

Full wwPDB X-ray Structure Validation Report (i)

Oct 20, 2024 – 08:30 PM EDT

PDB ID	:	9CQF
Title	:	CRYSTAL STRUCTURE OF APO C-TERMINAL HIS-TAG DOG
		HSP47(36-418) IN A C 2 2 21 CRYSTAL FORM
Authors	:	Sheriff, S.
Deposited on	:	2024-07-19
Resolution	:	2.93 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.93 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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	А	392	3% 91%	7% ••
1	В	392	<mark>3%</mark> 91%	8% ••
1	D	392	3% 	9% •
1	Е	392	3% 90%	6% ••
1	F	392	90%	9% •



Mol	Chain	Length	Quality of chain		
1	G	392	<mark>6%</mark> 90%	8%	•
1	Н	392	90%	9%	
1	Ι	392	91%	7%	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 48235 atoms, of which 24093 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.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace	
1	Δ	297	Total	С	Η	Ν	0	S	2002	0	0	
	A	301	6011	1914	3002	525	556	14	5002	0	0	
1	В	388	Total	С	Η	Ν	0	S	3016	0	0	
1	D	000	6037	1922	3016	528	557	14	5010	0	0	
1	л	300	Total	С	Η	Ν	Ο	\mathbf{S}	3028	0	0	
	D	030	6069	1933	3028	534	560	14	5028	0	0	
1	F	387	Total	С	Η	Ν	Ο	\mathbf{S}	3000	0	0	
L I		301	6018	1912	3009	525	558	14	5005	0	0	
1	F	388	Total	С	Η	Ν	Ο	\mathbf{S}	3020	0	0	
1	L	300	6051	1926	3020	530	561	14		0	U	
1	G	387	Total	\mathbf{C}	Η	Ν	0	\mathbf{S}	3007	0	0	
	G 30	G	301	6016	1913	3007	527	555	14	5007	0	0
1	н	297	Total	\mathbf{C}	Η	Ν	0	\mathbf{S}	3002	0	0	
	11	301	6006	1910	3002	525	555	14	5002	0	0	
1	1 T	387	Total	С	H	N	Ō	S	2000	0	0	
	1	301	6020	1916	3009	525	556	14	3009	U	U	

• Molecule 1 is a protein called Serpin H1.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	35	MET	-	initiating methionine	UNP C7C419
А	419	LEU	-	expression tag	UNP C7C419
А	420	GLU	-	expression tag	UNP C7C419
А	421	HIS	-	expression tag	UNP C7C419
А	422	HIS	-	expression tag	UNP C7C419
А	423	HIS	-	expression tag	UNP C7C419
А	424	HIS	-	expression tag	UNP C7C419
А	425	HIS	-	expression tag	UNP C7C419
А	426	HIS	-	expression tag	UNP C7C419
В	35	MET	-	initiating methionine	UNP C7C419
В	419	LEU	-	expression tag	UNP C7C419
В	420	GLU	-	expression tag	UNP C7C419
В	421	HIS	_	expression tag	UNP C7C419



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Chain	Residue	Modelled	Actual	Comment	Reference
В	422	HIS	-	expression tag	UNP C7C419
В	423	HIS	-	expression tag	UNP C7C419
В	424	HIS	-	expression tag	UNP C7C419
В	425	HIS	-	expression tag	UNP C7C419
В	426	HIS	-	expression tag	UNP C7C419
D	35	MET	-	initiating methionine	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
Е	35	MET	-	initiating methionine	UNP C7C419
Е	419	LEU	-	expression tag	UNP C7C419
Е	420	GLU	-	expression tag	UNP C7C419
Е	421	HIS	-	expression tag	UNP C7C419
Е	422	HIS	-	expression tag	UNP C7C419
Е	423	HIS	-	expression tag	UNP C7C419
Е	424	HIS	-	expression tag	UNP C7C419
Е	425	HIS	-	expression tag	UNP C7C419
Е	426	HIS	-	expression tag	UNP C7C419
F	35	MET	-	initiating methionine	UNP C7C419
F	419	LEU	-	expression tag	UNP C7C419
F	420	GLU	-	expression tag	UNP C7C419
F	421	HIS	-	expression tag	UNP C7C419
F	422	HIS	-	expression tag	UNP C7C419
F	423	HIS	-	expression tag	UNP C7C419
F	424	HIS	-	expression tag	UNP C7C419
F	425	HIS	-	expression tag	UNP C7C419
F	426	HIS	-	expression tag	UNP C7C419
G	35	MET	-	initiating methionine	UNP C7C419
G	419	LEU	-	expression tag	UNP C7C419
G	420	GLU	-	expression tag	UNP C7C419
G	421	HIS	-	expression tag	UNP C7C419
G	422	HIS	-	expression tag	UNP C7C419
G	423	HIS	-	expression tag	UNP C7C419
G	424	HIS	-	expression tag	UNP C7C419
G	425	HIS	-	expression tag	UNP C7C419
G	426	HIS	-	expression tag	UNP C7C419
H	35	MET	-	initiating methionine	UNP $C7C419$



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

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0
2	Е	2	Total O 2 2	0	0
2	\mathbf{F}	1	Total O 1 1	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 H1



H421 H1S H1S H1S H1S H1S H1S

• Molecule 1: Serpin H1



• Molecule 1: Serpin H1



PROTEIN DATA BANK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	117.78Å 129.94Å 501.93Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	250.97 - 2.93	Depositor
Resolution (A)	250.97 - 2.93	EDS
% Data completeness	$76.0\ (250.97-2.93)$	Depositor
(in resolution range)	$76.0\ (250.97-2.93)$	EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.06 (at 2.91 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
B B.	0.228 , 0.252	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.231 , 0.254	DCC
R_{free} test set	3075 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	71.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 83.0	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48235	wwPDB-VP
Average B, all atoms $(Å^2)$	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Bo	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.48	0/3070	0.65	1/4144~(0.0%)
1	В	0.43	0/3083	0.61	0/4162
1	D	0.46	0/3105	0.63	0/4192
1	Е	0.50	0/3069	0.65	0/4142
1	F	0.43	0/3094	0.61	0/4176
1	G	0.43	0/3070	0.62	0/4144
1	Н	0.40	0/3064	0.60	0/4136
1	Ι	0.39	0/3072	0.60	0/4147
All	All	0.44	0/24627	0.62	1/33243~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	419	LEU	N-CA-C	-5.42	96.36	111.00

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	А	3009	3002	3002	11	0
1	В	3021	3016	3016	8	0
1	D	3041	3028	3028	11	0
1	Е	3009	3009	3009	12	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3031	3020	3020	16	0
1	G	3009	3007	3007	11	0
1	Н	3004	3002	3002	12	0
1	Ι	3011	3009	3009	8	0
2	А	2	0	0	0	0
2	D	2	0	0	0	0
2	Е	2	0	0	0	0
2	F	1	0	0	0	0
All	All	24142	24093	24093	79	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 2.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:83:LEU:HD13	1:D:108:HIS:CD2	2.36	0.60
1:A:273:HIS:NE2	1:F:228:ARG:NH1	2.52	0.57
1:H:167:ARG:NH2	1:I:413:LYS:HZ1	2.03	0.57
1:F:83:LEU:HD13	1:F:108:HIS:CD2	2.43	0.53
1:F:252:LYS:HA	1:F:273:HIS:CE1	2.44	0.53
1:A:44:ALA:HB2	1:A:114:LEU:HD21	1.92	0.52
1:D:72:VAL:HG21	1:D:118:LEU:HD21	1.91	0.52
1:H:122:THR:O	1:H:127:THR:OG1	2.29	0.51
1:B:377:ARG:O	1:F:298:GLN:OE1	2.28	0.51
1:I:83:LEU:HD13	1:I:108:HIS:CD2	2.47	0.50
1:E:43:LEU:O	1:E:47:SER:OG	2.29	0.50
1:A:54:LEU:O	1:A:58:MET:HG3	2.13	0.49
1:D:83:LEU:CD1	1:D:108:HIS:CD2	2.94	0.49
1:F:413:LYS:CD	1:F:413:LYS:H	2.26	0.48
1:A:208:PRO:HD2	1:A:358:GLU:O	2.14	0.48
1:F:371:TYR:O	1:F:374:GLU:HB2	2.14	0.47
1:G:238:HIS:HB3	1:H:419:LEU:HD13	1.95	0.47
1:F:413:LYS:HZ2	1:G:171:GLN:HG3	1.80	0.47
1:E:83:LEU:HD12	1:E:108:HIS:CD2	2.49	0.47
1:F:238:HIS:HB3	1:I:419:LEU:HD13	1.97	0.47
1:F:281:LEU:HD23	1:F:389:ILE:HD12	1.97	0.47
1:B:54:LEU:O	1:B:58:MET:HG3	2.15	0.47
1:H:54:LEU:O	1:H:58:MET:HG3	2.14	0.47
1:I:281:LEU:HD23	1:I:389:ILE:HD12	1.97	0.47
1:G:179:GLN:HA	1:I:216:HIS:CE1	2.51	0.46



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:423:HIS:CD2	1:D:423:HIS:N	2.84	0.46
1:D:54:LEU:O	1:D:58:MET:HG3	2.15	0.46
1:H:281:LEU:HD23	1:H:389:ILE:HD12	1.98	0.46
1:A:242:LEU:HD23	1:A:371:TYR:CD2	2.50	0.46
1:I:54:LEU:O	1:I:58:MET:HG3	2.16	0.46
1:G:39:LYS:HG3	1:G:40:ALA:N	2.29	0.46
1:G:54:LEU:O	1:G:58:MET:HG3	2.17	0.45
1:B:281:LEU:HD23	1:B:389:ILE:HD12	1.97	0.45
1:E:281:LEU:HD23	1:E:389:ILE:HD12	1.97	0.45
1:F:54:LEU:O	1:F:58:MET:HG3	2.17	0.45
1:D:281:LEU:HD23	1:D:389:ILE:HD12	1.96	0.45
1:E:83:LEU:CD1	1:E:108:HIS:CD2	2.99	0.45
1:G:281:LEU:HD23	1:G:389:ILE:HD12	1.97	0.45
1:H:239:ARG:NH1	1:H:243:TYR:OH	2.42	0.45
1:E:253:LEU:HD22	1:E:281:LEU:HD11	1.99	0.44
1:A:222:ARG:NH1	1:A:383:TYR:OH	2.49	0.44
1:A:281:LEU:HD23	1:A:389:ILE:HD12	1.98	0.44
1:F:239:ARG:NH1	1:F:243:TYR:OH	2.45	0.44
1:E:343:LYS:HD2	1:E:344:LYS:O	2.17	0.44
1:E:133:ARG:HD3	1:E:135:TYR:CZ	2.53	0.44
1:B:133:ARG:HD3	1:B:135:TYR:CZ	2.54	0.43
1:F:83:LEU:CD1	1:F:108:HIS:CD2	3.01	0.43
1:H:368:GLN:O	1:H:369:ASP:CB	2.66	0.43
1:D:151:LYS:HE2	1:D:156:CYS:O	2.18	0.43
1:E:46:ARG:HG2	1:E:98:SER:O	2.18	0.43
1:I:133:ARG:HD3	1:I:135:TYR:CZ	2.54	0.43
1:E:177:ALA:CB	1:E:188:VAL:HG23	2.49	0.43
1:H:133:ARG:HD3	1:H:135:TYR:CZ	2.54	0.43
1:D:133:ARG:HD3	1:D:135:TYR:CZ	2.53	0.43
1:G:46:ARG:HG2	1:G:97:LEU:O	2.19	0.43
1:G:133:ARG:HD3	1:G:135:TYR:CZ	2.54	0.43
1:A:343:LYS:HD2	1:A:344:LYS:O	2.18	0.43
1:I:252:LYS:HA	1:I:273:HIS:CE1	2.54	0.43
1:D:252:LYS:HA	1:D:273:HIS:CE1	2.53	0.43
1:G:419:LEU:HD13	1:H:238:HIS:HB3	2.00	0.43
1:F:133:ARG:HD3	1:F:135:TYR:CZ	2.54	0.43
1:E:119:SER:HG	1:E:128:TRP:HD1	1.64	0.42
1:F:179:GLN:HA	1:H:216:HIS:CE1	2.54	0.42
1:A:133:ARG:HD3	1:A:135:TYR:CZ	2.54	0.42
1:B:216:HIS:CE1	1:E:179:GLN:HA	2.54	0.42
1:E:70:SER:H	1:E:353:HIS:CE1	2.38	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:222:ARG:NH1	1:H:383:TYR:OH	2.48	0.42
1:F:185:LEU:HD21	1:F:354:ALA:HB1	2.02	0.41
1:H:252:LYS:HA	1:H:273:HIS:CE1	2.55	0.41
1:G:271:MET:SD	1:G:384:ALA:HA	2.60	0.41
1:A:252:LYS:HA	1:A:273:HIS:CE1	2.56	0.41
1:F:150:SER:HG	1:F:158:HIS:CE1	2.38	0.41
1:G:343:LYS:NZ	1:G:343:LYS:HB3	2.37	0.40
1:A:271:MET:SD	1:A:384:ALA:HA	2.62	0.40
1:B:252:LYS:HA	1:B:273:HIS:CE1	2.55	0.40
1:B:274:HIS:CD2	1:B:274:HIS:H	2.39	0.40
1:D:177:ALA:CB	1:D:188:VAL:HG23	2.51	0.40
1:B:46:ARG:HG2	1:B:97:LEU:O	2.21	0.40
1:D:252:LYS:HA	1:D:273:HIS:ND1	2.36	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	Perc	entiles
1	А	385/392~(98%)	363 (94%)	21 (6%)	1 (0%)	37	65
1	В	386/392~(98%)	357~(92%)	25~(6%)	4 (1%)	13	38
1	D	388/392~(99%)	362~(93%)	25~(6%)	1 (0%)	37	65
1	Е	385/392~(98%)	354 (92%)	29~(8%)	2~(0%)	25	55
1	F	386/392~(98%)	361 (94%)	24 (6%)	1 (0%)	37	65
1	G	385/392~(98%)	355~(92%)	28 (7%)	2~(0%)	25	55
1	Н	385/392~(98%)	361 (94%)	22~(6%)	2~(0%)	25	55
1	Ι	385/392~(98%)	353~(92%)	29 (8%)	3 (1%)	16	44
All	All	3085/3136~(98%)	2866 (93%)	203 (7%)	16 (0%)	25	55



Mol	Chain	Res	Type
1	Е	371	TYR
1	А	344	LYS
1	В	367	ASP
1	В	373	ARG
1	Е	420	GLU
1	Ι	373	ARG
1	В	374	GLU
1	F	369	ASP
1	G	374	GLU
1	Н	369	ASP
1	Ι	375	GLU
1	D	373	ARG
1	В	413	LYS
1	G	370	ILE
1	Ι	275	VAL
1	Н	275	VAL

All (16) Ramachandran outliers are listed below:

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	Perce	entiles
1	А	318/337~(94%)	303~(95%)	15~(5%)	22	53
1	В	320/337~(95%)	303~(95%)	17 (5%)	19	48
1	D	322/337~(96%)	303~(94%)	19 (6%)	16	43
1	Ε	320/337~(95%)	301 (94%)	19 (6%)	16	43
1	F	322/337~(96%)	309~(96%)	13 (4%)	27	59
1	G	319/337~(95%)	303~(95%)	16 (5%)	20	50
1	Н	318/337~(94%)	304 (96%)	14 (4%)	24	55
1	Ι	319/337~(95%)	304 (95%)	15 (5%)	22	53
All	All	2558/2696~(95%)	2430 (95%)	128 (5%)	20	50

All (128) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	50	LEU
1	А	97	LEU
1	А	100	GLU
1	А	104	ASP
1	А	105	GLU
1	А	253	LEU
1	А	298	GLN
1	А	332	LYS
1	А	343	LYS
1	А	344	LYS
1	А	371	TYR
1	А	378	SER
1	А	401	LEU
1	А	412	ASP
1	А	419	LEU
1	В	97	LEU
1	В	100	GLU
1	В	104	ASP
1	В	105	GLU
1	В	249	GLU
1	В	253	LEU
1	В	274	HIS
1	В	276	GLU
1	В	298	GLN
1	В	332	LYS
1	В	343	LYS
1	В	376	LEU
1	В	378	SER
1	В	391	LEU
1	В	401	LEU
1	В	412	ASP
1	В	419	LEU
1	D	35	MET
1	D	39	LYS
1	D	43	LEU
1	D	97	LEU
1	D	100	GLU
1	D	104	ASP
1	D	105	GLU
1	D	253	LEU
1	D	298	GLN
1	D	332	LYS
1	D	343	LYS



Mol	Chain	Res	Type
1	D	344	LYS
1	D	376	LEU
1	D	378	SER
1	D	391	LEU
1	D	401	LEU
1	D	412	ASP
1	D	414	MET
1	D	415	ARG
1	Е	43	LEU
1	Е	46	ARG
1	Е	47	SER
1	Е	54	LEU
1	Е	97	LEU
1	Е	98	SER
1	Е	104	ASP
1	Е	119	SER
1	Е	145	ASP
1	Е	253	LEU
1	Е	265	SER
1	Е	298	GLN
1	Е	332	LYS
1	Е	343	LYS
1	Е	344	LYS
1	Е	378	SER
1	Е	391	LEU
1	Е	399	SER
1	Е	416	ASP
1	F	97	LEU
1	F	100	GLU
1	F	104	ASP
1	F	105	GLU
1	F	253	LEU
1	F	332	LYS
1	F	343	LYS
1	F	344	LYS
1	F	378	SER
1	F	391	LEU
1	F	401	LEU
1	F	412	ASP
1	F	413	LYS
1	G	83	LEU
1	G	97	LEU



Mol	Chain	Res	Type
1	G	100	GLU
1	G	104	ASP
1	G	105	GLU
1	G	253	LEU
1	G	298	GLN
1	G	332	LYS
1	G	344	LYS
1	G	376	LEU
1	G	378	SER
1	G	391	LEU
1	G	401	LEU
1	G	412	ASP
1	G	417	GLU
1	G	418	LEU
1	Н	97	LEU
1	Н	100	GLU
1	Н	104	ASP
1	Н	105	GLU
1	Н	253	LEU
1	Н	298	GLN
1	Н	332	LYS
1	Н	343	LYS
1	Н	344	LYS
1	Н	378	SER
1	Н	391	LEU
1	Н	401	LEU
1	Н	412	ASP
1	Н	413	LYS
1	Ι	97	LEU
1	Ι	100	GLU
1	Ι	104	ASP
1	Ι	105	GLU
1	Ι	253	LEU
1	Ι	274	HIS
1	Ι	298	GLN
1	Ι	332	LYS
1	Ι	343	LYS
1	Ι	376	LEU
1	Ι	378	SER
1	Ι	391	LEU
1	Ι	401	LEU
1	Ι	412	ASP



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Mol	Chain	Res	Type
1	Ι	413	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	171	GLN
1	А	353	HIS
1	В	171	GLN
1	В	274	HIS
1	В	353	HIS
1	D	171	GLN
1	D	353	HIS
1	D	423	HIS
1	Е	171	GLN
1	Е	353	HIS
1	F	353	HIS
1	G	171	GLN
1	G	353	HIS
1	Н	171	GLN
1	Н	353	HIS
1	Ι	171	GLN
1	Ι	353	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 (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	387/392~(98%)	0.04	12 (3%) 51 46	16, 31, 56, 70	0
1	В	388/392~(98%)	0.43	12 (3%) 51 46	18, 40, 65, 77	0
1	D	390/392~(99%)	0.18	11 (2%) 55 49	15, 34, 58, 72	0
1	Е	387/392~(98%)	-0.01	12 (3%) 51 46	16, 29, 51, 75	0
1	F	388/392~(98%)	0.28	15 (3%) 44 38	21, 38, 66, 80	0
1	G	387/392~(98%)	0.57	24 (6%) 28 24	19, 40, 64, 94	0
1	Н	387/392~(98%)	0.62	18 (4%) 37 32	24, 46, 73, 87	0
1	Ι	387/392~(98%)	0.92	43 (11%) 12 11	25, 53, 80, 104	0
All	All	3101/3136 (98%)	0.38	147 (4%) 37 32	15, 38, 69, 104	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	125	ASN	5.3
1	Ι	421	HIS	5.1
1	Ι	121	SER	4.7
1	F	345	ASP	4.5
1	Ι	78	LEU	4.2
1	Ι	198	ALA	4.2
1	Ι	348	LEU	4.0
1	F	163	PHE	3.9
1	Н	418	LEU	3.8
1	Ι	125	ASN	3.8
1	Ι	163	PHE	3.8
1	D	345	ASP	3.8
1	В	126	VAL	3.7
1	G	376	LEU	3.6
1	A	417	GLU	3.5
1	E	345	ASP	3.4



Mol	Chain	Res	Type	RSRZ
1	Е	123	ALA	3.4
1	Ι	326	LEU	3.4
1	Н	123	ALA	3.3
1	Е	118	LEU	3.3
1	Ι	321	LEU	3.3
1	F	121	SER	3.2
1	Ι	77	SER	3.2
1	Н	78	LEU	3.1
1	Ι	351	VAL	3.1
1	Е	122	THR	3.1
1	Ι	123	ALA	3.0
1	Ι	122	THR	3.0
1	Ι	281	LEU	3.0
1	G	270	LEU	3.0
1	F	35	MET	2.9
1	Ι	137	PRO	2.9
1	Ι	419	LEU	2.9
1	F	198	ALA	2.9
1	Ι	81	VAL	2.9
1	Н	368	GLN	2.9
1	F	122	THR	2.9
1	В	123	ALA	2.9
1	G	371	TYR	2.9
1	G	418	LEU	2.8
1	Ι	418	LEU	2.8
1	Н	97	LEU	2.8
1	Ι	134	LEU	2.8
1	Ι	329	ALA	2.8
1	А	371	TYR	2.8
1	Ι	420	GLU	2.8
1	В	163	PHE	2.8
1	В	348	LEU	2.7
1	G	123	ALA	2.7
1	Н	134	LEU	2.7
1	E	375	GLU	2.7
1	F	342	GLY	2.7
1	G	400	LEU	2.7
1	G	121	SER	2.7
1	G	375	GLU	2.7
1	А	369	ASP	2.7
1	Н	346	LEU	2.6
1	D	321	LEU	2.6



Mol	Chain	Res	Type	RSRZ
1	D	163	PHE	2.6
1	Ι	352	PHE	2.6
1	Ι	35	MET	2.6
1	В	420	GLU	2.6
1	G	321	LEU	2.6
1	G	163	PHE	2.6
1	D	122	THR	2.5
1	А	163	PHE	2.5
1	Ι	80	LEU	2.5
1	В	368	GLN	2.5
1	Ε	374	GLU	2.5
1	Е	121	SER	2.5
1	G	421	HIS	2.5
1	Η	420	GLU	2.5
1	А	418	LEU	2.5
1	G	102	LEU	2.5
1	Ι	93	ALA	2.4
1	В	371	TYR	2.4
1	G	62	GLN	2.4
1	Ι	378	SER	2.4
1	Н	270	LEU	2.4
1	G	125	ASN	2.4
1	А	345	ASP	2.4
1	В	421	HIS	2.4
1	D	39	LYS	2.4
1	Ι	154	TYR	2.4
1	Н	343	LYS	2.4
1	Ι	384	ALA	2.4
1	D	371	TYR	2.3
1	Ι	236	MET	2.3
1	Е	366	PHE	2.3
1	Н	352	PHE	2.3
1	G	285	LEU	2.3
1	Ι	136	GLY	2.3
1	Ι	197	GLY	2.3
1	Ι	374	GLU	2.3
1	Ι	90	ALA	2.3
1	D	373	ARG	2.3
1	D	125	ASN	2.3
1	Н	326	LEU	2.3
1	F	123	ALA	2.3
1	D	346	LEU	2.3



9CQF

Mol	Chain	Res	Type	RSRZ
1	F	36	LEU	2.3
1	Е	39	LYS	2.3
1	Е	370	ILE	2.2
1	G	382	PHE	2.2
1	F	339	ARG	2.2
1	Н	348	LEU	2.2
1	Н	419	LEU	2.2
1	А	372	GLY	2.2
1	А	421	HIS	2.2
1	G	63	ALA	2.2
1	G	35	MET	2.2
1	F	199	LEU	2.2
1	G	419	LEU	2.2
1	В	320	HIS	2.2
1	Н	329	ALA	2.2
1	А	134	LEU	2.2
1	Ι	118	LEU	2.2
1	Ι	161	ILE	2.2
1	В	366	PHE	2.2
1	G	373	ARG	2.2
1	D	90	ALA	2.2
1	Е	47	SER	2.2
1	F	197	GLY	2.1
1	Н	402	PHE	2.1
1	F	348	LEU	2.1
1	F	38	PRO	2.1
1	D	366	PHE	2.1
1	Ι	388	PHE	2.1
1	G	97	LEU	2.1
1	Н	93	ALA	2.1
1	Ι	277	PRO	2.1
1	Ι	89	THR	2.1
1	G	290	LEU	2.1
1	G	106	GLU	2.1
1	Ι	370	ILE	2.1
1	F	413	LYS	2.1
1	А	270	LEU	2.0
1	А	326	LEU	2.0
1	Н	369	ASP	2.0
1	А	168	SER	2.0
1	G	420	GLU	2.0
1	Ι	340	MET	2.0



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Mol	Chain	Res	Type	RSRZ
1	Ι	52	PHE	2.0
1	В	422	HIS	2.0
1	Ι	400	LEU	2.0
1	Е	419	LEU	2.0
1	Ι	156	CYS	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.

