Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2024 – 08:36 PM EDT

PDB ID	:	9CQE
Title	:	CRYSTAL STRUCTURE OF APO C-TERMINAL HIS-TAG DOG HSP47(36-418) IN A P 1 21 1 CRYSTAL FORM
Authors	:	Sheriff, S.
Deposited on	:	2024-07-19
Resolution	:	3.18 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:

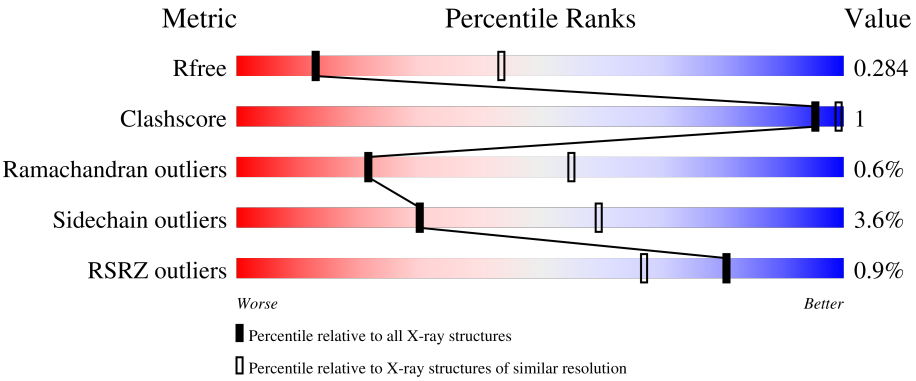
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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}	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	92% 5%
1	B	392	90% 7%
1	D	392	88% 9%
1	E	392	91% 7%
1	F	392	93%

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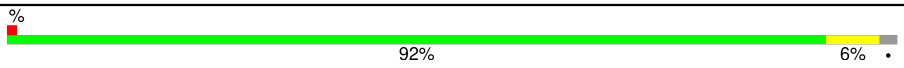
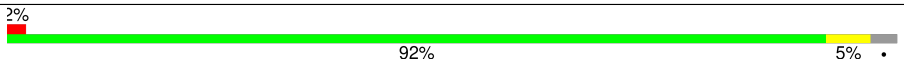
Mol	Chain	Length	Quality of chain
1	G	392	
1	H	392	
1	I	392	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 45775 atoms, of which 22579 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 H1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	H	N	O	S	2884	0	0
			5807	1853	2884	512	544	14			
1	B	382	Total	C	H	N	O	S	2887	0	0
			5821	1862	2887	513	545	14			
1	D	382	Total	C	H	N	O	S	2897	0	0
			5824	1863	2897	509	541	14			
1	E	381	Total	C	H	N	O	S	2786	0	0
			5660	1826	2786	500	535	13			
1	F	381	Total	C	H	N	O	S	2784	0	0
			5665	1828	2784	499	540	14			
1	G	384	Total	C	H	N	O	S	2805	0	0
			5708	1838	2805	511	541	13			
1	H	382	Total	C	H	N	O	S	2851	0	0
			5762	1848	2851	509	540	14			
1	I	381	Total	C	H	N	O	S	2685	0	0
			5528	1794	2685	499	537	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	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	-	initiating methionine	UNP C7C419
B	419	LEU	-	expression tag	UNP C7C419
B	420	GLU	-	expression tag	UNP C7C419
B	421	HIS	-	expression tag	UNP C7C419

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

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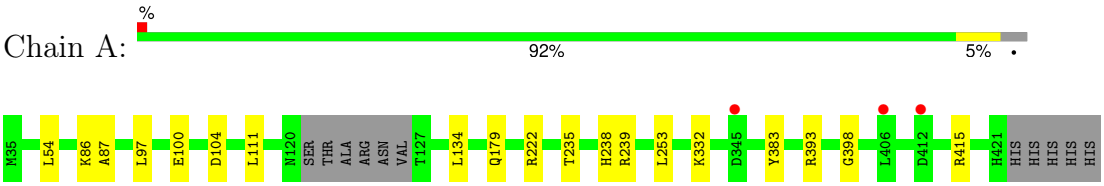
Chain	Residue	Modelled	Actual	Comment	Reference
H	419	LEU	-	expression tag	UNP C7C419
H	420	GLU	-	expression tag	UNP C7C419
H	421	HIS	-	expression tag	UNP C7C419
H	422	HIS	-	expression tag	UNP C7C419
H	423	HIS	-	expression tag	UNP C7C419
H	424	HIS	-	expression tag	UNP C7C419
H	425	HIS	-	expression tag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

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.

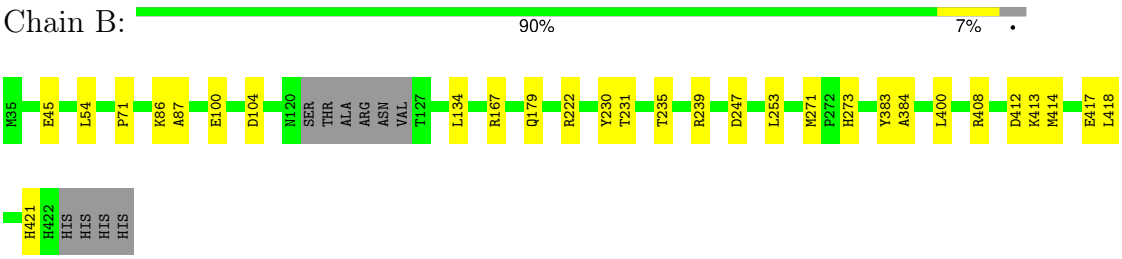
• Molecule 1: Serpin H1

Chain A:



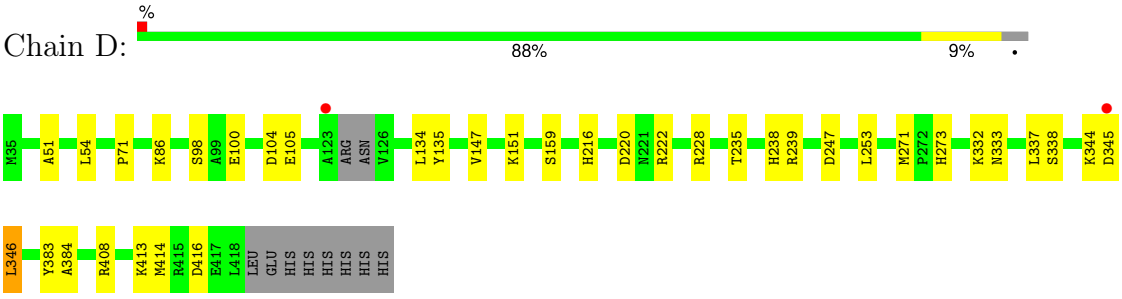
• Molecule 1: Serpin H1

Chain B:



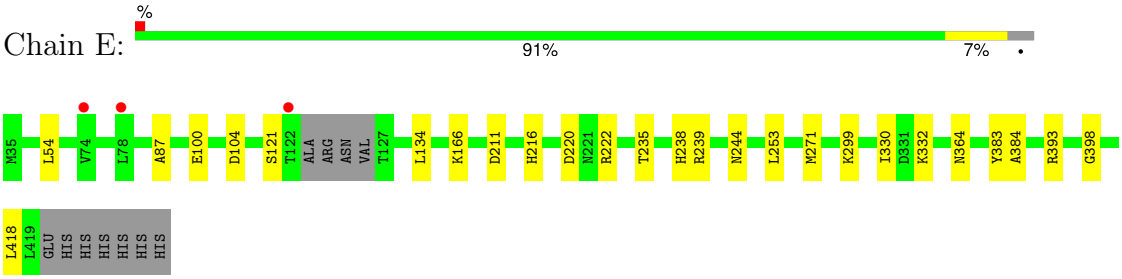
• Molecule 1: Serpin H1

Chain D:



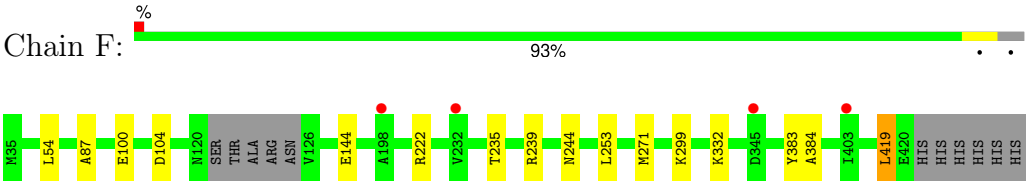
• Molecule 1: Serpin H1

Chain E:



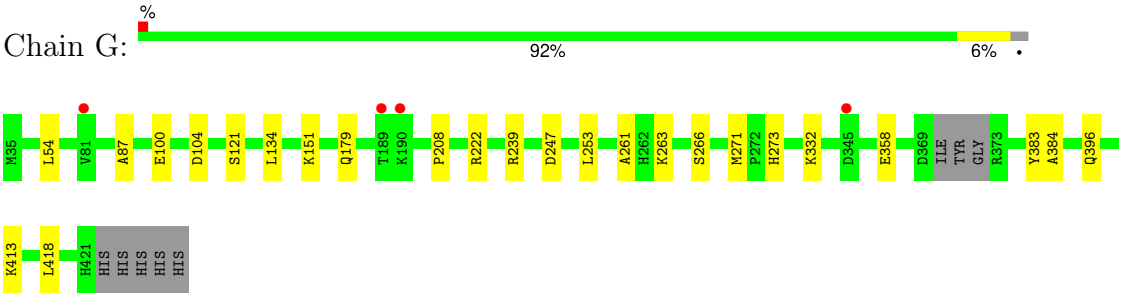
• Molecule 1: Serpin H1

Chain F:



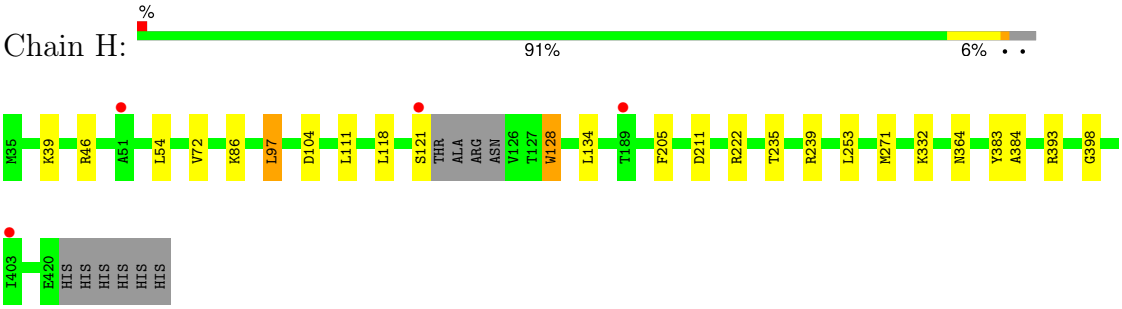
• Molecule 1: Serpin H1

Chain G:



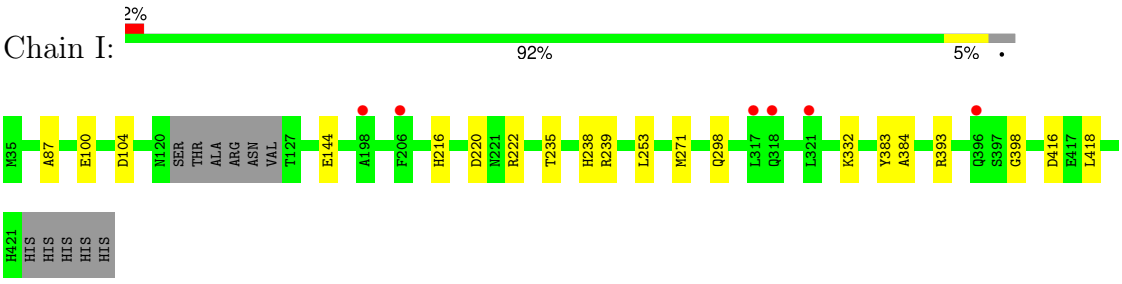
• Molecule 1: Serpin H1

Chain H:



• Molecule 1: Serpin H1

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	140.18Å 75.31Å 163.87Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	45.85 – 3.18 45.85 – 3.18	Depositor EDS
% Data completeness (in resolution range)	73.1 (45.85-3.18) 73.0 (45.85-3.18)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.263 , 0.288 0.262 , 0.284	Depositor DCC
R_{free} test set	2024 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	45775	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

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	0.37	0/2980	0.54	0/4026
1	B	0.37	0/2993	0.54	0/4046
1	D	0.41	0/2985	0.61	1/4033 (0.0%)
1	E	0.36	0/2932	0.54	0/3972
1	F	0.37	0/2939	0.54	0/3983
1	G	0.38	0/2961	0.56	0/4009
1	H	0.37	0/2969	0.55	0/4017
1	I	0.35	0/2901	0.54	0/3932
All	All	0.37	0/23660	0.55	1/32018 (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	D	346	LEU	N-CA-C	-5.02	97.45	111.00

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	2923	2884	2884	5	0
1	B	2934	2887	2885	10	0
1	D	2927	2897	2894	11	0
1	E	2874	2786	2782	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2881	2784	2784	3	0
1	G	2903	2805	2802	6	0
1	H	2911	2851	2851	8	0
1	I	2843	2685	2683	5	0
All	All	23196	22579	22565	49	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 1.

All (49) 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:F:244:ASN:OD1	1:F:299:LYS:HG3	1.74	0.88
1:B:230:TYR:OH	1:B:408:ARG:NH2	2.20	0.74
1:D:51:ALA:HB2	1:D:71:PRO:HB3	1.78	0.65
1:D:247:ASP:OD1	1:D:273:HIS:NE2	2.32	0.61
1:D:337:LEU:HD12	1:D:346:LEU:O	2.02	0.59
1:B:222:ARG:NH1	1:B:383:TYR:OH	2.36	0.58
1:H:222:ARG:NH1	1:H:383:TYR:OH	2.36	0.58
1:I:222:ARG:NH1	1:I:383:TYR:OH	2.36	0.58
1:G:222:ARG:NH1	1:G:383:TYR:OH	2.36	0.58
1:D:222:ARG:NH1	1:D:383:TYR:OH	2.37	0.58
1:A:222:ARG:NH1	1:A:383:TYR:OH	2.36	0.58
1:E:222:ARG:NH1	1:E:383:TYR:OH	2.37	0.56
1:F:222:ARG:NH1	1:F:383:TYR:OH	2.36	0.55
1:B:45:GLU:OE1	1:G:396:GLN:NE2	2.41	0.54
1:H:97:LEU:HD21	1:H:111:LEU:HD11	1.90	0.53
1:B:231:THR:O	1:B:414:MET:HB2	2.11	0.51
1:A:179:GLN:HA	1:D:216:HIS:CE1	2.46	0.50
1:B:167:ARG:NE	1:D:408:ARG:HH12	2.11	0.49
1:G:208:PRO:HD2	1:G:358:GLU:O	2.12	0.49
1:H:72:VAL:HG21	1:H:118:LEU:HD21	1.96	0.47
1:G:179:GLN:HA	1:I:216:HIS:CE1	2.50	0.46
1:G:271:MET:SD	1:G:384:ALA:HA	2.56	0.45
1:B:179:GLN:HA	1:E:216:HIS:CE1	2.53	0.43
1:B:71:PRO:HG2	1:B:400:LEU:O	2.19	0.43
1:D:86:LYS:HE3	1:D:338:SER:OG	2.18	0.43
1:D:220:ASP:OD1	1:D:238:HIS:NE2	2.44	0.43
1:B:271:MET:SD	1:B:384:ALA:HA	2.59	0.43
1:H:128:TRP:HA	1:H:205:PHE:O	2.19	0.42
1:I:271:MET:SD	1:I:384:ALA:HA	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:HB3	1:B:418:LEU:HD12	2.01	0.42
1:A:393:ARG:NH1	1:A:398:GLY:O	2.53	0.42
1:D:147:VAL:O	1:D:151:LYS:HB3	2.20	0.42
1:F:271:MET:SD	1:F:384:ALA:HA	2.59	0.42
1:E:211:ASP:O	1:E:364:ASN:HB2	2.21	0.41
1:B:247:ASP:OD1	1:B:273:HIS:NE2	2.44	0.41
1:D:135:TYR:HA	1:D:159:SER:O	2.20	0.41
1:H:271:MET:SD	1:H:384:ALA:HA	2.60	0.41
1:E:393:ARG:NH1	1:E:398:GLY:O	2.53	0.41
1:A:97:LEU:HD21	1:A:111:LEU:HD11	2.02	0.41
1:H:393:ARG:NH1	1:H:398:GLY:O	2.53	0.41
1:I:393:ARG:NH1	1:I:398:GLY:O	2.53	0.41
1:E:220:ASP:OD1	1:E:238:HIS:NE2	2.44	0.41
1:G:247:ASP:OD1	1:G:273:HIS:NE2	2.43	0.41
1:H:211:ASP:O	1:H:364:ASN:HB2	2.20	0.41
1:E:271:MET:SD	1:E:384:ALA:HA	2.61	0.41
1:D:271:MET:SD	1:D:384:ALA:HA	2.60	0.41
1:I:220:ASP:OD1	1:I:238:HIS:NE2	2.44	0.41
1:H:46:ARG:HG2	1:H:97:LEU:O	2.21	0.40
1:E:244:ASN:OD1	1:E:299:LYS:HG3	2.21	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	377/392 (96%)	357 (95%)	18 (5%)	2 (0%)	25 58
1	B	378/392 (96%)	359 (95%)	18 (5%)	1 (0%)	37 67
1	D	378/392 (96%)	355 (94%)	20 (5%)	3 (1%)	16 49
1	E	377/392 (96%)	359 (95%)	16 (4%)	2 (0%)	25 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	377/392 (96%)	355 (94%)	20 (5%)	2 (0%)	25	58
1	G	380/392 (97%)	356 (94%)	20 (5%)	4 (1%)	12	42
1	H	378/392 (96%)	356 (94%)	21 (6%)	1 (0%)	37	67
1	I	377/392 (96%)	359 (95%)	16 (4%)	2 (0%)	25	58
All	All	3022/3136 (96%)	2856 (94%)	149 (5%)	17 (1%)	22	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	416	ASP
1	F	419	LEU
1	G	121	SER
1	G	261	ALA
1	G	263	LYS
1	H	128	TRP
1	A	415	ARG
1	D	98	SER
1	F	87	ALA
1	I	416	ASP
1	A	87	ALA
1	B	87	ALA
1	D	345	ASP
1	E	87	ALA
1	G	87	ALA
1	I	87	ALA
1	E	121	SER

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	305/337 (90%)	296 (97%)	9 (3%)	36	64
1	B	306/337 (91%)	294 (96%)	12 (4%)	27	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	304/337 (90%)	290 (95%)	14 (5%)	23 53
1	E	292/337 (87%)	281 (96%)	11 (4%)	28 58
1	F	295/337 (88%)	286 (97%)	9 (3%)	35 63
1	G	294/337 (87%)	283 (96%)	11 (4%)	29 59
1	H	301/337 (89%)	290 (96%)	11 (4%)	29 59
1	I	282/337 (84%)	273 (97%)	9 (3%)	34 63
All	All	2379/2696 (88%)	2293 (96%)	86 (4%)	30 59

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	86	LYS
1	A	100	GLU
1	A	104	ASP
1	A	134	LEU
1	A	235	THR
1	A	239	ARG
1	A	253	LEU
1	A	332	LYS
1	B	54	LEU
1	B	86	LYS
1	B	100	GLU
1	B	104	ASP
1	B	134	LEU
1	B	235	THR
1	B	239	ARG
1	B	253	LEU
1	B	412	ASP
1	B	413	LYS
1	B	417	GLU
1	B	421	HIS
1	D	54	LEU
1	D	100	GLU
1	D	104	ASP
1	D	105	GLU
1	D	134	LEU
1	D	228	ARG
1	D	235	THR
1	D	239	ARG

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Mol	Chain	Res	Type
1	D	253	LEU
1	D	332	LYS
1	D	333	ASN
1	D	344	LYS
1	D	413	LYS
1	D	414	MET
1	E	54	LEU
1	E	100	GLU
1	E	104	ASP
1	E	134	LEU
1	E	166	LYS
1	E	235	THR
1	E	239	ARG
1	E	253	LEU
1	E	330	ILE
1	E	332	LYS
1	E	418	LEU
1	F	54	LEU
1	F	100	GLU
1	F	104	ASP
1	F	144	GLU
1	F	235	THR
1	F	239	ARG
1	F	253	LEU
1	F	332	LYS
1	F	419	LEU
1	G	54	LEU
1	G	100	GLU
1	G	104	ASP
1	G	134	LEU
1	G	151	LYS
1	G	239	ARG
1	G	253	LEU
1	G	266	SER
1	G	332	LYS
1	G	413	LYS
1	G	418	LEU
1	H	39	LYS
1	H	54	LEU
1	H	86	LYS
1	H	97	LEU
1	H	104	ASP

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Mol	Chain	Res	Type
1	H	121	SER
1	H	134	LEU
1	H	235	THR
1	H	239	ARG
1	H	253	LEU
1	H	332	LYS
1	I	100	GLU
1	I	104	ASP
1	I	144	GLU
1	I	235	THR
1	I	239	ARG
1	I	253	LEU
1	I	298	GLN
1	I	332	LYS
1	I	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	HIS
1	B	353	HIS
1	B	421	HIS
1	D	171	GLN
1	D	353	HIS
1	E	353	HIS
1	F	353	HIS
1	G	353	HIS
1	G	396	GLN
1	H	353	HIS
1	I	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

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	381/392 (97%)	-0.30	3 (0%) 82 70	19, 38, 64, 77	0
1	B	382/392 (97%)	-0.17	0 100 100	33, 51, 78, 90	0
1	D	382/392 (97%)	-0.28	2 (0%) 87 78	18, 35, 56, 78	0
1	E	381/392 (97%)	-0.14	3 (0%) 82 70	30, 52, 79, 95	0
1	F	381/392 (97%)	-0.10	4 (1%) 79 65	29, 47, 74, 82	0
1	G	384/392 (97%)	-0.09	4 (1%) 79 65	31, 52, 76, 91	0
1	H	382/392 (97%)	-0.26	4 (1%) 79 65	22, 39, 65, 80	0
1	I	381/392 (97%)	0.00	6 (1%) 70 55	30, 55, 93, 105	0
All	All	3054/3136 (97%)	-0.17	26 (0%) 81 67	18, 46, 77, 105	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	198	ALA	4.5
1	D	345	ASP	3.5
1	I	198	ALA	3.2
1	E	122	THR	3.1
1	F	345	ASP	3.1
1	G	345	ASP	3.0
1	H	403	ILE	3.0
1	I	396	GLN	2.8
1	A	412	ASP	2.8
1	H	189	THR	2.6
1	E	74	VAL	2.6
1	I	321	LEU	2.5
1	H	121	SER	2.4
1	F	232	VAL	2.3
1	I	318	GLN	2.2
1	I	206	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASP	2.2
1	G	189	THR	2.2
1	F	403	ILE	2.1
1	H	51	ALA	2.1
1	G	81	VAL	2.1
1	E	78	LEU	2.1
1	A	406	LEU	2.1
1	I	317	LEU	2.1
1	G	190	LYS	2.1
1	D	123	ALA	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.