



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:11 am GMT

PDB ID : 2CLT  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

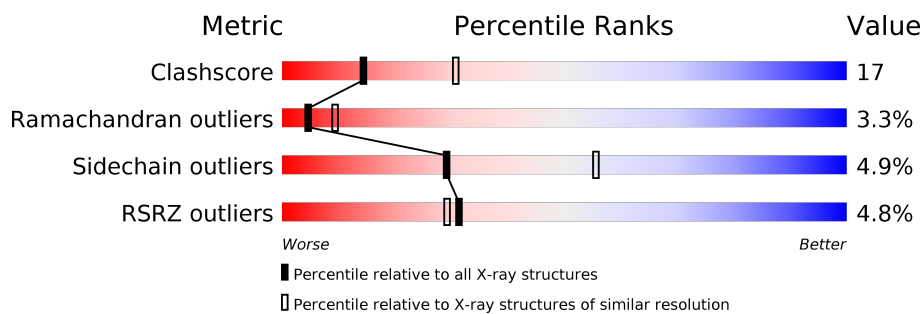
# 1 Overall quality at a glance

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	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>67%</div> <div>29%</div> <div>• •</div> </div>
1	B	367	<div> <div>7%</div> <div>68%</div> <div>28%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	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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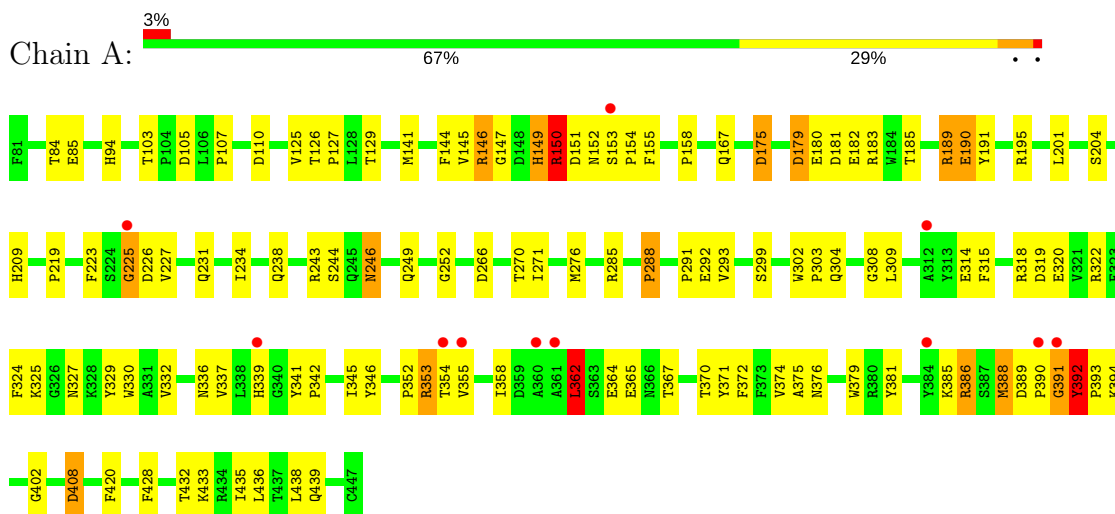
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	92	Total	O	0	0
			92	92		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	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) 92.1 (24.64-2.67)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.53	1/3010 (0.0%)	0.67	7/4091 (0.2%)
1	B	0.54	0/2981	0.65	5/4049 (0.1%)
All	All	0.54	1/5991 (0.0%)	0.66	12/8140 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	PRO	N-CD	10.12	1.62	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	288	PRO	CA-N-CD	-5.74	103.47	111.50
1	A	292	GLU	CA-CB-CG	5.67	125.87	113.40
1	A	105	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	105	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	181	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	266	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	389	ASP	CB-CG-OD2	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	179	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	151	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	181	ASP	CB-CG-OD2	5.20	122.98	118.30

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	92	0
1	B	2885	0	2644	102	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	192	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 17.

All (192) 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
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:276:MET:HE3	1:A:285:ARG:HE	1.54	0.73
1:A:145:VAL:HG21	1:A:149:HIS:CD2	2.24	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:CG	1:B:385:LYS:O	2.40	0.69
1:B:383:GLU:O	1:B:386:ARG:HG2	1.94	0.68
1:B:172:ILE:O	1:B:172:ILE:HG13	1.94	0.68
1:A:439:GLN:HG3	4:A:2102:HOH:O	1.94	0.67
1:A:85:GLU:CD	1:A:85:GLU:H	1.96	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:HD3	1:B:356:LYS:H	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TRP:CD1	1:A:332:VAL:HG11	2.39	0.58
1:A:389:ASP:HB2	1:A:392:TYR:HD2	1.69	0.58
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:381:TYR:OH	1:A:386:ARG:HA	2.05	0.57
1:A:183:ARG:HG3	1:B:335:GLN:HB2	1.86	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:HH11	1:A:195:ARG:HG3	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: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:85:GLU:N	1:A:85:GLU:CD	2.59	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:A:341:TYR:HA	1:A:342:PRO:C	2.27	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: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:HB3	1:B:386:ARG:NH2	2.24	0.52
1:B:392:TYR:O	1:B:394:LYS:N	2.39	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:HD12	1:B:358:ILE:N	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:352:PRO:C	1:A:354:THR:H	2.15	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: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:B:356:LYS:N	1:B:356:LYS:HD3	2.27	0.49
1:B:386:ARG:HB2	1:B:386:ARG:CZ	2.42	0.49
1:B:380:ARG:HD3	1:B:392:TYR:CZ	2.47	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:183:ARG:O	1:A:185:THR:HG23	2.14	0.47
1:A:180:GLU:C	1:A:182:GLU:H	2.18	0.47
1:B:380:ARG:HB2	1:B:392:TYR:CE2	2.50	0.47
1:B:209:HIS:HB3	1:B:219:PRO:HG3	1.96	0.47
1:A:436:LEU:HD12	1:A:436:LEU:N	2.30	0.47
1:A:152:ASN:C	1:A:154:PRO:HD3	2.34	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:432:THR:O	1:A:433:LYS:C	2.54	0.46
1:A:126:THR:HB	1:A:127:PRO:HD2	1.98	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: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:362:LEU:C	1:B:362:LEU:HD22	2.37	0.45
1:B:399:ASP:O	1:B:401:PRO:HD3	2.17	0.45
1:A:276:MET:HE3	1:A:285:ARG:NE	2.28	0.45
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:392:TYR:C	1:B:394:LYS:H	2.20	0.45
1:A:385:LYS:O	1:A:386:ARG:C	2.55	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TRP:CE3	1:A:388:MET:HE3	2.52	0.44
1:B:388:MET:O	1:B:389:ASP:O	2.35	0.44
1:A:149:HIS:O	1:A:150:ARG:CB	2.54	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:180:GLU:C	1:A:182:GLU:N	2.71	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:399:ASP:C	1:B:401:PRO:HD3	2.38	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:O	1:A:319:ASP:OD1	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: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: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: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:316:ALA:O	1:B:317:ASP:C	2.58	0.42
1:B:148:ASP:HA	1:B:154:PRO:HB3	2.00	0.42
1:B:172:ILE:O	1:B:172:ILE:CG1	2.67	0.42
1:B:281:ARG:HA	1:B:307:ASN:OD1	2.19	0.42
1:B:402:GLY:HA3	1:B:435:ILE:HD11	2.01	0.42
1:A:271:ILE:HG23	1:A:271:ILE:O	2.19	0.42
1:A:390:PRO:O	1:A:391:GLY:C	2.58	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:406:LYS:C	1:B:406:LYS:HD3	2.40	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:386:ARG:NH2	1:B:386:ARG:CB	2.83	0.42
1:B:96:THR:O	1:B:139:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:438:LEU:C	1:A:438:LEU:HD12	2.40	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:B:264:THR:HG22	1:B:422:GLY:C	2.41	0.41
1:A:103:THR:HB	1:A:144:PHE:CD2	2.56	0.41
1:B:231:GLN:HB2	1:B:252:GLY:O	2.20	0.41
1:B:388:MET:C	1:B:389:ASP:O	2.59	0.41
1:B:163:ALA:HB1	1:B:177:HIS:O	2.21	0.41
1:B:355:VAL:HG13	1:B:374:VAL:HG13	2.02	0.41
1:A:299:SER:O	1:A:303:PRO:HG3	2.20	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: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:374:VAL:O	1:A:375:ALA:C	2.57	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
1:A:438:LEU:O	1:A:438:LEU:HG	2.22	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	365/367 (100%)	319 (87%)	34 (9%)	12 (3%)	4	9
1	B	365/367 (100%)	314 (86%)	39 (11%)	12 (3%)	4	9
All	All	730/734 (100%)	633 (87%)	73 (10%)	24 (3%)	4	9

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
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%)	30	57
1	B	293/313 (94%)	278 (95%)	15 (5%)	28	53
All	All	590/626 (94%)	561 (95%)	29 (5%)	29	55

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	A	150	ARG
1	A	175	ASP
1	A	226	ASP
1	A	243	ARG
1	A	246	ASN
1	A	288	PRO
1	A	293	VAL
1	A	315	PHE
1	A	336	ASN
1	A	339	HIS
1	A	362	LEU
1	A	392	TYR
1	A	408	ASP
1	B	110	ASP
1	B	208	SER
1	B	213	ILE
1	B	216	LEU
1	B	222	THR
1	B	296	ASN
1	B	302	TRP
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	421	HIS
1	B	442	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates 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 [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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/367 (100%)	-0.02	11 (2%) 51 50	19, 40, 79, 88	0
1	B	367/367 (100%)	0.20	24 (6%) 20 17	20, 47, 81, 91	0
All	All	734/734 (100%)	0.09	35 (4%) 31 29	19, 44, 80, 91	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	ALA	5.8
1	B	288	PRO	4.9
1	B	289	PHE	4.6
1	B	312	ALA	3.9
1	B	390	PRO	3.7
1	B	366	ASN	3.5
1	A	384	TYR	3.4
1	B	410	VAL	3.2
1	B	267	ALA	3.2
1	B	153	SER	3.2
1	B	360	ALA	3.1
1	B	268	ILE	3.0
1	A	361	ALA	3.0
1	A	354	THR	2.9
1	A	355	VAL	2.9
1	A	339	HIS	2.8
1	A	391	GLY	2.7
1	B	290	TYR	2.6
1	B	432	THR	2.6
1	B	287	ASN	2.6
1	B	389	ASP	2.6
1	A	225	GLY	2.4
1	B	372	PHE	2.4
1	B	392	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	2.4
1	B	136	GLY	2.4
1	A	360	ALA	2.3
1	B	291	PRO	2.3
1	B	409	ALA	2.3
1	A	390	PRO	2.3
1	B	436	LEU	2.2
1	B	371	TYR	2.1
1	B	391	GLY	2.1
1	A	153	SER	2.0
1	B	248	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	1303	1/1	0.51	0.22	1.46	64,64,64,64	1
2	CA	A	1102	1/1	0.88	0.23	0.50	45,45,45,45	0
2	CA	B	1302	1/1	0.62	0.26	-0.13	57,57,57,57	0
2	CA	A	1103	1/1	0.71	0.11	-1.04	44,44,44,44	0
3	ZN	B	1401	1/1	0.98	0.09	-1.24	36,36,36,36	0
2	CA	A	1101	1/1	0.93	0.11	-1.49	28,28,28,28	0
3	ZN	A	1201	1/1	0.98	0.09	-1.89	40,40,40,40	0
2	CA	B	1301	1/1	0.86	0.11	-1.93	59,59,59,59	0
2	CA	A	1104	1/1	0.85	0.07	-2.58	47,47,47,47	0
2	CA	B	1304	1/1	0.95	0.06	-3.46	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1202	1/1	1.00	0.10	-	29,29,29,29	0
3	ZN	B	1402	1/1	0.99	0.11	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.