



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:59 PM UTC

PDB ID : 4AU2 / pdb_00004au2
Title : Crystal Structure of a Hsp47-collagen complex
Authors : Widmer, C.; Gebauer, J.M.; Brunstein, E.; Drogemuller, C.; Leeb, T.; Baumann, U.
Deposited on : 2012-05-13
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
Mogul : 2022.3.0, CSD as543be (2022)
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

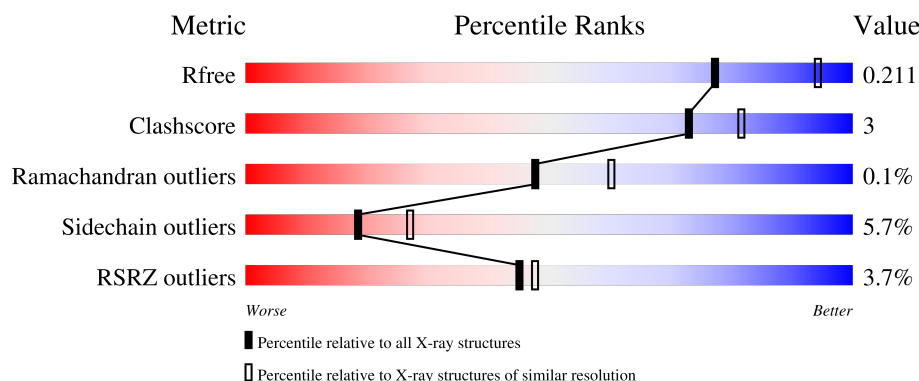
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	80% 12% 6%
1	B	392	80% 10% 10%
1	C	392	76% 10% 14%
1	D	392	79% 12% 8%
2	E	16	75% 12% 12%

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Mol	Chain	Length	Quality of chain
2	F	16	 75% 19% 6%
2	G	16	 6% 69% 19% 12%
2	H	16	 6% 75% 12% 12%
2	I	16	 6% 69% 25% 6%
2	J	16	 6% 56% 25% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11897 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	0	0	0
			2886	1839	501	532	14			
1	B	354	Total	C	N	O	S	0	0	0
			2778	1769	487	510	12			
1	C	338	Total	C	N	O	S	0	0	0
			2654	1692	461	488	13			
1	D	359	Total	C	N	O	S	0	0	0
			2814	1789	493	520	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP C7C419
A	419	LEU	-	expression tag	UNP C7C419
A	420	GLU	-	expression tag	UNP C7C419
A	421	HIS	-	expression tag	UNP C7C419
A	422	HIS	-	expression tag	UNP C7C419
A	423	HIS	-	expression tag	UNP C7C419
A	424	HIS	-	expression tag	UNP C7C419
A	425	HIS	-	expression tag	UNP C7C419
A	426	HIS	-	expression tag	UNP C7C419
B	35	MET	-	expression tag	UNP C7C419
B	419	LEU	-	expression tag	UNP C7C419
B	420	GLU	-	expression tag	UNP C7C419
B	421	HIS	-	expression tag	UNP C7C419
B	422	HIS	-	expression tag	UNP C7C419
B	423	HIS	-	expression tag	UNP C7C419
B	424	HIS	-	expression tag	UNP C7C419
B	425	HIS	-	expression tag	UNP C7C419
B	426	HIS	-	expression tag	UNP C7C419
C	35	MET	-	expression tag	UNP C7C419
C	419	LEU	-	expression tag	UNP C7C419

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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	GLU	-	expression tag	UNP C7C419
C	421	HIS	-	expression tag	UNP C7C419
C	422	HIS	-	expression tag	UNP C7C419
C	423	HIS	-	expression tag	UNP C7C419
C	424	HIS	-	expression tag	UNP C7C419
C	425	HIS	-	expression tag	UNP C7C419
C	426	HIS	-	expression tag	UNP C7C419
D	35	MET	-	expression tag	UNP C7C419
D	419	LEU	-	expression tag	UNP C7C419
D	420	GLU	-	expression tag	UNP C7C419
D	421	HIS	-	expression tag	UNP C7C419
D	422	HIS	-	expression tag	UNP C7C419
D	423	HIS	-	expression tag	UNP C7C419
D	424	HIS	-	expression tag	UNP C7C419
D	425	HIS	-	expression tag	UNP C7C419
D	426	HIS	-	expression tag	UNP C7C419

- Molecule 2 is a protein called 15ER COLLAGEN MODEL PEPTIDE 15-R8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	0	0	0
			90	59	17	14			
2	F	15	Total	C	N	O	0	0	0
			93	61	17	15			
2	G	14	Total	C	N	O	0	0	0
			86	56	16	14			
2	H	14	Total	C	N	O	0	0	0
			90	59	17	14			
2	I	15	Total	C	N	O	0	0	0
			93	61	17	15			
2	J	13	Total	C	N	O	0	0	0
			79	51	15	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	28	Total	O	0	0
			28	28		
3	C	43	Total	O	0	0
			43	43		

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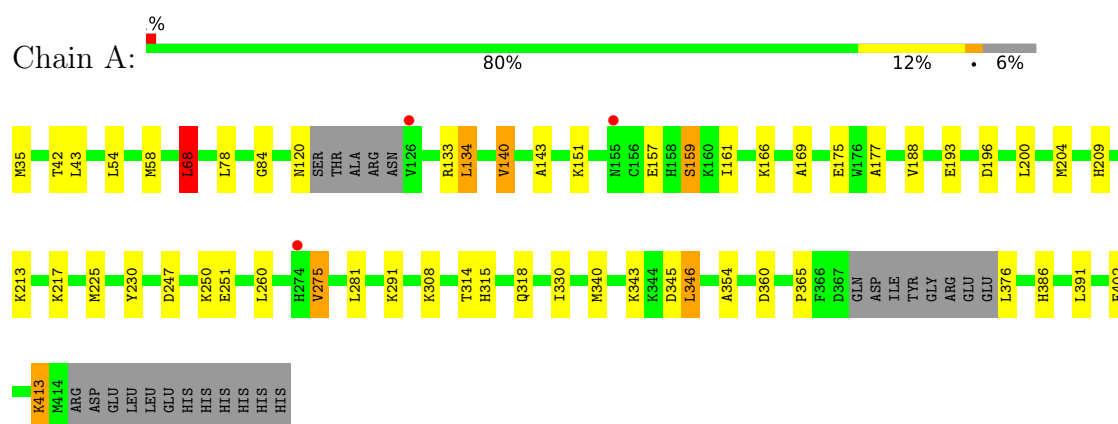
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	62	Total 62	O 62	0	0
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	20	Total 20	O 20	0	0

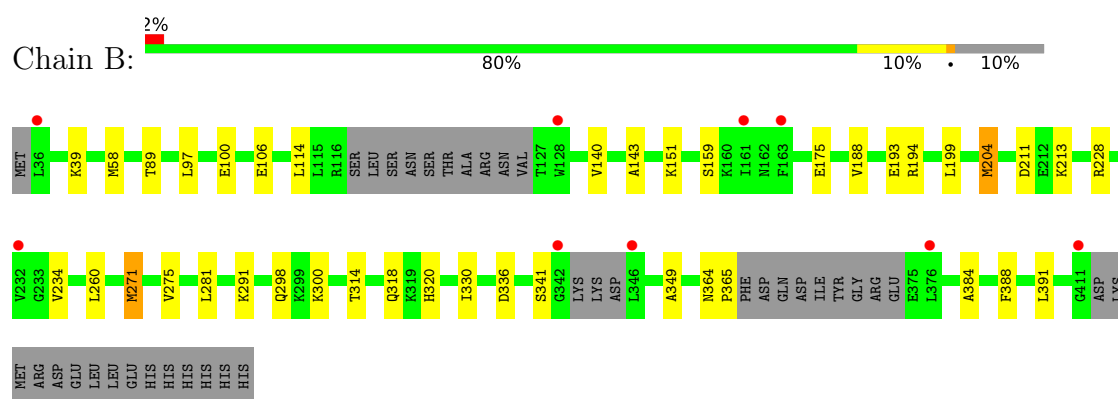
3 Residue-property plots [\(i\)](#)

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 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.

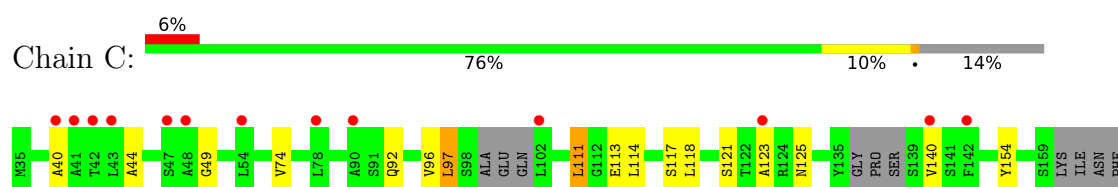
- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

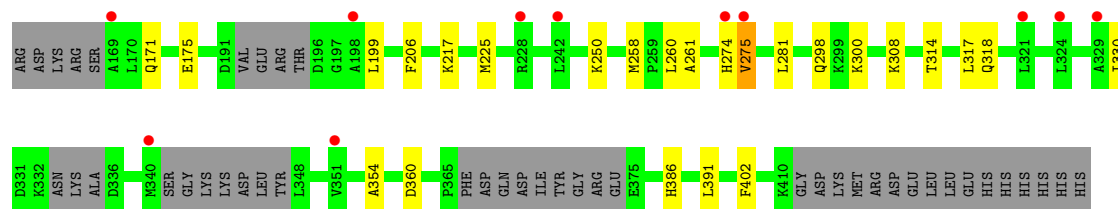


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)

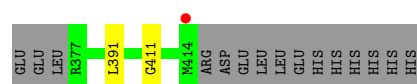
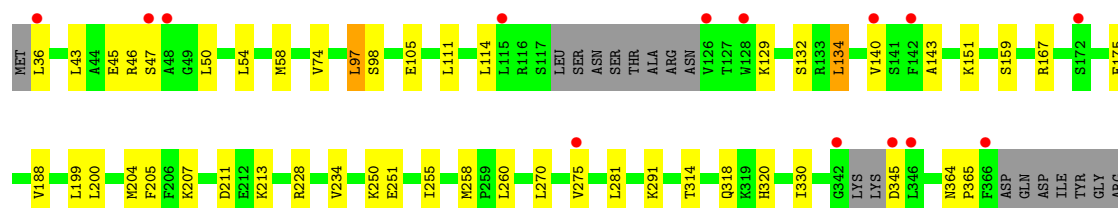
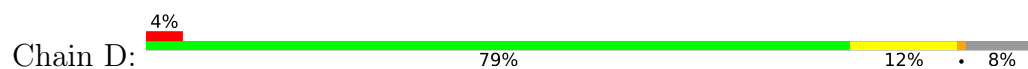


- Molecule 1: SERPIN PEPTIDASE INHIBITOR, CLADE H (HEAT SHOCK PROTEIN 47), MEMBER 1, (COLLAGEN BINDING PROTEIN 1)





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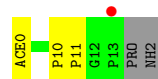
- Molecule 2: 15ER COLLAGEN MODEL PEPTIDE 15-R8



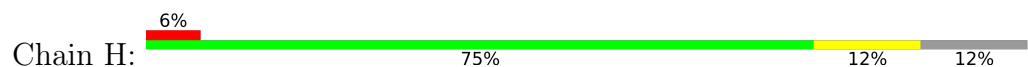
- Molecule 2: 15ER COLLAGEN MODEL PEPTIDE 15-R8



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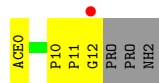
- Molecule 2: 15ER COLLAGEN MODEL PEPTIDE 15-R8

Chain I: 



- Molecule 2: 15ER COLLAGEN MODEL PEPTIDE 15-R8

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.50Å 92.78Å 100.46Å 95.24° 98.95° 96.73°	Depositor
Resolution (Å)	98.62 – 2.30 98.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (98.62-2.30) 96.4 (98.61-2.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.240 0.213 , 0.211	Depositor DCC
R_{free} test set	2802 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11897	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.84	0/2944	1.27	12/3968 (0.3%)
1	B	0.73	1/2834 (0.0%)	1.30	3/3821 (0.1%)
1	C	0.74	1/2703 (0.0%)	1.33	7/3641 (0.2%)
1	D	0.76	1/2870 (0.0%)	1.32	9/3869 (0.2%)
2	E	0.95	0/98	0.80	0/138
2	F	1.28	1/99 (1.0%)	0.85	0/141
2	G	1.29	1/91 (1.1%)	0.82	0/129
2	H	0.86	0/98	0.86	0/138
2	I	1.31	1/99 (1.0%)	0.82	0/141
2	J	1.28	1/83 (1.2%)	0.79	0/117
All	All	0.79	7/11919 (0.1%)	1.28	31/16103 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	0	ACE	C-N	-9.38	1.34	1.43
2	J	0	ACE	C-N	-8.94	1.34	1.43
1	B	271	MET	SD-CE	-8.87	1.57	1.79
2	F	0	ACE	C-N	-8.76	1.34	1.43
2	I	0	ACE	C-N	-8.42	1.35	1.43
1	D	258	MET	SD-CE	-7.42	1.61	1.79
1	C	258	MET	SD-CE	-6.69	1.62	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ALA	N-CA-C	-7.34	99.42	110.28
1	B	204	MET	N-CA-C	7.09	120.23	109.23
1	A	196	ASP	N-CA-C	6.95	121.93	113.17
1	C	250	LYS	N-CA-C	-6.44	98.77	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ALA	CA-C-N	-6.09	112.95	122.08
1	C	123	ALA	C-N-CA	-6.09	112.95	122.08
1	D	47	SER	CA-C-N	5.90	128.47	120.44
1	D	47	SER	C-N-CA	5.90	128.47	120.44
1	C	44	ALA	N-CA-C	5.79	118.34	111.33
1	A	120	ASN	CA-CB-CG	5.78	118.38	112.60
1	D	50	LEU	CA-C-N	5.57	128.06	120.54
1	D	50	LEU	C-N-CA	5.57	128.06	120.54
1	D	143	ALA	CA-C-N	5.48	127.94	120.54
1	D	143	ALA	C-N-CA	5.48	127.94	120.54
1	C	49	GLY	CA-C-N	5.46	128.61	120.31
1	C	49	GLY	C-N-CA	5.46	128.61	120.31
1	A	143	ALA	CA-C-N	5.45	127.89	120.54
1	A	143	ALA	C-N-CA	5.45	127.89	120.54
1	A	68	LEU	CD1-CG-CD2	-5.41	98.91	110.80
1	A	204	MET	N-CA-C	5.34	117.51	109.23
1	D	204	MET	N-CA-C	5.33	117.30	109.24
1	B	143	ALA	CA-C-N	5.31	127.71	120.54
1	B	143	ALA	C-N-CA	5.31	127.71	120.54
1	A	78	LEU	CA-C-N	5.27	125.83	119.98
1	A	78	LEU	C-N-CA	5.27	125.83	119.98
1	A	247	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	177	ALA	CA-C-N	5.14	127.12	120.44
1	A	177	ALA	C-N-CA	5.14	127.12	120.44
1	D	114	LEU	CA-C-N	5.06	127.33	120.44
1	D	114	LEU	C-N-CA	5.06	127.33	120.44
1	A	166	LYS	N-CA-C	5.03	116.76	111.28

There are no chirality outliers.

There are no planarity outliers.

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	2886	0	2919	23	0
1	B	2778	0	2799	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2654	0	2678	15	0
1	D	2814	0	2827	15	0
2	E	90	0	90	2	0
2	F	93	0	91	2	0
2	G	86	0	84	2	0
2	H	90	0	90	2	0
2	I	93	0	91	3	0
2	J	79	0	77	3	0
3	A	77	0	0	2	0
3	B	28	0	0	0	0
3	C	43	0	0	0	0
3	D	62	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	20	0	0	0	0
All	All	11897	0	11746	75	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 3.

All (75) 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:B:89:THR:HG21	1:B:336:ASP:H	1.37	0.88
1:B:271:MET:HE1	1:B:384:ALA:HA	1.58	0.85
1:B:89:THR:HG21	1:B:336:ASP:N	2.07	0.69
1:D:54:LEU:HD22	1:D:74:VAL:HG11	1.75	0.68
1:D:188:VAL:O	1:D:314:THR:HG21	1.95	0.67
1:A:42:THR:HG22	3:A:2003:HOH:O	1.97	0.64
1:D:134:LEU:HD12	1:D:200:LEU:HD13	1.80	0.63
1:B:188:VAL:O	1:B:314:THR:HG21	2.00	0.62
1:A:225:MET:HE3	1:A:275:VAL:HG22	1.81	0.61
1:A:275:VAL:HG13	1:A:386:HIS:HB2	1.83	0.60
1:B:271:MET:HE3	1:B:388:PHE:HB3	1.84	0.59
1:C:225:MET:HE3	1:C:275:VAL:HG22	1.84	0.59
1:C:275:VAL:HG13	1:C:386:HIS:HB2	1.84	0.59
1:B:271:MET:HE1	1:B:384:ALA:CA	2.32	0.57
1:C:298:GLN:HG3	1:C:300:LYS:HE2	1.88	0.56
1:A:209:HIS:HD2	3:A:2030:HOH:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:CE1	1:A:413:LYS:HB3	2.42	0.55
2:H:13:PRO:HG2	2:J:11:PRO:HB3	1.89	0.55
1:D:228:ARG:HG2	1:D:275:VAL:HG13	1.90	0.54
1:C:125:ASN:HA	1:C:261:ALA:HB3	1.90	0.53
1:B:213:LYS:HD3	1:B:365:PRO:HA	1.91	0.53
1:D:97:LEU:HD11	1:D:111:LEU:HD11	1.90	0.52
2:F:8:ARG:HE	2:G:10:PRO:HD3	1.74	0.52
1:B:298:GLN:HG3	1:B:300:LYS:HE2	1.92	0.52
1:A:84:GLY:HA3	1:A:340:MET:HG3	1.92	0.51
1:D:318:GLN:HG2	1:D:330:ILE:HD12	1.90	0.51
1:D:255:ILE:HD12	1:D:270:LEU:HD11	1.91	0.51
1:B:318:GLN:HG2	1:B:330:ILE:HD12	1.92	0.51
1:B:228:ARG:HG2	1:B:275:VAL:HG13	1.92	0.51
1:D:255:ILE:HB	1:D:270:LEU:HD13	1.93	0.51
1:D:213:LYS:HD3	1:D:365:PRO:HA	1.93	0.50
1:A:213:LYS:HD3	1:A:365:PRO:HA	1.92	0.50
1:A:54:LEU:O	1:A:58:MET:HG3	2.10	0.50
1:A:134:LEU:HG	1:A:200:LEU:HD13	1.94	0.50
1:D:250:LYS:HD3	1:D:251:GLU:HG2	1.94	0.50
2:E:11:PRO:HB3	2:F:10:PRO:HG2	1.95	0.49
1:C:97:LEU:HD21	1:C:111:LEU:HD11	1.94	0.48
1:A:225:MET:HE3	1:A:275:VAL:CG2	2.44	0.48
1:B:58:MET:HE3	1:B:320:HIS:CE1	2.48	0.48
1:A:58:MET:HE1	1:A:315:HIS:CG	2.49	0.47
1:C:318:GLN:HG2	1:C:330:ILE:HD12	1.95	0.47
1:C:111:LEU:HB3	1:C:154:TYR:HE1	1.78	0.47
1:A:133:ARG:HE	1:A:159:SER:HB2	1.79	0.47
1:A:340:MET:HE2	1:A:346:LEU:HD23	1.97	0.47
1:B:271:MET:CE	1:B:384:ALA:HA	2.38	0.46
1:A:250:LYS:HD3	1:A:251:GLU:HG2	1.97	0.46
1:C:308:LYS:NZ	1:C:360:ASP:OD1	2.47	0.46
1:A:308:LYS:NZ	1:A:360:ASP:OD1	2.49	0.45
1:C:74:VAL:HG22	1:C:317:LEU:HD21	1.98	0.45
1:A:314:THR:HG23	1:A:354:ALA:HB2	1.99	0.45
1:B:194:ARG:HB2	1:B:349:ALA:HB1	1.98	0.44
1:D:207:LYS:HE2	3:D:2031:HOH:O	2.16	0.44
1:C:206:PHE:CD1	1:C:402:PHE:CE2	3.06	0.44
1:C:206:PHE:CD1	1:C:402:PHE:HE2	2.36	0.44
1:A:188:VAL:O	1:A:314:THR:HG21	2.17	0.44
1:C:40:ALA:HB2	1:C:113:GLU:HB3	1.99	0.44
1:A:133:ARG:NH1	1:A:157:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:PRO:HB3	2:I:10:PRO:HG2	2.00	0.44
1:D:58:MET:HE3	1:D:320:HIS:CE1	2.52	0.43
1:A:68:LEU:HD12	1:A:402:PHE:HD1	1.83	0.43
1:A:140:VAL:HG23	1:A:345:ASP:OD2	2.19	0.43
1:A:68:LEU:HD13	1:A:68:LEU:HA	1.68	0.42
2:I:12:GLY:O	2:J:12:GLY:HA3	2.19	0.42
2:E:13:PRO:HG2	2:G:11:PRO:HB3	2.01	0.42
1:B:211:ASP:O	1:B:364:ASN:HB2	2.19	0.42
2:I:11:PRO:HA	2:J:10:PRO:O	2.20	0.42
1:D:46:ARG:HG3	1:D:98:SER:HB2	2.02	0.42
1:A:161:ILE:HD11	1:A:169:ALA:HA	2.03	0.41
1:C:314:THR:HG23	1:C:354:ALA:HB2	2.01	0.41
1:C:225:MET:HE3	1:C:275:VAL:CG2	2.48	0.41
1:A:68:LEU:HD12	1:A:402:PHE:CD1	2.55	0.41
1:D:211:ASP:O	1:D:364:ASN:HB2	2.21	0.40
1:C:92:GLN:O	1:C:96:VAL:HG23	2.22	0.40
1:D:129:LYS:HB2	1:D:205:PHE:HB3	2.04	0.40
1:B:39:LYS:HE2	1:B:106:GLU:HG2	2.02	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	361/392 (92%)	351 (97%)	10 (3%)	0	100	100
1	B	346/392 (88%)	336 (97%)	10 (3%)	0	100	100
1	C	322/392 (82%)	307 (95%)	15 (5%)	0	100	100
1	D	351/392 (90%)	340 (97%)	10 (3%)	1 (0%)	36	46
2	E	12/16 (75%)	12 (100%)	0	0	100	100
2	F	13/16 (81%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	12/16 (75%)	12 (100%)	0	0	100	100
2	H	12/16 (75%)	12 (100%)	0	0	100	100
2	I	13/16 (81%)	13 (100%)	0	0	100	100
2	J	11/16 (69%)	11 (100%)	0	0	100	100
All	All	1453/1664 (87%)	1407 (97%)	45 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	411	GLY

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	313/337 (93%)	292 (93%)	21 (7%)	15	21
1	B	298/337 (88%)	282 (95%)	16 (5%)	20	29
1	C	288/337 (86%)	272 (94%)	16 (6%)	19	28
1	D	302/337 (90%)	283 (94%)	19 (6%)	16	23
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
2	G	9/10 (90%)	9 (100%)	0	100	100
2	H	10/10 (100%)	10 (100%)	0	100	100
2	I	10/10 (100%)	10 (100%)	0	100	100
2	J	8/10 (80%)	8 (100%)	0	100	100
All	All	1258/1408 (89%)	1186 (94%)	72 (6%)	18	27

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET

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Mol	Chain	Res	Type
1	A	43	LEU
1	A	68	LEU
1	A	134	LEU
1	A	140	VAL
1	A	151	LYS
1	A	159	SER
1	A	175	GLU
1	A	193	GLU
1	A	217	LYS
1	A	260	LEU
1	A	275	VAL
1	A	281	LEU
1	A	291	LYS
1	A	318	GLN
1	A	330	ILE
1	A	343	LYS
1	A	346	LEU
1	A	376	LEU
1	A	391	LEU
1	A	413	LYS
1	B	97	LEU
1	B	100	GLU
1	B	114	LEU
1	B	140	VAL
1	B	151	LYS
1	B	159	SER
1	B	175	GLU
1	B	193	GLU
1	B	199	LEU
1	B	204	MET
1	B	234	VAL
1	B	260	LEU
1	B	281	LEU
1	B	291	LYS
1	B	341	SER
1	B	391	LEU
1	C	97	LEU
1	C	111	LEU
1	C	114	LEU
1	C	117	SER
1	C	118	LEU
1	C	121	SER

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Mol	Chain	Res	Type
1	C	140	VAL
1	C	171	GLN
1	C	175	GLU
1	C	199	LEU
1	C	217	LYS
1	C	260	LEU
1	C	274	HIS
1	C	275	VAL
1	C	281	LEU
1	C	391	LEU
1	D	36	LEU
1	D	43	LEU
1	D	45	GLU
1	D	97	LEU
1	D	105	GLU
1	D	132	SER
1	D	134	LEU
1	D	140	VAL
1	D	151	LYS
1	D	159	SER
1	D	167	ARG
1	D	175	GLU
1	D	199	LEU
1	D	234	VAL
1	D	260	LEU
1	D	281	LEU
1	D	291	LYS
1	D	345	ASP
1	D	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	162	ASN
1	A	179	GLN
1	A	216	HIS
1	A	254	GLN
1	A	396	GLN
1	B	56	GLN
1	B	162	ASN
1	B	209	HIS

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Mol	Chain	Res	Type
1	B	254	GLN
1	B	262	HIS
1	B	274	HIS
1	B	289	GLN
1	B	320	HIS
1	C	56	GLN
1	C	108	HIS
1	C	171	GLN
1	C	320	HIS
1	C	396	GLN
1	D	158	HIS
1	D	162	ASN
1	D	254	GLN
1	D	262	HIS
1	D	289	GLN
1	D	320	HIS

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](#)

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 ⓘ

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	367/392 (93%)	0.08	3 (0%) 82 83	30, 53, 89, 111	0
1	B	354/392 (90%)	0.54	9 (2%) 58 60	42, 84, 135, 168	0
1	C	338/392 (86%)	0.69	24 (7%) 22 24	45, 82, 131, 179	0
1	D	359/392 (91%)	0.41	15 (4%) 40 42	45, 66, 102, 134	0
2	E	14/16 (87%)	0.33	0 100 100	47, 56, 82, 89	0
2	F	14/16 (87%)	0.37	0 100 100	48, 56, 84, 89	0
2	G	13/16 (81%)	0.19	1 (7%) 19 21	47, 52, 85, 95	0
2	H	14/16 (87%)	0.38	1 (7%) 22 24	49, 57, 76, 85	0
2	I	14/16 (87%)	0.57	1 (7%) 22 24	49, 55, 92, 105	0
2	J	12/16 (75%)	0.52	1 (8%) 17 19	47, 54, 81, 101	0
All	All	1499/1664 (90%)	0.42	55 (3%) 45 48	30, 68, 123, 179	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	6.1
1	B	346	LEU	5.2
1	C	198	ALA	5.0
1	D	366	PHE	4.5
1	B	36	LEU	4.4
1	C	169	ALA	4.4
1	C	275	VAL	4.3
2	J	12	GLY	4.3
1	D	128	TRP	4.0
1	B	128	TRP	3.6
1	D	142	PHE	3.6
2	G	13	PRO	3.4
1	D	126	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	48	ALA	3.3
1	D	47	SER	3.3
1	D	414	MET	3.2
1	D	36	LEU	3.1
1	C	140	VAL	3.0
1	C	321	LEU	2.9
1	C	274	HIS	2.7
1	D	346	LEU	2.7
1	A	274	HIS	2.7
1	A	126	VAL	2.7
1	D	345	ASP	2.6
1	C	48	ALA	2.6
1	C	47	SER	2.6
1	D	172	SER	2.6
1	B	161	ILE	2.5
1	D	275	VAL	2.5
1	B	376	LEU	2.5
1	C	43	LEU	2.4
1	C	90	ALA	2.4
1	C	351	VAL	2.4
1	B	411	GLY	2.4
1	C	78	LEU	2.4
1	D	342	GLY	2.3
1	C	228	ARG	2.3
1	A	155	ASN	2.3
1	C	329	ALA	2.3
1	C	340	MET	2.3
1	D	140	VAL	2.2
1	C	142	PHE	2.2
1	C	54	LEU	2.2
1	C	242	LEU	2.2
1	B	163	PHE	2.2
1	B	232	VAL	2.1
1	C	41	ALA	2.1
1	C	102	LEU	2.1
1	C	324	LEU	2.1
1	C	42	THR	2.1
2	H	1	PRO	2.1
1	C	40	ALA	2.0
1	C	123	ALA	2.0
1	D	115	LEU	2.0
2	I	14	PRO	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 oligosaccharides 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.