



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 2CLT / pdb_00002clt
Title : Crystal structure of the active form (full-length) of human fibroblast collagenase.
Authors : Iyer, S.; Visse, R.; Nagase, H.; Acharya, K.R.
Deposited on : 2006-04-29
Resolution : 2.67 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

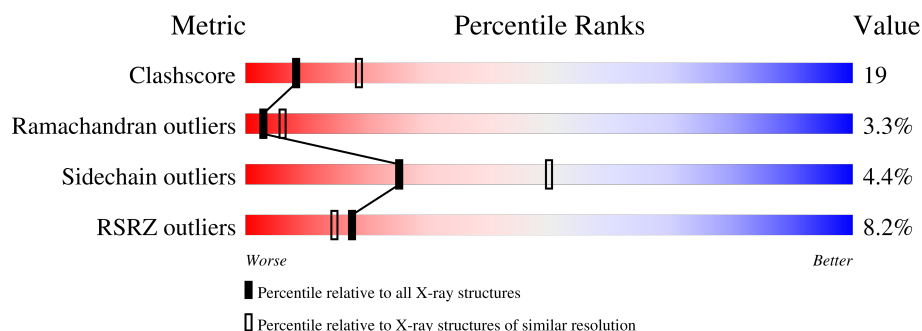
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	367	7% 63% 31% 5%
1	B	367	9% 62% 32% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6007 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 INTERSTITIAL COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2912	1868	498	537	9			
1	B	367	Total	C	N	O	S	0	0	0
			2885	1855	486	535	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	ALA	GLU	engineered mutation	UNP P03956
B	200	ALA	GLU	engineered mutation	UNP P03956

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	B	4	Total	Ca	0	0
			4	4		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		

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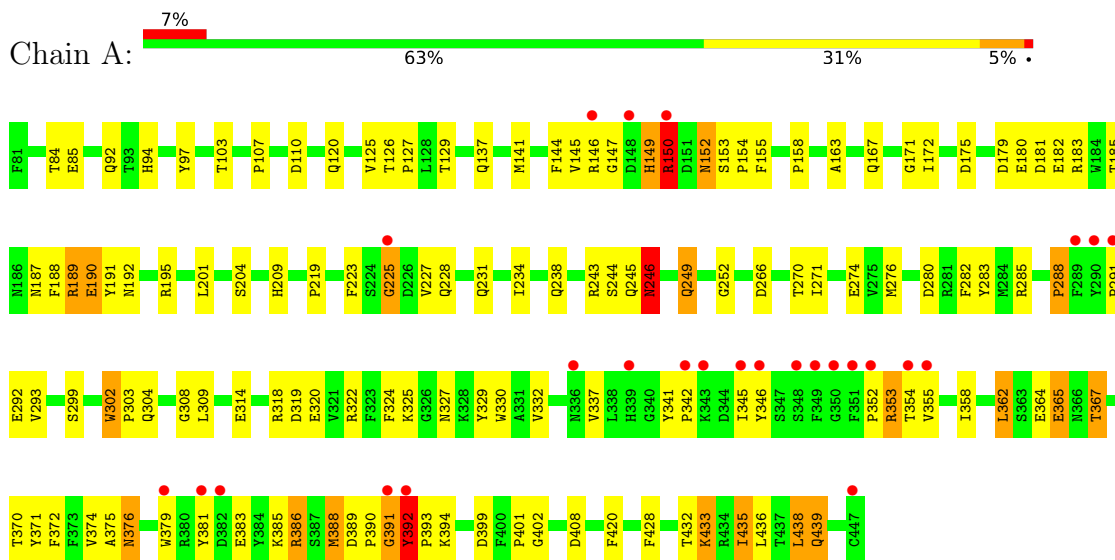
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	92	Total	O	0	0
			92	92		

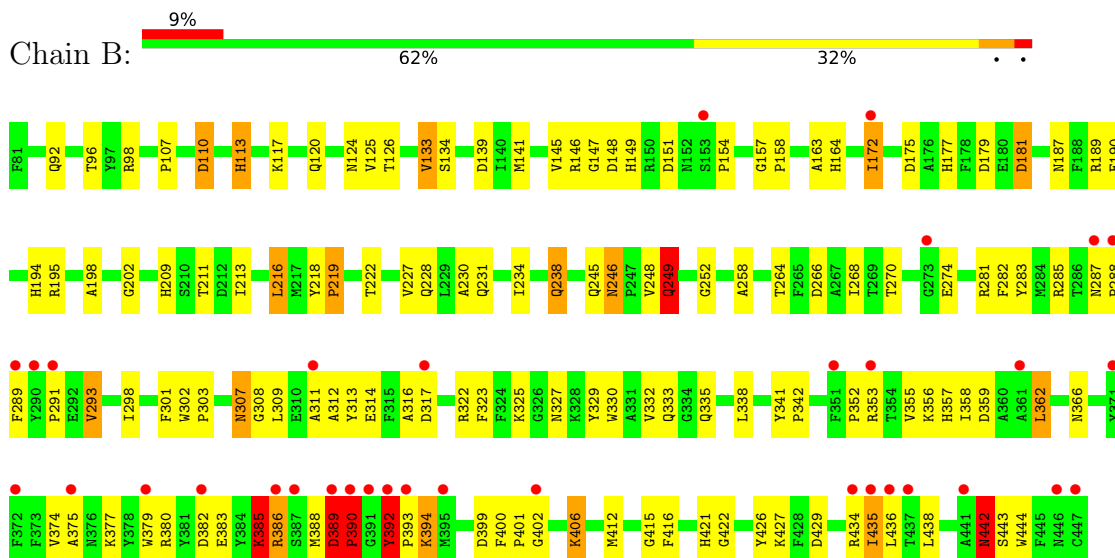
3 Residue-property plots

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 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.

• Molecule 1: INTERSTITIAL COLLAGENASE



• Molecule 1: INTERSTITIAL COLLAGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.49Å 138.49Å 110.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.64 – 2.67 24.64 – 2.67	Depositor EDS
% Data completeness (in resolution range)	88.2 (24.64-2.67) 92.0 (24.64-2.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.259 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6007	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.61	9/3010 (0.3%)	0.98	13/4091 (0.3%)
1	B	0.65	14/2981 (0.5%)	0.96	15/4049 (0.4%)
All	All	0.63	23/5991 (0.4%)	0.97	28/8140 (0.3%)

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	2
1	B	0	5
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	PRO	N-CD	10.19	1.62	1.47
1	B	92	GLN	CD-OE1	5.64	1.34	1.23
1	A	228	GLN	CD-OE1	5.51	1.34	1.23
1	B	124	ASN	CG-OD1	5.46	1.33	1.23
1	B	120	GLN	CD-OE1	5.44	1.33	1.23
1	B	228	GLN	CD-OE1	5.40	1.33	1.23
1	A	92	GLN	CD-OE1	5.40	1.33	1.23
1	B	113	HIS	ND1-CE1	5.39	1.38	1.32
1	B	307	ASN	CG-OD1	5.32	1.33	1.23
1	B	421	HIS	ND1-CE1	5.28	1.37	1.32
1	B	245	GLN	CD-OE1	5.28	1.33	1.23
1	B	187	ASN	CG-OD1	5.27	1.33	1.23
1	B	246	ASN	CG-OD1	5.25	1.33	1.23
1	A	120	GLN	CD-OE1	5.21	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ASN	CG-OD1	5.18	1.33	1.23
1	A	245	GLN	CD-OE1	5.17	1.33	1.23
1	A	376	ASN	CG-OD1	5.16	1.33	1.23
1	A	249	GLN	CD-OE1	5.13	1.33	1.23
1	B	238	GLN	CD-OE1	5.13	1.33	1.23
1	B	327	ASN	CG-OD1	5.08	1.33	1.23
1	B	249	GLN	CD-OE1	5.08	1.33	1.23
1	A	187	ASN	CG-OD1	5.05	1.33	1.23
1	B	442	ASN	CG-OD1	5.02	1.33	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ASP	CA-CB-CG	10.15	122.75	112.60
1	A	181	ASP	N-CA-C	-9.06	102.37	113.15
1	A	292	GLU	CB-CA-C	6.88	119.75	110.94
1	A	288	PRO	N-CA-C	-6.61	105.60	113.86
1	B	113	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	B	421	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	A	288	PRO	CA-N-CD	-6.09	103.47	112.00
1	A	302	TRP	CA-C-N	6.05	125.94	119.28
1	A	302	TRP	C-N-CA	6.05	125.94	119.28
1	A	292	GLU	CA-CB-CG	5.88	125.87	114.10
1	A	282	PHE	N-CA-C	5.87	118.76	110.14
1	B	113	HIS	CB-CG-ND1	5.72	131.28	122.70
1	B	421	HIS	CB-CG-ND1	5.69	131.24	122.70
1	A	171	GLY	N-CA-C	5.67	121.65	111.34
1	A	367	THR	N-CA-C	-5.61	107.68	114.75
1	A	163	ALA	N-CA-C	5.61	115.79	107.88
1	B	181	ASP	N-CA-C	-5.49	106.56	113.20
1	B	282	PHE	N-CA-C	5.44	118.14	110.14
1	B	218	TYR	CA-C-N	5.37	126.55	119.84
1	B	218	TYR	C-N-CA	5.37	126.55	119.84
1	B	202	GLY	N-CA-C	-5.34	106.32	112.73
1	B	211	THR	N-CA-C	-5.28	106.51	113.17
1	A	280	ASP	CB-CA-C	-5.28	110.50	116.63
1	B	400	PHE	CA-C-N	5.21	125.45	119.83
1	B	400	PHE	C-N-CA	5.21	125.45	119.83
1	B	366	ASN	N-CA-C	5.09	116.90	108.49
1	B	392	TYR	N-CA-C	5.09	121.06	109.81
1	A	245	GLN	N-CA-C	-5.04	107.16	113.15

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	HIS	Peptide
1	A	189	ARG	Peptide
1	B	172	ILE	Peptide
1	B	190	GLU	Peptide
1	B	385	LYS	Peptide
1	B	389	ASP	Peptide
1	B	390	PRO	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	2912	0	2671	104	0
1	B	2885	0	2644	112	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	106	0	0	3	0
4	B	92	0	0	3	0
All	All	6007	0	5315	214	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 19.

All (214) 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:146:ARG:HH21	1:A:180:GLU:HG3	1.08	1.09
1:B:389:ASP:HB3	1:B:390:PRO:HD2	1.46	0.95
1:B:385:LYS:O	1:B:385:LYS:HG2	1.67	0.91
1:A:146:ARG:NH2	1:A:180:GLU:HG3	1.85	0.91
1:A:149:HIS:O	1:A:150:ARG:HB2	1.72	0.86
1:A:94:HIS:HD1	1:A:129:THR:HG1	1.22	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:MET:HB2	1:A:175:ASP:OD1	1.81	0.81
1:B:389:ASP:CB	1:B:390:PRO:HD2	2.06	0.81
1:B:389:ASP:HB3	1:B:390:PRO:CD	2.11	0.80
1:B:382:ASP:OD2	1:B:385:LYS:HB3	1.85	0.76
1:A:155:PHE:CD1	1:A:179:ASP:HB2	2.22	0.75
1:B:289:PHE:O	1:B:291:PRO:HD3	1.89	0.73
1:A:145:VAL:HG21	1:A:149:HIS:CD2	2.24	0.72
1:A:85:GLU:CD	1:A:85:GLU:H	1.96	0.72
1:A:244:SER:OG	1:A:246:ASN:HB2	1.92	0.70
1:A:318:ARG:HB2	1:A:320:GLU:HG3	1.73	0.70
1:B:385:LYS:O	1:B:385:LYS:CG	2.40	0.69
1:B:383:GLU:O	1:B:386:ARG:HG2	1.94	0.68
1:A:276:MET:HE3	1:A:285:ARG:HE	1.58	0.68
1:B:172:ILE:HG13	1:B:172:ILE:O	1.94	0.68
1:A:439:GLN:HG3	4:A:2102:HOH:O	1.94	0.67
1:A:308:GLY:O	1:A:325:LYS:HD3	1.97	0.65
1:B:198:ALA:HB1	1:B:216:LEU:HD11	1.77	0.65
1:B:416:PHE:CE2	1:B:427:LYS:HE2	2.33	0.64
1:B:426:TYR:CD1	1:B:438:LEU:HD13	2.33	0.64
1:B:274:GLU:HG2	1:B:287:ASN:HA	1.80	0.64
1:B:117:LYS:HB3	1:B:194:HIS:CE1	2.32	0.64
1:A:341:TYR:HA	1:A:342:PRO:O	1.99	0.62
1:A:346:TYR:CE2	1:A:353:ARG:HA	2.35	0.62
1:A:402:GLY:HA3	1:A:435:ILE:HD12	1.81	0.61
1:A:304:GLN:HB2	1:A:337:VAL:HG21	1.82	0.61
1:B:113:HIS:HB2	4:B:2018:HOH:O	2.01	0.61
1:A:322:ARG:HD3	1:A:329:TYR:HE2	1.64	0.61
1:A:355:VAL:HG13	1:A:374:VAL:HG11	1.82	0.61
1:B:141:MET:HB2	1:B:175:ASP:OD1	2.01	0.60
1:B:356:LYS:H	1:B:356:LYS:HD3	1.64	0.60
1:B:412:MET:HE2	1:B:415:GLY:HA2	1.83	0.60
1:B:379:TRP:CH2	1:B:393:PRO:HG3	2.36	0.60
1:B:434:ARG:O	1:B:435:ILE:HG13	2.03	0.59
1:B:311:ALA:O	1:B:312:ALA:HB2	2.02	0.59
1:B:383:GLU:O	1:B:386:ARG:CG	2.49	0.59
1:B:330:TRP:CE2	1:B:342:PRO:HB3	2.37	0.59
1:B:389:ASP:CB	1:B:390:PRO:CD	2.78	0.59
1:A:85:GLU:CD	1:A:85:GLU:N	2.59	0.58
1:A:302:TRP:CD1	1:A:332:VAL:HG11	2.39	0.58
1:A:341:TYR:HA	1:A:342:PRO:C	2.27	0.58
1:A:389:ASP:HB2	1:A:392:TYR:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASN:O	1:A:345:ILE:HG12	2.03	0.58
1:A:381:TYR:HA	1:A:388:MET:HA	1.84	0.58
1:A:183:ARG:HG3	1:B:335:GLN:HB2	1.86	0.57
1:A:381:TYR:OH	1:A:386:ARG:HA	2.05	0.57
1:A:153:SER:N	1:A:154:PRO:HD3	2.20	0.56
1:A:155:PHE:CE1	1:A:179:ASP:HB2	2.40	0.56
1:B:246:ASN:OD1	1:B:248:VAL:HG22	2.05	0.56
1:B:426:TYR:CE1	1:B:438:LEU:HD13	2.40	0.56
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.70	0.56
1:A:392:TYR:H	1:A:393:PRO:HD3	1.70	0.56
1:A:379:TRP:CZ3	1:A:393:PRO:HG3	2.40	0.56
1:A:352:PRO:C	1:A:354:THR:H	2.15	0.55
1:B:125:VAL:HG23	1:B:126:THR:HG23	1.88	0.54
1:B:164:HIS:CD2	1:B:177:HIS:HB2	2.42	0.54
1:A:325:LYS:HB3	1:A:330:TRP:CZ3	2.43	0.53
1:A:392:TYR:N	1:A:393:PRO:HD3	2.24	0.53
1:B:234:ILE:O	1:B:238:GLN:HG3	2.07	0.53
1:A:209:HIS:HB3	1:A:219:PRO:HG3	1.89	0.53
1:B:270:THR:O	1:B:314:GLU:HB2	2.09	0.53
1:B:146:ARG:HG2	1:B:181:ASP:OD2	2.08	0.53
1:B:98:ARG:NE	1:B:134:SER:O	2.42	0.53
1:A:152:ASN:C	1:A:154:PRO:HD3	2.34	0.52
1:B:189:ARG:NE	4:B:2050:HOH:O	2.40	0.52
1:B:386:ARG:CB	1:B:386:ARG:CZ	2.87	0.52
1:B:386:ARG:NH2	1:B:386:ARG:HB3	2.24	0.52
1:B:392:TYR:O	1:B:394:LYS:N	2.39	0.52
1:A:180:GLU:C	1:A:182:GLU:H	2.18	0.52
1:A:370:THR:HG22	1:A:372:PHE:CE2	2.45	0.52
1:B:392:TYR:N	1:B:393:PRO:HD3	2.25	0.52
1:A:389:ASP:HB2	1:A:392:TYR:CD2	2.45	0.51
1:B:358:ILE:N	1:B:358:ILE:HD12	2.24	0.51
1:B:145:VAL:HG21	1:B:149:HIS:CD2	2.46	0.51
1:A:392:TYR:N	1:A:393:PRO:CD	2.74	0.51
1:A:432:THR:O	1:A:433:LYS:C	2.54	0.50
1:B:377:LYS:HG2	1:B:394:LYS:O	2.11	0.50
1:B:416:PHE:CD2	1:B:427:LYS:HE2	2.46	0.50
1:A:146:ARG:HE	1:A:180:GLU:HB3	1.75	0.50
1:B:98:ARG:HG3	1:B:133:VAL:O	2.11	0.50
1:B:362:LEU:HD22	1:B:362:LEU:C	2.37	0.50
1:A:195:ARG:HD3	1:A:227:VAL:HG22	1.93	0.50
1:A:145:VAL:HG23	1:A:155:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:TYR:O	1:A:394:LYS:N	2.42	0.49
1:A:379:TRP:CE3	1:A:388:MET:HE3	2.47	0.49
1:B:392:TYR:C	1:B:394:LYS:H	2.20	0.49
1:B:356:LYS:HD3	1:B:356:LYS:N	2.27	0.49
1:A:385:LYS:O	1:A:386:ARG:C	2.55	0.49
1:B:386:ARG:CZ	1:B:386:ARG:HB2	2.42	0.49
1:B:380:ARG:HD3	1:B:392:TYR:CZ	2.47	0.48
1:B:399:ASP:C	1:B:401:PRO:HD3	2.38	0.48
1:A:125:VAL:HG23	1:A:126:THR:HG23	1.96	0.48
1:B:266:ASP:HB3	1:B:309:LEU:O	2.13	0.48
1:B:268:ILE:O	4:B:2072:HOH:O	2.20	0.47
1:A:364:GLU:HB2	1:A:367:THR:OG1	2.13	0.47
1:A:304:GLN:HB2	1:A:337:VAL:CG2	2.45	0.47
1:A:180:GLU:C	1:A:182:GLU:N	2.71	0.47
1:B:316:ALA:O	1:B:317:ASP:C	2.58	0.47
1:A:183:ARG:O	1:A:185:THR:HG23	2.14	0.47
1:B:380:ARG:HB2	1:B:392:TYR:CE2	2.50	0.47
1:A:436:LEU:N	1:A:436:LEU:HD12	2.30	0.47
1:B:209:HIS:HB3	1:B:219:PRO:HG3	1.96	0.47
1:B:406:LYS:HD3	1:B:406:LYS:C	2.40	0.47
1:A:390:PRO:O	1:A:391:GLY:C	2.58	0.47
1:B:258:ALA:HB1	1:B:293:VAL:HG11	1.96	0.47
1:B:198:ALA:CB	1:B:216:LEU:HD11	2.42	0.46
1:A:183:ARG:NH2	1:A:190:GLU:O	2.47	0.46
1:A:352:PRO:O	1:A:354:THR:N	2.49	0.46
1:B:380:ARG:HD3	1:B:392:TYR:OH	2.15	0.46
1:A:179:ASP:O	1:A:182:GLU:HB2	2.16	0.46
1:A:438:LEU:C	1:A:438:LEU:HD12	2.40	0.46
1:A:126:THR:HB	1:A:127:PRO:HD2	1.98	0.46
1:B:264:THR:HG22	1:B:422:GLY:C	2.41	0.46
1:B:380:ARG:O	1:B:388:MET:SD	2.73	0.46
1:A:145:VAL:HG23	1:A:155:PHE:HE2	1.80	0.45
1:A:408:ASP:HB2	1:A:420:PHE:O	2.16	0.45
1:B:362:LEU:HD22	1:B:362:LEU:O	2.16	0.45
1:B:308:GLY:O	1:B:325:LYS:HD2	2.16	0.45
1:A:195:ARG:HG3	1:A:195:ARG:NH1	2.32	0.45
1:A:362:LEU:HD13	1:A:371:TYR:HB2	1.97	0.45
1:A:374:VAL:O	1:A:375:ALA:C	2.57	0.45
1:B:379:TRP:CZ2	1:B:393:PRO:HG3	2.52	0.45
1:A:428:PHE:CZ	1:A:433:LYS:HA	2.52	0.45
1:B:399:ASP:O	1:B:401:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:TRP:HE1	1:B:332:VAL:HG11	1.81	0.45
1:A:201:LEU:HA	1:A:204:SER:HB2	1.98	0.45
1:B:341:TYR:HB3	1:B:342:PRO:HA	1.99	0.44
1:A:182:GLU:HA	1:A:182:GLU:OE1	2.17	0.44
1:B:388:MET:O	1:B:389:ASP:O	2.35	0.44
1:B:388:MET:C	1:B:389:ASP:O	2.59	0.44
1:A:149:HIS:O	1:A:150:ARG:CB	2.54	0.44
1:A:364:GLU:O	1:A:365:GLU:C	2.60	0.44
1:A:330:TRP:H	1:A:330:TRP:HE3	1.66	0.44
1:A:381:TYR:HB2	1:A:388:MET:SD	2.58	0.44
1:A:266:ASP:HB3	1:A:309:LEU:O	2.17	0.44
1:B:248:VAL:CG2	1:B:249:GLN:N	2.81	0.44
1:B:380:ARG:HB2	1:B:392:TYR:CD2	2.52	0.44
1:B:434:ARG:O	1:B:435:ILE:CG1	2.66	0.44
1:A:234:ILE:O	1:A:238:GLN:HG3	2.18	0.43
1:A:270:THR:O	1:A:314:GLU:HB2	2.18	0.43
1:A:231:GLN:HB2	1:A:252:GLY:O	2.18	0.43
1:A:319:ASP:OD1	1:A:319:ASP:O	2.35	0.43
1:B:145:VAL:HG21	1:B:149:HIS:NE2	2.33	0.43
1:B:358:ILE:HG22	1:B:359:ASP:N	2.33	0.43
1:A:276:MET:CE	1:A:285:ARG:HE	2.29	0.43
1:A:352:PRO:C	1:A:354:THR:N	2.75	0.43
1:B:274:GLU:OE1	1:B:285:ARG:NH1	2.51	0.43
1:B:435:ILE:O	1:B:435:ILE:HG22	2.18	0.43
1:A:223:PHE:CE2	1:A:225:GLY:HA2	2.54	0.43
1:A:399:ASP:C	1:A:401:PRO:HD3	2.44	0.43
1:B:146:ARG:HD3	1:B:181:ASP:OD1	2.18	0.43
1:A:324:PHE:CD2	1:A:358:ILE:HD12	2.54	0.43
1:B:434:ARG:C	1:B:435:ILE:HG13	2.43	0.43
1:B:352:PRO:O	1:B:353:ARG:C	2.61	0.43
1:B:357:HIS:C	1:B:358:ILE:HD12	2.44	0.43
1:A:137:GLN:OE1	1:A:141:MET:HE2	2.19	0.43
1:B:429:ASP:HB2	1:B:436:LEU:CD1	2.49	0.43
1:A:84:THR:HG21	1:A:167:GLN:HG2	2.01	0.42
1:A:190:GLU:HA	1:A:191:TYR:HA	1.70	0.42
1:B:248:VAL:HG23	1:B:249:GLN:N	2.33	0.42
1:B:148:ASP:HA	1:B:154:PRO:HB3	2.00	0.42
1:B:443:SER:HG	1:B:444:TRP:CD1	2.37	0.42
1:A:188:PHE:CD1	1:A:188:PHE:C	2.97	0.42
1:A:192:ASN:OD1	1:A:192:ASN:C	2.62	0.42
1:B:281:ARG:HA	1:B:307:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ALA:O	1:B:231:GLN:C	2.61	0.42
1:B:402:GLY:HA3	1:B:435:ILE:HD11	2.01	0.42
1:A:271:ILE:O	1:A:271:ILE:HG23	2.19	0.42
1:A:276:MET:HE3	1:A:285:ARG:NE	2.30	0.42
1:A:362:LEU:C	1:A:362:LEU:HD22	2.45	0.42
1:B:96:THR:N	1:B:139:ASP:OD2	2.46	0.42
1:B:392:TYR:N	1:B:393:PRO:CD	2.82	0.42
1:B:274:GLU:HG2	1:B:288:PRO:HD3	2.01	0.42
1:B:309:LEU:HD22	1:B:323:PHE:HB3	2.00	0.42
1:B:96:THR:O	1:B:139:ASP:HB2	2.19	0.42
1:B:386:ARG:CB	1:B:386:ARG:NH2	2.83	0.42
1:A:158:PRO:HG3	1:B:301:PHE:HD1	1.85	0.42
1:A:183:ARG:O	1:A:183:ARG:HG2	2.18	0.41
1:A:352:PRO:HD2	1:A:379:TRP:CH2	2.55	0.41
1:A:383:GLU:C	1:A:385:LYS:H	2.28	0.41
1:B:416:PHE:CE2	1:B:436:LEU:HD22	2.55	0.41
1:A:189:ARG:HD2	4:A:2050:HOH:O	2.20	0.41
1:B:107:PRO:HD2	1:B:110:ASP:HB2	2.03	0.41
1:B:355:VAL:HG13	1:B:374:VAL:CG1	2.49	0.41
1:A:376:ASN:ND2	4:A:2093:HOH:O	2.54	0.41
1:B:311:ALA:HB2	1:B:358:ILE:HG22	2.03	0.41
1:A:379:TRP:HE3	1:A:388:MET:HE3	1.84	0.41
1:A:103:THR:HB	1:A:144:PHE:CD2	2.56	0.41
1:A:283:TYR:CD1	1:A:283:TYR:C	2.98	0.41
1:B:157:GLY:O	1:B:158:PRO:C	2.63	0.41
1:B:163:ALA:HB1	1:B:177:HIS:O	2.21	0.41
1:B:231:GLN:HB2	1:B:252:GLY:O	2.20	0.41
1:B:355:VAL:HG13	1:B:374:VAL:HG13	2.02	0.41
1:B:392:TYR:C	1:B:394:LYS:N	2.79	0.41
1:A:299:SER:O	1:A:303:PRO:HG3	2.20	0.41
1:B:148:ASP:OD1	1:B:148:ASP:C	2.64	0.41
1:B:195:ARG:HD3	1:B:227:VAL:HG22	2.02	0.41
1:B:258:ALA:CB	1:B:293:VAL:HG11	2.51	0.41
1:B:283:TYR:CD1	1:B:283:TYR:C	2.99	0.41
1:B:298:ILE:HD13	1:B:309:LEU:HD12	2.03	0.41
1:B:333:GLN:OE1	1:B:338:LEU:HD21	2.21	0.41
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.86	0.40
1:B:302:TRP:NE1	1:B:332:VAL:HG11	2.36	0.40
1:A:97:TYR:CD1	1:A:97:TYR:C	3.00	0.40
1:B:313:TYR:CZ	1:B:322:ARG:HG3	2.56	0.40
1:A:107:PRO:HD2	1:A:110:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:SER:C	1:A:246:ASN:H	2.29	0.40
1:A:438:LEU:O	1:A:438:LEU:HG	2.22	0.40
1:B:442:ASN:HD22	1:B:442:ASN:C	2.29	0.40

There are no symmetry-related clashes.

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	365/367 (100%)	319 (87%)	34 (9%)	12 (3%)	3	6
1	B	365/367 (100%)	314 (86%)	39 (11%)	12 (3%)	3	6
All	All	730/734 (100%)	633 (87%)	73 (10%)	24 (3%)	3	6

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	190	GLU
1	B	389	ASP
1	B	394	LYS
1	B	435	ILE
1	A	147	GLY
1	A	353	ARG
1	A	388	MET
1	A	391	GLY
1	B	390	PRO
1	A	365	GLU
1	A	386	ARG
1	B	151	ASP
1	B	375	ALA
1	A	249	GLN

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Mol	Chain	Res	Type
1	B	249	GLN
1	B	219	PRO
1	A	225	GLY
1	A	291	PRO
1	B	293	VAL
1	B	392	TYR
1	A	392	TYR
1	B	147	GLY
1	B	303	PRO

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	297/313 (95%)	283 (95%)	14 (5%)	23	47
1	B	293/313 (94%)	281 (96%)	12 (4%)	27	52
All	All	590/626 (94%)	564 (96%)	26 (4%)	25	50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	152	ASN
1	A	172	ILE
1	A	243	ARG
1	A	246	ASN
1	A	274	GLU
1	A	288	PRO
1	A	293	VAL
1	A	362	LEU
1	A	392	TYR
1	A	433	LYS
1	A	435	ILE
1	A	438	LEU
1	A	439	GLN

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	133	VAL
1	B	213	ILE
1	B	216	LEU
1	B	222	THR
1	B	329	TYR
1	B	362	LEU
1	B	385	LYS
1	B	386	ARG
1	B	392	TYR
1	B	406	LYS
1	B	442	ASN

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

Mol	Chain	Res	Type
1	A	167	GLN
1	B	161	ASN
1	B	376	ASN
1	B	439	GLN

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 [i](#)

Of 12 ligands modelled in this entry, 12 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	367/367 (100%)	0.36	26 (7%)	22 18	19, 40, 79, 88	0
1	B	367/367 (100%)	0.55	34 (9%)	14 12	20, 47, 81, 91	0
All	All	734/734 (100%)	0.45	60 (8%)	17 14	19, 44, 80, 91	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393	PRO	4.7
1	A	346	TYR	4.4
1	B	391	GLY	4.1
1	A	391	GLY	3.6
1	A	355	VAL	3.2
1	B	153	SER	3.2
1	B	288	PRO	3.1
1	A	379	TRP	3.1
1	B	289	PHE	3.1
1	B	287	ASN	3.0
1	B	446	ASN	3.0
1	B	317	ASP	3.0
1	B	353	ARG	3.0
1	A	342	PRO	3.0
1	A	291	PRO	2.9
1	A	348	SER	2.9
1	A	350	GLY	2.9
1	B	290	TYR	2.9
1	B	436	LEU	2.9
1	A	351	PHE	2.8
1	A	349	PHE	2.7
1	A	354	THR	2.7
1	A	343	LYS	2.7
1	A	352	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	390	PRO	2.7
1	A	146	ARG	2.7
1	A	290	TYR	2.6
1	A	225	GLY	2.6
1	B	441	ALA	2.5
1	A	148	ASP	2.5
1	B	435	ILE	2.5
1	B	437	THR	2.5
1	A	392	TYR	2.5
1	B	387	SER	2.4
1	A	289	PHE	2.4
1	B	351	PHE	2.4
1	B	392	TYR	2.4
1	A	339	HIS	2.4
1	A	382	ASP	2.4
1	A	381	TYR	2.3
1	B	371	TYR	2.3
1	A	336	ASN	2.2
1	B	395	MET	2.2
1	B	389	ASP	2.2
1	B	402	GLY	2.2
1	B	447	CYS	2.2
1	A	345	ILE	2.2
1	B	375	ALA	2.1
1	B	434	ARG	2.1
1	B	291	PRO	2.1
1	B	382	ASP	2.1
1	B	311	ALA	2.1
1	A	150	ARG	2.1
1	B	273	GLY	2.1
1	B	361	ALA	2.1
1	B	372	PHE	2.1
1	A	447	CYS	2.1
1	B	386	ARG	2.0
1	B	379	TRP	2.0
1	B	172	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	1303	1/1	0.58	0.24	64,64,64,64	1
2	CA	B	1302	1/1	0.70	0.17	57,57,57,57	0
2	CA	A	1102	1/1	0.88	0.12	45,45,45,45	0
2	CA	A	1103	1/1	0.88	0.09	44,44,44,44	0
2	CA	B	1301	1/1	0.90	0.09	59,59,59,59	0
2	CA	A	1104	1/1	0.97	0.05	47,47,47,47	0
2	CA	A	1101	1/1	0.97	0.04	28,28,28,28	0
2	CA	B	1304	1/1	0.97	0.05	50,50,50,50	0
3	ZN	B	1401	1/1	0.98	0.06	36,36,36,36	0
3	ZN	A	1201	1/1	0.99	0.06	40,40,40,40	0
3	ZN	B	1402	1/1	0.99	0.07	34,34,34,34	0
3	ZN	A	1202	1/1	1.00	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.