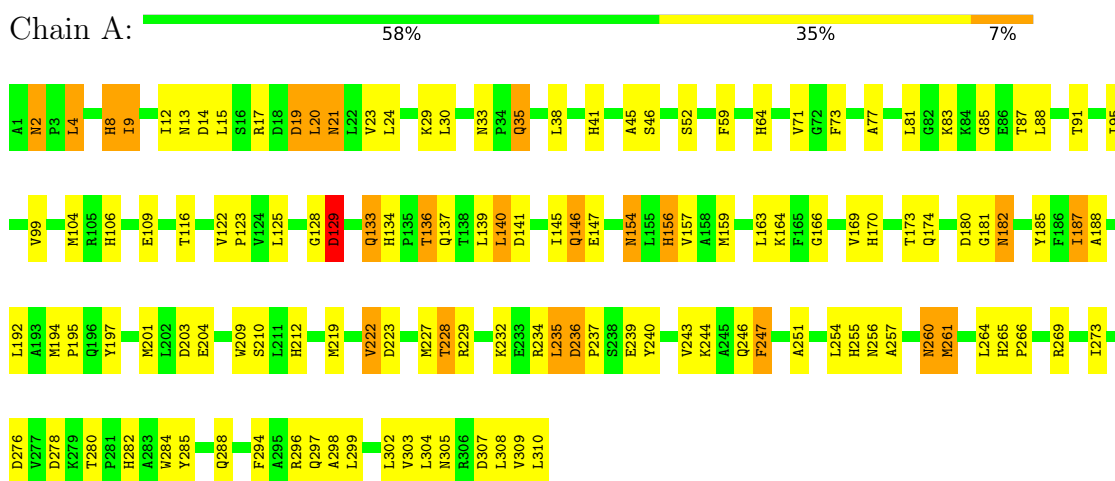
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

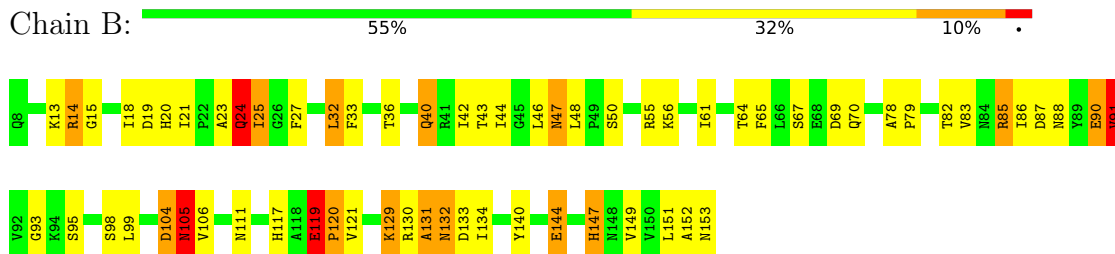
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: ASPARTATE TRANSCARBAMOYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	R 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.60 Å 100.60 Å 100.60 Å 81.40° 81.40° 81.40°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.252 , 0.344	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3409	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.01	13/2424 (0.5%)	1.76	48/3293 (1.5%)
2	B	0.96	4/1046 (0.4%)	1.96	27/1427 (1.9%)
All	All	0.99	17/3470 (0.5%)	1.82	75/4720 (1.6%)

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
2	B	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	SER	CA-C	7.43	1.56	1.52
1	A	170	HIS	CD2-NE2	-7.14	1.29	1.37
2	B	117	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	64	HIS	CD2-NE2	-7.09	1.30	1.37
2	B	147	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	8	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	265	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	134	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	282	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	156	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	265	HIS	CG-ND1	-5.62	1.32	1.38
1	A	255	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	8	HIS	CG-ND1	-5.41	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	HIS	CD2-NE2	-5.20	1.32	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASP	CA-CB-CG	10.95	123.55	112.60
1	A	222	VAL	N-CA-C	10.24	122.10	109.30
2	B	111	ASN	OD1-CG-ND2	-9.71	112.89	122.60
2	B	132	ASN	CA-CB-CG	9.55	122.15	112.60
1	A	222	VAL	N-CA-CB	-8.36	100.02	110.31
2	B	119	GLU	N-CA-C	7.72	122.80	109.82
1	A	219	MET	N-CA-C	7.70	119.67	111.28
1	A	106	HIS	O-C-N	-7.60	116.10	121.65
1	A	229	ARG	N-CA-C	7.54	121.32	110.24
2	B	27	PHE	N-CA-C	-7.03	103.55	111.14
1	A	8	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	278	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	20	LEU	N-CA-C	-6.96	103.78	111.36
1	A	255	HIS	CA-CB-CG	6.95	120.75	113.80
2	B	147	HIS	CB-CG-CD2	-6.95	122.17	131.20
1	A	180	ASP	N-CA-C	6.95	121.19	110.42
1	A	64	HIS	CB-CG-CD2	-6.81	122.35	131.20
2	B	117	HIS	CB-CG-CD2	-6.80	122.35	131.20
1	A	247	PHE	CA-CB-CG	-6.78	107.03	113.80
2	B	104	ASP	CA-CB-CG	-6.74	105.86	112.60
2	B	33	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	307	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	257	ALA	N-CA-C	6.28	119.09	110.24
1	A	52	SER	N-CA-C	-6.22	97.55	110.80
2	B	50	SER	N-CA-C	6.21	116.47	108.34
2	B	90	GLU	N-CA-C	6.15	118.65	108.99
2	B	140	TYR	N-CA-C	6.12	118.87	111.40
1	A	284	TRP	CG-CD2-CE3	6.12	140.02	133.90
2	B	152	ALA	O-C-N	6.11	128.69	122.09
1	A	212	HIS	CB-CG-CD2	-6.08	123.30	131.20
2	B	19	ASP	N-CA-C	6.06	118.62	109.41
2	B	131	ALA	N-CA-C	6.05	123.69	110.80
1	A	106	HIS	CA-CB-CG	5.96	119.76	113.80
2	B	91	VAL	N-CA-C	5.95	121.71	109.34
1	A	288	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	A	276	ASP	CA-CB-CG	5.91	118.51	112.60
2	B	36	THR	N-CA-CB	-5.91	101.47	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	LEU	N-CA-C	5.83	118.86	111.69
1	A	21	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	209	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	A	265	HIS	CB-CG-CD2	-5.81	123.65	131.20
2	B	20	HIS	N-CA-C	5.79	119.92	112.86
2	B	144	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	256	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	B	83	VAL	N-CA-C	-5.74	97.41	109.34
1	A	210	SER	CA-CB-OG	5.72	122.54	111.10
1	A	104	MET	N-CA-C	5.70	117.93	108.13
1	A	294	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	265	HIS	CA-C-N	5.64	125.31	119.56
1	A	265	HIS	C-N-CA	5.64	125.31	119.56
2	B	111	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	235	LEU	N-CA-C	5.44	119.29	111.02
1	A	106	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	156	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	170	HIS	O-C-N	5.38	127.84	122.03
2	B	85	ARG	N-CA-C	5.37	118.02	110.23
1	A	203	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	24	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	35	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	228	THR	CA-CB-OG1	-5.32	101.63	109.60
1	A	197	TYR	N-CA-C	-5.31	106.97	113.50
2	B	56	LYS	N-CA-C	5.31	118.14	109.59
1	A	73	PHE	N-CA-C	5.30	116.57	108.52
2	B	117	HIS	CB-CG-ND1	5.28	130.62	122.70
1	A	8	HIS	CB-CG-ND1	5.28	130.61	122.70
1	A	284	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	A	71	VAL	O-C-N	-5.22	117.55	123.03
1	A	33	ASN	CA-C-N	5.21	125.20	119.89
1	A	33	ASN	C-N-CA	5.21	125.20	119.89
1	A	133	GLN	N-CA-C	5.13	118.43	110.17
1	A	246	GLN	OE1-CD-NE2	-5.10	117.50	122.60
2	B	61	ILE	O-C-N	-5.10	117.29	122.95
1	A	19	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	8	HIS	N-CA-C	-5.06	101.06	109.46
2	B	47	ASN	CA-CB-CG	-5.04	107.56	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	119	GLU	Peptide
2	B	78	ALA	Peptide

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	2378	0	2362	50	0
2	B	1030	0	950	29	0
3	B	1	0	0	0	0
All	All	3409	0	3312	79	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 12.

All (79) 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:9:ILE:HD11	1:A:125:LEU:HG	1.54	0.88
2:B:105:ASN:HD22	2:B:106:VAL:H	1.29	0.81
2:B:129:LYS:NZ	2:B:132:ASN:HD22	1.84	0.75
1:A:2:ASN:HD22	1:A:4:LEU:H	1.40	0.69
1:A:251:ALA:HA	1:A:254:LEU:HD23	1.75	0.68
1:A:9:ILE:H	1:A:9:ILE:HD13	1.61	0.64
2:B:129:LYS:HE2	2:B:132:ASN:HB3	1.82	0.62
2:B:23:ALA:HB1	2:B:24:GLN:NE2	2.14	0.61
1:A:136:THR:HB	1:A:296:ARG:NH1	2.15	0.61
1:A:13:ASN:HD21	1:A:174:GLN:HB3	1.66	0.61
1:A:154:ASN:HD22	1:A:181:GLY:HA3	1.66	0.60
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.82	0.60
2:B:129:LYS:HB3	2:B:134:ILE:HA	1.83	0.60
1:A:194:MET:SD	1:A:195:PRO:HD2	2.42	0.60
2:B:129:LYS:HZ3	2:B:132:ASN:HD22	1.50	0.59
2:B:105:ASN:ND2	2:B:106:VAL:H	2.01	0.57
1:A:91:THR:O	1:A:95:ILE:HG12	2.05	0.56
1:A:236:ASP:HB3	1:A:239:GLU:HB3	1.87	0.56
1:A:243:VAL:HG22	1:A:247:PHE:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:O	1:A:23:VAL:HG23	2.07	0.55
1:A:269:ARG:HH11	1:A:273:ILE:HG22	1.71	0.55
2:B:21:ILE:HD12	2:B:21:ILE:H	1.72	0.55
1:A:163:LEU:HD12	1:A:188:ALA:HB2	1.90	0.54
2:B:105:ASN:HD22	2:B:106:VAL:N	2.04	0.54
1:A:232:LYS:NZ	1:A:237:PRO:HA	2.23	0.54
1:A:141:ASP:O	1:A:145:ILE:HG23	2.08	0.53
1:A:154:ASN:HA	1:A:182:ASN:H	1.74	0.53
1:A:305:ASN:HD22	1:A:308:LEU:HD12	1.75	0.52
2:B:119:GLU:HB3	2:B:121:VAL:HG22	1.92	0.51
1:A:95:ILE:O	1:A:99:VAL:HG22	2.11	0.51
1:A:269:ARG:NH1	1:A:273:ILE:HG22	2.25	0.51
1:A:192:LEU:HD21	1:A:234:ARG:HB3	1.92	0.51
1:A:145:ILE:HG22	1:A:264:LEU:HD11	1.93	0.51
2:B:13:LYS:HA	2:B:86:ILE:HD11	1.94	0.50
2:B:18:ILE:HG22	2:B:21:ILE:HD11	1.92	0.50
2:B:40:GLN:O	2:B:42:ILE:HG13	2.12	0.49
2:B:67:SER:HB3	2:B:70:GLN:HG3	1.95	0.48
2:B:14:ARG:H	2:B:86:ILE:HG12	1.79	0.47
1:A:235:LEU:O	1:A:236:ASP:HB2	2.14	0.47
1:A:232:LYS:HZ2	1:A:237:PRO:HA	1.80	0.47
1:A:261:MET:C	1:A:261:MET:SD	2.98	0.47
2:B:129:LYS:CE	2:B:132:ASN:HB3	2.45	0.46
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.51	0.46
1:A:128:GLY:HA2	1:A:133:GLN:O	2.15	0.46
2:B:85:ARG:HD2	2:B:87:ASP:CB	2.46	0.45
1:A:154:ASN:ND2	1:A:181:GLY:HA3	2.32	0.45
1:A:4:LEU:HD23	1:A:302:LEU:HD23	1.99	0.44
1:A:187:ILE:HG22	1:A:247:PHE:CE1	2.52	0.44
2:B:85:ARG:O	2:B:91:VAL:HA	2.17	0.44
2:B:99:LEU:HD21	2:B:130:ARG:HA	2.00	0.44
1:A:166:GLY:O	1:A:169:VAL:HG22	2.17	0.43
1:A:240:TYR:O	1:A:244:LYS:HB2	2.18	0.43
1:A:9:ILE:HD12	1:A:303:VAL:HG21	2.00	0.43
2:B:14:ARG:HA	2:B:86:ILE:HG23	2.00	0.43
2:B:129:LYS:HZ2	2:B:132:ASN:HD22	1.63	0.43
1:A:38:LEU:HD11	1:A:305:ASN:HD21	1.83	0.42
1:A:122:VAL:HA	1:A:123:PRO:HD2	1.94	0.42
2:B:119:GLU:HA	2:B:120:PRO:HD2	1.88	0.42
2:B:86:ILE:HG13	2:B:90:GLU:HA	2.00	0.42
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.01	0.42
2:B:129:LYS:HG3	2:B:131:ALA:H	1.84	0.42
1:A:260:ASN:ND2	1:A:260:ASN:H	2.17	0.42
1:A:146:GLN:HG3	1:A:147:GLU:N	2.35	0.42
1:A:223:ASP:O	1:A:261:MET:HA	2.19	0.42
2:B:42:ILE:O	2:B:44:ILE:HG13	2.20	0.41
2:B:21:ILE:CG2	2:B:25:ILE:HB	2.50	0.41
1:A:8:HIS:ND1	1:A:123:PRO:HA	2.35	0.41
1:A:9:ILE:HD13	1:A:9:ILE:N	2.32	0.41
1:A:20:LEU:HD12	1:A:139:LEU:HD21	2.01	0.41
2:B:15:GLY:H	2:B:86:ILE:HG23	1.84	0.41
2:B:65:PHE:CZ	2:B:85:ARG:HD3	2.55	0.41
2:B:147:HIS:O	2:B:151:LEU:HB2	2.21	0.41
1:A:298:ALA:O	1:A:302:LEU:HD13	2.21	0.41
1:A:30:LEU:HD13	1:A:297:GLN:HE21	1.85	0.40
1:A:137:GLN:O	1:A:140:LEU:HG	2.21	0.40
1:A:156:HIS:HB3	1:A:185:TYR:HE2	1.86	0.40
1:A:227:MET:O	1:A:266:PRO:HD2	2.22	0.40
1:A:164:LYS:HA	1:A:195:PRO:HD3	2.02	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	308/310 (99%)	278 (90%)	24 (8%)	6 (2%)	6	8
2	B	144/146 (99%)	102 (71%)	28 (19%)	14 (10%)	0	0
All	All	452/456 (99%)	380 (84%)	52 (12%)	20 (4%)	2	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	236	ASP
2	B	40	GLN
2	B	55	ARG
2	B	79	PRO
2	B	91	VAL
2	B	133	ASP
1	A	77	ALA
2	B	25	ILE
2	B	14	ARG
2	B	46	LEU
2	B	105	ASN
2	B	129	LYS
1	A	129	ASP
2	B	120	PRO
1	A	85	GLY
2	B	88	ASN
2	B	43	THR
2	B	93	GLY
1	A	309	VAL

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	251/261 (96%)	214 (85%)	37 (15%)	3	4
2	B	100/130 (77%)	86 (86%)	14 (14%)	3	4
All	All	351/391 (90%)	300 (86%)	51 (14%)	3	4

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	LEU
1	A	9	ILE
1	A	14	ASP

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	17	ARG
1	A	21	ASN
1	A	24	LEU
1	A	29	LYS
1	A	35	GLN
1	A	46	SER
1	A	81	LEU
1	A	83	LYS
1	A	87	THR
1	A	88	LEU
1	A	109	GLU
1	A	116	THR
1	A	129	ASP
1	A	136	THR
1	A	140	LEU
1	A	146	GLN
1	A	154	ASN
1	A	157	VAL
1	A	159	MET
1	A	173	THR
1	A	187	ILE
1	A	201	MET
1	A	204	GLU
1	A	222	VAL
1	A	228	THR
1	A	260	ASN
1	A	261	MET
1	A	280	THR
1	A	285	TYR
1	A	299	LEU
1	A	304	LEU
1	A	310	LEU
2	B	24	GLN
2	B	32	LEU
2	B	47	ASN
2	B	48	LEU
2	B	64	THR
2	B	69	ASP
2	B	82	THR
2	B	95	SER
2	B	104	ASP

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Mol	Chain	Res	Type
2	B	105	ASN
2	B	119	GLU
2	B	144	GLU
2	B	149	VAL
2	B	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	GLN
1	A	13	ASN
1	A	64	HIS
1	A	106	HIS
1	A	108	GLN
1	A	134	HIS
1	A	154	ASN
1	A	255	HIS
1	A	297	GLN
1	A	305	ASN
2	B	70	GLN
2	B	73	GLN
2	B	105	ASN
2	B	113	ASN
2	B	132	ASN
2	B	147	HIS
2	B	153	ASN

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 1 ligands modelled in this entry, 1 is 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 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.