



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:30 AM UTC

PDB ID : 1AZZ / pdb_00001azz
Title : FIDDLER CRAB COLLAGENASE COMPLEXED TO ECOTIN
Authors : Perona, J.J.; Fletterick, R.J.
Deposited on : 1997-11-24
Resolution : 2.30 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

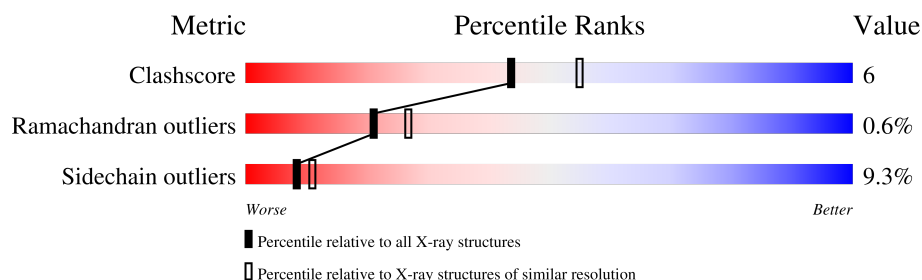
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	226	75% 20% .
1	B	226	73% 24% .
2	C	142	77% 16% . .
2	D	142	68% 24% . . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5527 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 COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1653	1043	267	334	9			
1	B	226	Total	C	N	O	S	0	0	0
			1653	1043	267	334	9			

- Molecule 2 is a protein called ECOTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	0
			1048	671	175	196	6			
2	D	138	Total	C	N	O	S	0	0	0
			1033	661	173	193	6			

- Molecule 3 is water.

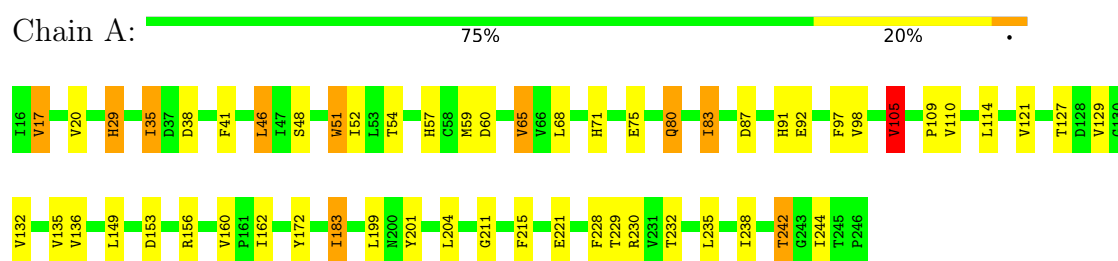
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	47	Total	O	0	0
			47	47		
3	C	22	Total	O	0	0
			22	22		
3	D	19	Total	O	0	0
			19	19		

3 Residue-property plots [i](#)

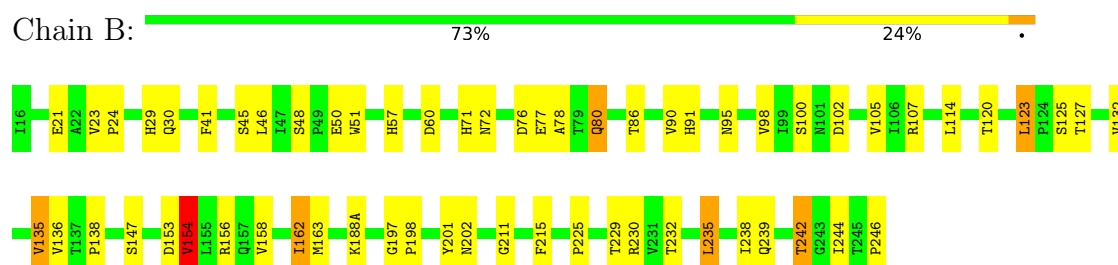
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

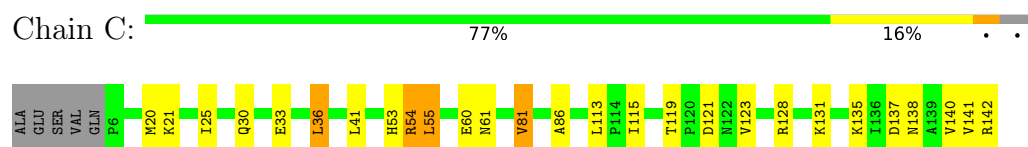
• Molecule 1: COLLAGENASE



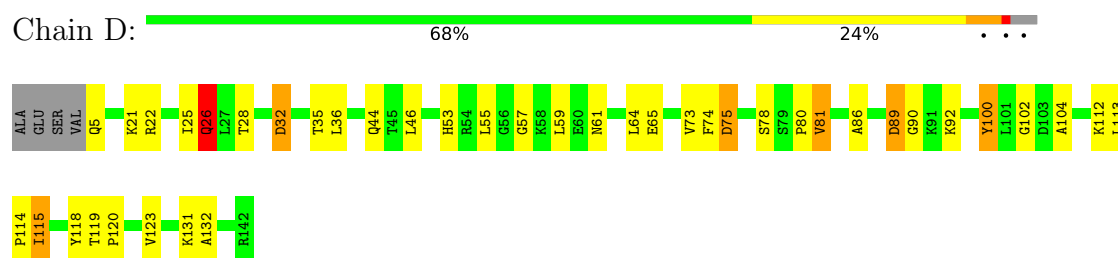
• Molecule 1: COLLAGENASE



• Molecule 2: ECOTIN



• Molecule 2: ECOTIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.11Å 89.11Å 291.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	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	0.91	6/1691 (0.4%)	1.59	18/2322 (0.8%)
1	B	0.92	6/1691 (0.4%)	1.59	22/2322 (0.9%)
2	C	0.78	1/1070 (0.1%)	1.51	4/1455 (0.3%)
2	D	0.81	1/1055 (0.1%)	1.63	20/1441 (1.4%)
All	All	0.87	14/5507 (0.3%)	1.58	64/7540 (0.8%)

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	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	VAL	CA-CB	7.18	1.62	1.54
1	A	71	HIS	CD2-NE2	-7.06	1.30	1.37
1	A	65	VAL	CA-CB	7.00	1.62	1.54
1	B	91	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	91	HIS	CD2-NE2	-6.96	1.30	1.37
2	D	53	HIS	CD2-NE2	-6.70	1.30	1.37
2	C	53	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	57	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	57	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	29	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	71	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	57	HIS	CG-ND1	-6.03	1.31	1.38
1	A	29	HIS	CD2-NE2	-5.42	1.31	1.37
1	B	57	HIS	CG-ND1	-5.09	1.32	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	VAL	N-CA-CB	-8.59	100.99	112.16
2	D	32	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	98	VAL	N-CA-CB	-7.40	102.55	112.16
2	D	112	LYS	CA-CB-CG	7.25	128.61	114.10
1	A	105	VAL	N-CA-CB	-7.23	99.58	111.44
2	D	81	VAL	N-CA-CB	-7.20	100.37	112.47
1	A	160	VAL	N-CA-CB	-7.06	101.32	111.21
1	B	80	GLN	OE1-CD-NE2	-6.99	115.61	122.60
2	C	81	VAL	N-CA-CB	-6.95	100.80	112.47
1	A	20	VAL	N-CA-CB	-6.90	102.86	112.52
1	B	76	ASP	CA-CB-CG	6.84	119.44	112.60
1	B	102	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	242	THR	N-CA-CB	-6.78	98.99	110.51
2	D	92	LYS	N-CA-C	-6.66	97.69	108.41
1	B	156	ARG	CG-CD-NE	-6.62	97.44	112.00
1	B	71	HIS	N-CA-C	-6.50	103.41	112.12
1	B	242	THR	N-CA-CB	-6.48	101.22	110.81
1	A	91	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	215	PHE	CA-CB-CG	6.45	120.25	113.80
2	D	53	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	B	91	HIS	CB-CG-CD2	-6.32	122.98	131.20
2	D	90	GLY	O-C-N	6.20	130.16	123.58
1	A	105	VAL	CB-CA-C	6.07	119.85	110.50
2	D	26	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	129	VAL	CB-CA-C	5.96	119.72	111.19
2	C	53	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	B	154	VAL	N-CA-CB	-5.88	98.92	111.37
2	D	61	ASN	OD1-CG-ND2	-5.80	116.80	122.60
2	D	100	TYR	N-CA-C	-5.76	100.44	109.25
2	D	112	LYS	CB-CA-C	-5.66	100.17	110.63
1	B	107	ARG	CA-CB-CG	-5.61	102.89	114.10
1	B	215	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	57	HIS	CA-CB-CG	5.55	119.35	113.80
2	D	104	ALA	N-CA-C	5.52	119.27	112.54
1	B	86	THR	CA-CB-OG1	-5.51	101.33	109.60
1	B	23	VAL	N-CA-C	-5.51	103.55	108.95
1	B	51	TRP	CE2-CD2-CG	-5.50	100.59	107.20
2	C	60	GLU	CA-CB-CG	5.49	125.07	114.10
1	B	230	ARG	CA-CB-CG	5.46	125.02	114.10
1	A	87	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	172	TYR	N-CA-C	5.41	120.01	113.41
2	D	81	VAL	CB-CA-C	5.38	118.65	110.90
1	B	51	TRP	CG-CD2-CE3	5.35	139.25	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	D	90	GLY	CA-C-O	5.27	127.34	121.86
1	B	78	ALA	N-CA-C	5.23	118.92	112.54
1	B	98	VAL	CB-CA-C	5.21	118.00	111.65
2	D	89	ASP	N-CA-CB	5.18	119.25	110.49
1	A	153	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	71	HIS	CB-CG-CD2	-5.14	124.52	131.20
2	D	21	LYS	N-CA-C	-5.13	101.50	109.24
2	C	61	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	51	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	A	51	TRP	CE2-CD2-CG	-5.09	101.09	107.20
2	D	32	ASP	CA-C-O	5.08	125.82	120.54
2	D	61	ASN	CB-CG-ND2	5.07	124.00	116.40
1	B	202	ASN	N-CA-C	5.06	118.58	111.90
1	A	35	ILE	CA-CB-CG2	-5.05	101.91	110.50
1	B	51	TRP	CB-CG-CD1	-5.04	119.33	126.90
1	A	75	GLU	CA-CB-CG	-5.04	104.02	114.10
2	D	115	ILE	N-CA-C	-5.03	101.34	108.58
2	D	75	ASP	CA-CB-CG	-5.02	107.58	112.60
1	B	105	VAL	N-CA-CB	-5.01	103.47	111.58
2	D	90	GLY	N-CA-C	5.00	117.37	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	5	GLN	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	1653	0	1571	23	0
1	B	1653	0	1571	18	0
2	C	1048	0	1021	14	0
2	D	1033	0	981	14	0
3	A	52	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	47	0	0	1	0
3	C	22	0	0	0	0
3	D	19	0	0	0	0
All	All	5527	0	5144	64	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 6.

All (64) 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)
2:D:119:THR:HB	2:D:123:VAL:HG23	1.61	0.81
1:A:83:ILE:HD11	1:A:109:PRO:HD2	1.65	0.77
1:A:48:SER:HB3	1:A:244:ILE:HD11	1.66	0.76
2:D:44:GLN:HG3	2:D:123:VAL:HG12	1.73	0.71
1:B:242:THR:HG22	1:B:244:ILE:HG12	1.76	0.67
1:A:97:PHE:O	2:C:54:ARG:HD2	1.94	0.67
2:C:128:ARG:HD3	2:D:132:ALA:HB1	1.77	0.65
1:B:136:VAL:HG12	1:B:201:TYR:HB2	1.82	0.61
1:A:136:VAL:HG12	1:A:201:TYR:HB2	1.80	0.61
1:A:54:THR:HG21	1:A:59:MET:HE3	1.85	0.58
1:A:48:SER:CB	1:A:244:ILE:HD11	2.35	0.56
1:A:132:VAL:HA	1:A:162:ILE:HG22	1.89	0.54
2:D:26:GLN:NE2	2:D:114:PRO:HB3	2.23	0.53
1:A:17:VAL:HG11	1:A:221:GLU:HG2	1.90	0.53
2:D:35:THR:OG1	2:D:131:LYS:NZ	2.42	0.52
1:B:21:GLU:HG3	1:B:154:VAL:HG13	1.92	0.52
1:B:123:LEU:HD22	1:B:244:ILE:HG22	1.91	0.52
1:A:17:VAL:CG1	1:A:221:GLU:HG2	2.40	0.52
1:B:30:GLN:NE2	1:B:198:PRO:HD2	2.25	0.51
2:C:135:LYS:NZ	2:C:137:ASP:HB2	2.25	0.51
2:C:119:THR:HB	2:C:123:VAL:CG2	2.42	0.50
1:B:238:ILE:O	1:B:242:THR:HB	2.11	0.50
2:C:30:GLN:HG3	2:C:36:LEU:HD21	1.94	0.49
2:C:119:THR:HB	2:C:123:VAL:HG22	1.93	0.49
1:A:29:HIS:CG	1:A:121:VAL:HB	2.47	0.49
1:B:72:ASN:HA	1:B:153:ASP:O	2.12	0.49
2:D:36:LEU:HD23	2:D:131:LYS:HG3	1.94	0.48
2:D:57:GLY:HA3	2:D:74:PHE:CE1	2.49	0.48
1:A:211:GLY:HA2	1:A:229:THR:O	2.14	0.47
2:D:119:THR:HB	2:D:123:VAL:CG2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:LYS:HB2	2:C:121:ASP:HA	1.97	0.47
1:B:163:MET:SD	1:B:225:PRO:HB3	2.55	0.46
2:C:30:GLN:HB2	2:C:33:GLU:HG2	1.98	0.46
2:C:140:VAL:HG12	2:C:142:ARG:HG3	1.97	0.45
1:A:238:ILE:O	1:A:242:THR:HB	2.16	0.45
1:A:46:LEU:HD22	1:A:48:SER:O	2.16	0.45
1:B:158:VAL:HG21	1:B:188(A):LYS:HB3	1.97	0.45
1:B:211:GLY:HA2	1:B:229:THR:O	2.17	0.45
1:A:48:SER:HB3	1:A:244:ILE:CD1	2.44	0.44
1:A:156:ARG:HD3	3:A:247:HOH:O	2.16	0.44
2:D:100:TYR:CZ	2:D:102:GLY:HA2	2.52	0.43
1:B:232:THR:HA	1:B:235:LEU:HD22	2.00	0.43
1:A:183:ILE:HB	1:A:228:PHE:HE1	1.84	0.43
1:A:68:LEU:O	1:A:80:GLN:HA	2.19	0.43
1:B:41:PHE:HB3	2:D:86:ALA:HB3	2.00	0.43
1:A:232:THR:HA	1:A:235:LEU:HG	2.01	0.42
1:B:95:ASN:HB3	1:B:100:SER:OG	2.20	0.42
1:A:46:LEU:HD23	1:A:52:ILE:HD13	2.01	0.42
1:B:197:GLY:HA3	3:B:259:HOH:O	2.19	0.42
1:A:51:TRP:CE3	1:A:105:VAL:HG13	2.54	0.42
2:D:25:ILE:HB	2:D:115:ILE:HB	2.02	0.42
1:A:41:PHE:HB3	2:C:86:ALA:HB3	2.00	0.42
1:B:45:SER:OG	1:B:198:PRO:HB3	2.20	0.41
1:B:138:PRO:HD2	1:B:158:VAL:O	2.20	0.41
1:A:230:ARG:NH2	3:A:297:HOH:O	2.52	0.41
1:A:92:GLU:H	1:A:92:GLU:CD	2.29	0.41
2:C:142:ARG:OXT	2:D:22:ARG:NH1	2.54	0.41
2:D:55:LEU:HD13	2:D:80:PRO:HG3	2.01	0.41
1:B:132:VAL:HA	1:B:162:ILE:HG13	2.03	0.41
2:C:25:ILE:HB	2:C:115:ILE:HB	2.03	0.41
2:D:22:ARG:HD3	2:D:118:TYR:CZ	2.56	0.41
1:B:77:GLU:HB2	1:B:80:GLN:HG3	2.02	0.41
2:C:20:MET:HA	2:C:119:THR:O	2.21	0.41
2:C:54:ARG:HG3	2:C:55:LEU:N	2.36	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	224/226 (99%)	216 (96%)	6 (3%)	2 (1%)	14	17
1	B	224/226 (99%)	213 (95%)	10 (4%)	1 (0%)	30	38
2	C	135/142 (95%)	131 (97%)	4 (3%)	0	100	100
2	D	136/142 (96%)	130 (96%)	5 (4%)	1 (1%)	18	23
All	All	719/736 (98%)	690 (96%)	25 (4%)	4 (1%)	21	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	B	60	ASP
2	D	89	ASP
1	A	38	ASP

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	179/179 (100%)	165 (92%)	14 (8%)	11	16
1	B	179/179 (100%)	162 (90%)	17 (10%)	8	10
2	C	109/125 (87%)	100 (92%)	9 (8%)	10	14
2	D	104/125 (83%)	91 (88%)	13 (12%)	4	5
All	All	571/608 (94%)	518 (91%)	53 (9%)	8	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	35	ILE
1	A	46	LEU
1	A	65	VAL
1	A	83	ILE
1	A	105	VAL
1	A	110	VAL
1	A	114	LEU
1	A	127	THR
1	A	135	VAL
1	A	149	LEU
1	A	183	ILE
1	A	199	LEU
1	A	204	LEU
1	B	24	PRO
1	B	46	LEU
1	B	48	SER
1	B	50	GLU
1	B	90	VAL
1	B	114	LEU
1	B	120	THR
1	B	123	LEU
1	B	125	SER
1	B	127	THR
1	B	135	VAL
1	B	147	SER
1	B	154	VAL
1	B	162	ILE
1	B	235	LEU
1	B	239	GLN
1	B	246	PRO
2	C	36	LEU
2	C	41	LEU
2	C	54	ARG
2	C	55	LEU
2	C	81	VAL
2	C	113	LEU
2	C	131	LYS
2	C	138	ASN
2	C	141	VAL
2	D	26	GLN
2	D	28	THR

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Mol	Chain	Res	Type
2	D	32	ASP
2	D	46	LEU
2	D	59	LEU
2	D	64	LEU
2	D	65	GLU
2	D	73	VAL
2	D	75	ASP
2	D	78	SER
2	D	81	VAL
2	D	113	LEU
2	D	120	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	101	ASN
1	B	30	GLN
1	B	80	GLN
1	B	101	ASN
2	C	23	GLN
2	C	26	GLN
2	D	26	GLN
2	D	122	ASN

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 oligosaccharides 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.