



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:52 AM UTC

PDB ID : 9CQG / pdb_00009cQG
Title : CRYSTAL STRUCTURE OF APO C-TERMINAL HIS-TAG DOG
HSP47(36-418) IN A P 1 CRYSTAL FORM
Authors : Sheriff, S.
Deposited on : 2024-07-19
Resolution : 2.47 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
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

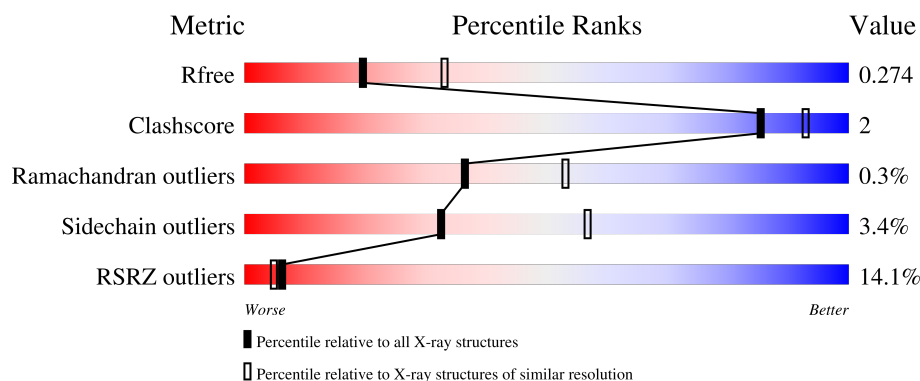
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	10% 93% 6% ..
1	B	392	10% 92% 8% .
1	D	392	8% 90% 8% .
1	E	392	26% 91% 9%
1	F	392	8% 93% 6% ..

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Mol	Chain	Length	Quality of chain
1	G	392	22% 91% 8%
1	H	392	10% 92% 7%
1	I	392	17% 90% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48565 atoms, of which 24169 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	390	Total	C	H	N	O	S	3013	0	0
			6052	1932	3013	531	562	14			
1	B	392	Total	C	H	N	O	S	3047	0	0
			6115	1949	3047	541	564	14			
1	D	387	Total	C	H	N	O	S	2999	0	0
			6008	1915	2999	523	557	14			
1	E	392	Total	C	H	N	O	S	3037	0	0
			6098	1945	3037	538	564	14			
1	F	390	Total	C	H	N	O	S	3035	0	0
			6081	1937	3035	536	559	14			
1	G	391	Total	C	H	N	O	S	2991	0	0
			6027	1925	2991	533	564	14			
1	H	390	Total	C	H	N	O	S	3020	0	0
			6061	1934	3020	530	563	14			
1	I	391	Total	C	H	N	O	S	3027	0	0
			6078	1938	3027	538	561	14			

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

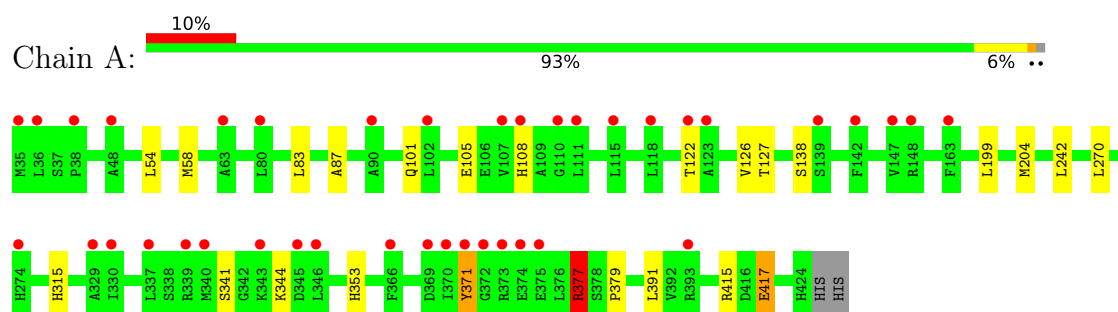
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	7	Total O 7 7	0	0
2	D	4	Total O 4 4	0	0
2	E	8	Total O 8 8	0	0
2	F	4	Total O 4 4	0	0
2	G	5	Total O 5 5	0	0
2	H	1	Total O 1 1	0	0
2	I	4	Total O 4 4	0	0

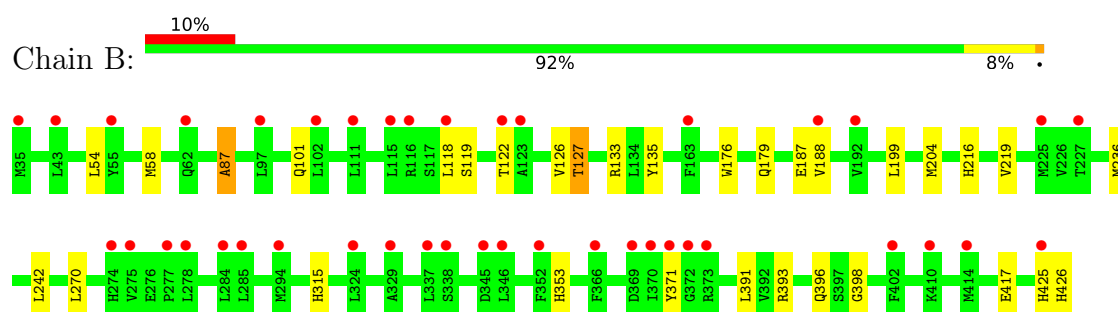
3 Residue-property plots [i](#)

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.

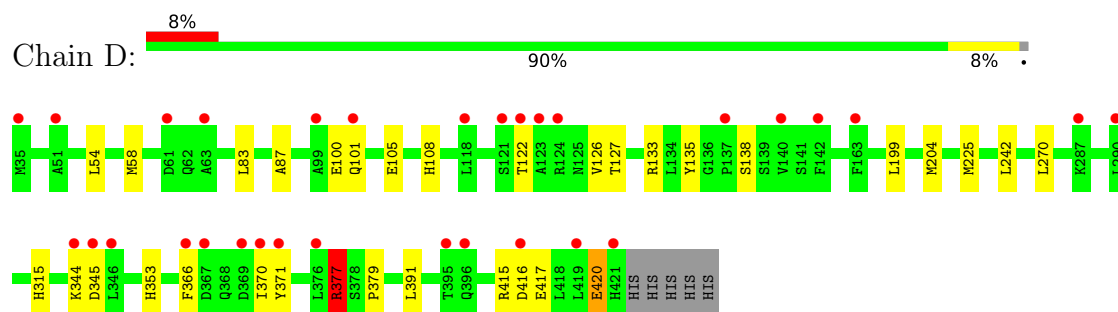
• Molecule 1: Serpin H1



• Molecule 1: Serpin H1

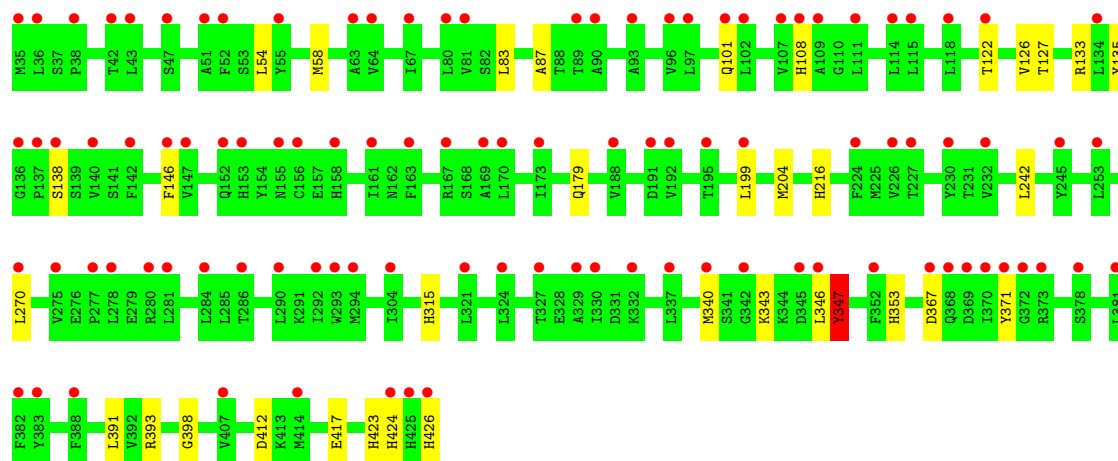


• Molecule 1: Serpin H1

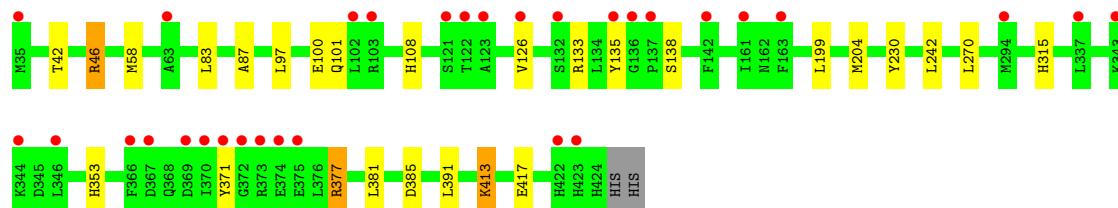
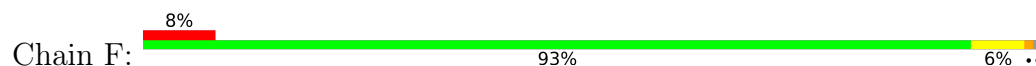


• Molecule 1: Serpin H1

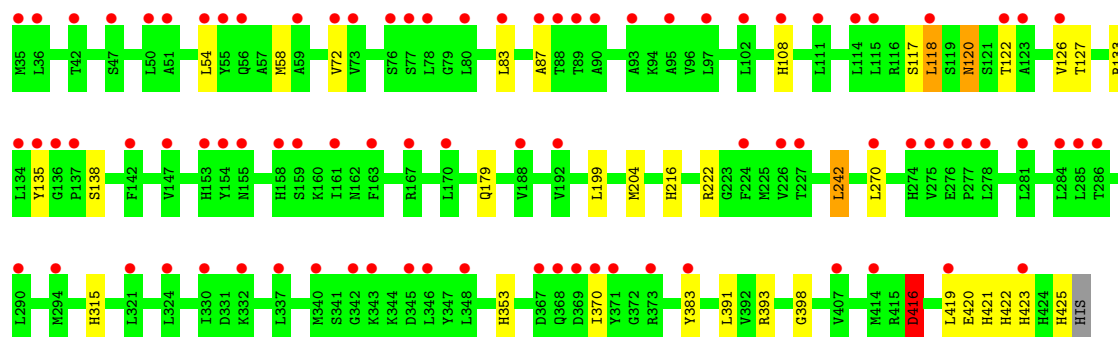
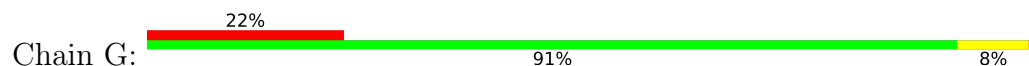




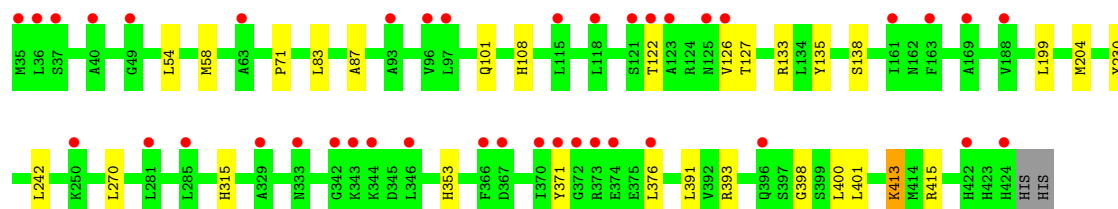
• Molecule 1: Serpin H1



• Molecule 1: Serpin H1

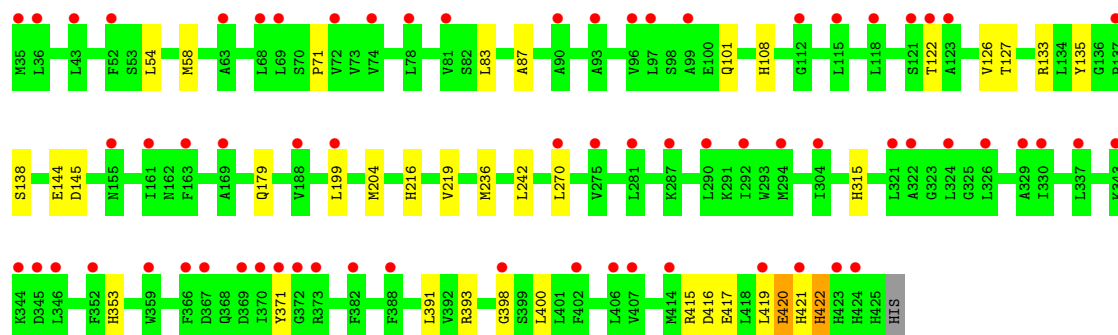


• Molecule 1: Serpin H1



● Molecule 1: Serpin H1

Chain I:  17% 90% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.30Å 92.00Å 123.58Å 85.23° 70.69° 83.23°	Depositor
Resolution (Å)	116.50 – 2.47 116.50 – 2.47	Depositor EDS
% Data completeness (in resolution range)	69.4 (116.50-2.47) 69.4 (116.50-2.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.243 , 0.264 (Not available) , 0.274	Depositor DCC
R_{free} test set	4465 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48565	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 ⓘ

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	0.79	3/3104 (0.1%)	1.03	1/4193 (0.0%)
1	B	0.81	2/3135 (0.1%)	1.04	1/4233 (0.0%)
1	D	0.79	2/3071 (0.1%)	1.03	0/4147
1	E	0.77	2/3128 (0.1%)	1.02	0/4224
1	F	0.78	2/3111 (0.1%)	1.02	0/4200
1	G	0.75	1/3101 (0.0%)	1.04	3/4190 (0.1%)
1	H	0.75	1/3105 (0.0%)	1.00	0/4193
1	I	0.76	2/3117 (0.1%)	1.04	6/4209 (0.1%)
All	All	0.78	15/24872 (0.1%)	1.03	11/33589 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ALA	CA-C	7.05	1.62	1.52
1	D	87	ALA	CA-C	6.73	1.61	1.52
1	I	87	ALA	CA-C	6.57	1.61	1.52
1	E	87	ALA	CA-C	6.29	1.61	1.52
1	G	87	ALA	CA-C	6.28	1.61	1.52
1	A	87	ALA	CA-C	6.21	1.61	1.52
1	H	87	ALA	CA-C	6.20	1.61	1.52
1	F	377	ARG	CA-C	6.02	1.60	1.52
1	D	377	ARG	CA-C	5.89	1.60	1.52
1	A	371	TYR	CA-C	5.79	1.56	1.52
1	A	377	ARG	CA-C	5.74	1.60	1.52
1	B	87	ALA	CA-C	5.49	1.60	1.52
1	B	127	THR	CA-C	5.47	1.60	1.52
1	E	347	TYR	CA-C	5.44	1.60	1.52
1	I	419	LEU	CA-C	5.16	1.59	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	ASN	CA-CB-CG	8.18	120.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	416	ASP	CA-CB-CG	7.00	119.60	112.60
1	I	419	LEU	CA-C-N	6.87	132.46	122.77
1	I	419	LEU	C-N-CA	6.87	132.46	122.77
1	I	145	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	188	VAL	N-CA-C	-6.11	105.18	110.74
1	I	144	GLU	CA-C-N	6.01	128.25	120.44
1	I	144	GLU	C-N-CA	6.01	128.25	120.44
1	A	417	GLU	CB-CG-CD	5.25	121.52	112.60
1	G	370	ILE	N-CA-C	-5.17	105.50	110.72
1	I	420	GLU	N-CA-C	-5.11	99.96	108.34

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	3039	3013	3013	9	0
1	B	3068	3047	3047	15	0
1	D	3009	2999	2999	12	0
1	E	3061	3037	3037	16	0
1	F	3046	3035	3035	12	0
1	G	3036	2991	2991	20	0
1	H	3041	3020	3020	13	0
1	I	3051	3027	3027	16	0
2	A	12	0	0	0	0
2	B	7	0	0	0	0
2	D	4	0	0	0	0
2	E	8	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	1	0	0	0	0
2	I	4	0	0	0	0
All	All	24396	24169	24169	105	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 (105) 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:E:58:MET:HE1	1:E:315:HIS:ND1	2.06	0.71
1:H:58:MET:HE1	1:H:315:HIS:ND1	2.06	0.70
1:I:58:MET:HE1	1:I:315:HIS:ND1	2.07	0.70
1:A:58:MET:HE1	1:A:315:HIS:ND1	2.07	0.69
1:D:58:MET:HE1	1:D:315:HIS:ND1	2.07	0.69
1:G:58:MET:HE1	1:G:315:HIS:ND1	2.07	0.68
1:H:230:TYR:OH	1:H:413:LYS:HD2	1.95	0.67
1:B:204:MET:HE1	1:B:353:HIS:CE1	2.35	0.61
1:F:42:THR:O	1:F:46:ARG:HD2	2.02	0.59
1:F:58:MET:HE1	1:F:315:HIS:ND1	2.16	0.59
1:F:385:ASP:OD2	1:G:422:HIS:HD2	1.87	0.58
1:H:122:THR:O	1:H:127:THR:OG1	2.21	0.58
1:E:122:THR:O	1:E:127:THR:OG1	2.22	0.57
1:I:421:HIS:O	1:I:422:HIS:HB2	2.05	0.56
1:B:58:MET:HE1	1:B:315:HIS:CD2	2.41	0.56
1:I:421:HIS:O	1:I:422:HIS:CB	2.56	0.54
1:D:122:THR:O	1:D:127:THR:OG1	2.26	0.53
1:G:423:HIS:ND1	1:G:425:HIS:CE1	2.76	0.53
1:G:117:SER:O	1:G:120:ASN:OD1	2.27	0.51
1:E:424:HIS:CE1	1:E:426:HIS:CD2	2.99	0.50
1:G:222:ARG:NH1	1:G:383:TYR:OH	2.38	0.50
1:G:122:THR:O	1:G:127:THR:OG1	2.30	0.50
1:E:346:LEU:O	1:E:347:TYR:O	2.29	0.49
1:H:58:MET:HE1	1:H:315:HIS:CG	2.46	0.49
1:A:122:THR:O	1:A:127:THR:OG1	2.31	0.49
1:F:58:MET:HE1	1:F:315:HIS:CG	2.47	0.49
1:I:122:THR:O	1:I:127:THR:OG1	2.30	0.49
1:A:58:MET:HE1	1:A:315:HIS:CG	2.48	0.49
1:G:179:GLN:HA	1:I:216:HIS:CE1	2.47	0.48
1:B:216:HIS:CE1	1:E:179:GLN:HA	2.47	0.48
1:G:58:MET:HE1	1:G:315:HIS:CG	2.48	0.48
1:D:58:MET:HE1	1:D:315:HIS:CG	2.48	0.47
1:E:58:MET:HE1	1:E:315:HIS:CG	2.48	0.47
1:G:83:LEU:HD13	1:G:108:HIS:CD2	2.49	0.47
1:B:58:MET:HE1	1:B:315:HIS:CG	2.50	0.47
1:I:58:MET:HE1	1:I:315:HIS:CG	2.49	0.47
1:H:393:ARG:NH1	1:H:398:GLY:O	2.47	0.47
1:B:58:MET:HE1	1:B:315:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:LEU:HD13	1:E:108:HIS:CD2	2.50	0.47
1:F:83:LEU:HD13	1:F:108:HIS:CD2	2.50	0.47
1:A:83:LEU:HD13	1:A:108:HIS:CD2	2.49	0.47
1:H:83:LEU:HD13	1:H:108:HIS:CD2	2.49	0.47
1:I:83:LEU:HD13	1:I:108:HIS:CD2	2.50	0.47
1:G:216:HIS:CE1	1:I:179:GLN:HA	2.50	0.46
1:D:83:LEU:HD13	1:D:108:HIS:CD2	2.50	0.46
1:E:54:LEU:O	1:E:58:MET:HG3	2.16	0.46
1:I:54:LEU:O	1:I:58:MET:HG3	2.16	0.46
1:B:58:MET:CE	1:B:315:HIS:CE1	3.00	0.45
1:A:54:LEU:O	1:A:58:MET:HG3	2.16	0.45
1:I:71:PRO:HG2	1:I:400:LEU:O	2.16	0.45
1:G:83:LEU:CD1	1:G:108:HIS:CD2	3.00	0.45
1:H:230:TYR:HH	1:H:413:LYS:HD2	1.80	0.45
1:A:83:LEU:CD1	1:A:108:HIS:CD2	2.99	0.45
1:G:54:LEU:O	1:G:58:MET:HG3	2.16	0.45
1:H:71:PRO:HD2	1:H:401:LEU:O	2.17	0.45
1:H:54:LEU:O	1:H:58:MET:HG3	2.17	0.45
1:H:83:LEU:CD1	1:H:108:HIS:CD2	3.00	0.45
1:D:344:LYS:HG2	1:D:345:ASP:N	2.31	0.44
1:I:83:LEU:CD1	1:I:108:HIS:CD2	3.01	0.44
1:F:46:ARG:HB3	1:F:97:LEU:O	2.17	0.44
1:I:393:ARG:NH1	1:I:398:GLY:O	2.51	0.44
1:E:83:LEU:CD1	1:E:108:HIS:CD2	3.00	0.44
1:A:377:ARG:O	1:A:379:PRO:HD3	2.18	0.44
1:F:83:LEU:CD1	1:F:108:HIS:CD2	3.01	0.44
1:F:381:LEU:HD11	1:G:421:HIS:CE1	2.53	0.43
1:D:225:MET:HE1	1:E:423:HIS:CE1	2.53	0.43
1:D:54:LEU:O	1:D:58:MET:HG3	2.18	0.43
1:E:146:PHE:CE2	1:E:340:MET:HG3	2.54	0.43
1:F:204:MET:HE1	1:F:353:HIS:CE1	2.54	0.43
1:G:204:MET:HE1	1:G:353:HIS:CE1	2.54	0.43
1:A:204:MET:HE1	1:A:353:HIS:CE1	2.53	0.42
1:A:270:LEU:HD12	1:A:270:LEU:N	2.35	0.42
1:B:425:HIS:O	1:B:426:HIS:HB2	2.19	0.42
1:D:83:LEU:CD1	1:D:108:HIS:CD2	3.01	0.42
1:B:133:ARG:HD3	1:B:135:TYR:CZ	2.54	0.42
1:D:204:MET:HE1	1:D:353:HIS:CE1	2.55	0.42
1:E:270:LEU:HD12	1:E:270:LEU:N	2.35	0.42
1:B:270:LEU:HD12	1:B:270:LEU:N	2.35	0.42
1:H:270:LEU:HD12	1:H:270:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:ARG:NH1	1:E:398:GLY:O	2.51	0.42
1:I:204:MET:HE1	1:I:353:HIS:CE1	2.55	0.42
1:D:270:LEU:N	1:D:270:LEU:HD12	2.35	0.42
1:G:270:LEU:HD12	1:G:270:LEU:N	2.35	0.42
1:H:204:MET:HE1	1:H:353:HIS:CE1	2.54	0.42
1:E:204:MET:HE1	1:E:353:HIS:CE1	2.54	0.42
1:E:133:ARG:HD3	1:E:135:TYR:CZ	2.55	0.41
1:F:270:LEU:HD12	1:F:270:LEU:N	2.35	0.41
1:B:393:ARG:NH1	1:B:398:GLY:O	2.53	0.41
1:G:72:VAL:HG21	1:G:118:LEU:HD21	2.01	0.41
1:G:133:ARG:HD3	1:G:135:TYR:CZ	2.55	0.41
1:G:416:ASP:O	1:G:419:LEU:HG	2.20	0.41
1:B:425:HIS:ND1	1:G:242:LEU:HD11	2.35	0.41
1:B:122:THR:O	1:B:127:THR:OG1	2.38	0.41
1:F:230:TYR:CE1	1:F:413:LYS:HG3	2.56	0.41
1:H:133:ARG:HD3	1:H:135:TYR:CZ	2.55	0.41
1:B:179:GLN:HA	1:E:216:HIS:CE1	2.56	0.41
1:B:219:VAL:HA	1:B:236:MET:O	2.21	0.41
1:D:133:ARG:HD3	1:D:135:TYR:CZ	2.56	0.41
1:D:377:ARG:O	1:D:379:PRO:HD3	2.21	0.41
1:F:133:ARG:HD3	1:F:135:TYR:CZ	2.56	0.41
1:I:133:ARG:HD3	1:I:135:TYR:CZ	2.55	0.41
1:I:219:VAL:HA	1:I:236:MET:O	2.21	0.41
1:I:270:LEU:N	1:I:270:LEU:HD12	2.35	0.41
1:B:133:ARG:HB2	1:B:176:TRP:CZ2	2.56	0.40
1:G:393:ARG:NH1	1:G:398:GLY:O	2.54	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	388/392 (99%)	360 (93%)	26 (7%)	2 (0%)	24	40
1	B	390/392 (100%)	364 (93%)	25 (6%)	1 (0%)	36	53
1	D	385/392 (98%)	350 (91%)	32 (8%)	3 (1%)	16	28
1	E	390/392 (100%)	359 (92%)	29 (7%)	2 (0%)	24	40
1	F	388/392 (99%)	362 (93%)	25 (6%)	1 (0%)	36	53
1	G	389/392 (99%)	363 (93%)	26 (7%)	0	100	100
1	H	388/392 (99%)	362 (93%)	26 (7%)	0	100	100
1	I	389/392 (99%)	364 (94%)	24 (6%)	1 (0%)	36	53
All	All	3107/3136 (99%)	2884 (93%)	213 (7%)	10 (0%)	36	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	347	TYR
1	I	422	HIS
1	A	377	ARG
1	B	87	ALA
1	D	377	ARG
1	F	377	ARG
1	D	420	GLU
1	E	367	ASP
1	A	344	LYS
1	D	370	ILE

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	322/337 (96%)	311 (97%)	11 (3%)	32	57
1	B	326/337 (97%)	314 (96%)	12 (4%)	30	54
1	D	319/337 (95%)	305 (96%)	14 (4%)	25	47
1	E	325/337 (96%)	314 (97%)	11 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	323/337 (96%)	312 (97%)	11 (3%)	32	57
1	G	320/337 (95%)	312 (98%)	8 (2%)	42	66
1	H	322/337 (96%)	311 (97%)	11 (3%)	32	57
1	I	323/337 (96%)	312 (97%)	11 (3%)	32	57
All	All	2580/2696 (96%)	2491 (97%)	89 (3%)	32	57

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	105	GLU
1	A	126	VAL
1	A	138	SER
1	A	199	LEU
1	A	242	LEU
1	A	341	SER
1	A	371	TYR
1	A	391	LEU
1	A	415	ARG
1	A	417	GLU
1	B	54	LEU
1	B	101	GLN
1	B	118	LEU
1	B	119	SER
1	B	126	VAL
1	B	187	GLU
1	B	199	LEU
1	B	242	LEU
1	B	371	TYR
1	B	391	LEU
1	B	396	GLN
1	B	417	GLU
1	D	100	GLU
1	D	101	GLN
1	D	105	GLU
1	D	126	VAL
1	D	138	SER
1	D	199	LEU
1	D	242	LEU
1	D	366	PHE
1	D	371	TYR

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Mol	Chain	Res	Type
1	D	391	LEU
1	D	415	ARG
1	D	416	ASP
1	D	417	GLU
1	D	420	GLU
1	E	101	GLN
1	E	126	VAL
1	E	138	SER
1	E	199	LEU
1	E	242	LEU
1	E	343	LYS
1	E	347	TYR
1	E	371	TYR
1	E	391	LEU
1	E	412	ASP
1	E	417	GLU
1	F	46	ARG
1	F	100	GLU
1	F	101	GLN
1	F	126	VAL
1	F	138	SER
1	F	199	LEU
1	F	242	LEU
1	F	371	TYR
1	F	391	LEU
1	F	413	LYS
1	F	417	GLU
1	G	118	LEU
1	G	126	VAL
1	G	138	SER
1	G	199	LEU
1	G	242	LEU
1	G	391	LEU
1	G	416	ASP
1	G	420	GLU
1	H	101	GLN
1	H	126	VAL
1	H	138	SER
1	H	199	LEU
1	H	242	LEU
1	H	371	TYR
1	H	376	LEU

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Mol	Chain	Res	Type
1	H	391	LEU
1	H	400	LEU
1	H	413	LYS
1	H	415	ARG
1	I	101	GLN
1	I	126	VAL
1	I	138	SER
1	I	199	LEU
1	I	242	LEU
1	I	371	TYR
1	I	391	LEU
1	I	415	ARG
1	I	416	ASP
1	I	417	GLU
1	I	420	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	353	HIS
1	B	158	HIS
1	B	353	HIS
1	B	421	HIS
1	B	422	HIS
1	B	426	HIS
1	D	353	HIS
1	E	353	HIS
1	F	101	GLN
1	F	318	GLN
1	F	353	HIS
1	F	422	HIS
1	G	162	ASN
1	G	353	HIS
1	G	422	HIS
1	G	425	HIS
1	H	171	GLN
1	H	353	HIS
1	H	422	HIS
1	I	171	GLN
1	I	353	HIS
1	I	422	HIS

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Mol	Chain	Res	Type
1	I	425	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, 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	390/392 (99%)	0.65	39 (10%)	12 10	15, 31, 59, 72	0
1	B	392/392 (100%)	0.88	41 (10%)	11 9	15, 36, 56, 72	0
1	D	387/392 (98%)	0.69	31 (8%)	18 16	16, 32, 56, 72	0
1	E	392/392 (100%)	1.35	102 (26%)	1 1	15, 40, 63, 82	0
1	F	390/392 (99%)	0.66	31 (7%)	18 16	17, 32, 62, 75	0
1	G	391/392 (99%)	1.22	87 (22%)	2 2	15, 41, 73, 91	0
1	H	390/392 (99%)	0.87	40 (10%)	12 10	19, 37, 62, 77	0
1	I	391/392 (99%)	1.18	68 (17%)	4 3	20, 41, 63, 76	0
All	All	3123/3136 (99%)	0.94	439 (14%)	6 5	15, 36, 63, 91	0

All (439) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	118	LEU	5.2
1	E	163	PHE	5.0
1	I	345	ASP	4.9
1	B	371	TYR	4.7
1	I	371	TYR	4.6
1	A	345	ASP	4.5
1	I	321	LEU	4.5
1	D	345	ASP	4.4
1	F	123	ALA	4.4
1	E	371	TYR	4.4
1	E	167	ARG	4.3
1	G	122	THR	4.3
1	E	346	LEU	4.3
1	I	370	ILE	4.2
1	D	371	TYR	4.1
1	E	370	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	51	ALA	4.0
1	G	371	TYR	4.0
1	D	140	VAL	4.0
1	H	373	ARG	4.0
1	G	93	ALA	3.9
1	I	163	PHE	3.9
1	I	369	ASP	3.9
1	E	81	VAL	3.8
1	E	278	LEU	3.8
1	H	374	GLU	3.7
1	D	419	LEU	3.7
1	E	102	LEU	3.7
1	I	346	LEU	3.7
1	H	342	GLY	3.7
1	G	80	LEU	3.7
1	G	102	LEU	3.7
1	A	373	ARG	3.6
1	E	55	TYR	3.6
1	E	138	SER	3.6
1	B	163	PHE	3.6
1	E	372	GLY	3.6
1	F	126	VAL	3.6
1	H	63	ALA	3.6
1	E	140	VAL	3.5
1	H	367	ASP	3.5
1	D	421	HIS	3.5
1	E	373	ARG	3.4
1	I	372	GLY	3.4
1	F	163	PHE	3.4
1	F	136	GLY	3.4
1	H	123	ALA	3.4
1	F	373	ARG	3.4
1	D	123	ALA	3.4
1	G	348	LEU	3.3
1	E	90	ALA	3.3
1	G	161	ILE	3.3
1	A	369	ASP	3.3
1	H	396	GLN	3.3
1	E	284	LEU	3.3
1	E	122	THR	3.3
1	E	321	LEU	3.3
1	G	419	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	226	VAL	3.3
1	I	419	LEU	3.2
1	E	142	PHE	3.2
1	E	290	LEU	3.2
1	H	370	ILE	3.2
1	E	111	LEU	3.1
1	E	192	VAL	3.1
1	E	109	ALA	3.1
1	E	108	HIS	3.1
1	A	118	LEU	3.1
1	G	163	PHE	3.1
1	B	122	THR	3.1
1	G	115	LEU	3.1
1	G	35	MET	3.0
1	H	35	MET	3.0
1	I	118	LEU	3.0
1	E	369	ASP	3.0
1	I	96	VAL	3.0
1	E	329	ALA	3.0
1	I	99	ALA	3.0
1	A	374	GLU	3.0
1	B	115	LEU	3.0
1	H	163	PHE	3.0
1	I	122	THR	3.0
1	A	340	MET	3.0
1	I	68	LEU	3.0
1	I	366	PHE	3.0
1	D	101	GLN	3.0
1	E	294	MET	3.0
1	I	123	ALA	3.0
1	E	115	LEU	3.0
1	G	97	LEU	3.0
1	I	97	LEU	3.0
1	E	155	ASN	3.0
1	H	126	VAL	2.9
1	G	369	ASP	2.9
1	G	192	VAL	2.9
1	I	423	HIS	2.9
1	H	122	THR	2.9
1	G	324	LEU	2.9
1	I	36	LEU	2.9
1	D	367	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	112	GLY	2.9
1	F	370	ILE	2.9
1	G	111	LEU	2.9
1	H	346	LEU	2.9
1	D	163	PHE	2.9
1	F	371	TYR	2.9
1	I	281	LEU	2.8
1	A	163	PHE	2.8
1	E	352	PHE	2.8
1	B	35	MET	2.8
1	E	191	ASP	2.8
1	E	188	VAL	2.8
1	A	63	ALA	2.8
1	E	170	LEU	2.8
1	E	146	PHE	2.8
1	E	153	HIS	2.8
1	G	142	PHE	2.8
1	G	155	ASN	2.8
1	E	275	VAL	2.8
1	E	97	LEU	2.8
1	A	35	MET	2.8
1	E	340	MET	2.8
1	G	414	MET	2.8
1	F	422	HIS	2.8
1	I	275	VAL	2.7
1	B	337	LEU	2.7
1	G	285	LEU	2.7
1	B	274	HIS	2.7
1	A	372	GLY	2.7
1	B	370	ILE	2.7
1	A	111	LEU	2.7
1	E	152	GLN	2.7
1	E	161	ILE	2.7
1	E	232	VAL	2.7
1	E	281	LEU	2.7
1	G	340	MET	2.7
1	E	89	THR	2.7
1	I	398	GLY	2.7
1	E	67	ILE	2.7
1	D	344	LYS	2.7
1	B	97	LEU	2.7
1	D	118	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	73	VAL	2.7
1	I	329	ALA	2.7
1	E	367	ASP	2.6
1	B	366	PHE	2.6
1	E	292	ILE	2.6
1	H	343	LYS	2.6
1	E	36	LEU	2.6
1	G	275	VAL	2.6
1	A	90	ALA	2.6
1	G	42	THR	2.6
1	H	371	TYR	2.6
1	G	423	HIS	2.6
1	E	345	ASP	2.6
1	G	330	ILE	2.6
1	B	414	MET	2.6
1	B	284	LEU	2.6
1	E	199	LEU	2.6
1	G	346	LEU	2.6
1	I	78	LEU	2.6
1	I	199	LEU	2.6
1	E	42	THR	2.6
1	E	63	ALA	2.6
1	G	277	PRO	2.6
1	G	370	ILE	2.6
1	B	346	LEU	2.6
1	G	134	LEU	2.6
1	G	72	VAL	2.6
1	E	414	MET	2.6
1	F	161	ILE	2.6
1	A	366	PHE	2.6
1	D	366	PHE	2.6
1	G	321	LEU	2.6
1	E	368	GLN	2.6
1	H	188	VAL	2.6
1	I	74	VAL	2.6
1	A	329	ALA	2.6
1	D	63	ALA	2.6
1	B	373	ARG	2.5
1	B	369	ASP	2.5
1	G	136	GLY	2.5
1	I	402	PHE	2.5
1	I	290	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.5
1	E	286	THR	2.5
1	G	55	TYR	2.5
1	B	345	ASP	2.5
1	A	115	LEU	2.5
1	B	43	LEU	2.5
1	I	324	LEU	2.5
1	H	424	HIS	2.5
1	G	373	ARG	2.5
1	H	372	GLY	2.5
1	E	253	LEU	2.5
1	I	69	LEU	2.5
1	F	344	LYS	2.5
1	B	192	VAL	2.5
1	E	107	VAL	2.5
1	I	63	ALA	2.5
1	G	77	SER	2.5
1	D	370	ILE	2.5
1	A	80	LEU	2.5
1	B	324	LEU	2.5
1	G	54	LEU	2.5
1	G	83	LEU	2.5
1	F	423	HIS	2.5
1	A	107	VAL	2.5
1	I	72	VAL	2.5
1	A	48	ALA	2.5
1	D	287	LYS	2.4
1	G	154	TYR	2.4
1	I	343	LYS	2.4
1	D	124	ARG	2.4
1	G	147	VAL	2.4
1	B	329	ALA	2.4
1	H	329	ALA	2.4
1	E	227	THR	2.4
1	B	410	LYS	2.4
1	D	369	ASP	2.4
1	E	330	ILE	2.4
1	I	367	ASP	2.4
1	G	281	LEU	2.4
1	G	158	HIS	2.4
1	A	148	ARG	2.4
1	E	35	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	125	ASN	2.4
1	F	137	PRO	2.4
1	H	250	LYS	2.4
1	F	372	GLY	2.4
1	G	170	LEU	2.4
1	G	274	HIS	2.4
1	A	371	TYR	2.4
1	D	99	ALA	2.4
1	E	93	ALA	2.4
1	G	87	ALA	2.4
1	I	90	ALA	2.4
1	A	343	LYS	2.4
1	A	36	LEU	2.4
1	E	80	LEU	2.4
1	G	278	LEU	2.4
1	E	245	TYR	2.4
1	D	35	MET	2.4
1	G	224	PHE	2.4
1	H	96	VAL	2.4
1	G	47	SER	2.3
1	B	285	LEU	2.3
1	I	294	MET	2.3
1	A	142	PHE	2.3
1	F	142	PHE	2.3
1	F	366	PHE	2.3
1	B	275	VAL	2.3
1	H	169	ALA	2.3
1	G	89	THR	2.3
1	G	227	THR	2.3
1	E	378	SER	2.3
1	G	167	ARG	2.3
1	H	121	SER	2.3
1	E	114	LEU	2.3
1	G	118	LEU	2.3
1	G	343	LYS	2.3
1	G	135	TYR	2.3
1	F	375	GLU	2.3
1	A	123	ALA	2.3
1	D	51	ALA	2.3
1	E	137	PRO	2.3
1	E	293	TRP	2.3
1	A	330	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	134	LEU	2.3
1	F	102	LEU	2.3
1	H	285	LEU	2.3
1	H	344	LYS	2.3
1	E	224	PHE	2.3
1	B	55	TYR	2.3
1	B	277	PRO	2.3
1	E	277	PRO	2.3
1	F	63	ALA	2.3
1	G	137	PRO	2.3
1	B	111	LEU	2.3
1	H	376	LEU	2.3
1	I	304	ILE	2.3
1	B	402	PHE	2.3
1	E	388	PHE	2.3
1	H	366	PHE	2.3
1	I	352	PHE	2.3
1	G	407	VAL	2.3
1	E	38	PRO	2.3
1	E	230	TYR	2.3
1	G	51	ALA	2.2
1	G	95	ALA	2.2
1	E	425	HIS	2.2
1	E	381	LEU	2.2
1	F	132	SER	2.2
1	G	78	LEU	2.2
1	G	114	LEU	2.2
1	G	337	LEU	2.2
1	I	414	MET	2.2
1	G	367	ASP	2.2
1	E	382	PHE	2.2
1	G	90	ALA	2.2
1	I	93	ALA	2.2
1	G	368	GLN	2.2
1	I	421	HIS	2.2
1	F	343	LYS	2.2
1	G	332	LYS	2.2
1	B	118	LEU	2.2
1	B	294	MET	2.2
1	I	35	MET	2.2
1	F	374	GLU	2.2
1	I	388	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	188	VAL	2.2
1	G	123	ALA	2.2
1	B	62	GLN	2.2
1	E	158	HIS	2.2
1	B	227	THR	2.2
1	D	396	GLN	2.2
1	A	346	LEU	2.2
1	E	337	LEU	2.2
1	F	337	LEU	2.2
1	I	270	LEU	2.2
1	A	370	ILE	2.2
1	B	338	SER	2.2
1	E	280	ARG	2.2
1	I	137	PRO	2.2
1	B	123	ALA	2.2
1	F	35	MET	2.2
1	G	294	MET	2.2
1	D	395	THR	2.2
1	G	88	THR	2.2
1	E	43	LEU	2.2
1	E	324	LEU	2.2
1	E	383	TYR	2.2
1	H	115	LEU	2.2
1	I	359	TRP	2.2
1	E	64	VAL	2.1
1	E	96	VAL	2.1
1	I	188	VAL	2.1
1	G	59	ALA	2.1
1	G	153	HIS	2.1
1	B	278	LEU	2.1
1	E	195	THR	2.1
1	H	36	LEU	2.1
1	H	97	LEU	2.1
1	I	406	LEU	2.1
1	H	161	ILE	2.1
1	F	369	ASP	2.1
1	E	169	ALA	2.1
1	H	40	ALA	2.1
1	A	337	LEU	2.1
1	B	102	LEU	2.1
1	B	372	GLY	2.1
1	D	290	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	270	LEU	2.1
1	G	290	LEU	2.1
1	H	118	LEU	2.1
1	A	375	GLU	2.1
1	G	383	TYR	2.1
1	D	416	ASP	2.1
1	F	121	SER	2.1
1	F	367	ASP	2.1
1	H	37	SER	2.1
1	D	137	PRO	2.1
1	G	108	HIS	2.1
1	H	422	HIS	2.1
1	I	424	HIS	2.1
1	E	147	VAL	2.1
1	G	56	GLN	2.1
1	I	81	VAL	2.1
1	I	155	ASN	2.1
1	A	102	LEU	2.1
1	F	346	LEU	2.1
1	F	122	THR	2.1
1	H	49	GLY	2.1
1	I	115	LEU	2.1
1	A	393	ARG	2.1
1	I	373	ARG	2.1
1	G	76	SER	2.1
1	E	426	HIS	2.1
1	B	188	VAL	2.1
1	G	126	VAL	2.1
1	H	93	ALA	2.1
1	I	322	ALA	2.1
1	D	346	LEU	2.1
1	D	376	LEU	2.1
1	G	50	LEU	2.1
1	I	326	LEU	2.1
1	E	136	GLY	2.1
1	G	342	GLY	2.1
1	A	122	THR	2.1
1	D	122	THR	2.1
1	G	286	THR	2.1
1	I	161	ILE	2.1
1	I	292	ILE	2.1
1	G	345	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	121	SER	2.1
1	E	156	CYS	2.1
1	D	142	PHE	2.0
1	I	52	PHE	2.0
1	A	339	ARG	2.0
1	B	116	ARG	2.0
1	F	103	ARG	2.0
1	E	270	LEU	2.0
1	G	36	LEU	2.0
1	H	281	LEU	2.0
1	H	333	ASN	2.0
1	I	43	LEU	2.0
1	G	276	GLU	2.0
1	E	304	ILE	2.0
1	E	332	LYS	2.0
1	I	287	LYS	2.0
1	D	61	ASP	2.0
1	A	38	PRO	2.0
1	D	121	SER	2.0
1	E	47	SER	2.0
1	F	294	MET	2.0
1	G	159	SER	2.0
1	A	274	HIS	2.0
1	B	425	HIS	2.0
1	E	424	HIS	2.0
1	E	101	GLN	2.0
1	A	147	VAL	2.0
1	B	352	PHE	2.0
1	E	52	PHE	2.0
1	E	407	VAL	2.0
1	G	226	VAL	2.0
1	I	382	PHE	2.0
1	I	407	VAL	2.0
1	G	284	LEU	2.0
1	I	169	ALA	2.0
1	I	337	LEU	2.0
1	A	110	GLY	2.0
1	E	342	GLY	2.0
1	I	344	LYS	2.0
1	E	173	ILE	2.0
1	E	327	THR	2.0
1	I	330	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	225	MET	2.0
1	A	108	HIS	2.0
1	F	135	TYR	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.