Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 12:47 pm GMT

PDB ID	:	7BEE
Title	:	Crystal structure of a Hsp47-collagen peptide complex
Authors	:	Abraham, E.T.; Gebauer, J.M.; Baumann, U.
Deposited on	:	2020-12-23
Resolution	:	1.94 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

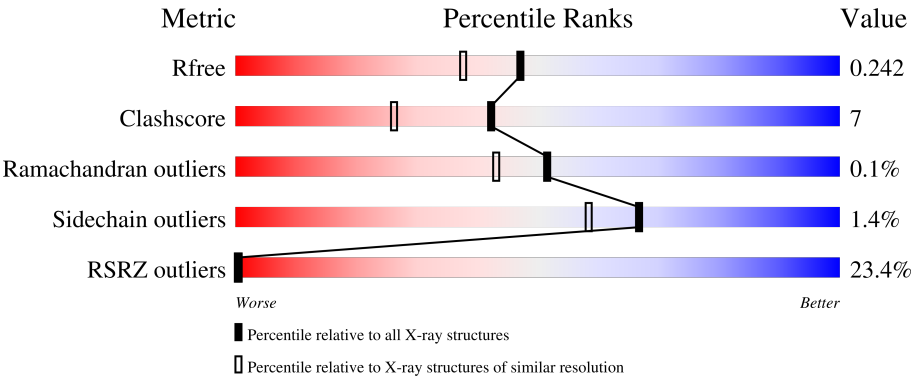
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.94 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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	21% 84% 12% ·
1	B	392	23% 84% 9% · 5%
2	C	22	23% 86% 9% 5%
2	D	22	23% 82% 9% 9%
2	E	22	14% 73% 14% 5% 9%

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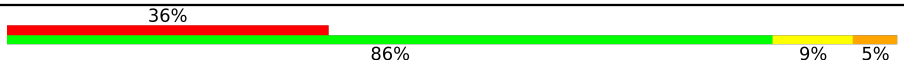
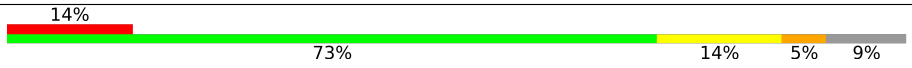
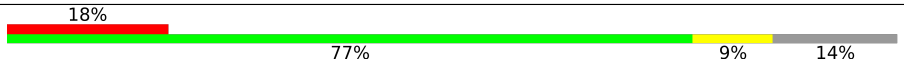
Mol	Chain	Length	Quality of chain
2	F	22	
2	G	22	
2	H	22	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7032 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 Collagen-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2982	1893	522	554	13			
1	B	373	Total	C	N	O	S	0	0	0
			2938	1867	514	543	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	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
B	35	MET	-	initiating methionine	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 2 is a protein called 21er collagen model peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	0	0	0
			133	89	23	21			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	0	0	0
			126	84	22	20			
2	E	20	Total	C	N	O	0	0	0
			126	84	22	20			
2	F	22	Total	C	N	O	0	0	0
			137	91	24	22			
2	G	20	Total	C	N	O	0	0	0
			126	84	22	20			
2	H	19	Total	C	N	O	0	0	0
			119	79	21	19			

- Molecule 3 is water.

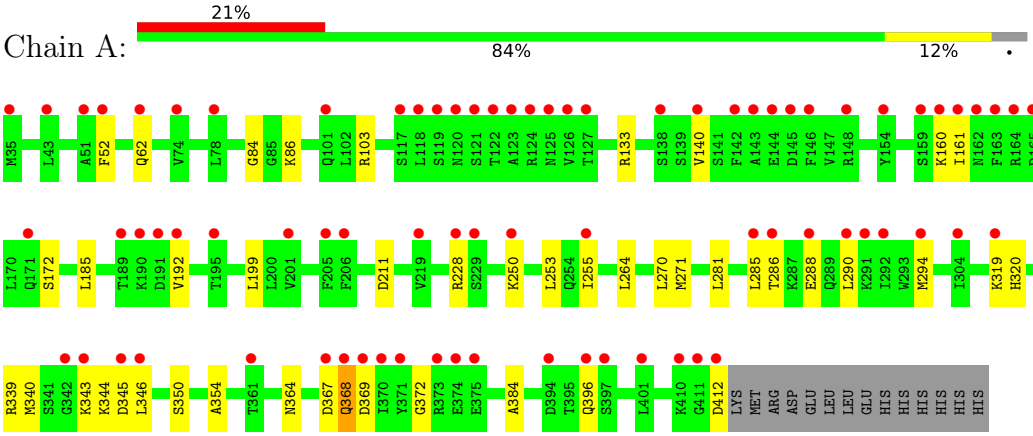
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	143	Total	O	0	0
			143	143		
3	C	6	Total	O	0	0
			6	6		
3	D	17	Total	O	0	0
			17	17		
3	E	7	Total	O	0	0
			7	7		
3	F	9	Total	O	0	0
			9	9		
3	G	7	Total	O	0	0
			7	7		
3	H	11	Total	O	0	0
			11	11		

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.

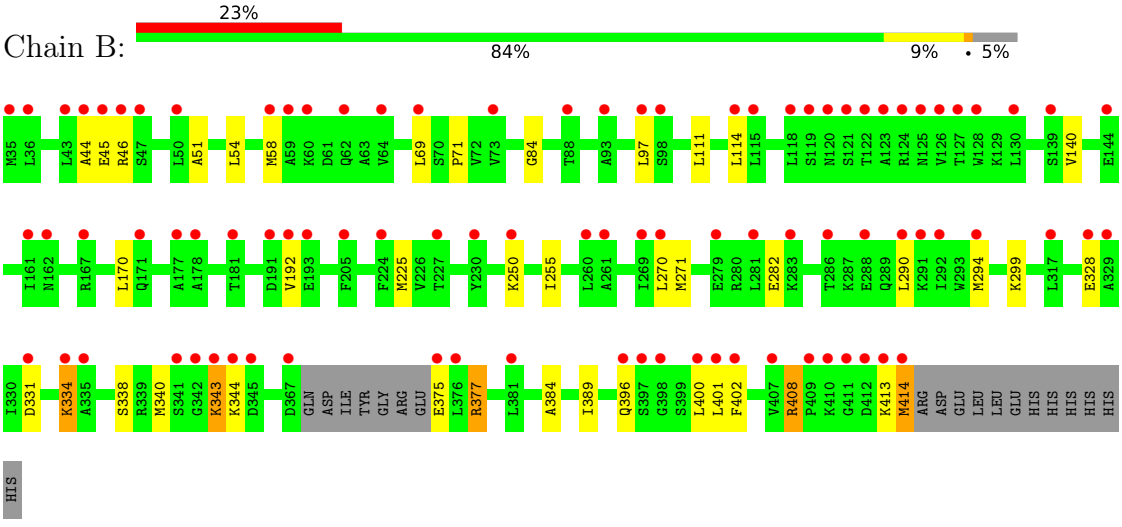
• Molecule 1: Collagen-binding protein

Chain A:



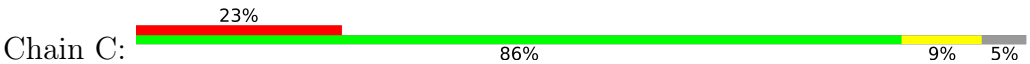
• Molecule 1: Collagen-binding protein

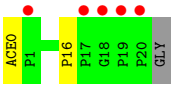
Chain B:



• Molecule 2: 21er collagen model peptide

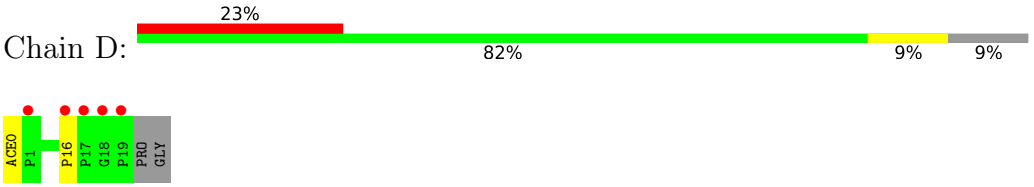
Chain C:





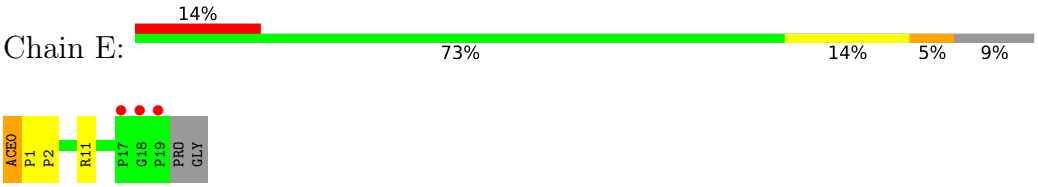
• Molecule 2: 21er collagen model peptide

Chain D:



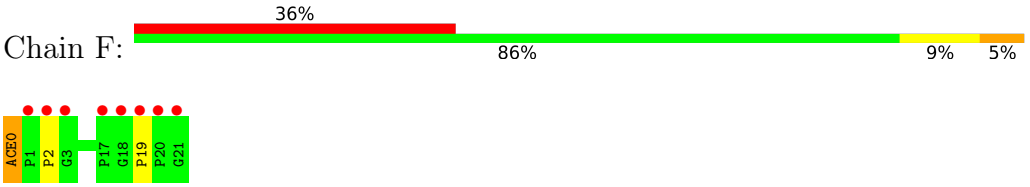
• Molecule 2: 21er collagen model peptide

Chain E:



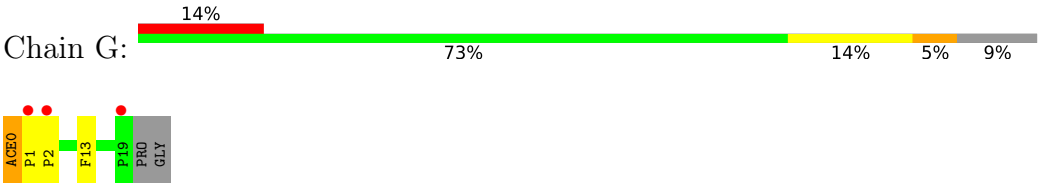
• Molecule 2: 21er collagen model peptide

Chain F:



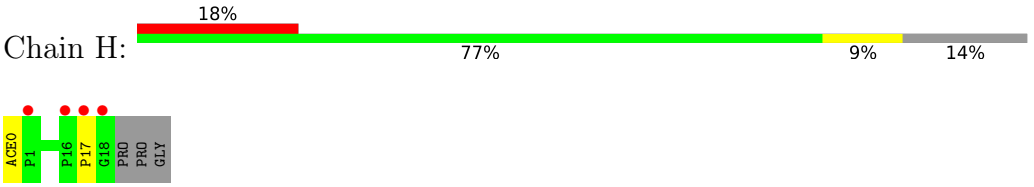
• Molecule 2: 21er collagen model peptide

Chain G:



• Molecule 2: 21er collagen model peptide

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.68Å 96.68Å 187.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.81 – 1.94 46.81 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.81-1.94) 99.8 (46.81-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, R_{free}	0.207 , 0.242 0.207 , 0.242	Depositor DCC
R_{free} test set	3838 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7032	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.42	0/3043	0.61	0/4105
1	B	0.43	0/2997	0.60	2/4040 (0.0%)
2	C	0.35	0/143	0.70	1/203 (0.5%)
2	D	0.35	0/135	0.85	1/191 (0.5%)
2	E	0.37	0/135	0.65	1/191 (0.5%)
2	F	0.38	0/147	1.12	3/208 (1.4%)
2	G	0.39	0/135	0.80	1/191 (0.5%)
2	H	0.40	0/127	1.13	2/179 (1.1%)
All	All	0.42	0/6862	0.65	11/9308 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	0	ACE	O-C-N	11.22	142.42	121.10
2	H	0	ACE	O-C-N	-10.82	100.54	121.10
2	D	0	ACE	O-C-N	-9.60	102.86	121.10
2	F	0	ACE	C-N-CD	8.48	146.21	128.40
2	H	0	ACE	C-N-CD	-8.01	102.98	120.60
2	G	0	ACE	C-N-CD	7.30	143.73	128.40
1	B	401	LEU	CA-CB-CG	6.22	129.60	115.30
2	C	0	ACE	O-C-N	5.97	132.45	121.10
2	E	0	ACE	O-C-N	-5.83	110.03	121.10
1	B	408	ARG	CG-CD-NE	-5.21	100.86	111.80
2	F	0	ACE	C-N-CA	-5.07	100.69	122.00

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	2982	0	3006	48	0
1	B	2938	0	2973	39	0
2	C	133	0	127	1	0
2	D	126	0	120	7	0
2	E	126	0	120	3	0
2	F	137	0	130	3	0
2	G	126	0	120	4	0
2	H	119	0	113	1	0
3	A	145	0	0	2	0
3	B	143	0	0	2	0
3	C	6	0	0	0	0
3	D	17	0	0	0	0
3	E	7	0	0	0	0
3	F	9	0	0	0	0
3	G	7	0	0	0	0
3	H	11	0	0	0	0
All	All	7032	0	6709	93	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 7.

All (93) 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:331:ASP:OD2	1:B:334:LYS:HE3	1.36	1.22
1:B:331:ASP:CG	1:B:334:LYS:HE3	1.69	1.09
1:B:54:LEU:HG	1:B:58:MET:HE1	1.37	1.01
1:A:343:LYS:HZ3	1:A:345:ASP:H	1.15	0.92
1:A:343:LYS:NZ	1:A:345:ASP:H	1.69	0.90
1:A:228:ARG:NH2	2:D:16:PRO:HB3	1.86	0.89
1:B:331:ASP:OD2	1:B:334:LYS:CE	2.20	0.88
1:A:255:ILE:CD1	1:A:270:LEU:HG	2.04	0.86
1:A:86:LYS:NZ	1:A:338:SER:OG	2.09	0.84
1:B:54:LEU:HG	1:B:58:MET:CE	2.08	0.83
1:A:343:LYS:HZ1	1:A:346:LEU:N	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:NH2	2:D:16:PRO:HG3	1.94	0.82
1:A:319:LYS:NZ	1:A:320:HIS:NE2	2.27	0.82
1:A:255:ILE:HD12	1:A:270:LEU:HG	1.63	0.79
1:A:228:ARG:NH2	2:D:16:PRO:CG	2.48	0.77
1:A:228:ARG:NH2	2:D:16:PRO:CB	2.49	0.75
1:B:44:ALA:HA	1:B:114:LEU:HD11	1.68	0.75
1:B:282:GLU:OE1	3:B:501:HOH:O	2.05	0.74
1:B:396:GLN:NE2	3:B:502:HOH:O	2.23	0.71
1:B:58:MET:CE	1:B:69:LEU:HD11	2.21	0.71
1:A:228:ARG:CZ	2:D:16:PRO:HB3	2.21	0.70
1:B:58:MET:HE3	1:B:69:LEU:HD11	1.74	0.68
1:B:44:ALA:HB2	1:B:114:LEU:HD21	1.77	0.66
1:B:331:ASP:CB	1:B:334:LYS:HE3	2.26	0.66
1:B:338:SER:HB3	1:B:344:LYS:HB2	1.76	0.66
1:B:375:GLU:N	1:B:377:ARG:HE	1.95	0.65
1:A:286:THR:OG1	1:A:288:GLU:HG2	1.96	0.65
3:A:580:HOH:O	2:E:0:ACE:H1	1.96	0.64
1:B:54:LEU:O	1:B:58:MET:HE2	1.98	0.63
1:A:343:LYS:NZ	1:A:345:ASP:N	2.46	0.62
1:A:161:ILE:HD11	2:F:0:ACE:H2	1.82	0.61
1:A:133:ARG:NH1	3:A:501:HOH:O	2.22	0.61
1:A:343:LYS:NZ	1:A:346:LEU:H	2.00	0.60
1:A:86:LYS:HG2	1:A:339:ARG:HE	1.66	0.60
1:A:228:ARG:HH22	2:D:16:PRO:HG3	1.67	0.60
1:A:369:ASP:CG	1:A:372:GLY:H	2.05	0.60
1:A:228:ARG:HH21	2:D:16:PRO:CG	2.16	0.58
1:A:343:LYS:NZ	1:A:346:LEU:N	2.51	0.58
1:A:319:LYS:HZ2	1:A:320:HIS:CD2	2.23	0.57
1:B:51:ALA:HB2	1:B:71:PRO:HB3	1.87	0.57
1:A:319:LYS:NZ	1:A:320:HIS:CD2	2.73	0.56
1:A:264:LEU:HD22	1:A:396:GLN:HE21	1.71	0.56
1:A:250:LYS:H	1:A:250:LYS:HE2	1.70	0.55
1:B:140:VAL:HG13	1:B:343:LYS:HE3	1.87	0.55
1:B:140:VAL:HG22	1:B:343:LYS:CE	2.38	0.54
1:A:199:LEU:HD22	1:A:350:SER:HB2	1.90	0.53
1:B:54:LEU:CG	1:B:58:MET:HE1	2.26	0.52
1:B:45:GLU:OE2	1:B:46:ARG:HD3	2.10	0.52
1:A:228:ARG:HG2	1:A:228:ARG:O	2.10	0.52
1:B:45:GLU:OE2	1:B:46:ARG:NH1	2.41	0.51
1:A:84:GLY:HA3	1:A:340:MET:HG3	1.92	0.51
1:A:52:PHE:CZ	1:A:286:THR:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:O	1:A:368:GLN:C	2.49	0.50
1:A:253:LEU:HD22	1:A:281:LEU:HD11	1.92	0.50
1:B:375:GLU:N	1:B:377:ARG:HH21	2.09	0.50
1:A:52:PHE:HZ	1:A:285:LEU:O	1.95	0.50
1:B:44:ALA:CA	1:B:114:LEU:HD11	2.41	0.48
1:A:338:SER:HB3	1:A:344:LYS:HG3	1.96	0.48
1:B:331:ASP:CG	1:B:334:LYS:CE	2.62	0.47
1:B:58:MET:HE1	1:B:69:LEU:HD11	1.96	0.46
1:B:282:GLU:HG3	1:B:389:ILE:HD11	1.98	0.46
1:B:271:MET:SD	1:B:384:ALA:HA	2.56	0.46
1:A:367:ASP:OD2	1:A:368:GLN:N	2.49	0.45
1:A:160:LYS:O	1:A:161:ILE:HD12	2.17	0.45
1:A:140:VAL:HG11	1:A:346:LEU:HD22	1.99	0.45
1:B:225:MET:CE	2:G:13:PHE:HE2	2.30	0.44
1:B:255:ILE:HD12	1:B:270:LEU:HG	2.00	0.44
2:F:2:PRO:HA	2:G:1:PRO:O	2.18	0.44
1:A:192:VAL:HG11	1:A:199:LEU:HD11	1.98	0.44
1:B:97:LEU:HD21	1:B:111:LEU:HD11	2.00	0.43
1:A:185:LEU:HD21	1:A:354:ALA:HB1	2.00	0.43
1:B:328:GLU:HG3	1:B:334:LYS:HG3	2.00	0.43
1:A:211:ASP:O	1:A:364:ASN:HB2	2.19	0.43
1:B:51:ALA:HB3	1:B:400:LEU:HD23	2.00	0.43
1:A:271:MET:SD	1:A:384:ALA:HA	2.59	0.42
1:A:290:LEU:O	1:A:294:MET:HG3	2.19	0.42
2:C:16:PRO:HD3	2:E:11:ARG:HD3	2.02	0.42
1:A:343:LYS:HZ1	1:A:345:ASP:C	2.22	0.42
1:B:331:ASP:HB3	1:B:334:LYS:CD	2.50	0.42
1:B:71:PRO:HD3	1:B:402:PHE:HA	2.02	0.42
1:A:319:LYS:HZ2	1:A:320:HIS:CE1	2.32	0.42
2:G:1:PRO:HA	2:G:2:PRO:HD3	1.96	0.41
1:B:413:LYS:HD2	1:B:414:MET:N	2.35	0.41
2:E:1:PRO:HA	2:E:2:PRO:HD3	1.95	0.41
1:B:290:LEU:HG	1:B:294:MET:SD	2.60	0.41
1:B:84:GLY:HA3	1:B:340:MET:HG3	2.02	0.41
1:B:170:LEU:HD21	1:B:192:VAL:HG23	2.03	0.41
1:A:172:SER:OG	2:G:0:ACE:H2	2.21	0.41
1:A:344:LYS:HE2	1:A:344:LYS:HB3	1.84	0.41
1:A:369:ASP:OD2	1:A:372:GLY:N	2.54	0.41
1:A:62:GLN:H	1:A:62:GLN:HG2	1.77	0.41
1:B:377:ARG:HD2	1:B:377:ARG:H	1.86	0.40
2:F:19:PRO:HG2	2:H:17:PRO:HB3	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	376/392 (96%)	364 (97%)	11 (3%)	1 (0%)	41 32
1	B	369/392 (94%)	363 (98%)	6 (2%)	0	100 100
2	C	19/22 (86%)	19 (100%)	0	0	100 100
2	D	18/22 (82%)	18 (100%)	0	0	100 100
2	E	18/22 (82%)	18 (100%)	0	0	100 100
2	F	20/22 (91%)	20 (100%)	0	0	100 100
2	G	18/22 (82%)	18 (100%)	0	0	100 100
2	H	17/22 (77%)	17 (100%)	0	0	100 100
All	All	855/916 (93%)	837 (98%)	17 (2%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN

5.3.2 Protein sidechains (i)

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	323/337 (96%)	320 (99%)	3 (1%)	78 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	319/337 (95%)	312 (98%)	7 (2%)	52 39
2	C	14/14 (100%)	14 (100%)	0	100 100
2	D	13/14 (93%)	13 (100%)	0	100 100
2	E	13/14 (93%)	13 (100%)	0	100 100
2	F	14/14 (100%)	14 (100%)	0	100 100
2	G	13/14 (93%)	13 (100%)	0	100 100
2	H	12/14 (86%)	12 (100%)	0	100 100
All	All	721/758 (95%)	711 (99%)	10 (1%)	67 58

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	166	LYS
1	A	412	ASP
1	B	250	LYS
1	B	299	LYS
1	B	334	LYS
1	B	343	LYS
1	B	377	ARG
1	B	408	ARG
1	B	414	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	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 monosaccharides 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 (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^{th} 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	378/392 (96%)	1.60	84 (22%)	0	0	27, 41, 92, 159	0
1	B	373/392 (95%)	1.48	91 (24%)	0	0	28, 43, 76, 113	0
2	C	20/22 (90%)	1.67	5 (25%)	0	0	29, 40, 100, 102	0
2	D	19/22 (86%)	1.53	5 (26%)	0	0	30, 38, 79, 101	0
2	E	19/22 (86%)	1.74	3 (15%)	2	2	32, 38, 79, 90	0
2	F	21/22 (95%)	1.92	8 (38%)	0	0	31, 48, 100, 114	0
2	G	19/22 (86%)	1.05	3 (15%)	2	2	32, 43, 83, 93	0
2	H	18/22 (81%)	1.43	4 (22%)	0	0	34, 41, 75, 99	0
All	All	867/916 (94%)	1.54	203 (23%)	0	0	27, 42, 85, 159	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	20.5
1	A	123	ALA	17.1
1	A	369	ASP	10.5
1	A	374	GLU	10.1
2	E	19	PRO	9.9
1	A	370	ILE	9.8
1	A	126	VAL	8.7
1	A	169	ALA	7.8
1	A	368	GLN	7.6
1	A	411	GLY	7.5
1	A	371	TYR	7.5
1	A	163	PHE	7.4
2	C	20	PRO	7.2
1	B	398	GLY	7.1
1	A	367	ASP	7.0
1	B	119	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	120	ASN	6.6
1	A	122	THR	6.4
2	F	19	PRO	6.2
1	B	118	LEU	6.1
1	A	124	ARG	5.8
1	B	342	GLY	5.7
1	B	334	LYS	5.6
1	A	167	ARG	5.6
2	C	19	PRO	5.6
2	F	1	PRO	5.6
1	A	396	GLN	5.6
2	H	18	GLY	5.4
2	E	17	PRO	5.4
2	H	17	PRO	5.3
1	B	193	GLU	5.3
1	B	412	ASP	5.2
1	B	414	MET	5.2
1	A	118	LEU	5.1
1	B	122	THR	5.1
1	A	145	ASP	4.9
1	B	115	LEU	4.9
2	D	19	PRO	4.9
1	B	413	LYS	4.8
1	A	191	ASP	4.8
1	A	228	ARG	4.7
1	B	396	GLN	4.7
1	B	367	ASP	4.7
1	B	345	ASP	4.6
2	D	1	PRO	4.6
1	A	292	ILE	4.6
2	F	2	PRO	4.5
2	F	20	PRO	4.5
1	A	52	PHE	4.5
1	B	401	LEU	4.4
1	A	168	SER	4.4
1	B	411	GLY	4.4
2	C	18	GLY	4.3
2	E	18	GLY	4.3
1	B	410	LYS	4.2
1	A	345	ASP	4.2
1	B	344	LYS	4.2
2	F	18	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	SER	4.2
1	B	341	SER	4.1
1	B	36	LEU	4.1
1	B	35	MET	4.1
1	B	288	GLU	4.1
1	B	343	LYS	4.1
1	B	121	SER	4.0
1	B	126	VAL	4.0
1	B	128	TRP	4.0
1	A	161	ILE	3.9
1	A	190	LYS	3.8
1	A	394	ASP	3.8
1	B	230	TYR	3.8
1	B	120	ASN	3.8
1	A	148	ARG	3.8
1	A	343	LYS	3.7
1	B	114	LEU	3.7
2	D	18	GLY	3.6
2	D	17	PRO	3.6
1	A	291	LYS	3.6
2	C	17	PRO	3.5
1	A	397	SER	3.5
1	B	123	ALA	3.5
2	D	16	PRO	3.4
1	B	124	ARG	3.4
1	A	62	GLN	3.4
1	A	164	ARG	3.3
2	C	1	PRO	3.3
1	B	44	ALA	3.3
1	A	117	SER	3.3
2	G	1	PRO	3.3
1	A	285	LEU	3.3
1	B	98	SER	3.2
1	A	255	ILE	3.2
1	B	130	LEU	3.2
1	B	192	VAL	3.2
1	B	50	LEU	3.2
1	A	286	THR	3.2
1	A	119	SER	3.2
1	B	73	VAL	3.2
1	B	260	LEU	3.1
1	B	409	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	292	ILE	3.1
1	A	319	LYS	3.1
1	B	181	THR	3.1
1	B	283	LYS	3.0
1	A	330	ILE	3.0
1	B	88	THR	3.0
1	A	159	SER	3.0
1	B	171	GLN	3.0
1	B	279	GLU	3.0
1	A	166	LYS	3.0
1	B	375	GLU	3.0
1	B	250	LYS	3.0
1	B	97	LEU	2.9
1	A	146	PHE	2.9
2	H	1	PRO	2.9
1	A	144	GLU	2.9
1	A	192	VAL	2.9
1	B	397	SER	2.9
2	G	19	PRO	2.9
1	B	402	PHE	2.8
1	A	43	LEU	2.8
2	H	16	PRO	2.8
1	B	291	LYS	2.8
1	B	58	MET	2.7
1	B	69	LEU	2.7
1	A	206	PHE	2.7
1	A	143	ALA	2.7
1	B	290	LEU	2.7
1	A	189	THR	2.7
1	A	74	VAL	2.7
1	A	288	GLU	2.7
1	A	410	LYS	2.7
1	A	127	THR	2.7
1	A	160	LYS	2.6
1	B	46	ARG	2.6
1	B	286	THR	2.6
1	A	346	LEU	2.6
1	A	250	LYS	2.6
1	A	138	SER	2.6
1	A	373	ARG	2.6
1	A	51	ALA	2.6
2	G	2	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	127	THR	2.6
1	B	59	ALA	2.5
1	A	162	ASN	2.5
1	B	162	ASN	2.5
1	B	317	LEU	2.5
1	A	205	PHE	2.4
1	B	400	LEU	2.4
1	B	45	GLU	2.4
1	B	161	ILE	2.4
1	B	294	MET	2.4
2	F	17	PRO	2.4
1	A	342	GLY	2.4
1	B	64	VAL	2.4
1	B	328	GLU	2.4
1	B	270	LEU	2.4
1	A	229	SER	2.4
1	A	412	ASP	2.4
1	B	177	ALA	2.4
1	B	125	ASN	2.4
1	B	331	ASP	2.3
1	A	125	ASN	2.3
1	A	375	GLU	2.3
1	A	361	THR	2.3
1	B	139	SER	2.3
1	A	35	MET	2.3
1	A	290	LEU	2.3
1	A	304	ILE	2.3
1	A	195	THR	2.3
1	A	337	LEU	2.3
1	B	144	GLU	2.3
2	F	3	GLY	2.3
1	A	219	VAL	2.3
1	B	93	ALA	2.3
1	A	171	GLN	2.3
1	A	78	LEU	2.3
1	B	62	GLN	2.2
1	B	261	ALA	2.2
1	A	101	GLN	2.2
1	B	191	ASP	2.2
1	B	407	VAL	2.2
1	B	43	LEU	2.2
2	F	21	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	60	LYS	2.2
1	B	227	THR	2.2
1	B	329	ALA	2.2
1	A	165	ASP	2.2
1	B	281	LEU	2.1
1	B	205	PHE	2.1
1	B	335	ALA	2.1
1	B	376	LEU	2.1
1	A	294	MET	2.1
1	B	269	ILE	2.1
1	A	401	LEU	2.1
1	A	154	TYR	2.1
1	B	381	LEU	2.1
1	A	140	VAL	2.0
1	A	142	PHE	2.0
1	B	178	ALA	2.0
1	A	201	VAL	2.0
1	B	167	ARG	2.0
1	B	224	PHE	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 monosaccharides 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.