



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:39 AM EDT

PDB ID : 9CQF / pdb_00009cqf
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 ⓘ 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

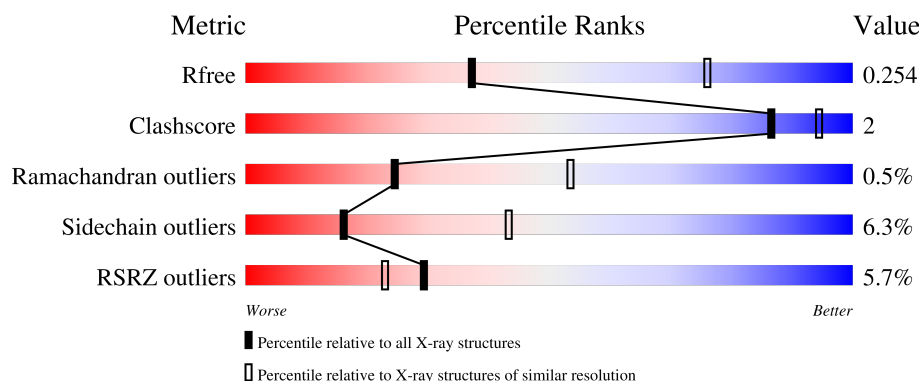
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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 $\leq 5\%$. 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	4% 88% 10% ..
1	B	392	4% 88% 10% ..
1	D	392	3% 87% 12% .
1	E	392	3% 88% 9% ..
1	F	392	4% 88% 11% .

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Mol	Chain	Length	Quality of chain
1	G	392	7% 88% 10% ..
1	H	392	7% 87% 11% ..
1	I	392	13% 89% 9% ..

2 Entry composition

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.

- Molecule 1 is a protein called Serpin H1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	H	N	O	S	3002	0	0
			6011	1914	3002	525	556	14			
1	B	388	Total	C	H	N	O	S	3016	0	0
			6037	1922	3016	528	557	14			
1	D	390	Total	C	H	N	O	S	3028	0	0
			6069	1933	3028	534	560	14			
1	E	387	Total	C	H	N	O	S	3009	0	0
			6018	1912	3009	525	558	14			
1	F	388	Total	C	H	N	O	S	3020	0	0
			6051	1926	3020	530	561	14			
1	G	387	Total	C	H	N	O	S	3007	0	0
			6016	1913	3007	527	555	14			
1	H	387	Total	C	H	N	O	S	3002	0	0
			6006	1910	3002	525	555	14			
1	I	387	Total	C	H	N	O	S	3009	0	0
			6020	1916	3009	525	556	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

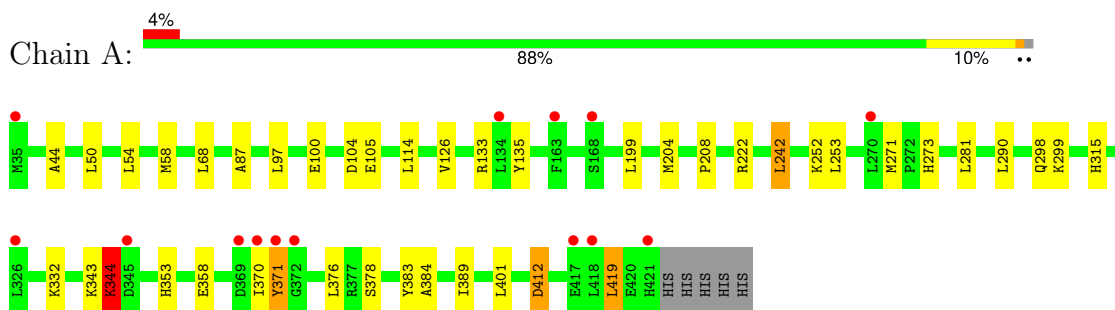
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0
2	E	2	Total O 2 2	0	0
2	F	1	Total O 1 1	0	0

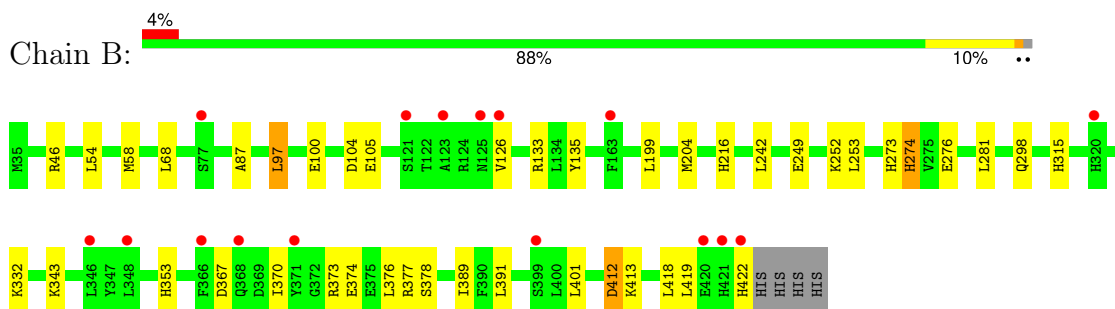
3 Residue-property plots [i](#)

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.

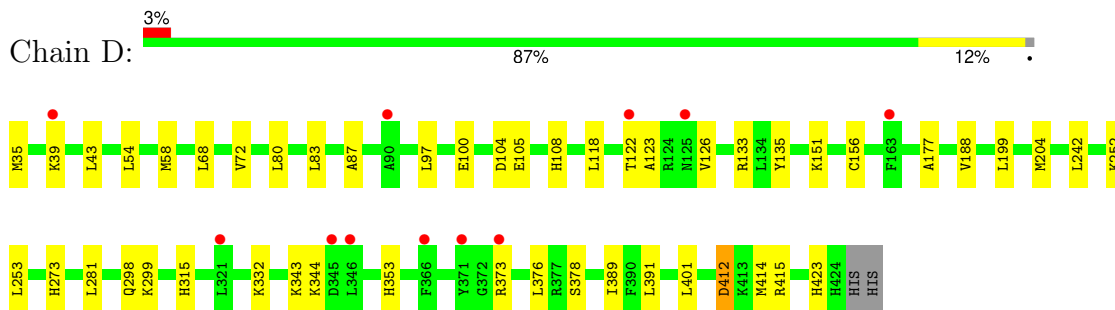
• Molecule 1: Serpin H1



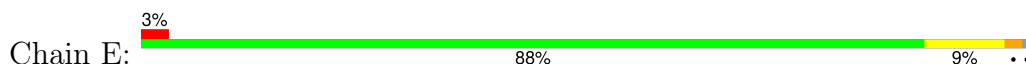
• Molecule 1: Serpin H1

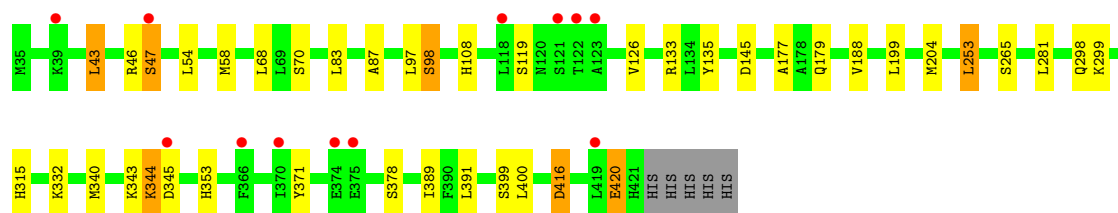


• Molecule 1: Serpin H1

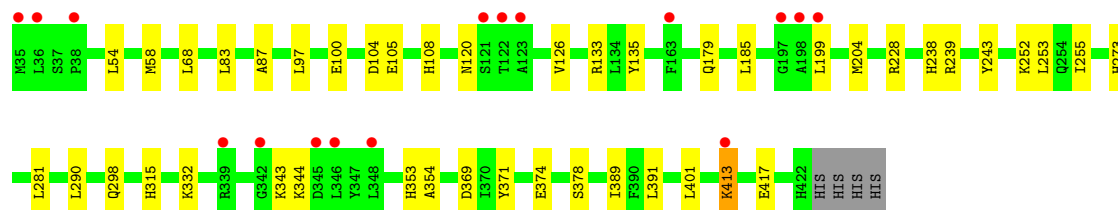
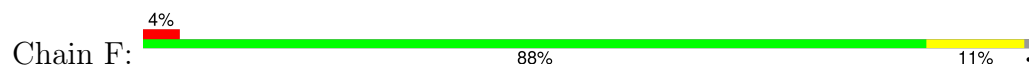


• Molecule 1: Serpin H1

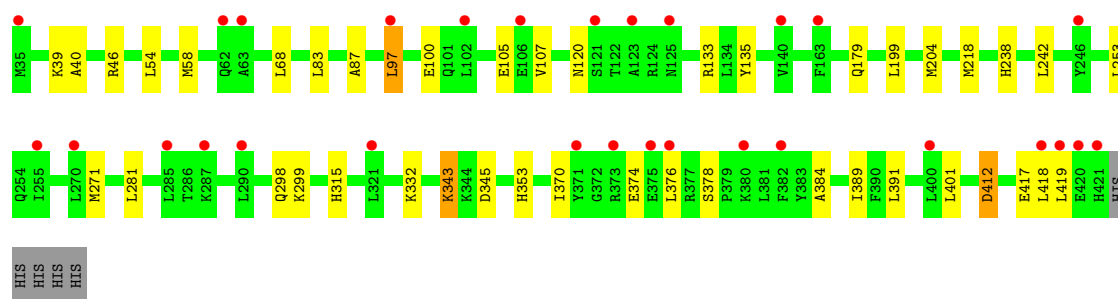
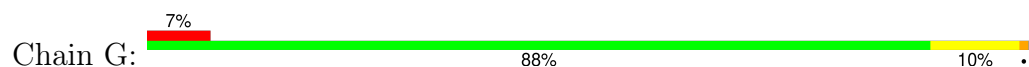




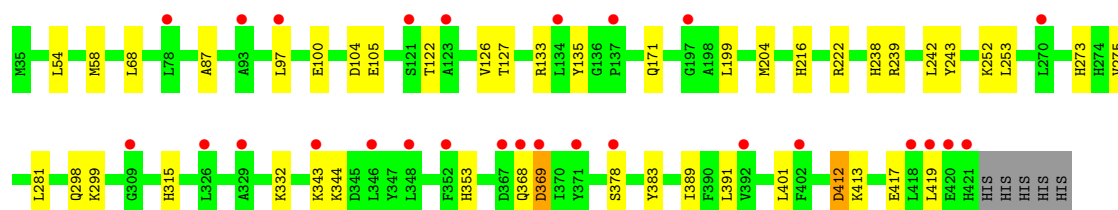
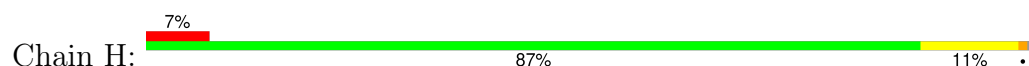
• Molecule 1: Serpin H1



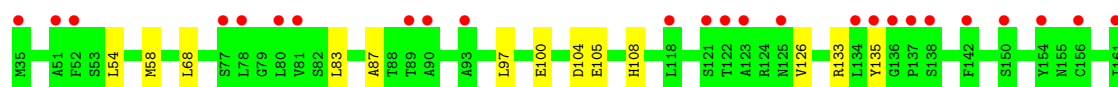
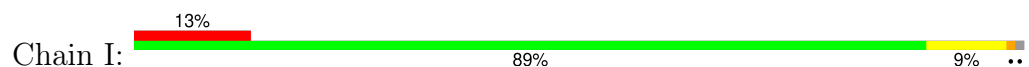
• Molecule 1: Serpin H1

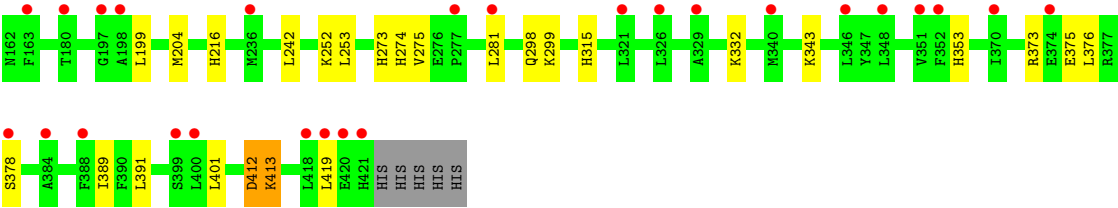


• Molecule 1: Serpin H1



• Molecule 1: Serpin H1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.78Å 129.94Å 501.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	250.97 – 2.93 250.97 – 2.93	Depositor EDS
% Data completeness (in resolution range)	76.0 (250.97-2.93) 76.0 (250.97-2.93)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.228 , 0.252 0.231 , 0.254	Depositor 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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	0.84	2/3070 (0.1%)	1.06	4/4144 (0.1%)
1	B	0.78	3/3083 (0.1%)	1.03	2/4162 (0.0%)
1	D	0.83	2/3105 (0.1%)	1.05	3/4192 (0.1%)
1	E	0.86	3/3069 (0.1%)	1.07	2/4142 (0.0%)
1	F	0.78	2/3094 (0.1%)	1.03	2/4176 (0.0%)
1	G	0.77	3/3070 (0.1%)	1.04	3/4144 (0.1%)
1	H	0.75	2/3064 (0.1%)	1.02	2/4136 (0.0%)
1	I	0.74	1/3072 (0.0%)	1.01	2/4147 (0.0%)
All	All	0.80	18/24627 (0.1%)	1.04	20/33243 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	87	ALA	CA-C	9.51	1.61	1.53
1	A	87	ALA	CA-C	9.33	1.61	1.53
1	I	87	ALA	CA-C	9.20	1.61	1.53
1	F	87	ALA	CA-C	9.07	1.61	1.53
1	B	87	ALA	CA-C	8.39	1.60	1.53
1	D	87	ALA	CA-C	8.38	1.60	1.53
1	G	87	ALA	CA-C	8.35	1.60	1.53
1	E	87	ALA	CA-C	6.82	1.59	1.53
1	E	126	VAL	CA-C	6.06	1.59	1.52
1	G	345	ASP	CA-C	5.88	1.60	1.52
1	A	126	VAL	CA-C	5.63	1.58	1.52
1	H	126	VAL	CA-C	5.61	1.58	1.52
1	B	370	ILE	CA-C	5.50	1.58	1.52
1	E	345	ASP	CA-C	5.45	1.60	1.52
1	F	126	VAL	CA-C	5.30	1.58	1.52
1	B	126	VAL	CA-C	5.25	1.58	1.52
1	G	345	ASP	C-N	5.02	1.40	1.33
1	D	123	ALA	CA-C	5.00	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASP	CA-CB-CG	8.56	121.16	112.60
1	E	416	ASP	CA-CB-CG	7.79	120.39	112.60
1	I	412	ASP	CA-CB-CG	7.55	120.15	112.60
1	G	412	ASP	CA-CB-CG	7.28	119.88	112.60
1	H	412	ASP	CA-CB-CG	7.12	119.72	112.60
1	D	412	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	412	ASP	CA-CB-CG	6.29	118.89	112.60
1	F	120	ASN	CA-CB-CG	5.88	118.48	112.60
1	G	120	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	370	ILE	N-CA-C	-5.84	106.12	111.67
1	E	126	VAL	CB-CA-C	5.72	116.14	111.05
1	A	126	VAL	CB-CA-C	5.56	116.00	111.05
1	B	126	VAL	CB-CA-C	5.50	115.95	111.05
1	A	419	LEU	N-CA-C	-5.47	96.36	107.41
1	F	126	VAL	CB-CA-C	5.47	115.92	111.05
1	D	126	VAL	CB-CA-C	5.44	115.89	111.05
1	H	126	VAL	CB-CA-C	5.36	115.82	111.05
1	G	107	VAL	N-CA-C	-5.34	105.88	110.74
1	I	126	VAL	CB-CA-C	5.26	115.73	111.05
1	D	122	THR	N-CA-C	5.03	116.90	110.61

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	3009	3002	3002	14	0
1	B	3021	3016	3016	11	0
1	D	3041	3028	3028	14	0
1	E	3009	3009	3009	14	0
1	F	3031	3020	3020	17	0
1	G	3009	3007	3007	14	0
1	H	3004	3002	3002	17	0
1	I	3011	3009	3009	12	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	1	0	0	0	0
All	All	24142	24093	24093	102	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 (102) 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:D:58:MET:HE1	1:D:315:HIS:ND1	2.14	0.62
1:A:58:MET:HE1	1:A:315:HIS:ND1	2.15	0.62
1:F:58:MET:HE1	1:F:315:HIS:ND1	2.14	0.62
1:H:58:MET:HE1	1:H:315:HIS:ND1	2.15	0.61
1:E:58:MET:HE1	1:E:315:HIS:ND1	2.15	0.61
1:I:58:MET:HE1	1:I:315:HIS:ND1	2.16	0.61
1:G:58:MET:HE1	1:G:315:HIS:ND1	2.16	0.61
1:D:83:LEU:HD13	1:D:108:HIS:CD2	2.36	0.60
1:B:58:MET:HE1	1:B:315:HIS:ND1	2.16	0.59
1:A:273:HIS:NE2	1:F:228:ARG:NH1	2.52	0.57
1:E:58:MET:HE1	1:E:315:HIS:CG	2.40	0.56
1:A:58:MET:HE1	1:A:315:HIS:CG	2.42	0.54
1:D:58:MET:HE1	1:D:315:HIS:CG	2.42	0.54
1:F:58:MET:HE1	1:F:315:HIS:CG	2.42	0.54
1:B:58:MET:HE1	1:B:315:HIS:CG	2.43	0.54
1:I:58:MET:HE1	1:I:315:HIS:CG	2.43	0.54
1:E:204:MET:HE1	1:E:353:HIS:CE1	2.43	0.54
1:H:58:MET:HE1	1:H:315:HIS:CG	2.42	0.54
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:G:58:MET:HE1	1:G:315:HIS:CG	2.44	0.52
1:G:204:MET:HE1	1:G:353:HIS:CE1	2.45	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:B:204:MET:HE1	1:B:353:HIS:CE1	2.46	0.51
1:I:204:MET:HE1	1:I:353:HIS:CE1	2.46	0.50
1:H:204:MET:HE1	1:H:353:HIS:CE1	2.45	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MET:HE1	1:A:353:HIS:CE1	2.47	0.50
1:A:54:LEU:O	1:A:58:MET:HG3	2.13	0.49
1:F:204:MET:HE1	1:F:353:HIS:CE1	2.46	0.49
1:D:83:LEU:CD1	1:D:108:HIS:CD2	2.94	0.49
1:D:204:MET:HE1	1:D:353:HIS:CE1	2.47	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: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
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:171:GLN:HE21	1:I:413:LYS:HZ1	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:343:LYS:NZ	1:G:343:LYS:HB3	2.37	0.40
1:H:171:GLN:NE2	1:I:413:LYS:HZ1	2.18	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:G:218:MET:HE1	1:H:417:GLU:O	2.20	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 ⓘ

5.3.1 Protein backbone ⓘ

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	385/392 (98%)	363 (94%)	21 (6%)	1 (0%)	36	64
1	B	386/392 (98%)	357 (92%)	25 (6%)	4 (1%)	12	37
1	D	388/392 (99%)	362 (93%)	25 (6%)	1 (0%)	36	64
1	E	385/392 (98%)	354 (92%)	29 (8%)	2 (0%)	24	53
1	F	386/392 (98%)	361 (94%)	24 (6%)	1 (0%)	36	64
1	G	385/392 (98%)	355 (92%)	28 (7%)	2 (0%)	24	53
1	H	385/392 (98%)	361 (94%)	22 (6%)	2 (0%)	24	53
1	I	385/392 (98%)	353 (92%)	29 (8%)	3 (1%)	16	43
All	All	3085/3136 (98%)	2866 (93%)	203 (7%)	16 (0%)	24	53

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	371	TYR
1	A	344	LYS
1	B	367	ASP
1	B	373	ARG
1	E	420	GLU
1	I	373	ARG
1	B	374	GLU
1	F	369	ASP
1	G	374	GLU
1	H	369	ASP
1	I	375	GLU
1	D	373	ARG
1	B	413	LYS
1	G	370	ILE
1	I	275	VAL
1	H	275	VAL

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	318/337 (94%)	298 (94%)	20 (6%)	16	43
1	B	320/337 (95%)	298 (93%)	22 (7%)	14	39
1	D	322/337 (96%)	298 (92%)	24 (8%)	12	35
1	E	320/337 (95%)	298 (93%)	22 (7%)	14	39
1	F	322/337 (96%)	305 (95%)	17 (5%)	20	50
1	G	319/337 (95%)	300 (94%)	19 (6%)	17	45
1	H	318/337 (94%)	300 (94%)	18 (6%)	18	48
1	I	319/337 (95%)	300 (94%)	19 (6%)	17	45
All	All	2558/2696 (95%)	2397 (94%)	161 (6%)	16	43

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	68	LEU
1	A	97	LEU
1	A	100	GLU
1	A	104	ASP
1	A	105	GLU
1	A	199	LEU
1	A	242	LEU
1	A	253	LEU
1	A	290	LEU
1	A	298	GLN
1	A	299	LYS
1	A	332	LYS
1	A	344	LYS
1	A	371	TYR
1	A	376	LEU
1	A	378	SER
1	A	401	LEU
1	A	412	ASP
1	A	419	LEU
1	B	68	LEU
1	B	97	LEU
1	B	100	GLU
1	B	104	ASP
1	B	105	GLU
1	B	199	LEU
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	249	GLU
1	B	253	LEU
1	B	274	HIS
1	B	276	GLU
1	B	298	GLN
1	B	332	LYS
1	B	343	LYS
1	B	376	LEU
1	B	378	SER
1	B	391	LEU
1	B	401	LEU
1	B	412	ASP
1	B	418	LEU
1	B	419	LEU
1	B	422	HIS
1	D	35	MET
1	D	39	LYS
1	D	43	LEU
1	D	68	LEU
1	D	80	LEU
1	D	97	LEU
1	D	100	GLU
1	D	104	ASP
1	D	105	GLU
1	D	199	LEU
1	D	242	LEU
1	D	253	LEU
1	D	298	GLN
1	D	299	LYS
1	D	332	LYS
1	D	343	LYS
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	E	43	LEU
1	E	47	SER
1	E	54	LEU

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Mol	Chain	Res	Type
1	E	68	LEU
1	E	97	LEU
1	E	98	SER
1	E	119	SER
1	E	145	ASP
1	E	199	LEU
1	E	253	LEU
1	E	265	SER
1	E	298	GLN
1	E	299	LYS
1	E	332	LYS
1	E	340	MET
1	E	344	LYS
1	E	378	SER
1	E	391	LEU
1	E	399	SER
1	E	400	LEU
1	E	416	ASP
1	E	420	GLU
1	F	68	LEU
1	F	97	LEU
1	F	100	GLU
1	F	104	ASP
1	F	105	GLU
1	F	199	LEU
1	F	253	LEU
1	F	255	ILE
1	F	290	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	413	LYS
1	F	417	GLU
1	G	68	LEU
1	G	83	LEU
1	G	97	LEU
1	G	100	GLU
1	G	105	GLU
1	G	199	LEU

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Mol	Chain	Res	Type
1	G	242	LEU
1	G	253	LEU
1	G	298	GLN
1	G	299	LYS
1	G	332	LYS
1	G	343	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	H	68	LEU
1	H	97	LEU
1	H	100	GLU
1	H	104	ASP
1	H	105	GLU
1	H	199	LEU
1	H	242	LEU
1	H	253	LEU
1	H	298	GLN
1	H	299	LYS
1	H	332	LYS
1	H	343	LYS
1	H	344	LYS
1	H	378	SER
1	H	391	LEU
1	H	401	LEU
1	H	412	ASP
1	H	413	LYS
1	I	68	LEU
1	I	97	LEU
1	I	100	GLU
1	I	104	ASP
1	I	105	GLU
1	I	199	LEU
1	I	242	LEU
1	I	253	LEU
1	I	274	HIS
1	I	298	GLN
1	I	299	LYS

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Mol	Chain	Res	Type
1	I	332	LYS
1	I	343	LYS
1	I	376	LEU
1	I	378	SER
1	I	391	LEU
1	I	401	LEU
1	I	412	ASP
1	I	413	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	262	HIS
1	A	320	HIS
1	A	353	HIS
1	B	171	GLN
1	B	274	HIS
1	B	320	HIS
1	B	353	HIS
1	B	396	GLN
1	D	125	ASN
1	D	171	GLN
1	D	320	HIS
1	D	353	HIS
1	D	396	GLN
1	D	423	HIS
1	E	171	GLN
1	E	320	HIS
1	E	353	HIS
1	F	244	ASN
1	F	320	HIS
1	F	353	HIS
1	F	364	ASN
1	F	422	HIS
1	G	171	GLN
1	G	320	HIS
1	G	353	HIS
1	G	396	GLN
1	H	125	ASN
1	H	171	GLN
1	H	320	HIS

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Mol	Chain	Res	Type
1	H	353	HIS
1	H	396	GLN
1	I	108	HIS
1	I	125	ASN
1	I	171	GLN
1	I	320	HIS
1	I	353	HIS
1	I	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 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	387/392 (98%)	0.19	14 (3%)	46	37	16, 31, 56, 70	0
1	B	388/392 (98%)	0.57	16 (4%)	41	33	18, 40, 65, 77	0
1	D	390/392 (99%)	0.32	11 (2%)	55	45	15, 34, 58, 72	0
1	E	387/392 (98%)	0.14	12 (3%)	51	41	16, 29, 51, 75	0
1	F	388/392 (98%)	0.42	16 (4%)	41	33	21, 38, 66, 80	0
1	G	387/392 (98%)	0.70	29 (7%)	20	16	19, 40, 64, 94	0
1	H	387/392 (98%)	0.76	27 (6%)	22	18	24, 46, 73, 87	0
1	I	387/392 (98%)	1.05	51 (13%)	7	6	25, 53, 80, 104	0
All	All	3101/3136 (98%)	0.52	176 (5%)	29	23	15, 38, 69, 104	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	ASN	5.3
1	I	421	HIS	5.1
1	I	121	SER	4.8
1	F	345	ASP	4.5
1	I	78	LEU	4.3
1	I	198	ALA	4.3
1	I	348	LEU	4.1
1	F	163	PHE	4.0
1	H	418	LEU	4.0
1	I	163	PHE	3.9
1	I	125	ASN	3.9
1	D	345	ASP	3.8
1	B	126	VAL	3.8
1	G	376	LEU	3.8
1	E	345	ASP	3.5
1	E	123	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	417	GLU	3.5
1	I	326	LEU	3.5
1	E	118	LEU	3.4
1	I	321	LEU	3.4
1	H	123	ALA	3.4
1	F	121	SER	3.3
1	I	77	SER	3.3
1	H	78	LEU	3.2
1	I	351	VAL	3.2
1	E	122	THR	3.2
1	I	123	ALA	3.1
1	I	122	THR	3.1
1	I	281	LEU	3.1
1	G	270	LEU	3.1
1	F	35	MET	3.1
1	I	137	PRO	3.1
1	I	419	LEU	3.1
1	F	198	ALA	3.0
1	I	81	VAL	3.0
1	G	371	TYR	3.0
1	H	368	GLN	3.0
1	F	122	THR	3.0
1	G	418	LEU	3.0
1	I	418	LEU	3.0
1	B	123	ALA	3.0
1	H	97	LEU	2.9
1	I	134	LEU	2.9
1	A	371	TYR	2.9
1	B	163	PHE	2.9
1	I	329	ALA	2.9
1	B	348	LEU	2.9
1	H	134	LEU	2.8
1	I	420	GLU	2.8
1	G	123	ALA	2.8
1	F	342	GLY	2.8
1	G	400	LEU	2.8
1	E	375	GLU	2.8
1	D	163	PHE	2.8
1	I	352	PHE	2.8
1	H	346	LEU	2.8
1	A	369	ASP	2.8
1	G	121	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	321	LEU	2.7
1	I	35	MET	2.7
1	G	375	GLU	2.7
1	G	163	PHE	2.7
1	G	321	LEU	2.7
1	A	163	PHE	2.7
1	B	420	GLU	2.7
1	D	122	THR	2.6
1	I	80	LEU	2.6
1	A	418	LEU	2.6
1	G	102	LEU	2.6
1	B	368	GLN	2.6
1	E	121	SER	2.6
1	G	421	HIS	2.6
1	B	371	TYR	2.6
1	E	374	GLU	2.6
1	H	270	LEU	2.5
1	H	420	GLU	2.5
1	I	93	ALA	2.5
1	I	378	SER	2.5
1	I	154	TYR	2.5
1	G	62	GLN	2.5
1	G	125	ASN	2.5
1	B	421	HIS	2.5
1	A	345	ASP	2.5
1	D	371	TYR	2.5
1	E	366	PHE	2.5
1	H	352	PHE	2.5
1	I	236	MET	2.5
1	I	384	ALA	2.5
1	D	39	LYS	2.5
1	G	285	LEU	2.4
1	I	136	GLY	2.4
1	I	197	GLY	2.4
1	H	343	LYS	2.4
1	I	90	ALA	2.4
1	H	326	LEU	2.4
1	D	125	ASN	2.4
1	G	382	PHE	2.4
1	I	374	GLU	2.4
1	D	346	LEU	2.4
1	F	36	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	373	ARG	2.4
1	F	123	ALA	2.4
1	H	348	LEU	2.4
1	H	419	LEU	2.4
1	E	370	ILE	2.4
1	A	372	GLY	2.3
1	G	35	MET	2.3
1	A	421	HIS	2.3
1	F	199	LEU	2.3
1	G	419	LEU	2.3
1	E	39	LYS	2.3
1	B	366	PHE	2.3
1	G	63	ALA	2.3
1	A	134	LEU	2.3
1	I	118	LEU	2.3
1	B	320	HIS	2.3
1	F	339	ARG	2.3
1	H	402	PHE	2.3
1	H	329	ALA	2.3
1	I	161	ILE	2.3
1	F	197	GLY	2.3
1	D	366	PHE	2.3
1	I	388	PHE	2.3
1	D	90	ALA	2.3
1	F	348	LEU	2.3
1	E	47	SER	2.3
1	F	38	PRO	2.3
1	G	97	LEU	2.2
1	G	373	ARG	2.2
1	I	277	PRO	2.2
1	H	93	ALA	2.2
1	G	290	LEU	2.2
1	I	89	THR	2.2
1	I	370	ILE	2.2
1	I	52	PHE	2.2
1	A	270	LEU	2.2
1	A	326	LEU	2.2
1	G	106	GLU	2.2
1	H	369	ASP	2.2
1	I	340	MET	2.2
1	I	156	CYS	2.2
1	A	168	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	400	LEU	2.2
1	B	422	HIS	2.1
1	F	413	LYS	2.1
1	E	419	LEU	2.1
1	G	246	TYR	2.1
1	G	420	GLU	2.1
1	H	137	PRO	2.1
1	H	197	GLY	2.1
1	B	121	SER	2.1
1	I	399	SER	2.1
1	B	346	LEU	2.1
1	H	309	GLY	2.1
1	I	180	THR	2.1
1	I	135	TYR	2.1
1	B	77	SER	2.1
1	H	121	SER	2.1
1	H	421	HIS	2.1
1	I	142	PHE	2.1
1	H	367	ASP	2.1
1	I	51	ALA	2.1
1	H	371	TYR	2.1
1	B	399	SER	2.0
1	H	378	SER	2.0
1	G	255	ILE	2.0
1	G	380	LYS	2.0
1	H	392	VAL	2.0
1	I	138	SER	2.0
1	I	150	SER	2.0
1	F	346	LEU	2.0
1	I	346	LEU	2.0
1	A	370	ILE	2.0
1	G	287	LYS	2.0
1	A	35	MET	2.0
1	G	140	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.