



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 PM GMT

PDB ID : 4RSQ  
Title : 2.9A resolution structure of SRPN2 (K198C/E359C) from Anopheles gambiae  
Authors : Lovell, S.; Battaile, K.P.; Zhang, X.; Meekins, D.A.; An, C.; Michel, K.  
Deposited on : 2014-11-10  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

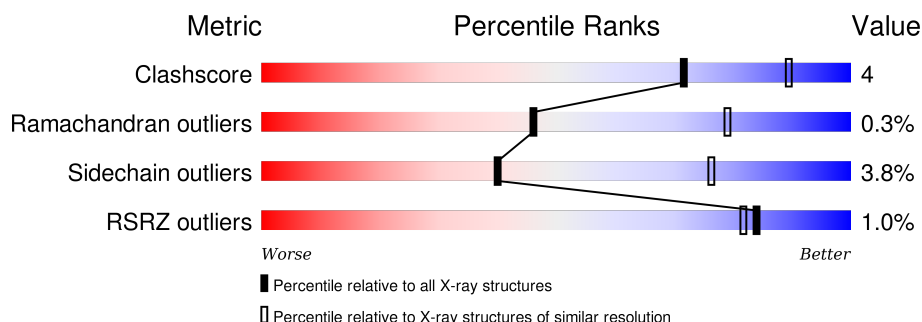
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	397	<div> <div>76%</div> <div>13%</div> <div>10%</div> </div>
1	B	397	<div> <div>82%</div> <div>7%</div> <div>11%</div> </div>
1	C	397	<div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
1	D	397	<div> <div>2%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
1	E	397	<div> <div>80%</div> <div>9%</div> <div>10%</div> </div>
1	F	397	<div> <div>79%</div> <div>9%</div> <div>11%</div> </div>
1	G	397	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	397	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>76%13%10%</div></div></div>
1	I	397	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>73%14%10%</div></div></div>
1	J	397	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>76%13%11%</div></div></div>
1	K	397	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>80%10%10%</div></div></div>
1	L	397	<div><div><div></div><div></div><div></div></div><div>76%12%10%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33765 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serpin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2827	1813	468	538	8			
1	B	355	Total	C	N	O	S	0	0	0
			2800	1800	460	532	8			
1	C	354	Total	C	N	O	S	0	0	0
			2816	1806	464	538	8			
1	D	355	Total	C	N	O	S	0	0	0
			2801	1797	463	533	8			
1	E	356	Total	C	N	O	S	0	0	0
			2816	1808	467	533	8			
1	F	353	Total	C	N	O	S	0	0	0
			2804	1802	461	533	8			
1	G	357	Total	C	N	O	S	0	0	0
			2829	1815	468	538	8			
1	H	357	Total	C	N	O	S	0	0	0
			2814	1807	465	534	8			
1	I	356	Total	C	N	O	S	0	0	0
			2814	1808	466	532	8			
1	J	355	Total	C	N	O	S	0	0	0
			2817	1808	465	536	8			
1	K	356	Total	C	N	O	S	0	0	0
			2807	1803	463	533	8			
1	L	356	Total	C	N	O	S	0	0	0
			2820	1807	468	537	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	EXPRESSION TAG	UNP Q005N3
A	14	GLY	-	EXPRESSION TAG	UNP Q005N3
A	15	HIS	-	EXPRESSION TAG	UNP Q005N3
A	16	HIS	-	EXPRESSION TAG	UNP Q005N3
A	17	HIS	-	EXPRESSION TAG	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	EXPRESSION TAG	UNP Q005N3
A	19	HIS	-	EXPRESSION TAG	UNP Q005N3
A	20	HIS	-	EXPRESSION TAG	UNP Q005N3
A	21	GLY	-	EXPRESSION TAG	UNP Q005N3
A	198	CYS	LYS	engineered mutation	UNP Q005N3
A	359	CYS	GLU	engineered mutation	UNP Q005N3
B	13	MET	-	EXPRESSION TAG	UNP Q005N3
B	14	GLY	-	EXPRESSION TAG	UNP Q005N3
B	15	HIS	-	EXPRESSION TAG	UNP Q005N3
B	16	HIS	-	EXPRESSION TAG	UNP Q005N3
B	17	HIS	-	EXPRESSION TAG	UNP Q005N3
B	18	HIS	-	EXPRESSION TAG	UNP Q005N3
B	19	HIS	-	EXPRESSION TAG	UNP Q005N3
B	20	HIS	-	EXPRESSION TAG	UNP Q005N3
B	21	GLY	-	EXPRESSION TAG	UNP Q005N3
B	198	CYS	LYS	engineered mutation	UNP Q005N3
B	359	CYS	GLU	engineered mutation	UNP Q005N3
C	13	MET	-	EXPRESSION TAG	UNP Q005N3
C	14	GLY	-	EXPRESSION TAG	UNP Q005N3
C	15	HIS	-	EXPRESSION TAG	UNP Q005N3
C	16	HIS	-	EXPRESSION TAG	UNP Q005N3
C	17	HIS	-	EXPRESSION TAG	UNP Q005N3
C	18	HIS	-	EXPRESSION TAG	UNP Q005N3
C	19	HIS	-	EXPRESSION TAG	UNP Q005N3
C	20	HIS	-	EXPRESSION TAG	UNP Q005N3
C	21	GLY	-	EXPRESSION TAG	UNP Q005N3
C	198	CYS	LYS	engineered mutation	UNP Q005N3
C	359	CYS	GLU	engineered mutation	UNP Q005N3
D	13	MET	-	EXPRESSION TAG	UNP Q005N3
D	14	GLY	-	EXPRESSION TAG	UNP Q005N3
D	15	HIS	-	EXPRESSION TAG	UNP Q005N3
D	16	HIS	-	EXPRESSION TAG	UNP Q005N3
D	17	HIS	-	EXPRESSION TAG	UNP Q005N3
D	18	HIS	-	EXPRESSION TAG	UNP Q005N3
D	19	HIS	-	EXPRESSION TAG	UNP Q005N3
D	20	HIS	-	EXPRESSION TAG	UNP Q005N3
D	21	GLY	-	EXPRESSION TAG	UNP Q005N3
D	198	CYS	LYS	engineered mutation	UNP Q005N3
D	359	CYS	GLU	engineered mutation	UNP Q005N3
E	13	MET	-	EXPRESSION TAG	UNP Q005N3
E	14	GLY	-	EXPRESSION TAG	UNP Q005N3
E	15	HIS	-	EXPRESSION TAG	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	-	EXPRESSION TAG	UNP Q005N3
E	17	HIS	-	EXPRESSION TAG	UNP Q005N3
E	18	HIS	-	EXPRESSION TAG	UNP Q005N3
E	19	HIS	-	EXPRESSION TAG	UNP Q005N3
E	20	HIS	-	EXPRESSION TAG	UNP Q005N3
E	21	GLY	-	EXPRESSION TAG	UNP Q005N3
E	198	CYS	LYS	engineered mutation	UNP Q005N3
E	359	CYS	GLU	engineered mutation	UNP Q005N3
F	13	MET	-	EXPRESSION TAG	UNP Q005N3
F	14	GLY	-	EXPRESSION TAG	UNP Q005N3
F	15	HIS	-	EXPRESSION TAG	UNP Q005N3
F	16	HIS	-	EXPRESSION TAG	UNP Q005N3
F	17	HIS	-	EXPRESSION TAG	UNP Q005N3
F	18	HIS	-	EXPRESSION TAG	UNP Q005N3
F	19	HIS	-	EXPRESSION TAG	UNP Q005N3
F	20	HIS	-	EXPRESSION TAG	UNP Q005N3
F	21	GLY	-	EXPRESSION TAG	UNP Q005N3
F	198	CYS	LYS	engineered mutation	UNP Q005N3
F	359	CYS	GLU	engineered mutation	UNP Q005N3
G	13	MET	-	EXPRESSION TAG	UNP Q005N3
G	14	GLY	-	EXPRESSION TAG	UNP Q005N3
G	15	HIS	-	EXPRESSION TAG	UNP Q005N3
G	16	HIS	-	EXPRESSION TAG	UNP Q005N3
G	17	HIS	-	EXPRESSION TAG	UNP Q005N3
G	18	HIS	-	EXPRESSION TAG	UNP Q005N3
G	19	HIS	-	EXPRESSION TAG	UNP Q005N3
G	20	HIS	-	EXPRESSION TAG	UNP Q005N3
G	21	GLY	-	EXPRESSION TAG	UNP Q005N3
G	198	CYS	LYS	engineered mutation	UNP Q005N3
G	359	CYS	GLU	engineered mutation	UNP Q005N3
H	13	MET	-	EXPRESSION TAG	UNP Q005N3
H	14	GLY	-	EXPRESSION TAG	UNP Q005N3
H	15	HIS	-	EXPRESSION TAG	UNP Q005N3
H	16	HIS	-	EXPRESSION TAG	UNP Q005N3
H	17	HIS	-	EXPRESSION TAG	UNP Q005N3
H	18	HIS	-	EXPRESSION TAG	UNP Q005N3
H	19	HIS	-	EXPRESSION TAG	UNP Q005N3
H	20	HIS	-	EXPRESSION TAG	UNP Q005N3
H	21	GLY	-	EXPRESSION TAG	UNP Q005N3
H	198	CYS	LYS	engineered mutation	UNP Q005N3
H	359	CYS	GLU	engineered mutation	UNP Q005N3
I	13	MET	-	EXPRESSION TAG	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	14	GLY	-	EXPRESSION TAG	UNP Q005N3
I	15	HIS	-	EXPRESSION TAG	UNP Q005N3
I	16	HIS	-	EXPRESSION TAG	UNP Q005N3
I	17	HIS	-	EXPRESSION TAG	UNP Q005N3
I	18	HIS	-	EXPRESSION TAG	UNP Q005N3
I	19	HIS	-	EXPRESSION TAG	UNP Q005N3
I	20	HIS	-	EXPRESSION TAG	UNP Q005N3
I	21	GLY	-	EXPRESSION TAG	UNP Q005N3
I	198	CYS	LYS	engineered mutation	UNP Q005N3
I	359	CYS	GLU	engineered mutation	UNP Q005N3
J	13	MET	-	EXPRESSION TAG	UNP Q005N3
J	14	GLY	-	EXPRESSION TAG	UNP Q005N3
J	15	HIS	-	EXPRESSION TAG	UNP Q005N3
J	16	HIS	-	EXPRESSION TAG	UNP Q005N3
J	17	HIS	-	EXPRESSION TAG	UNP Q005N3
J	18	HIS	-	EXPRESSION TAG	UNP Q005N3
J	19	HIS	-	EXPRESSION TAG	UNP Q005N3
J	20	HIS	-	EXPRESSION TAG	UNP Q005N3
J	21	GLY	-	EXPRESSION TAG	UNP Q005N3
J	198	CYS	LYS	engineered mutation	UNP Q005N3
J	359	CYS	GLU	engineered mutation	UNP Q005N3
K	13	MET	-	EXPRESSION TAG	UNP Q005N3
K	14	GLY	-	EXPRESSION TAG	UNP Q005N3
K	15	HIS	-	EXPRESSION TAG	UNP Q005N3
K	16	HIS	-	EXPRESSION TAG	UNP Q005N3
K	17	HIS	-	EXPRESSION TAG	UNP Q005N3
K	18	HIS	-	EXPRESSION TAG	UNP Q005N3
K	19	HIS	-	EXPRESSION TAG	UNP Q005N3
K	20	HIS	-	EXPRESSION TAG	UNP Q005N3
K	21	GLY	-	EXPRESSION TAG	UNP Q005N3
K	198	CYS	LYS	engineered mutation	UNP Q005N3
K	359	CYS	GLU	engineered mutation	UNP Q005N3
L	13	MET	-	EXPRESSION TAG	UNP Q005N3
L	14	GLY	-	EXPRESSION TAG	UNP Q005N3
L	15	HIS	-	EXPRESSION TAG	UNP Q005N3
L	16	HIS	-	EXPRESSION TAG	UNP Q005N3
L	17	HIS	-	EXPRESSION TAG	UNP Q005N3
L	18	HIS	-	EXPRESSION TAG	UNP Q005N3
L	19	HIS	-	EXPRESSION TAG	UNP Q005N3
L	20	HIS	-	EXPRESSION TAG	UNP Q005N3
L	21	GLY	-	EXPRESSION TAG	UNP Q005N3
L	198	CYS	LYS	engineered mutation	UNP Q005N3

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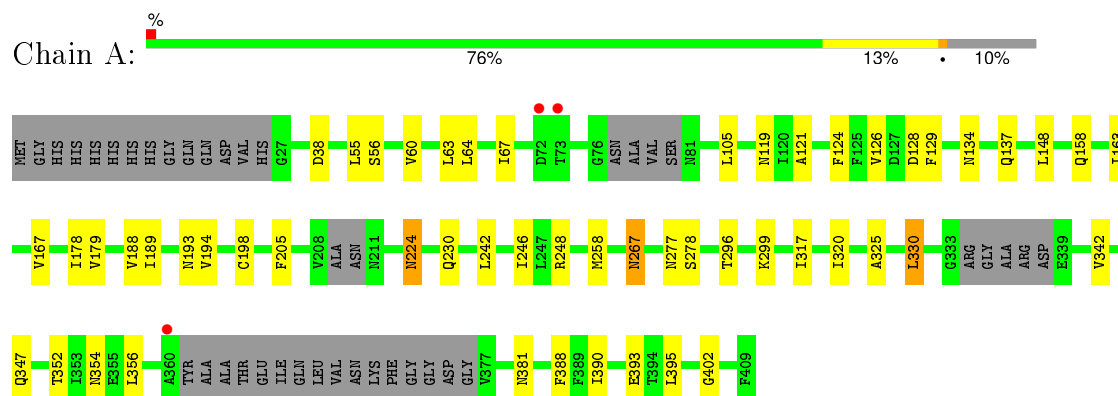
Chain	Residue	Modelled	Actual	Comment	Reference
L	359	CYS	GLU	engineered mutation	UNP Q005N3



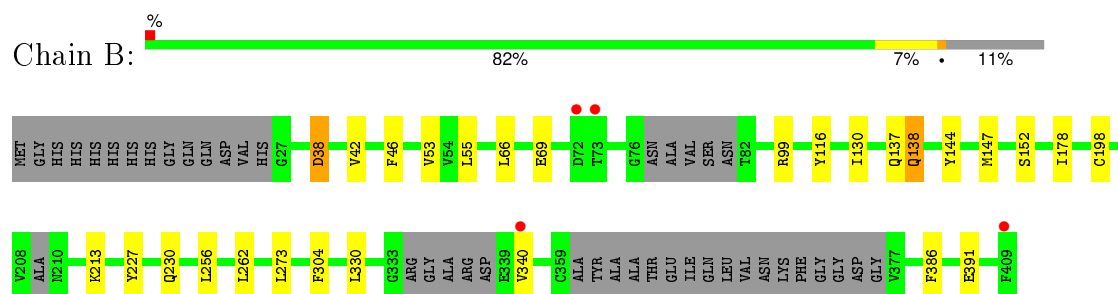
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

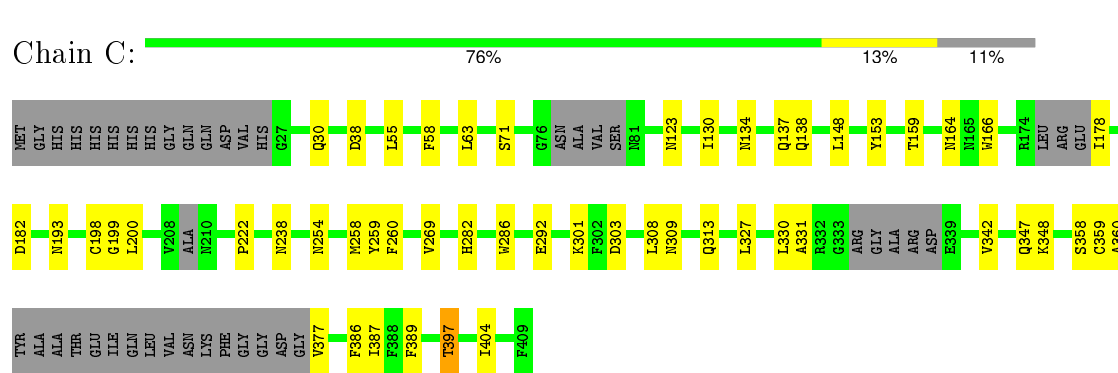
#### • Molecule 1: Serpin 2



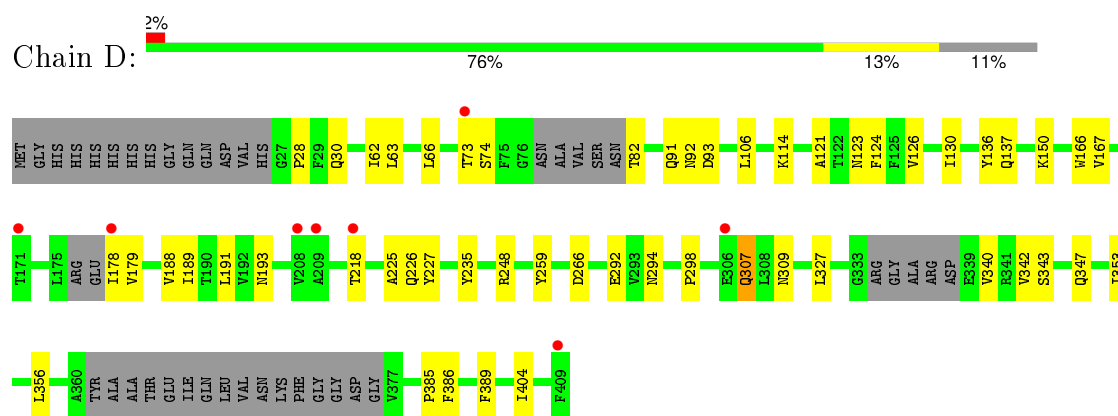
#### • Molecule 1: Serpin 2



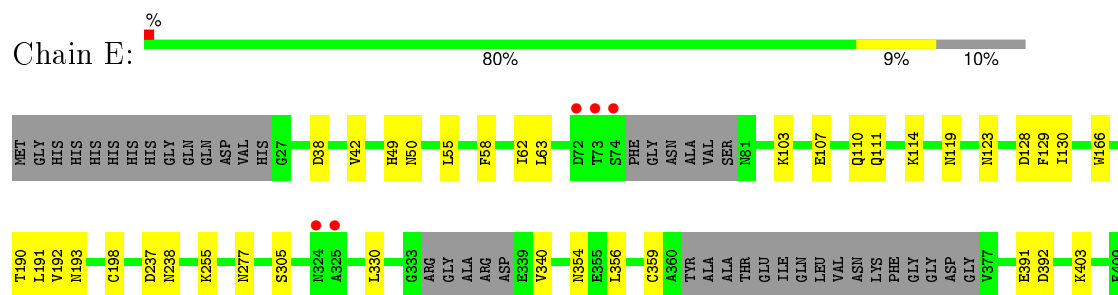
#### • Molecule 1: Serpin 2



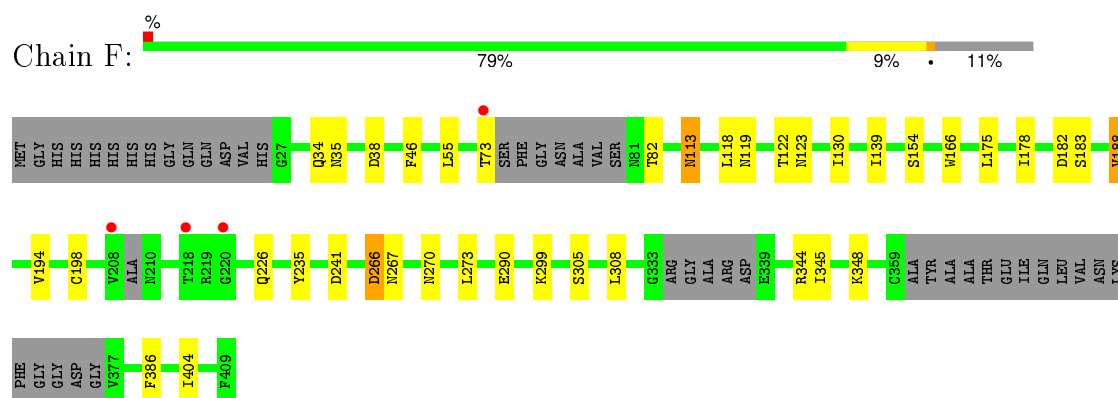
#### • Molecule 1: Serpin 2



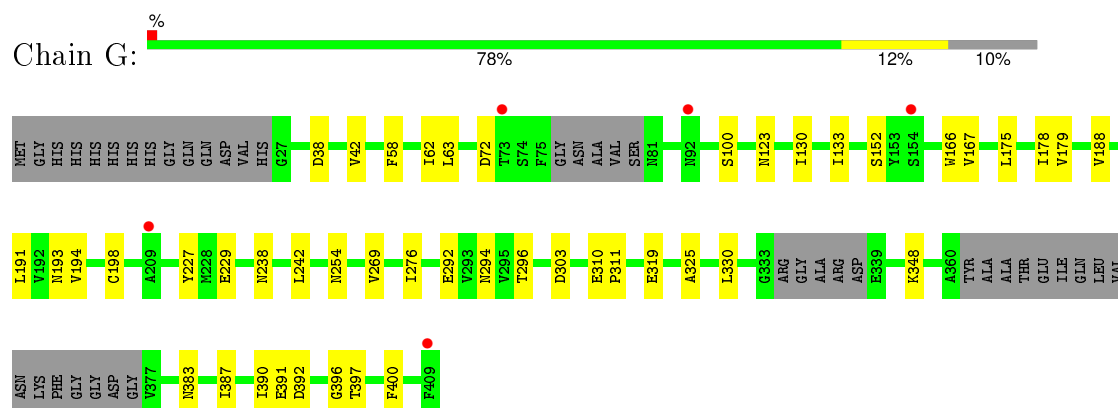
- Molecule 1: Serpin 2



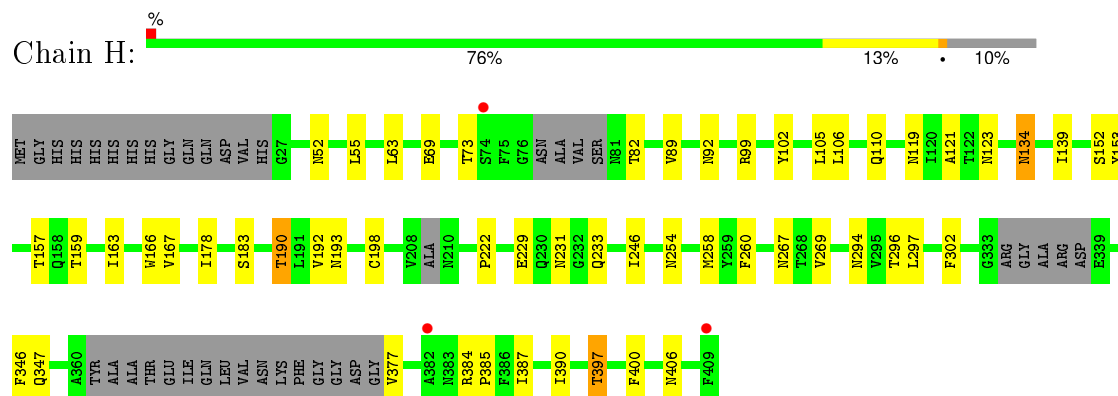
- Molecule 1: Serpin 2



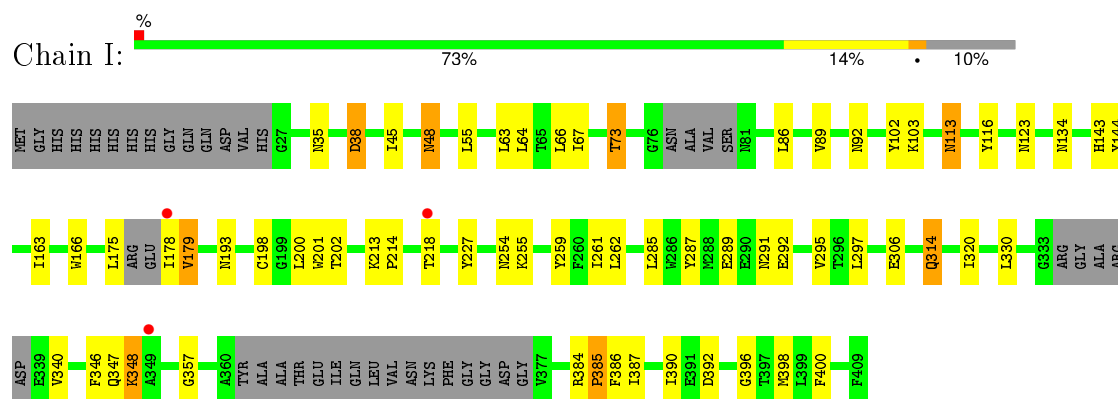
- Molecule 1: Serpin 2



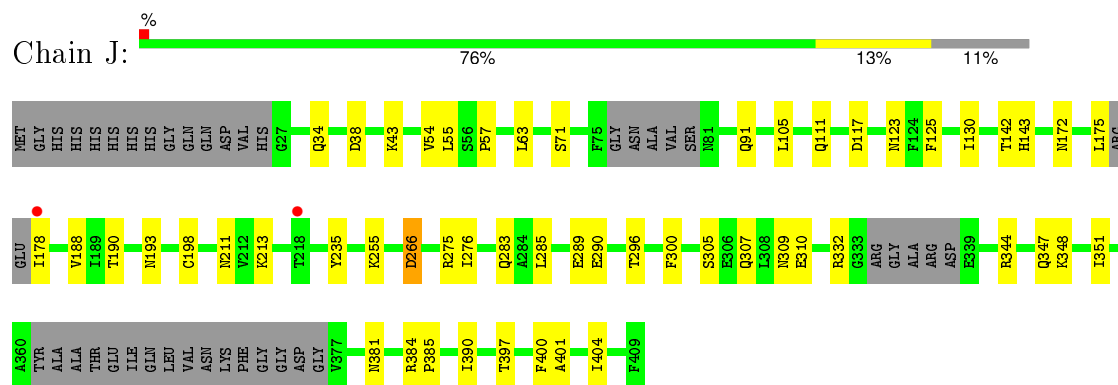
- Molecule 1: Serpin 2



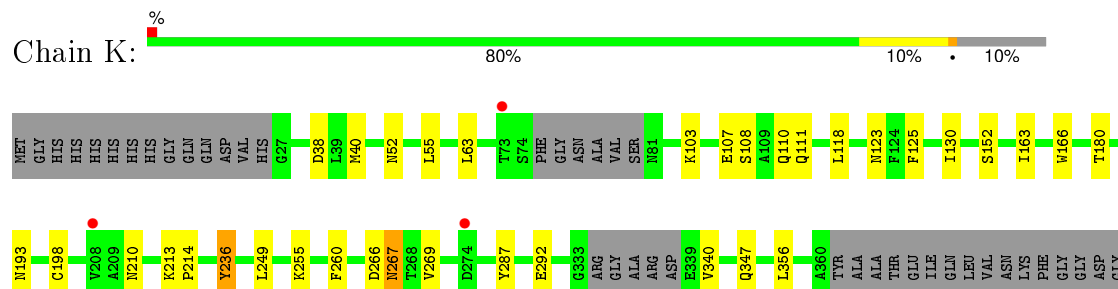
- Molecule 1: Serpin 2

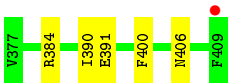


- Molecule 1: Serpin 2

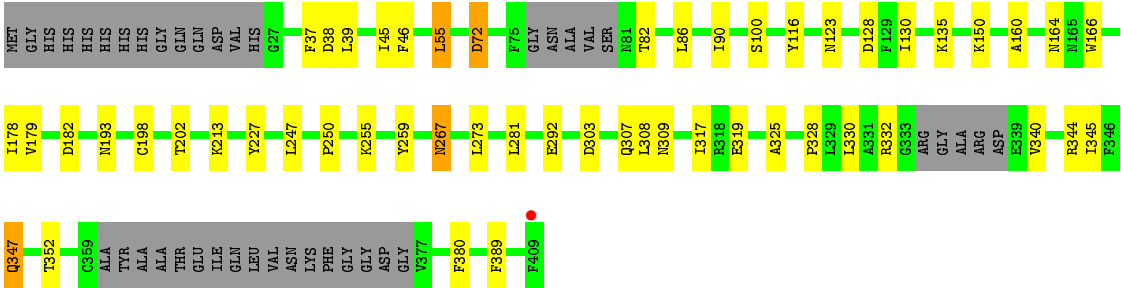


- Molecule 1: Serpin 2





● Molecule 1: Serpin 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.92Å 164.39Å 186.18Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	47.82 – 2.90 47.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.82-2.90) 99.3 (47.82-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.255 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 8.6	EDS
Estimated twinning fraction	0.445 for H, K, L 0.555 for H, -K, -L 0.427 for h,-k,-l	Xtriage
Reported twinning fraction	0.445 for H, K, L 0.555 for H, -K, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 129620 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2202e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2890	0.54	0/3928
1	B	0.35	0/2863	0.54	0/3894
1	C	0.37	0/2878	0.56	0/3909
1	D	0.37	0/2863	0.55	0/3892
1	E	0.38	0/2880	0.56	0/3918
1	F	0.34	0/2867	0.52	0/3898
1	G	0.34	0/2893	0.52	0/3935
1	H	0.35	0/2877	0.55	0/3913
1	I	0.37	0/2877	0.54	0/3911
1	J	0.37	0/2880	0.55	0/3916
1	K	0.36	0/2871	0.55	0/3908
1	L	0.36	0/2883	0.55	0/3923
All	All	0.36	0/34522	0.54	0/46945

There are no bond length outliers.

There are no bond angle outliers.

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	2827	0	2699	30	0
1	B	2800	0	2658	14	0
1	C	2816	0	2689	24	0
1	D	2801	0	2672	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2816	0	2688	17	0
1	F	2804	0	2673	18	0
1	G	2829	0	2698	20	0
1	H	2814	0	2676	30	0
1	I	2814	0	2692	34	0
1	J	2817	0	2690	28	0
1	K	2807	0	2668	16	0
1	L	2820	0	2690	30	0
All	All	33765	0	32193	282	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 4.

All (282) 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:63:LEU:HD21	1:E:193:ASN:HB2	1.65	0.77
1:A:63:LEU:HD21	1:A:193:ASN:HB2	1.65	0.77
1:G:130:ILE:HD11	1:G:188:VAL:HG12	1.69	0.74
1:G:178:ILE:HG23	1:G:179:VAL:HG13	1.70	0.73
1:K:130:ILE:HD11	1:K:340:VAL:HG11	1.72	0.71
1:L:130:ILE:O	1:L:150:LYS:NZ	2.23	0.71
1:F:130:ILE:HD11	1:F:188:VAL:HG12	1.71	0.70
1:A:178:ILE:HG23	1:A:179:VAL:HG13	1.74	0.70
1:I:175:LEU:HD13	1:I:348:LYS:HG2	1.77	0.67
1:D:73:THR:HG21	1:D:82:THR:HB	1.76	0.67
1:K:123:ASN:HB2	1:K:166:TRP:CZ2	2.30	0.67
1:F:73:THR:HG21	1:F:82:THR:HB	1.76	0.66
1:E:63:LEU:HD22	1:E:191:LEU:HD11	1.78	0.66
1:J:332:ARG:NH1	1:K:287:TYR:O	2.29	0.66
1:L:308:LEU:HD12	1:L:345:ILE:HG22	1.78	0.66
1:I:193:ASN:HD22	1:I:347:GLN:HG3	1.62	0.64
1:I:123:ASN:HB2	1:I:166:TRP:CZ2	2.32	0.64
1:J:123:ASN:OD1	1:J:125:PHE:CZ	2.51	0.64
1:A:248:ARG:NE	1:A:393:GLU:OE1	2.26	0.63
1:I:48:ASN:HD22	1:I:48:ASN:N	1.97	0.63
1:H:63:LEU:HD11	1:H:193:ASN:HB2	1.81	0.63
1:G:229:GLU:HG3	1:G:296:THR:HG23	1.80	0.62
1:C:259:TYR:HB2	1:C:389:PHE:CE1	2.34	0.62
1:I:175:LEU:HD22	1:I:348:LYS:HE3	1.80	0.62
1:I:178:ILE:HD11	1:I:346:PHE:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:390:ILE:HD12	1:I:400:PHE:CD1	2.34	0.62
1:L:130:ILE:HD11	1:L:340:VAL:HG11	1.83	0.61
1:D:130:ILE:HD11	1:D:188:VAL:HG12	1.81	0.61
1:H:123:ASN:HB2	1:H:166:TRP:CZ2	2.36	0.60
1:I:63:LEU:HD21	1:I:193:ASN:HB2	1.84	0.60
1:G:123:ASN:HB2	1:G:166:TRP:CZ2	2.37	0.60
1:J:55:LEU:HD23	1:J:401:ALA:O	2.02	0.60
1:J:193:ASN:HD22	1:J:347:GLN:HG3	1.66	0.60
1:I:67:ILE:HD13	1:I:320:ILE:HD12	1.84	0.59
1:H:152:SER:O	1:H:159:THR:OG1	2.18	0.59
1:A:67:ILE:HD13	1:A:320:ILE:HD12	1.84	0.59
1:J:63:LEU:HD21	1:J:193:ASN:HB2	1.83	0.59
1:E:103:LYS:NZ	1:E:107:GLU:OE2	2.34	0.59
1:K:55:LEU:HB2	1:K:347:GLN:HE22	1.68	0.59
1:H:269:VAL:HG13	1:H:387:ILE:HD11	1.85	0.59
1:J:130:ILE:HD11	1:J:188:VAL:HG12	1.86	0.58
1:H:106:LEU:HD22	1:H:110:GLN:HE21	1.67	0.58
1:A:126:VAL:HG22	1:A:189:ILE:HG12	1.86	0.58
1:H:153:TYR:OH	1:H:190:THR:OG1	2.22	0.58
1:G:269:VAL:HG13	1:G:387:ILE:HD11	1.86	0.58
1:H:63:LEU:HD11	1:H:193:ASN:CB	2.35	0.57
1:D:178:ILE:HG23	1:D:179:VAL:HG13	1.86	0.57
1:F:266:ASP:OD1	1:F:266:ASP:N	2.36	0.57
1:K:390:ILE:HD12	1:K:400:PHE:CD2	2.39	0.57
1:C:178:ILE:HD12	1:C:348:LYS:HB2	1.87	0.56
1:J:178:ILE:HD12	1:J:348:LYS:HB2	1.88	0.56
1:J:175:LEU:HD22	1:J:348:LYS:HE2	1.88	0.56
1:G:63:LEU:HB3	1:G:191:LEU:HD21	1.86	0.56
1:D:62:ILE:HD12	1:D:106:LEU:HD11	1.88	0.56
1:I:262:LEU:HD12	1:I:386:PHE:HB3	1.89	0.55
1:A:330:LEU:C	1:A:330:LEU:HD23	2.26	0.55
1:D:66:LEU:O	1:D:136:TYR:OH	2.25	0.55
1:L:213:LYS:HB2	1:L:227:TYR:CE1	2.43	0.54
1:L:116:TYR:OH	1:L:255:LYS:HD2	2.06	0.54
1:B:46:PHE:HD2	1:B:273:LEU:HD11	1.73	0.54
1:F:308:LEU:HD12	1:F:345:ILE:HG22	1.89	0.54
1:L:193:ASN:HD22	1:L:347:GLN:CG	2.20	0.53
1:D:193:ASN:HD22	1:D:347:GLN:HG3	1.74	0.53
1:H:260:PHE:CE2	1:H:297:LEU:HD13	2.43	0.53
1:C:258:MET:SD	1:C:260:PHE:CZ	3.02	0.53
1:B:38:ASP:O	1:B:42:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:390:ILE:HD12	1:J:400:PHE:CD2	2.43	0.53
1:D:259:TYR:HB2	1:D:389:PHE:CE1	2.44	0.53
1:F:175:LEU:HD22	1:F:348:LYS:HE2	1.90	0.53
1:C:137:GLN:HE22	1:C:148:LEU:H	1.57	0.52
1:G:319:GLU:O	1:G:325:ALA:HB2	2.08	0.52
1:D:73:THR:HG21	1:D:82:THR:CB	2.39	0.52
1:I:314:GLN:HE21	1:I:314:GLN:HA	1.74	0.52
1:L:72:ASP:OD1	1:L:72:ASP:C	2.47	0.52
1:I:175:LEU:HD13	1:I:348:LYS:CG	2.39	0.52
1:D:28:PRO:HG2	1:D:235:TYR:CE2	2.46	0.51
1:H:73:THR:HG21	1:H:82:THR:HB	1.92	0.51
1:B:53:VAL:HG13	1:B:304:PHE:CE2	2.45	0.51
1:L:330:LEU:HD23	1:L:330:LEU:C	2.31	0.51
1:H:390:ILE:HD12	1:H:400:PHE:CD1	2.46	0.51
1:B:66:LEU:HD21	1:B:144:TYR:HB2	1.93	0.51
1:G:63:LEU:HD21	1:G:193:ASN:HB2	1.92	0.51
1:B:69:GLU:OE2	1:B:99:ARG:NE	2.35	0.51
1:A:134:ASN:O	1:A:137:GLN:HB3	2.10	0.51
1:B:213:LYS:HB2	1:B:227:TYR:CD2	2.46	0.51
1:J:38:ASP:OD2	1:J:57:PRO:HB2	2.11	0.50
1:L:178:ILE:HG23	1:L:179:VAL:HG13	1.93	0.50
1:A:267:ASN:N	1:A:267:ASN:OD1	2.44	0.50
1:I:89:VAL:O	1:I:102:TYR:OH	2.21	0.50
1:G:227:TYR:OH	1:G:383:ASN:HA	2.12	0.50
1:I:64:LEU:HB3	1:I:86:LEU:HD22	1.94	0.50
1:L:308:LEU:HD12	1:L:345:ILE:CG2	2.41	0.49
1:E:63:LEU:HD21	1:E:193:ASN:CB	2.39	0.49
1:D:130:ILE:HD11	1:D:188:VAL:CG1	2.41	0.49
1:L:39:LEU:HD21	1:L:281:LEU:HD22	1.94	0.49
1:D:167:VAL:HG21	1:D:178:ILE:CG2	2.41	0.49
1:H:178:ILE:HD13	1:H:192:VAL:HG13	1.95	0.49
1:A:64:LEU:HD22	1:A:317:ILE:HD13	1.94	0.49
1:K:103:LYS:NZ	1:K:107:GLU:OE2	2.44	0.49
1:C:309:ASN:O	1:C:313:GLN:HG3	2.12	0.49
1:L:309:ASN:HD21	1:L:344:ARG:HA	1.76	0.49
1:A:242:LEU:HD12	1:A:246:ILE:HD11	1.94	0.49
1:L:46:PHE:HD2	1:L:273:LEU:HD11	1.78	0.48
1:C:308:LEU:HD11	1:C:347:GLN:HB2	1.94	0.48
1:K:125:PHE:CE2	1:K:163:ILE:HG23	2.48	0.48
1:I:45:ILE:HD12	1:I:306:GLU:OE1	2.13	0.48
1:G:167:VAL:HG13	1:G:194:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:LEU:HD13	1:G:348:LYS:HG2	1.95	0.48
1:L:213:LYS:HB2	1:L:227:TYR:CD1	2.48	0.48
1:G:391:GLU:HA	1:G:397:THR:O	2.13	0.48
1:L:45:ILE:HG21	1:L:55:LEU:HD22	1.95	0.48
1:E:123:ASN:HB2	1:E:166:TRP:CZ2	2.49	0.48
1:F:123:ASN:HB2	1:F:166:TRP:CZ2	2.48	0.48
1:J:190:THR:HG23	1:J:344:ARG:HB2	1.95	0.48
1:L:193:ASN:HD22	1:L:347:GLN:HG2	1.78	0.48
1:A:388:PHE:CZ	1:A:402:GLY:HA3	2.49	0.47
1:I:113:ASN:N	1:I:113:ASN:HD22	2.12	0.47
1:I:103:LYS:HD3	1:I:143:HIS:HA	1.96	0.47
1:L:123:ASN:HB2	1:L:166:TRP:CZ2	2.50	0.47
1:C:130:ILE:HG23	1:C:331:ALA:HB1	1.97	0.47
1:H:384:ARG:HB2	1:H:385:PRO:CD	2.44	0.47
1:L:247:LEU:HD22	1:L:380:PHE:CD2	2.50	0.47
1:I:163:ILE:HG21	1:I:179:VAL:HG21	1.96	0.47
1:H:105:LEU:HD23	1:H:397:THR:HG23	1.96	0.47
1:E:114:LYS:HA	1:I:200:LEU:HD11	1.96	0.47
1:I:116:TYR:OH	1:I:255:LYS:HD2	2.15	0.47
1:A:224:ASN:N	1:A:224:ASN:HD22	2.13	0.47
1:L:319:GLU:O	1:L:325:ALA:HB2	2.14	0.47
1:D:123:ASN:HB2	1:D:166:TRP:CZ2	2.49	0.47
1:G:330:LEU:HD23	1:G:330:LEU:C	2.35	0.47
1:H:384:ARG:HB2	1:H:385:PRO:HD2	1.97	0.47
1:C:359:CYS:O	1:C:360:ALA:HB2	2.15	0.47
1:F:386:PHE:CZ	1:F:404:ILE:HG13	2.50	0.47
1:E:190:THR:HG22	1:E:192:VAL:HG23	1.97	0.46
1:H:55:LEU:HB2	1:H:347:GLN:HE22	1.80	0.46
1:K:193:ASN:HD22	1:K:347:GLN:HG3	1.80	0.46
1:C:269:VAL:HG13	1:C:387:ILE:HD11	1.97	0.46
1:C:153:TYR:CE1	1:C:159:THR:HG21	2.51	0.46
1:I:384:ARG:HB2	1:I:385:PRO:HD2	1.98	0.46
1:J:296:THR:HB	1:J:381:ASN:HA	1.97	0.46
1:I:390:ILE:HD12	1:I:400:PHE:CG	2.51	0.46
1:A:296:THR:HB	1:A:381:ASN:HA	1.97	0.46
1:L:267:ASN:HD22	1:L:267:ASN:N	2.14	0.46
1:D:124:PHE:CE1	1:D:191:LEU:HD13	2.51	0.46
1:A:258:MET:HE3	1:A:390:ILE:HD11	1.99	0.45
1:K:108:SER:O	1:K:255:LYS:HD3	2.16	0.45
1:J:142:THR:HB	1:J:143:HIS:CD2	2.51	0.45
1:C:198:CYS:HA	1:C:358:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:TYR:CE1	1:F:290:GLU:HG3	2.51	0.45
1:A:105:LEU:HG	1:A:395:LEU:HD13	1.99	0.45
1:D:309:ASN:ND2	1:D:343:SER:O	2.49	0.45
1:H:246:ILE:HA	1:H:260:PHE:O	2.17	0.45
1:A:56:SER:O	1:A:60:VAL:HG23	2.16	0.45
1:A:163:ILE:O	1:A:167:VAL:HG23	2.17	0.45
1:A:193:ASN:HD22	1:A:347:GLN:HG3	1.82	0.45
1:I:48:ASN:ND2	1:I:48:ASN:N	2.64	0.45
1:A:67:ILE:HG12	1:A:342:VAL:HG21	1.98	0.45
1:J:390:ILE:HD12	1:J:400:PHE:CG	2.52	0.45
1:F:130:ILE:HD11	1:F:188:VAL:CG1	2.42	0.45
1:H:167:VAL:HG21	1:H:178:ILE:HG22	1.99	0.45
1:H:69:GLU:OE2	1:H:99:ARG:NE	2.50	0.45
1:F:118:LEU:HD23	1:F:119:ASN:N	2.32	0.44
1:H:229:GLU:HG2	1:H:296:THR:HG23	1.98	0.44
1:F:35:ASN:HA	1:F:38:ASP:OD1	2.17	0.44
1:C:330:LEU:C	1:C:330:LEU:HD23	2.37	0.44
1:B:262:LEU:HD12	1:B:386:PHE:HB3	1.98	0.44
1:H:89:VAL:O	1:H:102:TYR:OH	2.34	0.44
1:G:130:ILE:HD11	1:G:188:VAL:CG1	2.43	0.44
1:D:307:GLN:HE21	1:D:309:ASN:HB2	1.82	0.44
1:E:237:ASP:OD1	1:E:238:ASN:N	2.50	0.44
1:L:160:ALA:O	1:L:164:ASN:ND2	2.50	0.44
1:L:72:ASP:HB3	1:L:328:PRO:HG3	1.98	0.44
1:J:34:GLN:HE22	1:J:91:GLN:HE22	1.66	0.44
1:C:258:MET:SD	1:C:260:PHE:CE1	3.11	0.44
1:L:259:TYR:HB2	1:L:389:PHE:CE1	2.52	0.44
1:D:130:ILE:HD13	1:D:189:ILE:HD11	2.00	0.44
1:J:175:LEU:HD13	1:J:348:LYS:HG2	2.00	0.44
1:D:121:ALA:HB1	1:D:166:TRP:CZ2	2.52	0.44
1:E:58:PHE:CE2	1:E:62:ILE:HD11	2.52	0.44
1:J:43:LYS:NZ	1:J:276:ILE:O	2.48	0.44
1:J:123:ASN:OD1	1:J:125:PHE:CE1	2.71	0.44
1:F:308:LEU:HD12	1:F:345:ILE:CG2	2.47	0.44
1:D:298:PRO:O	1:D:353:ILE:HD11	2.18	0.44
1:F:194:VAL:HG12	1:F:348:LYS:HB3	2.00	0.44
1:B:330:LEU:C	1:B:330:LEU:HD23	2.38	0.44
1:H:119:ASN:ND2	1:H:121:ALA:HB2	2.31	0.44
1:D:63:LEU:HD21	1:D:193:ASN:HB2	2.00	0.44
1:B:330:LEU:HD23	1:B:330:LEU:O	2.17	0.44
1:C:63:LEU:HD21	1:C:193:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:THR:HG22	1:L:86:LEU:HD12	1.99	0.44
1:I:213:LYS:HB3	1:I:214:PRO:HD2	1.99	0.44
1:C:134:ASN:HD21	1:C:138:GLN:NE2	2.16	0.44
1:G:310:GLU:HB3	1:G:311:PRO:HD3	2.00	0.43
1:G:242:LEU:HD22	1:G:276:ILE:HG13	1.99	0.43
1:C:58:PHE:CD1	1:C:397:THR:CG2	3.01	0.43
1:C:327:LEU:HD11	1:C:342:VAL:HG23	2.00	0.43
1:B:116:TYR:CE2	1:B:256:LEU:HD11	2.52	0.43
1:I:213:LYS:HB2	1:I:227:TYR:CE1	2.53	0.43
1:G:58:PHE:CZ	1:G:62:ILE:HD11	2.54	0.43
1:G:390:ILE:HB	1:G:400:PHE:HB2	2.00	0.43
1:C:199:GLY:O	1:C:200:LEU:HD23	2.17	0.43
1:H:258:MET:SD	1:H:260:PHE:CZ	3.11	0.43
1:E:330:LEU:HD23	1:E:330:LEU:C	2.39	0.43
1:G:133:ILE:HD13	1:I:287:TYR:CD1	2.53	0.43
1:F:226:GLN:HB3	1:F:299:LYS:HE3	2.01	0.43
1:F:183:SER:O	1:F:344:ARG:NH1	2.52	0.43
1:A:330:LEU:O	1:A:330:LEU:HD23	2.19	0.42
1:K:110:GLN:O	1:K:111:GLN:C	2.57	0.42
1:I:261:ILE:HB	1:I:387:ILE:HB	2.01	0.42
1:I:330:LEU:HD23	1:I:330:LEU:C	2.40	0.42
1:I:66:LEU:HD21	1:I:144:TYR:HB2	1.99	0.42
1:A:137:GLN:HE22	1:A:148:LEU:H	1.68	0.42
1:D:386:PHE:CE1	1:D:404:ILE:HG13	2.54	0.42
1:D:225:ALA:HB3	1:D:227:TYR:CE1	2.54	0.42
1:J:266:ASP:N	1:J:266:ASP:OD1	2.51	0.42
1:F:46:PHE:HD2	1:F:273:LEU:HD11	1.84	0.42
1:I:35:ASN:HA	1:I:38:ASP:OD1	2.19	0.42
1:J:289:GLU:CD	1:L:332:ARG:HH22	2.22	0.42
1:I:201:TRP:CD1	1:I:357:GLY:HA2	2.54	0.42
1:J:105:LEU:HD23	1:J:397:THR:OG1	2.20	0.42
1:A:167:VAL:HG13	1:A:194:VAL:HG11	2.02	0.42
1:K:52:ASN:ND2	1:K:406:ASN:O	2.41	0.42
1:L:37:PHE:CE1	1:L:317:ILE:HD11	2.55	0.42
1:L:308:LEU:HD11	1:L:347:GLN:HB2	2.02	0.42
1:B:138:GLN:HG2	1:C:30:GLN:HE22	1.85	0.42
1:K:236:TYR:CD1	1:K:236:TYR:C	2.93	0.42
1:A:277:ASN:O	1:A:278:SER:C	2.58	0.42
1:D:327:LEU:HD11	1:D:342:VAL:HG23	2.02	0.42
1:H:55:LEU:HD23	1:H:55:LEU:N	2.34	0.42
1:L:86:LEU:O	1:L:90:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PHE:CE1	1:C:404:ILE:HG21	2.54	0.42
1:H:52:ASN:HB3	1:H:302:PHE:CZ	2.55	0.42
1:K:267:ASN:OD1	1:K:267:ASN:N	2.53	0.42
1:A:188:VAL:HG12	1:A:189:ILE:HG13	2.02	0.41
1:A:330:LEU:CD2	1:A:330:LEU:C	2.88	0.41
1:E:255:LYS:CG	1:E:392:ASP:OD1	2.68	0.41
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.90	0.41
1:I:392:ASP:O	1:I:396:GLY:N	2.51	0.41
1:E:63:LEU:HD22	1:E:191:LEU:CD1	2.48	0.41
1:C:164:ASN:HD21	1:C:178:ILE:N	2.18	0.41
1:G:392:ASP:O	1:G:396:GLY:N	2.52	0.41
1:J:384:ARG:HB2	1:J:385:PRO:HD2	2.01	0.41
1:B:130:ILE:HG12	1:B:340:VAL:HG11	2.03	0.41
1:H:119:ASN:HD21	1:H:121:ALA:HB2	1.85	0.41
1:E:130:ILE:HD11	1:E:340:VAL:HG11	2.02	0.41
1:A:55:LEU:HB2	1:A:347:GLN:NE2	2.35	0.41
1:H:178:ILE:HD11	1:H:346:PHE:HB3	2.02	0.41
1:H:134:ASN:ND2	1:H:134:ASN:C	2.73	0.41
1:J:285:LEU:O	1:L:135:LYS:NZ	2.52	0.41
1:H:163:ILE:O	1:H:167:VAL:HG23	2.20	0.41
1:K:213:LYS:HB3	1:K:214:PRO:HD2	2.03	0.41
1:D:30:GLN:HB3	1:F:139:ILE:HD11	2.02	0.41
1:J:307:GLN:HE21	1:J:309:ASN:HB2	1.86	0.41
1:D:248:ARG:HD2	1:D:259:TYR:CZ	2.55	0.41
1:A:299:LYS:HG2	1:A:354:ASN:HA	2.01	0.41
1:K:249:LEU:HD12	1:K:260:PHE:CE1	2.56	0.41
1:E:38:ASP:O	1:E:42:VAL:HG23	2.21	0.41
1:C:123:ASN:HB2	1:C:166:TRP:CZ2	2.55	0.41
1:D:130:ILE:O	1:D:150:LYS:NZ	2.42	0.41
1:C:327:LEU:HD13	1:C:330:LEU:HD13	2.03	0.41
1:I:259:TYR:CE2	1:I:285:LEU:HD22	2.56	0.41
1:J:300:PHE:CE1	1:J:404:ILE:HD11	2.55	0.41
1:B:46:PHE:CD2	1:B:273:LEU:HD11	2.55	0.41
1:A:205:PHE:CD2	1:A:230:GLN:HG2	2.56	0.41
1:C:282:HIS:O	1:C:286:TRP:HB2	2.20	0.41
1:E:110:GLN:O	1:E:111:GLN:C	2.59	0.41
1:L:202:THR:HB	1:L:250:PRO:HG2	2.03	0.41
1:B:137:GLN:HE22	1:B:147:MET:HA	1.86	0.41
1:D:91:GLN:O	1:D:93:ASP:N	2.53	0.41
1:A:119:ASN:HD21	1:A:121:ALA:HB2	1.86	0.41
1:F:113:ASN:HD22	1:F:113:ASN:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ASN:OD1	1:E:356:LEU:N	2.50	0.40
1:H:231:ASN:HD21	1:H:294:ASN:HD21	1.68	0.40
1:H:139:ILE:HD13	1:H:139:ILE:HA	1.90	0.40
1:J:211:ASN:OD1	1:J:213:LYS:NZ	2.54	0.40
1:A:124:PHE:HB2	1:A:148:LEU:HG	2.02	0.40
1:J:235:TYR:CE1	1:J:290:GLU:HG3	2.55	0.40
1:I:295:VAL:CG1	1:I:297:LEU:HG	2.51	0.40
1:D:385:PRO:HA	1:D:404:ILE:O	2.21	0.40
1:E:49:HIS:O	1:E:403:LYS:NZ	2.40	0.40
1:K:63:LEU:HD21	1:K:193:ASN:HB2	2.03	0.40
1:J:54:VAL:HG21	1:J:351:ILE:HB	2.03	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	346/397 (87%)	335 (97%)	10 (3%)	1 (0%)	46	79
1	B	345/397 (87%)	325 (94%)	19 (6%)	1 (0%)	46	79
1	C	342/397 (86%)	327 (96%)	14 (4%)	1 (0%)	46	79
1	D	345/397 (87%)	326 (94%)	17 (5%)	2 (1%)	30	67
1	E	348/397 (88%)	326 (94%)	22 (6%)	0	100	100
1	F	343/397 (86%)	329 (96%)	13 (4%)	1 (0%)	46	79
1	G	349/397 (88%)	335 (96%)	14 (4%)	0	100	100
1	H	347/397 (87%)	334 (96%)	10 (3%)	3 (1%)	21	57
1	I	346/397 (87%)	324 (94%)	19 (6%)	3 (1%)	21	57
1	J	345/397 (87%)	325 (94%)	20 (6%)	0	100	100
1	K	348/397 (88%)	333 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	348/397 (88%)	340 (98%)	8 (2%)	0	100	100
All	All	4152/4764 (87%)	3959 (95%)	181 (4%)	12 (0%)	46	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	ASN
1	H	92	ASN
1	D	74	SER
1	H	222	PRO
1	I	92	ASN
1	A	325	ALA
1	I	73	THR
1	C	222	PRO
1	B	178	ILE
1	F	178	ILE
1	I	385	PRO
1	H	406	ASN

### 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	305/349 (87%)	295 (97%)	10 (3%)	45	80
1	B	299/349 (86%)	292 (98%)	7 (2%)	58	87
1	C	305/349 (87%)	294 (96%)	11 (4%)	42	78
1	D	300/349 (86%)	290 (97%)	10 (3%)	45	80
1	E	302/349 (86%)	292 (97%)	10 (3%)	45	80
1	F	302/349 (86%)	289 (96%)	13 (4%)	35	71
1	G	304/349 (87%)	293 (96%)	11 (4%)	42	78
1	H	301/349 (86%)	291 (97%)	10 (3%)	45	80
1	I	302/349 (86%)	284 (94%)	18 (6%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	304/349 (87%)	293 (96%)	11 (4%)	42	78
1	K	300/349 (86%)	285 (95%)	15 (5%)	30	65
1	L	304/349 (87%)	291 (96%)	13 (4%)	35	71
All	All	3628/4188 (87%)	3489 (96%)	139 (4%)	40	76

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	128	ASP
1	A	129	PHE
1	A	158	GLN
1	A	198	CYS
1	A	224	ASN
1	A	267	ASN
1	A	330	LEU
1	A	352	THR
1	A	356	LEU
1	B	38	ASP
1	B	55	LEU
1	B	138	GLN
1	B	152	SER
1	B	198	CYS
1	B	230	GLN
1	B	391	GLU
1	C	38	ASP
1	C	55	LEU
1	C	71	SER
1	C	182	ASP
1	C	238	ASN
1	C	254	ASN
1	C	292	GLU
1	C	301	LYS
1	C	303	ASP
1	C	377	VAL
1	C	397	THR
1	D	114	LYS
1	D	126	VAL
1	D	137	GLN
1	D	218	THR
1	D	226	GLN

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Mol	Chain	Res	Type
1	D	266	ASP
1	D	292	GLU
1	D	294	ASN
1	D	307	GLN
1	D	340	VAL
1	E	50	ASN
1	E	55	LEU
1	E	119	ASN
1	E	128	ASP
1	E	129	PHE
1	E	198	CYS
1	E	277	ASN
1	E	305	SER
1	E	359	CYS
1	E	391	GLU
1	F	34	GLN
1	F	55	LEU
1	F	113	ASN
1	F	122	THR
1	F	154	SER
1	F	182	ASP
1	F	188	VAL
1	F	198	CYS
1	F	241	ASP
1	F	266	ASP
1	F	267	ASN
1	F	270	ASN
1	F	305	SER
1	G	38	ASP
1	G	42	VAL
1	G	72	ASP
1	G	100	SER
1	G	152	SER
1	G	198	CYS
1	G	238	ASN
1	G	254	ASN
1	G	292	GLU
1	G	294	ASN
1	G	303	ASP
1	H	134	ASN
1	H	157	THR
1	H	183	SER

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Mol	Chain	Res	Type
1	H	190	THR
1	H	198	CYS
1	H	233	GLN
1	H	254	ASN
1	H	267	ASN
1	H	377	VAL
1	H	397	THR
1	I	38	ASP
1	I	48	ASN
1	I	55	LEU
1	I	73	THR
1	I	113	ASN
1	I	134	ASN
1	I	179	VAL
1	I	198	CYS
1	I	202	THR
1	I	218	THR
1	I	254	ASN
1	I	289	GLU
1	I	291	ASN
1	I	292	GLU
1	I	314	GLN
1	I	340	VAL
1	I	348	LYS
1	I	398	MET
1	J	71	SER
1	J	111	GLN
1	J	117	ASP
1	J	172	ASN
1	J	198	CYS
1	J	255	LYS
1	J	266	ASP
1	J	275	ARG
1	J	283	GLN
1	J	305	SER
1	J	310	GLU
1	K	38	ASP
1	K	40	MET
1	K	118	LEU
1	K	152	SER
1	K	180	THR
1	K	198	CYS

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Mol	Chain	Res	Type
1	K	210	ASN
1	K	236	TYR
1	K	266	ASP
1	K	267	ASN
1	K	269	VAL
1	K	292	GLU
1	K	356	LEU
1	K	384	ARG
1	K	391	GLU
1	L	38	ASP
1	L	55	LEU
1	L	72	ASP
1	L	100	SER
1	L	128	ASP
1	L	182	ASP
1	L	198	CYS
1	L	267	ASN
1	L	292	GLU
1	L	303	ASP
1	L	307	GLN
1	L	347	GLN
1	L	352	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	137	GLN
1	A	141	ASN
1	A	165	ASN
1	A	193	ASN
1	A	224	ASN
1	A	270	ASN
1	A	347	GLN
1	A	378	GLN
1	B	34	GLN
1	B	91	GLN
1	B	172	ASN
1	B	193	ASN
1	B	238	ASN
1	B	245	GLN
1	B	378	GLN

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Mol	Chain	Res	Type
1	B	406	ASN
1	C	30	GLN
1	C	34	GLN
1	C	104	GLN
1	C	134	ASN
1	C	137	GLN
1	C	233	GLN
1	C	238	ASN
1	C	254	ASN
1	C	264	ASN
1	C	267	ASN
1	C	294	ASN
1	C	307	GLN
1	C	347	GLN
1	D	193	ASN
1	D	238	ASN
1	D	264	ASN
1	D	267	ASN
1	D	291	ASN
1	D	294	ASN
1	D	378	GLN
1	E	34	GLN
1	E	50	ASN
1	E	91	GLN
1	E	104	GLN
1	E	119	ASN
1	E	141	ASN
1	E	193	ASN
1	E	233	GLN
1	E	245	GLN
1	E	254	ASN
1	E	270	ASN
1	E	277	ASN
1	E	313	GLN
1	E	347	GLN
1	E	378	GLN
1	F	104	GLN
1	F	113	ASN
1	F	254	ASN
1	F	270	ASN
1	F	291	ASN
1	F	378	GLN

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Mol	Chain	Res	Type
1	G	104	GLN
1	G	123	ASN
1	G	137	GLN
1	G	141	ASN
1	G	170	HIS
1	G	193	ASN
1	G	238	ASN
1	G	254	ASN
1	G	291	ASN
1	G	294	ASN
1	G	347	GLN
1	G	378	GLN
1	H	34	GLN
1	H	91	GLN
1	H	110	GLN
1	H	119	ASN
1	H	134	ASN
1	H	141	ASN
1	H	145	HIS
1	H	193	ASN
1	H	231	ASN
1	H	245	GLN
1	H	270	ASN
1	H	294	ASN
1	H	313	GLN
1	H	347	GLN
1	H	378	GLN
1	I	48	ASN
1	I	104	GLN
1	I	111	GLN
1	I	113	ASN
1	I	137	GLN
1	I	141	ASN
1	I	145	HIS
1	I	193	ASN
1	I	270	ASN
1	I	314	GLN
1	I	347	GLN
1	I	378	GLN
1	I	383	ASN
1	J	34	GLN
1	J	104	GLN

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Mol	Chain	Res	Type
1	J	123	ASN
1	J	134	ASN
1	J	170	HIS
1	J	193	ASN
1	J	226	GLN
1	J	254	ASN
1	J	270	ASN
1	J	307	GLN
1	J	347	GLN
1	K	30	GLN
1	K	34	GLN
1	K	104	GLN
1	K	165	ASN
1	K	193	ASN
1	K	210	ASN
1	K	313	GLN
1	K	347	GLN
1	K	378	GLN
1	L	34	GLN
1	L	91	GLN
1	L	104	GLN
1	L	137	GLN
1	L	141	ASN
1	L	193	ASN
1	L	270	ASN
1	L	313	GLN
1	L	347	GLN
1	L	378	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/397 (89%)	0.06	3 (0%) 87 86	24, 38, 62, 90	0
1	B	355/397 (89%)	0.11	4 (1%) 82 80	27, 43, 65, 90	0
1	C	354/397 (89%)	0.01	0 100 100	18, 36, 58, 98	0
1	D	355/397 (89%)	0.14	8 (2%) 64 59	21, 41, 66, 94	0
1	E	356/397 (89%)	0.09	5 (1%) 78 76	23, 40, 65, 87	0
1	F	353/397 (88%)	0.10	4 (1%) 82 80	32, 45, 65, 89	0
1	G	357/397 (89%)	0.08	5 (1%) 78 76	24, 43, 63, 85	0
1	H	357/397 (89%)	0.15	3 (0%) 87 86	24, 46, 69, 95	0
1	I	356/397 (89%)	0.11	3 (0%) 87 86	24, 43, 69, 84	0
1	J	355/397 (89%)	0.08	2 (0%) 90 89	23, 42, 66, 88	0
1	K	356/397 (89%)	0.15	4 (1%) 82 80	26, 43, 75, 96	0
1	L	356/397 (89%)	0.03	1 (0%) 94 94	24, 40, 56, 83	0
All	All	4266/4764 (89%)	0.09	42 (0%) 84 82	18, 42, 66, 98	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	THR	4.3
1	B	73	THR	4.3
1	G	73	THR	3.6
1	B	72	ASP	3.5
1	I	218	THR	3.2
1	D	409	PHE	3.2
1	J	218	THR	3.1
1	D	208	VAL	3.1
1	K	208	VAL	3.1
1	B	409	PHE	3.0
1	K	409	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	72	ASP	2.9
1	J	178	ILE	2.9
1	K	73	THR	2.9
1	D	209	ALA	2.7
1	D	73	THR	2.7
1	D	218	THR	2.7
1	E	73	THR	2.6
1	H	409	PHE	2.6
1	I	178	ILE	2.6
1	G	409	PHE	2.6
1	F	208	VAL	2.5
1	E	325	ALA	2.5
1	E	324	ASN	2.4
1	D	178	ILE	2.3
1	A	72	ASP	2.3
1	F	220	GLY	2.3
1	B	340	VAL	2.3
1	F	218	THR	2.2
1	G	154	SER	2.2
1	D	171	THR	2.2
1	I	349	ALA	2.2
1	F	73	THR	2.2
1	H	74	SER	2.1
1	E	74	SER	2.1
1	A	360	ALA	2.1
1	L	409	PHE	2.1
1	G	92	ASN	2.1
1	K	274	ASP	2.0
1	G	209	ALA	2.0
1	H	382	ALA	2.0
1	D	306	GLU	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 ⓘ

There are no carbohydrates 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.