



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4AU3  
Title : Crystal Structure of a Hsp47-collagen complex  
Authors : Widmer, C.; Gebauer, J.M.; Brunstein, E.; Rodenbaum, S.; Zaucke, F.; Drogemüller, C.; Leeb, T.; Baumann, U.  
Deposited on : 2012-05-14  
Resolution : 2.78 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

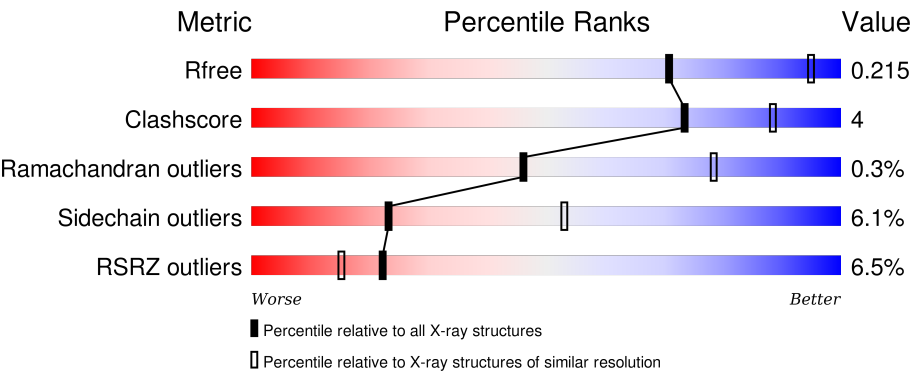
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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))
R <sub>free</sub>	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	392	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>84%9%• 6%</div></div>
1	C	392	<div><div>14%</div><div></div><div></div><div></div><div></div></div> <div>79%15%• 6%</div>

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Mol	Chain	Length	Quality of chain
3	F	20	 80% 20%
3	G	20	 70% 5% 25%
3	H	20	 80% 5% 15%
3	I	20	 70% 10% 20%
3	J	20	 65% 10% 25%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12171 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 SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	Se	0	0	0
			2886	1839	501	532	1	13			
1	C	370	Total	C	N	O	S	Se	0	0	0
			2911	1854	505	538	1	13			
1	D	372	Total	C	N	O	S	Se	0	0	0
			2926	1861	513	538	1	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MSE	-	EXPRESSION TAG	UNP E2RHY7
A	419	LEU	-	EXPRESSION TAG	UNP E2RHY7
A	420	GLU	-	EXPRESSION TAG	UNP E2RHY7
A	421	HIS	-	EXPRESSION TAG	UNP E2RHY7
A	422	HIS	-	EXPRESSION TAG	UNP E2RHY7
A	423	HIS	-	EXPRESSION TAG	UNP E2RHY7
A	424	HIS	-	EXPRESSION TAG	UNP E2RHY7
A	425	HIS	-	EXPRESSION TAG	UNP E2RHY7
A	426	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	35	MSE	-	EXPRESSION TAG	UNP E2RHY7
C	419	LEU	-	EXPRESSION TAG	UNP E2RHY7
C	420	GLU	-	EXPRESSION TAG	UNP E2RHY7
C	421	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	422	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	423	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	424	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	425	HIS	-	EXPRESSION TAG	UNP E2RHY7
C	426	HIS	-	EXPRESSION TAG	UNP E2RHY7
D	35	MSE	-	EXPRESSION TAG	UNP E2RHY7
D	419	LEU	-	EXPRESSION TAG	UNP E2RHY7
D	420	GLU	-	EXPRESSION TAG	UNP E2RHY7
D	421	HIS	-	EXPRESSION TAG	UNP E2RHY7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	422	HIS	-	EXPRESSION TAG	UNP E2RHY7
D	423	HIS	-	EXPRESSION TAG	UNP E2RHY7
D	424	HIS	-	EXPRESSION TAG	UNP E2RHY7
D	425	HIS	-	EXPRESSION TAG	UNP E2RHY7
D	426	HIS	-	EXPRESSION TAG	UNP E2RHY7

- Molecule 2 is a protein called SERPYIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	Se	0	0	0
			2856	1817	498	527	1	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	MSE	-	EXPRESSION TAG	UNP E2RHY7
B	419	LEU	-	EXPRESSION TAG	UNP E2RHY7
B	420	GLU	-	EXPRESSION TAG	UNP E2RHY7
B	421	HIS	-	EXPRESSION TAG	UNP E2RHY7
B	422	HIS	-	EXPRESSION TAG	UNP E2RHY7
B	423	HIS	-	EXPRESSION TAG	UNP E2RHY7
B	424	HIS	-	EXPRESSION TAG	UNP E2RHY7
B	425	HIS	-	EXPRESSION TAG	UNP E2RHY7
B	426	HIS	-	EXPRESSION TAG	UNP E2RHY7

- Molecule 3 is a protein called 18ER COLLAGEN MODEL PEPTIDE 15-R8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	15	Total	C	N	O	0	0	0
			94	61	18	15			
3	F	16	Total	C	N	O	0	0	0
			101	66	19	16			
3	G	15	Total	C	N	O	0	0	0
			94	61	18	15			
3	H	17	Total	C	N	O	0	0	0
			108	71	20	17			
3	I	16	Total	C	N	O	0	0	0
			101	66	19	16			
3	J	15	Total	C	N	O	0	0	0
			94	61	18	15			

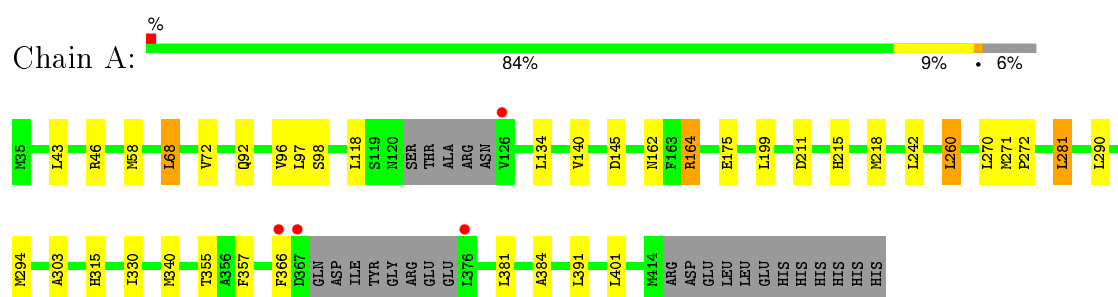
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	EXPRESSION TAG	UNP Q96A83
E	19	NH2	-	EXPRESSION TAG	UNP Q96A83
F	0	ACE	-	EXPRESSION TAG	UNP Q96A83
F	19	NH2	-	EXPRESSION TAG	UNP Q96A83
G	0	ACE	-	EXPRESSION TAG	UNP Q96A83
G	19	NH2	-	EXPRESSION TAG	UNP Q96A83
H	0	ACE	-	EXPRESSION TAG	UNP Q96A83
H	19	NH2	-	EXPRESSION TAG	UNP Q96A83
I	0	ACE	-	EXPRESSION TAG	UNP Q96A83
I	19	NH2	-	EXPRESSION TAG	UNP Q96A83
J	0	ACE	-	EXPRESSION TAG	UNP Q96A83
J	19	NH2	-	EXPRESSION TAG	UNP Q96A83

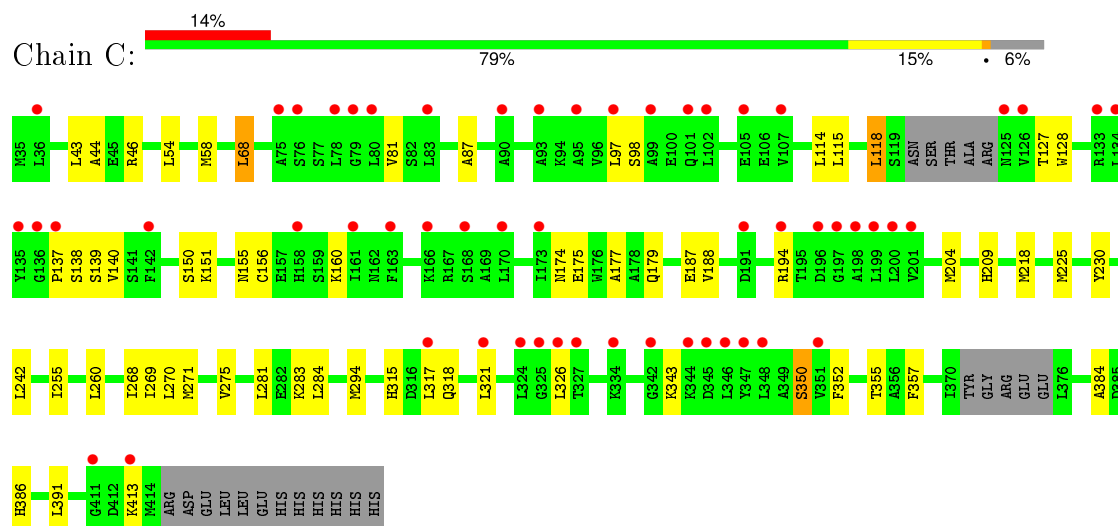
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

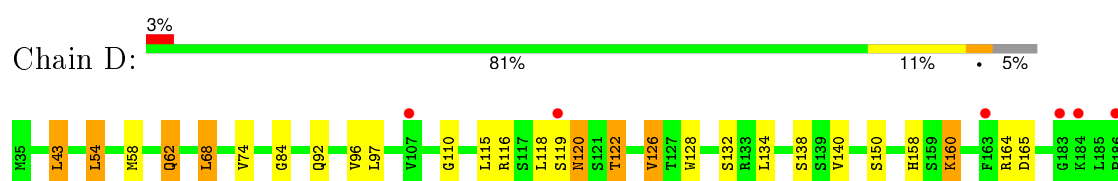
- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

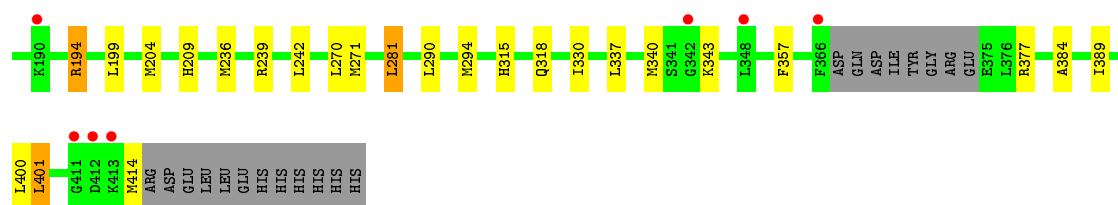


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

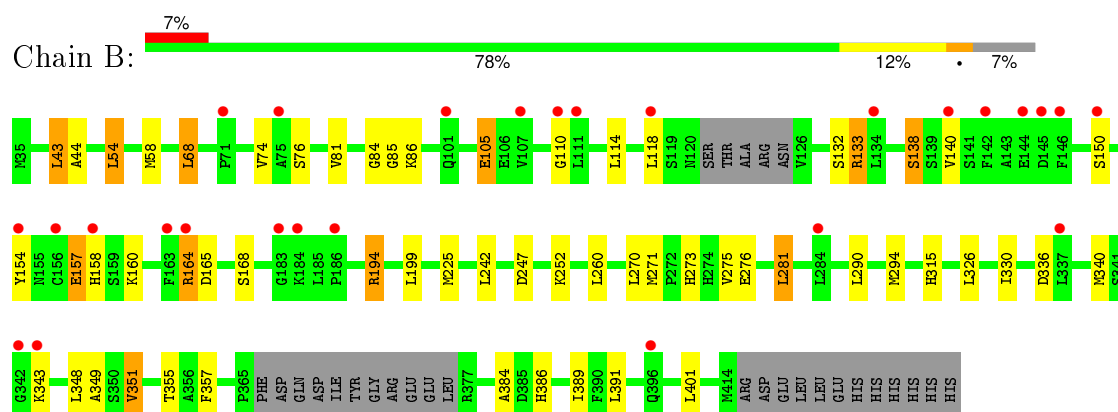


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

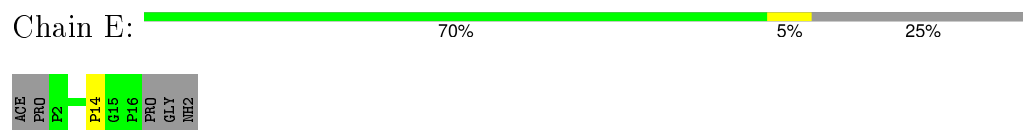




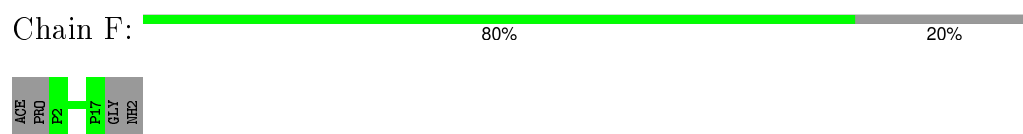
- Molecule 2: SERPYIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47 ), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)



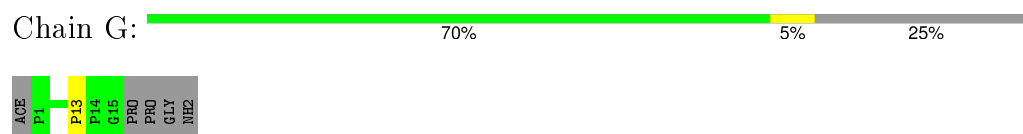
- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8



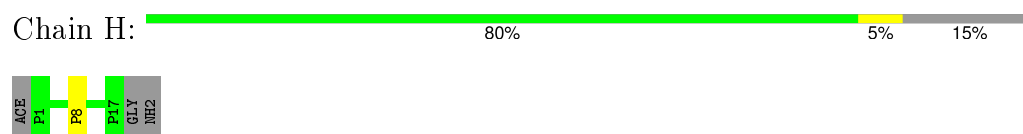
- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8



- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8



- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8



- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8



Chain I:  70% 10% 20%



- Molecule 3: 18ER COLLAGEN MODEL PEPTIDE 15-R8

Chain J:  65% 10% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.26 Å   101.26 Å   366.98 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	91.74 – 2.78 91.75 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.7 (91.74-2.78) 97.8 (91.75-2.68)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.69 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.203   ,   0.234 0.216   ,   0.215	Depositor DCC
$R_{free}$ test set	1332 reflections (2.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 53747 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.54	0/2932	0.73	0/3932
1	C	0.50	0/2957	0.72	0/3966
1	D	0.49	0/2973	0.73	1/3988 (0.0%)
2	B	0.49	0/2901	0.73	0/3889
3	E	0.44	0/102	0.43	0/143
3	F	0.45	0/110	0.48	0/155
3	G	0.52	0/102	0.44	0/143
3	H	0.55	0/118	0.44	0/167
3	I	0.44	0/110	0.48	0/155
3	J	0.54	0/102	0.46	0/143
All	All	0.51	0/12407	0.72	1/16681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	ARG	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2886	0	2919	15	0
1	C	2911	0	2942	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2926	0	2965	22	0
2	B	2856	0	2883	31	0
3	E	94	0	91	1	0
3	F	101	0	98	0	0
3	G	94	0	93	1	0
3	H	108	0	107	1	0
3	I	101	0	100	2	0
3	J	94	0	93	2	0
All	All	12171	0	12291	99	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 4.

All (99) 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:C:230:TYR:HE1	1:C:413:LYS:HB3	1.47	0.77
1:D:43:LEU:HD23	1:D:110:GLY:HA3	1.68	0.74
1:C:58:MSE:HE1	1:C:315:HIS:HB3	1.70	0.73
1:A:72:VAL:HG21	1:A:118:LEU:HD21	1.71	0.73
1:A:58:MSE:HE1	1:A:315:HIS:HB3	1.76	0.68
1:C:174:ASN:ND2	1:C:187:GLU:HG3	2.10	0.66
1:A:162:ASN:OD1	1:A:164:ARG:HB2	1.97	0.64
1:D:58:MSE:HE1	1:D:315:HIS:HB3	1.79	0.63
1:C:68:LEU:HD11	1:C:357:PHE:HB2	1.81	0.61
2:B:165:ASP:HB2	1:C:284:LEU:HD21	1.83	0.60
1:A:68:LEU:HD11	1:A:357:PHE:HB2	1.84	0.60
1:C:128:TRP:CH2	1:C:204:MSE:HG2	2.38	0.59
2:B:133:ARG:HD2	2:B:157:GLU:HB2	1.84	0.58
2:B:68:LEU:HD11	2:B:357:PHE:HB2	1.86	0.58
1:D:116:ARG:O	1:D:120:ASN:HB2	2.05	0.57
1:C:174:ASN:HD21	1:C:187:GLU:HG3	1.68	0.56
2:B:225:MSE:CE	2:B:275:VAL:HG21	2.35	0.56
1:D:115:LEU:O	1:D:119:SER:HB2	2.06	0.56
1:D:68:LEU:HD11	1:D:357:PHE:HB2	1.88	0.56
1:C:118:LEU:HB3	1:C:128:TRP:CD1	2.42	0.55
2:B:54:LEU:HD12	2:B:74:VAL:HG11	1.88	0.55
1:D:126:VAL:CG2	1:D:209:HIS:H	2.19	0.54
2:B:138:SER:HA	2:B:160:LYS:HB3	1.90	0.53
1:D:150:SER:HG	1:D:158:HIS:CE1	2.27	0.53
1:D:84:GLY:HA3	1:D:340:MSE:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:VAL:HG13	2:B:386:HIS:HB2	1.92	0.52
2:B:247:ASP:OD1	2:B:273:HIS:NE2	2.43	0.51
2:B:84:GLY:HA3	2:B:340:MSE:HG3	1.91	0.51
2:B:43:LEU:HD23	2:B:110:GLY:HA3	1.92	0.51
2:B:252:LYS:HA	2:B:273:HIS:CE1	2.46	0.51
1:D:128:TRP:HE1	1:D:204:MSE:HG2	1.74	0.51
1:C:46:ARG:HD3	1:C:98:SER:HB2	1.93	0.51
1:D:126:VAL:HG22	1:D:209:HIS:H	1.76	0.51
1:C:268:ILE:HG12	1:C:294:MSE:HE2	1.92	0.50
2:B:225:MSE:HE3	2:B:275:VAL:HG21	1.92	0.50
1:C:137:PRO:C	1:C:139:SER:H	2.15	0.50
2:B:194:ARG:HB2	2:B:349:ALA:HB1	1.93	0.50
1:A:134:LEU:HD13	1:A:340:MSE:HE3	1.94	0.50
1:C:150:SER:HB3	1:C:156:CYS:HB3	1.93	0.50
1:C:230:TYR:HE1	1:C:413:LYS:CB	2.22	0.49
1:D:194:ARG:H	1:D:194:ARG:HE	1.58	0.49
1:C:275:VAL:HG13	1:C:386:HIS:HB2	1.95	0.48
2:B:290:LEU:HG	2:B:294:MSE:HE2	1.94	0.48
1:C:350:SER:HB3	1:C:352:PHE:CE1	2.49	0.48
2:B:281:LEU:HD13	2:B:389:ILE:HD12	1.95	0.48
2:B:76:SER:HB2	2:B:154:TYR:CD1	2.48	0.47
1:D:271:MSE:SE	1:D:384:ALA:HA	2.65	0.47
1:C:118:LEU:HD22	1:C:128:TRP:HE1	1.80	0.47
1:C:271:MSE:SE	1:C:384:ALA:HA	2.65	0.46
1:D:337:LEU:O	1:D:340:MSE:HB2	2.16	0.46
1:C:177:ALA:HB2	1:C:188:VAL:HG23	1.98	0.46
1:A:46:ARG:HD3	1:A:98:SER:HB2	1.98	0.46
1:D:62:GLN:HE21	1:D:62:GLN:H	1.65	0.45
1:D:54:LEU:HD12	1:D:74:VAL:HG11	1.98	0.45
1:C:151:LYS:HA	1:C:155:ASN:HA	1.99	0.45
2:B:225:MSE:HE3	2:B:275:VAL:CG2	2.47	0.45
1:A:271:MSE:SE	1:A:384:ALA:HA	2.66	0.45
3:H:8:PRO:HA	3:I:7:PRO:O	2.17	0.45
2:B:76:SER:HB2	2:B:154:TYR:HD1	1.81	0.45
1:C:218:MSE:HG2	3:J:2:PRO:HG2	1.98	0.45
1:A:290:LEU:HG	1:A:294:MSE:HE2	1.97	0.45
2:B:58:MSE:HE1	2:B:315:HIS:HB3	2.00	0.44
1:A:211:ASP:HB2	1:A:260:LEU:O	2.17	0.44
1:A:303:ALA:HB3	1:A:381:LEU:HD23	1.99	0.44
1:A:134:LEU:HD22	1:A:340:MSE:HE1	1.99	0.43
1:C:127:THR:HG21	1:C:209:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HB3	1:A:218:MSE:CG	2.49	0.43
1:A:92:GLN:O	1:A:96:VAL:HG23	2.18	0.43
2:B:81:VAL:HG11	2:B:326:LEU:HD11	2.00	0.43
1:A:68:LEU:HD13	1:A:355:THR:HB	2.00	0.43
1:A:272:PRO:HD3	1:A:281:LEU:HD12	2.00	0.43
1:D:290:LEU:HG	1:D:294:MSE:HE2	2.00	0.43
2:B:164:ARG:HD2	1:C:283:LYS:O	2.19	0.43
2:B:105:GLU:OE1	2:B:105:GLU:HA	2.18	0.42
2:B:348:LEU:HD21	2:B:351:VAL:HG13	2.02	0.42
2:B:271:MSE:SE	2:B:384:ALA:HA	2.68	0.42
2:B:85:GLY:HA2	2:B:336:ASP:O	2.19	0.42
1:C:317:LEU:O	1:C:321:LEU:HG	2.19	0.42
1:D:92:GLN:O	1:D:96:VAL:HG23	2.20	0.42
2:B:225:MSE:CE	2:B:275:VAL:CG2	2.97	0.42
1:C:225:MSE:HE3	1:C:275:VAL:CG2	2.50	0.42
1:C:68:LEU:HD13	1:C:355:THR:HB	2.01	0.41
1:D:54:LEU:HA	1:D:54:LEU:HD23	1.88	0.41
3:E:14:PRO:HA	3:G:13:PRO:O	2.20	0.41
1:C:81:VAL:HG11	1:C:326:LEU:HD11	2.02	0.41
1:C:255:ILE:HA	1:C:269:ILE:O	2.21	0.41
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.90	0.41
1:C:44:ALA:HB2	1:C:114:LEU:HD21	2.03	0.41
1:C:54:LEU:HA	1:C:54:LEU:HD23	1.82	0.41
1:C:115:LEU:O	1:C:118:LEU:HD23	2.21	0.41
2:B:68:LEU:HD13	2:B:355:THR:HB	2.02	0.41
1:D:118:LEU:O	1:D:122:THR:HG23	2.20	0.41
2:B:150:SER:OG	2:B:158:HIS:NE2	2.54	0.41
1:D:281:LEU:HD13	1:D:389:ILE:HD12	2.03	0.41
1:D:138:SER:HA	1:D:160:LYS:HG2	2.02	0.41
1:D:122:THR:HG21	1:D:401:LEU:HD21	2.02	0.40
2:B:114:LEU:O	2:B:118:LEU:HG	2.21	0.40
3:I:16:PRO:O	3:J:15:GLY:HA3	2.21	0.40
2:B:44:ALA:HB2	2:B:114:LEU:HD21	2.04	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	361/392 (92%)	350 (97%)	10 (3%)	1 (0%)	46	78
1	C	364/392 (93%)	346 (95%)	16 (4%)	2 (0%)	34	68
1	D	368/392 (94%)	349 (95%)	17 (5%)	2 (0%)	34	68
2	B	358/392 (91%)	348 (97%)	10 (3%)	0	100	100
3	E	13/20 (65%)	13 (100%)	0	0	100	100
3	F	14/20 (70%)	14 (100%)	0	0	100	100
3	G	13/20 (65%)	13 (100%)	0	0	100	100
3	H	15/20 (75%)	15 (100%)	0	0	100	100
3	I	14/20 (70%)	14 (100%)	0	0	100	100
3	J	13/20 (65%)	13 (100%)	0	0	100	100
All	All	1533/1688 (91%)	1475 (96%)	53 (4%)	5 (0%)	46	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	165	ASP
1	A	366	PHE
1	C	138	SER
1	C	87	ALA
1	D	377	ARG

### 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	313/324 (97%)	298 (95%)	15 (5%)	31	64
1	C	316/324 (98%)	299 (95%)	17 (5%)	27	59
1	D	317/324 (98%)	292 (92%)	25 (8%)	15	38
2	B	309/325 (95%)	285 (92%)	24 (8%)	16	38
3	E	10/12 (83%)	10 (100%)	0	100	100
3	F	11/12 (92%)	11 (100%)	0	100	100
3	G	10/12 (83%)	10 (100%)	0	100	100
3	H	12/12 (100%)	12 (100%)	0	100	100
3	I	11/12 (92%)	11 (100%)	0	100	100
3	J	10/12 (83%)	10 (100%)	0	100	100
All	All	1319/1369 (96%)	1238 (94%)	81 (6%)	23	53

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	68	LEU
1	A	97	LEU
1	A	140	VAL
1	A	145	ASP
1	A	164	ARG
1	A	175	GLU
1	A	199	LEU
1	A	242	LEU
1	A	260	LEU
1	A	270	LEU
1	A	281	LEU
1	A	330	ILE
1	A	391	LEU
1	A	401	LEU
2	B	43	LEU
2	B	54	LEU
2	B	68	LEU
2	B	86	LYS
2	B	105	GLU
2	B	132	SER
2	B	133	ARG
2	B	138	SER
2	B	140	VAL

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Mol	Chain	Res	Type
2	B	157	GLU
2	B	164	ARG
2	B	168	SER
2	B	194	ARG
2	B	199	LEU
2	B	242	LEU
2	B	260	LEU
2	B	270	LEU
2	B	276	GLU
2	B	281	LEU
2	B	330	ILE
2	B	343	LYS
2	B	351	VAL
2	B	391	LEU
2	B	401	LEU
1	C	43	LEU
1	C	68	LEU
1	C	97	LEU
1	C	118	LEU
1	C	140	VAL
1	C	160	LYS
1	C	175	GLU
1	C	179	GLN
1	C	194	ARG
1	C	242	LEU
1	C	260	LEU
1	C	270	LEU
1	C	281	LEU
1	C	318	GLN
1	C	343	LYS
1	C	350	SER
1	C	391	LEU
1	D	43	LEU
1	D	54	LEU
1	D	62	GLN
1	D	68	LEU
1	D	97	LEU
1	D	120	ASN
1	D	122	THR
1	D	126	VAL
1	D	132	SER
1	D	134	LEU

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Mol	Chain	Res	Type
1	D	140	VAL
1	D	160	LYS
1	D	194	ARG
1	D	199	LEU
1	D	236	MSE
1	D	239	ARG
1	D	242	LEU
1	D	270	LEU
1	D	281	LEU
1	D	318	GLN
1	D	330	ILE
1	D	343	LYS
1	D	400	LEU
1	D	401	LEU
1	D	414	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	ASN
1	D	62	GLN
1	D	262	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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	354/392 (90%)	0.07	4 (1%) 82 77	35, 55, 89, 130	0
1	C	357/392 (91%)	0.70	55 (15%) 3 2	33, 82, 153, 179	0
1	D	359/392 (91%)	0.31	13 (3%) 46 39	41, 79, 139, 166	0
2	B	351/392 (89%)	0.52	27 (7%) 16 10	42, 82, 127, 178	0
3	E	15/20 (75%)	0.21	0 100 100	47, 60, 89, 98	0
3	F	16/20 (80%)	0.21	0 100 100	49, 60, 91, 95	0
3	G	15/20 (75%)	0.14	0 100 100	39, 51, 86, 97	0
3	H	17/20 (85%)	-0.05	0 100 100	37, 46, 75, 83	0
3	I	16/20 (80%)	0.00	0 100 100	41, 51, 86, 94	0
3	J	15/20 (75%)	0.03	0 100 100	33, 48, 78, 98	0
All	All	1515/1688 (89%)	0.38	99 (6%) 22 15	33, 70, 138, 179	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	LYS	8.9
2	B	342	GLY	8.1
1	A	366	PHE	7.6
2	B	343	LYS	6.7
1	C	348	LEU	6.1
1	C	134	LEU	5.7
1	C	198	ALA	5.4
2	B	158	HIS	5.3
1	C	321	LEU	5.2
1	C	83	LEU	5.0
1	D	412	ASP	4.9
1	C	97	LEU	4.9
1	D	163	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	366	PHE	4.3
1	C	200	LEU	4.2
1	C	325	GLY	4.2
1	C	99	ALA	3.9
1	C	78	LEU	3.8
1	C	326	LEU	3.8
1	D	342	GLY	3.7
1	C	327	THR	3.7
2	B	142	PHE	3.7
1	D	107	VAL	3.6
2	B	145	ASP	3.6
1	C	93	ALA	3.5
1	C	101	GLN	3.4
1	C	324	LEU	3.4
1	C	201	VAL	3.4
2	B	163	PHE	3.4
1	C	102	LEU	3.4
2	B	107	VAL	3.4
1	A	376	LEU	3.3
1	C	168	SER	3.2
1	C	137	PRO	3.1
1	C	199	LEU	3.1
1	C	107	VAL	3.1
1	C	342	GLY	3.1
1	C	194	ARG	3.1
2	B	146	PHE	3.1
2	B	134	LEU	3.1
1	C	344	LYS	3.0
1	C	142	PHE	2.9
1	C	317	LEU	2.9
2	B	111	LEU	2.9
2	B	118	LEU	2.9
1	C	135	TYR	2.9
2	B	140	VAL	2.9
1	C	346	LEU	2.8
2	B	337	LEU	2.8
1	D	186	PRO	2.8
1	C	126	VAL	2.7
2	B	150	SER	2.7
2	B	110	GLY	2.7
1	C	36	LEU	2.7
1	C	163	PHE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	184	LYS	2.6
1	C	133	ARG	2.6
1	C	79	GLY	2.5
1	C	351	VAL	2.5
1	C	166	LYS	2.5
1	C	125	ASN	2.5
1	C	196	ASP	2.5
2	B	154	TYR	2.5
1	C	90	ALA	2.4
1	C	95	ALA	2.4
1	C	334	LYS	2.4
1	C	80	LEU	2.4
2	B	396	GLN	2.4
1	C	345	ASP	2.4
2	B	186	PRO	2.3
1	C	411	GLY	2.3
1	D	190	LYS	2.3
1	C	75	ALA	2.3
1	D	183	GLY	2.3
2	B	144	GLU	2.3
1	C	173	ILE	2.3
1	D	411	GLY	2.3
1	C	136	GLY	2.2
1	C	158	HIS	2.2
1	C	191	ASP	2.2
2	B	156	CYS	2.2
2	B	284	LEU	2.2
1	C	161	ILE	2.1
1	C	197	GLY	2.1
1	C	413	LYS	2.1
2	B	101	GLN	2.1
2	B	71	PRO	2.1
1	C	170	LEU	2.1
1	D	119	SER	2.1
1	C	105	GLU	2.1
1	D	184	LYS	2.1
1	C	347	TYR	2.1
1	C	76	SER	2.1
1	A	126	VAL	2.1
2	B	164	ARG	2.1
2	B	75	ALA	2.0
2	B	183	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	348	LEU	2.0
1	A	367	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.