



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:33 AM UTC

PDB ID : 4RSQ / pdb_00004rsq
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

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

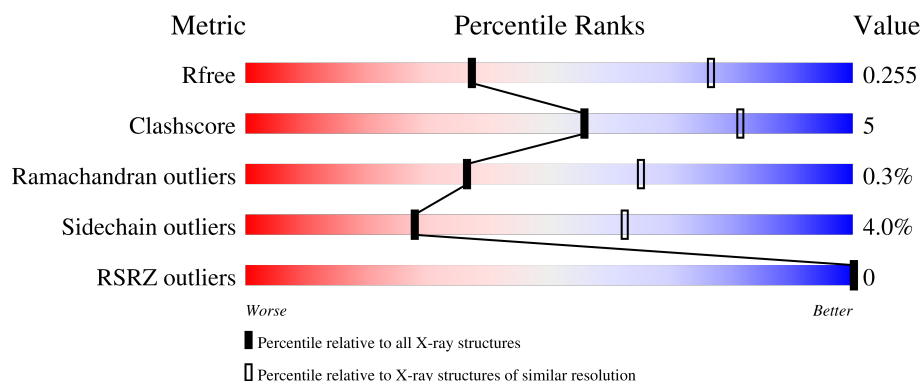
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

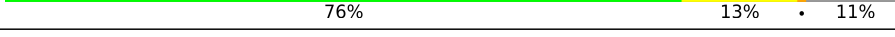
The reported resolution of this entry is 2.90 Å.

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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	

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Mol	Chain	Length	Quality of chain
1	F	397	 79%9% • 11%
1	G	397	 78%12% • 10%
1	H	397	 74%15% • 10%
1	I	397	 73%15% • 10%
1	J	397	 74%14% • 11%
1	K	397	 79%10% • 10%
1	L	397	 76%12% • 10%

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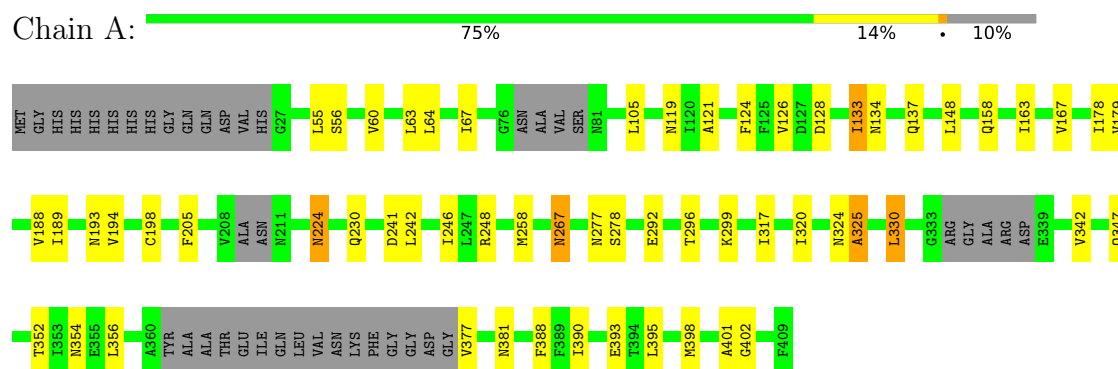
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Chain	Residue	Modelled	Actual	Comment	Reference
L	359	CYS	GLU	engineered mutation	UNP Q005N3

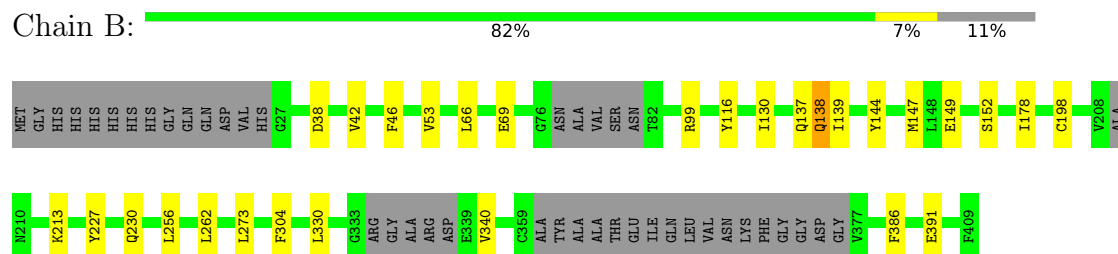
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

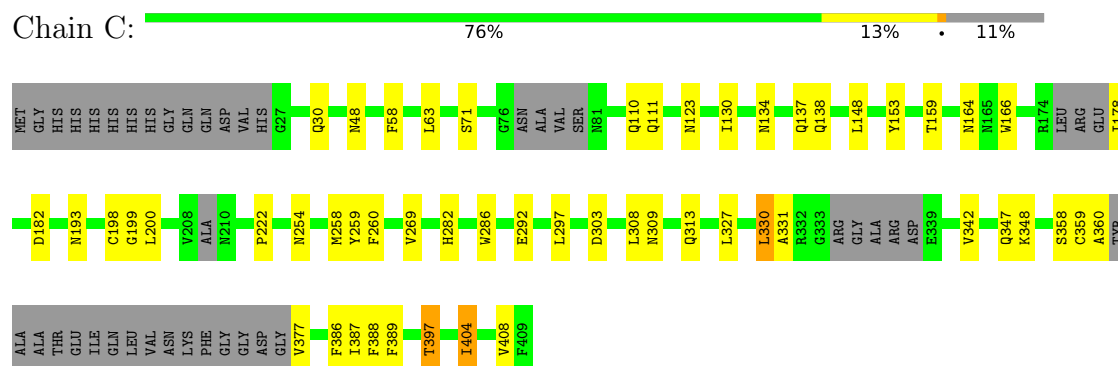
• Molecule 1: Serpin 2



• Molecule 1: Serpin 2

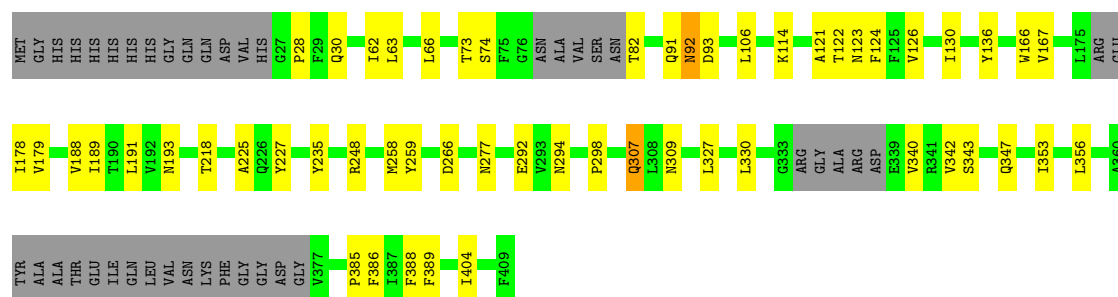


• Molecule 1: Serpin 2



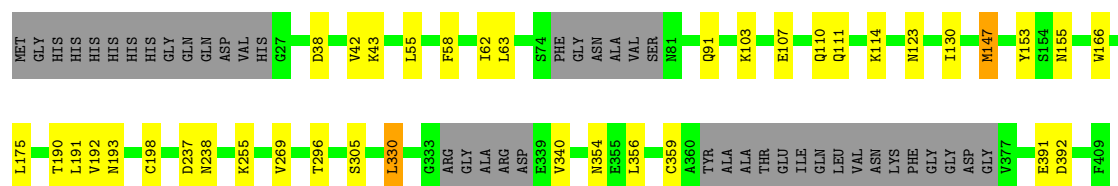
• Molecule 1: Serpin 2

Chain D:  76% 13% 11%



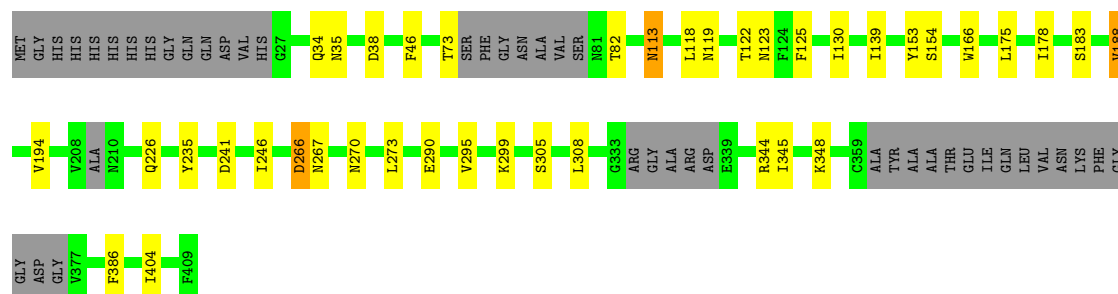
• Molecule 1: Serpin 2

Chain E:  80% 9% 10%



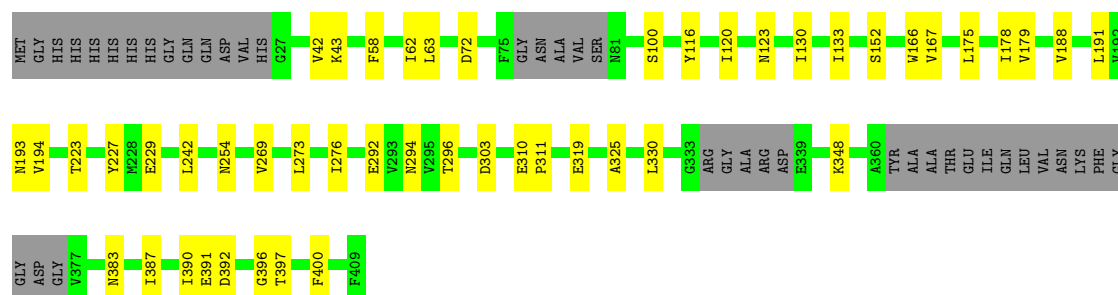
• Molecule 1: Serpin 2

Chain F:  79% 9% 11%



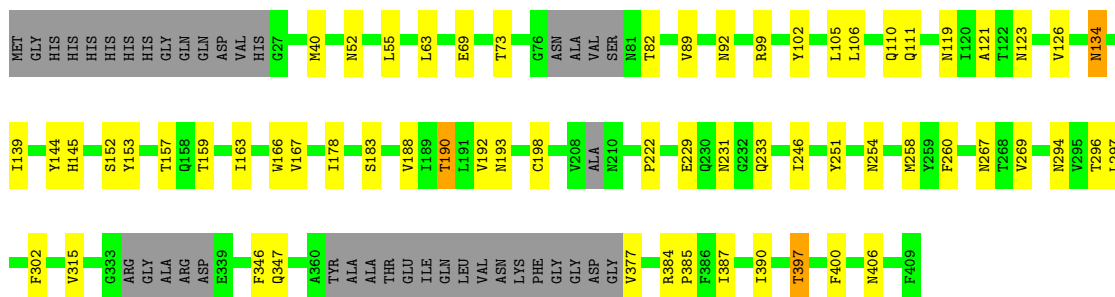
• Molecule 1: Serpin 2

Chain G:  78% 12% 10%



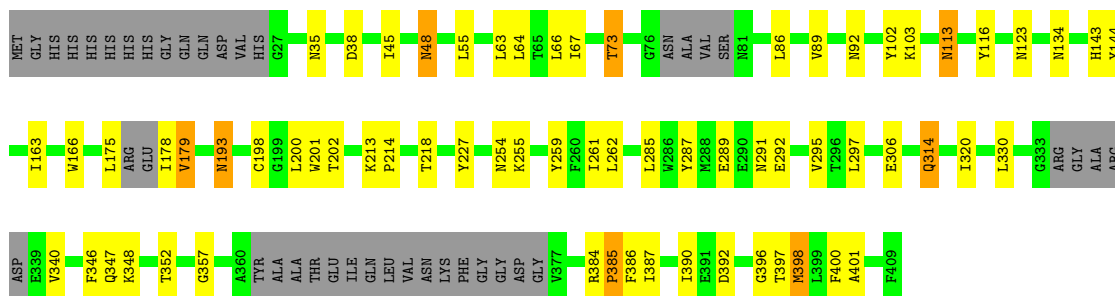
• Molecule 1: Serpin 2

Chain H: 74% 15% • 10%



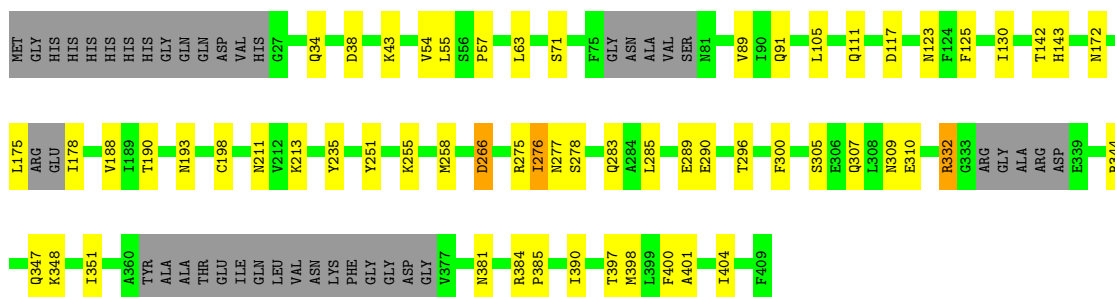
- Molecule 1: Serpin 2

Chain I: 73% 15% • 10%

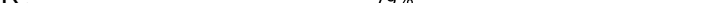


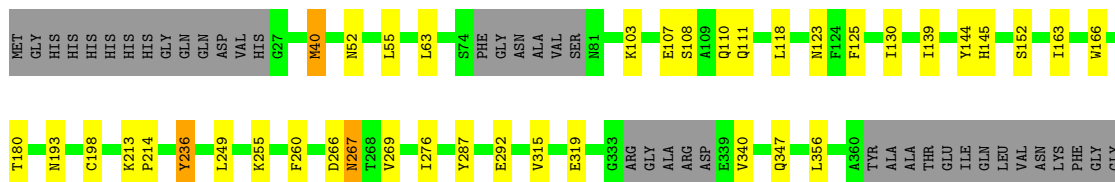
- Molecule 1: Serpin 2

Chain J:  74% 14% • 11%



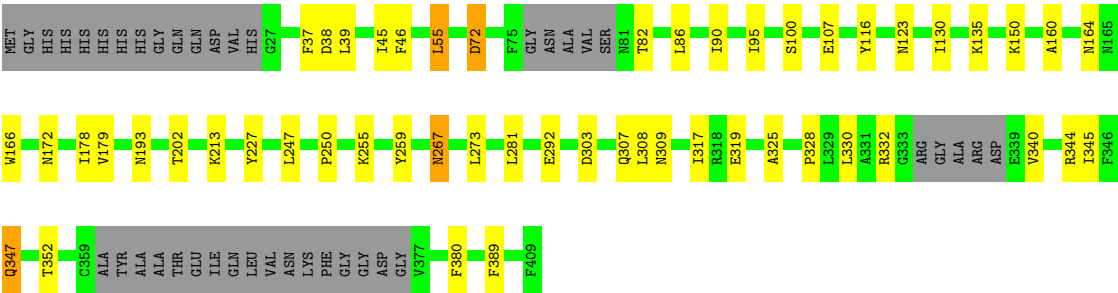
- Molecule 1: Serpin 2

Chain K:  79% 10% • 10%





● Molecule 1: Serpin 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.255 0.196 , 0.255	Depositor DCC
R_{free} test set	6286 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 15.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
Reported twinning fraction	0.445 for H, K, L 0.555 for h,-k,-l	Depositor
Outliers	0 of 129620 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33765	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.50	0/2890	0.77	1/3928 (0.0%)
1	B	0.47	0/2863	0.73	0/3894
1	C	0.50	0/2878	0.75	0/3909
1	D	0.50	0/2863	0.74	0/3892
1	E	0.51	0/2880	0.75	0/3918
1	F	0.45	0/2867	0.70	0/3898
1	G	0.47	0/2893	0.71	0/3935
1	H	0.48	0/2877	0.74	0/3913
1	I	0.51	0/2877	0.75	0/3911
1	J	0.50	0/2880	0.74	0/3916
1	K	0.49	0/2871	0.76	0/3908
1	L	0.49	0/2883	0.76	0/3923
All	All	0.49	0/34522	0.74	1/46945 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ILE	N-CA-CB	5.17	116.74	110.95

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	2827	0	2699	34	0
1	B	2800	0	2658	14	0
1	C	2816	0	2689	26	0
1	D	2801	0	2672	30	0
1	E	2816	0	2688	18	0
1	F	2804	0	2673	19	0
1	G	2829	0	2698	22	0
1	H	2814	0	2676	34	0
1	I	2814	0	2692	36	0
1	J	2817	0	2690	32	0
1	K	2807	0	2668	18	0
1	L	2820	0	2690	32	0
All	All	33765	0	32193	308	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 5.

All (308) 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:A:398:MET:HE2	1:A:401:ALA:HB2	1.73	0.70
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:N	1:I:48:ASN:HD22	1.97	0.63
1:H:63:LEU:HD11	1:H:193:ASN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:TYR:HB2	1:C:389:PHE:CE1	2.34	0.62
1:G:229:GLU:HG3	1:G:296:THR:HG23	1.80	0.62
1:K:40:MET:HE3	1:K:315:VAL:HB	1.82	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
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:G:123:ASN:HB2	1:G:166:TRP:CZ2	2.37	0.60
1:I:63:LEU:HD21	1:I:193:ASN:HB2	1.84	0.60
1:A:330:LEU:C	1:A:330:LEU:HD23	2.26	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:H:152:SER:O	1:H:159:THR:OG1	2.18	0.59
1:I:67:ILE:HD13	1:I:320:ILE:HD12	1.84	0.59
1:A:67:ILE:HD13	1:A:320:ILE:HD12	1.84	0.59
1:E:103:LYS:NZ	1:E:107:GLU:OE2	2.34	0.59
1:J:63:LEU:HD21	1:J:193:ASN:HB2	1.83	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:H:106:LEU:HD22	1:H:110:GLN:HE21	1.67	0.58
1:J:130:ILE:HD11	1:J:188:VAL:HG12	1.86	0.58
1:A:126:VAL:HG22	1:A:189:ILE:HG12	1.86	0.58
1:G:269:VAL:HG13	1:G:387:ILE:HD11	1.86	0.58
1:H:153:TYR:OH	1:H:190:THR:OG1	2.22	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:L:72:ASP:C	1:L:72:ASP:OD1	2.47	0.56
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:G:63:LEU:HB3	1:G:191:LEU:HD21	1.86	0.56
1:J:175:LEU:HD22	1:J:348:LYS:HE2	1.88	0.56
1:D:62:ILE:HD12	1:D:106:LEU:HD11	1.88	0.56
1:L:330:LEU:C	1:L:330:LEU:HD23	2.31	0.56
1:I:262:LEU:HD12	1:I:386:PHE:HB3	1.89	0.55
1:J:398:MET:HE2	1:J:401:ALA:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:258:MET:SD	1:C:260:PHE:CZ	3.02	0.53
1:H:260:PHE:CE2	1:H:297:LEU:HD13	2.43	0.53
1:B:38:ASP:O	1:B:42:VAL:HG23	2.09	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:J:390:ILE:HD12	1:J:400:PHE:CD2	2.43	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:H:40:MET:HE3	1:H:315:VAL:HB	1.91	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:G:330:LEU:C	1:G:330:LEU:HD23	2.35	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:B:66:LEU:HD21	1:B:144:TYR:HB2	1.93	0.51
1:H:390:ILE:HD12	1:H:400:PHE:CD1	2.46	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:OD1	1:A:267:ASN:N	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:C:258:MET:HE2	1:C:388:PHE:CD1	2.47	0.49
1:C:330:LEU:C	1:C:330:LEU:HD23	2.37	0.49
1:L:308:LEU:HD12	1:L:345:ILE:CG2	2.41	0.49
1:D:130:ILE:HD11	1:D:188:VAL:CG1	2.41	0.49
1:E:63:LEU:HD21	1:E:193:ASN:CB	2.39	0.49
1:L:39:LEU:HD21	1:L:281:LEU:HD22	1.94	0.49
1:A:64:LEU:HD22	1:A:317:ILE:HD13	1.94	0.49
1:D:167:VAL:HG21	1:D:178:ILE:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:ILE:HD13	1:H:192:VAL:HG13	1.95	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:A:398:MET:HE2	1:A:401:ALA:CB	2.42	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:B:330:LEU:C	1:B:330:LEU:HD23	2.38	0.48
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:I:45:ILE:HD12	1:I:306:GLU:OE1	2.13	0.48
1:K:125:PHE:CE2	1:K:163:ILE:HG23	2.48	0.48
1:G:167:VAL:HG13	1:G:194:VAL:HG11	1.96	0.48
1:G:175:LEU:HD13	1:G:348:LYS:HG2	1.95	0.48
1:G:391:GLU:HA	1:G:397:THR:O	2.13	0.48
1:L:213:LYS:HB2	1:L:227:TYR:CD1	2.48	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:45:ILE:HG21	1:L:55:LEU:HD22	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:H:251:TYR:OH	1:H:258:MET:HE3	2.14	0.47
1:E:330:LEU:C	1:E:330:LEU:HD23	2.39	0.47
1:I:103:LYS:HD3	1:I:143:HIS:HA	1.96	0.47
1:I:113:ASN:N	1:I:113:ASN:HD22	2.12	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:J:289:GLU:CD	1:L:332:ARG:HH22	2.22	0.47
1:A:224:ASN:N	1:A:224:ASN:HD22	2.13	0.47
1:E:114:LYS:HA	1:I:200:LEU:HD11	1.96	0.47
1:H:105:LEU:HD23	1:H:397:THR:HG23	1.96	0.47
1:I:116:TYR:OH	1:I:255:LYS:HD2	2.15	0.47
1:I:163:ILE:HG21	1:I:179:VAL:HG21	1.96	0.47
1:L:247:LEU:HD22	1:L:380:PHE:CD2	2.50	0.47
1:L:319:GLU:O	1:L:325:ALA:HB2	2.14	0.47
1:K:236:TYR:CD1	1:K:236:TYR:C	2.93	0.47
1:A:277:ASN:O	1:A:278:SER:C	2.58	0.47
1:D:123:ASN:HB2	1:D:166:TRP:CZ2	2.49	0.47
1:C:359:CYS:O	1:C:360:ALA:HB2	2.15	0.47
1:F:125:PHE:O	1:F:153:TYR:OH	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:PHE:CZ	1:F:404:ILE:HG13	2.50	0.47
1:H:384:ARG:HB2	1:H:385:PRO:HD2	1.97	0.47
1:I:398:MET:HE2	1:I:401:ALA:HB2	1.97	0.47
1:I:330:LEU:HD23	1:I:330:LEU:C	2.40	0.46
1:K:110:GLN:O	1:K:111:GLN:C	2.57	0.46
1:E:190:THR:HG22	1:E:192:VAL:HG23	1.97	0.46
1:A:330:LEU:C	1:A:330:LEU:CD2	2.88	0.46
1:H:55:LEU:HB2	1:H:347:GLN:HE22	1.80	0.46
1:C:269:VAL:HG13	1:C:387:ILE:HD11	1.97	0.46
1:K:193:ASN:HD22	1:K:347:GLN:HG3	1.80	0.46
1:C:153:TYR:CE1	1:C:159:THR:HG21	2.51	0.46
1:H:134:ASN:C	1:H:134:ASN:ND2	2.73	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:A:296:THR:HB	1:A:381:ASN:HA	1.97	0.46
1:I:390:ILE:HD12	1:I:400:PHE:CG	2.51	0.46
1:D:124:PHE:CE1	1:D:191:LEU:HD13	2.51	0.46
1:L:267:ASN:N	1:L:267:ASN:HD22	2.14	0.46
1:C:198:CYS:HA	1:C:358:SER:O	2.17	0.45
1:E:110:GLN:O	1:E:111:GLN:C	2.59	0.45
1:J:142:THR:HB	1:J:143:HIS:CD2	2.51	0.45
1:K:108:SER:O	1:K:255:LYS:HD3	2.16	0.45
1:A:105:LEU:HG	1:A:395:LEU:HD13	1.99	0.45
1:A:258:MET:HE3	1:A:390:ILE:HD11	1.98	0.45
1:D:309:ASN:ND2	1:D:343:SER:O	2.49	0.45
1:F:235:TYR:CE1	1:F:290:GLU:HG3	2.51	0.45
1:A:56:SER:O	1:A:60:VAL:HG23	2.16	0.45
1:H:246:ILE:HA	1:H:260:PHE:O	2.17	0.45
1:A:163:ILE:O	1:A:167:VAL:HG23	2.17	0.45
1:A:67:ILE:HG12	1:A:342:VAL:HG21	1.98	0.45
1:A:193:ASN:HD22	1:A:347:GLN:HG3	1.82	0.45
1:I:48:ASN:N	1:I:48:ASN:ND2	2.64	0.45
1:L:123:ASN:HD22	1:L:166:TRP:NE1	2.14	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:69:GLU:OE2	1:H:99:ARG:NE	2.50	0.45
1:H:167:VAL:HG21	1:H:178:ILE:HG22	1.99	0.45
1:F:35:ASN:HA	1:F:38:ASP:OD1	2.17	0.44
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:J:43:LYS:NZ	1:J:276:ILE:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD12	1:B:386:PHE:HB3	1.98	0.44
1:C:110:GLN:O	1:C:111:GLN:C	2.60	0.44
1:H:89:VAL:O	1:H:102:TYR:OH	2.34	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:G:130:ILE:HD11	1:G:188:VAL:CG1	2.43	0.44
1:L:160:ALA:O	1:L:164:ASN:ND2	2.50	0.44
1:J:34:GLN:HE22	1:J:91:GLN:HE22	1.66	0.44
1:L:72:ASP:HB3	1:L:328:PRO:HG3	1.98	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:121:ALA:HB1	1:D:166:TRP:CZ2	2.52	0.44
1:D:130:ILE:HD13	1:D:189:ILE:HD11	2.00	0.44
1:E:58:PHE:CE2	1:E:62:ILE:HD11	2.52	0.44
1:J:175:LEU:HD13	1:J:348:LYS:HG2	2.00	0.44
1:D:298:PRO:O	1:D:353:ILE:HD11	2.18	0.44
1:F:308:LEU:HD12	1:F:345:ILE:CG2	2.47	0.44
1:J:123:ASN:OD1	1:J:125:PHE:CE1	2.71	0.44
1:F:194:VAL:HG12	1:F:348:LYS:HB3	2.00	0.44
1:G:116:TYR:CD1	1:G:116:TYR:C	2.96	0.44
1:H:119:ASN:ND2	1:H:121:ALA:HB2	2.31	0.44
1:J:398:MET:HE2	1:J:401:ALA:CB	2.47	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
1:C:134:ASN:HD21	1:C:138:GLN:NE2	2.16	0.44
1:D:63:LEU:HD21	1:D:193:ASN:HB2	2.00	0.44
1:I:213:LYS:HB3	1:I:214:PRO:HD2	1.99	0.44
1:K:144:TYR:O	1:K:145:HIS:C	2.60	0.44
1:L:82:THR:HG22	1:L:86:LEU:HD12	1.99	0.44
1:D:330:LEU:HD23	1:D:330:LEU:C	2.43	0.43
1:G:310:GLU:HB3	1:G:311:PRO:HD3	2.00	0.43
1:C:58:PHE:CD1	1:C:397:THR:CG2	3.01	0.43
1:G:242:LEU:HD22	1:G:276:ILE:HG13	1.99	0.43
1:B:116:TYR:CE2	1:B:256:LEU:HD11	2.52	0.43
1:C:327:LEU:HD11	1:C:342:VAL:HG23	2.00	0.43
1:C:199:GLY:O	1:C:200:LEU:HD23	2.17	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:I:213:LYS:HB2	1:I:227:TYR:CE1	2.53	0.43
1:D:91:GLN:O	1:D:92:ASN:C	2.62	0.43
1:D:258:MET:HE2	1:D:388:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:ILE:HD13	1:I:287:TYR:CD1	2.53	0.43
1:H:258:MET:SD	1:H:260:PHE:CZ	3.11	0.43
1:E:153:TYR:C	1:E:155:ASN:H	2.27	0.43
1:F:183:SER:O	1:F:344:ARG:NH1	2.52	0.43
1:F:226:GLN:HB3	1:F:299:LYS:HE3	2.01	0.43
1:A:324:ASN:O	1:A:325:ALA:C	2.60	0.43
1:H:110:GLN:O	1:H:111:GLN:C	2.62	0.43
1:A:330:LEU:HD23	1:A:330:LEU:O	2.19	0.42
1:I:66:LEU:HD21	1:I:144:TYR:HB2	1.99	0.42
1:I:261:ILE:HB	1:I:387:ILE:HB	2.01	0.42
1:A:137:GLN:HE22	1:A:148:LEU:H	1.68	0.42
1:D:225:ALA:HB3	1:D:227:TYR:CE1	2.54	0.42
1:D:386:PHE:CE1	1:D:404:ILE:HG13	2.54	0.42
1:F:46:PHE:HD2	1:F:273:LEU:HD11	1.84	0.42
1:J:266:ASP:OD1	1:J:266:ASP:N	2.51	0.42
1:J:285:LEU:O	1:L:135:LYS:NZ	2.52	0.42
1:G:43:LYS:NZ	1:G:273:LEU:O	2.35	0.42
1:I:35:ASN:HA	1:I:38:ASP:OD1	2.19	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:B:138:GLN:HG2	1:C:30:GLN:HE22	1.85	0.42
1:L:308:LEU:HD11	1:L:347:GLN:HB2	2.02	0.42
1:D:327:LEU:HD11	1:D:342:VAL:HG23	2.02	0.42
1:E:147:MET:HE3	1:E:147:MET:HB2	1.96	0.42
1:J:251:TYR:OH	1:J:258:MET:HE3	2.20	0.42
1:H:55:LEU:HD23	1:H:55:LEU:N	2.34	0.42
1:H:144:TYR:O	1:H:145:HIS:C	2.63	0.42
1:C:386:PHE:CE1	1:C:404:ILE:HG21	2.54	0.42
1:I:396:GLY:O	1:I:397:THR:C	2.62	0.42
1:L:86:LEU:O	1:L:90:ILE:HG12	2.20	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:D:356:LEU:HD23	1:D:356:LEU:HA	1.90	0.41
1:E:255:LYS:CG	1:E:392:ASP:OD1	2.68	0.41
1:I:392:ASP:O	1:I:396:GLY:N	2.51	0.41
1:C:164:ASN:HD21	1:C:178:ILE:N	2.18	0.41
1:E:63:LEU:HD22	1:E:191:LEU:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:392:ASP:O	1:G:396:GLY:N	2.52	0.41
1:B:130:ILE:HG12	1:B:340:VAL:HG11	2.03	0.41
1:J:384:ARG:HB2	1:J:385:PRO:HD2	2.01	0.41
1:E:130:ILE:HD11	1:E:340:VAL:HG11	2.02	0.41
1:H:119:ASN:HD21	1:H:121:ALA:HB2	1.85	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:A:241:ASP:C	1:A:241:ASP:OD1	2.64	0.41
1:D:30:GLN:HB3	1:F:139:ILE:HD11	2.02	0.41
1:H:163:ILE:O	1:H:167:VAL:HG23	2.20	0.41
1:J:307:GLN:HE21	1:J:309:ASN:HB2	1.86	0.41
1:K:213:LYS:HB3	1:K:214:PRO:HD2	2.03	0.41
1:L:37:PHE:O	1:L:38:ASP:C	2.64	0.41
1:A:299:LYS:HG2	1:A:354:ASN:HA	2.01	0.41
1:C:123:ASN:HB2	1:C:166:TRP:CZ2	2.55	0.41
1:D:248:ARG:HD2	1:D:259:TYR:CZ	2.55	0.41
1:E:38:ASP:O	1:E:42:VAL:HG23	2.21	0.41
1:K:249:LEU:HD12	1:K:260:PHE:CE1	2.56	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:277:ASN:O	1:J:278:SER:C	2.64	0.41
1:J:300:PHE:CE1	1:J:404:ILE:HD11	2.55	0.41
1:A:205:PHE:CD2	1:A:230:GLN:HG2	2.56	0.41
1:B:46:PHE:CD2	1:B:273:LEU:HD11	2.55	0.41
1:B:137:GLN:HE22	1:B:147:MET:HA	1.86	0.41
1:C:282:HIS:O	1:C:286:TRP:HB2	2.20	0.41
1:L:202:THR:HB	1:L:250:PRO:HG2	2.03	0.41
1:A:119:ASN:HD21	1:A:121:ALA:HB2	1.86	0.41
1:D:91:GLN:O	1:D:93:ASP:N	2.53	0.41
1:E:354:ASN:OD1	1:E:356:LEU:N	2.50	0.40
1:F:113:ASN:HD22	1:F:113:ASN:N	2.19	0.40
1:H:139:ILE:HD13	1:H:139:ILE:HA	1.90	0.40
1:H:231:ASN:HD21	1:H:294:ASN:HD21	1.68	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:I:295:VAL:CG1	1:I:297:LEU:HG	2.51	0.40
1:J:235:TYR:CE1	1:J:290:GLU:HG3	2.55	0.40
1:D:385:PRO:HA	1:D:404:ILE:O	2.21	0.40
1:J:54:VAL:HG21	1:J:351:ILE:HB	2.03	0.40
1:K:63:LEU:HD21	1:K:193:ASN:HB2	2.03	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	346/397 (87%)	335 (97%)	10 (3%)	1 (0%)	36	65
1	B	345/397 (87%)	325 (94%)	19 (6%)	1 (0%)	36	65
1	C	342/397 (86%)	327 (96%)	14 (4%)	1 (0%)	36	65
1	D	345/397 (87%)	326 (94%)	17 (5%)	2 (1%)	21	51
1	E	348/397 (88%)	326 (94%)	22 (6%)	0	100	100
1	F	343/397 (86%)	329 (96%)	13 (4%)	1 (0%)	36	65
1	G	349/397 (88%)	335 (96%)	14 (4%)	0	100	100
1	H	347/397 (87%)	334 (96%)	10 (3%)	3 (1%)	14	41
1	I	346/397 (87%)	324 (94%)	19 (6%)	3 (1%)	14	41
1	J	345/397 (87%)	325 (94%)	20 (6%)	0	100	100
1	K	348/397 (88%)	333 (96%)	15 (4%)	0	100	100
1	L	348/397 (88%)	340 (98%)	8 (2%)	0	100	100
All	All	4152/4764 (87%)	3959 (95%)	181 (4%)	12 (0%)	36	65

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%)	294 (96%)	11 (4%)	31	65
1	B	299/349 (86%)	292 (98%)	7 (2%)	44	76
1	C	305/349 (87%)	293 (96%)	12 (4%)	28	63
1	D	300/349 (86%)	290 (97%)	10 (3%)	33	67
1	E	302/349 (86%)	290 (96%)	12 (4%)	28	62
1	F	302/349 (86%)	290 (96%)	12 (4%)	28	62
1	G	304/349 (87%)	294 (97%)	10 (3%)	33	67
1	H	301/349 (86%)	289 (96%)	12 (4%)	28	62
1	I	302/349 (86%)	284 (94%)	18 (6%)	17	47
1	J	304/349 (87%)	290 (95%)	14 (5%)	24	57
1	K	300/349 (86%)	284 (95%)	16 (5%)	20	52
1	L	304/349 (87%)	292 (96%)	12 (4%)	28	63
All	All	3628/4188 (87%)	3482 (96%)	146 (4%)	28	62

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	A	133	ILE
1	A	158	GLN
1	A	198	CYS
1	A	224	ASN
1	A	267	ASN
1	A	292	GLU
1	A	330	LEU
1	A	352	THR
1	A	356	LEU
1	A	377	VAL
1	B	138	GLN
1	B	139	ILE
1	B	149	GLU

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Mol	Chain	Res	Type
1	B	152	SER
1	B	198	CYS
1	B	230	GLN
1	B	391	GLU
1	C	48	ASN
1	C	71	SER
1	C	182	ASP
1	C	254	ASN
1	C	292	GLU
1	C	297	LEU
1	C	303	ASP
1	C	330	LEU
1	C	377	VAL
1	C	397	THR
1	C	404	ILE
1	C	408	VAL
1	D	114	LYS
1	D	122	THR
1	D	126	VAL
1	D	218	THR
1	D	266	ASP
1	D	277	ASN
1	D	292	GLU
1	D	294	ASN
1	D	307	GLN
1	D	340	VAL
1	E	43	LYS
1	E	55	LEU
1	E	91	GLN
1	E	147	MET
1	E	175	LEU
1	E	198	CYS
1	E	269	VAL
1	E	296	THR
1	E	305	SER
1	E	330	LEU
1	E	359	CYS
1	E	391	GLU
1	F	34	GLN
1	F	113	ASN
1	F	122	THR
1	F	154	SER

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Mol	Chain	Res	Type
1	F	188	VAL
1	F	241	ASP
1	F	246	ILE
1	F	266	ASP
1	F	267	ASN
1	F	270	ASN
1	F	295	VAL
1	F	305	SER
1	G	42	VAL
1	G	72	ASP
1	G	100	SER
1	G	120	ILE
1	G	152	SER
1	G	223	THR
1	G	254	ASN
1	G	292	GLU
1	G	294	ASN
1	G	303	ASP
1	H	126	VAL
1	H	134	ASN
1	H	157	THR
1	H	183	SER
1	H	188	VAL
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	48	ASN
1	I	55	LEU
1	I	73	THR
1	I	113	ASN
1	I	134	ASN
1	I	179	VAL
1	I	193	ASN
1	I	198	CYS
1	I	202	THR
1	I	218	THR
1	I	254	ASN
1	I	289	GLU

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Mol	Chain	Res	Type
1	I	291	ASN
1	I	292	GLU
1	I	314	GLN
1	I	340	VAL
1	I	352	THR
1	I	398	MET
1	J	71	SER
1	J	89	VAL
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	276	ILE
1	J	283	GLN
1	J	305	SER
1	J	310	GLU
1	J	332	ARG
1	K	40	MET
1	K	118	LEU
1	K	139	ILE
1	K	152	SER
1	K	180	THR
1	K	198	CYS
1	K	236	TYR
1	K	266	ASP
1	K	267	ASN
1	K	269	VAL
1	K	276	ILE
1	K	292	GLU
1	K	319	GLU
1	K	356	LEU
1	K	384	ARG
1	K	391	GLU
1	L	55	LEU
1	L	72	ASP
1	L	95	ILE
1	L	100	SER
1	L	107	GLU
1	L	172	ASN

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Mol	Chain	Res	Type
1	L	267	ASN
1	L	292	GLU
1	L	303	ASP
1	L	307	GLN
1	L	347	GLN
1	L	352	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (155) 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	291	ASN
1	A	313	GLN
1	A	347	GLN
1	B	30	GLN
1	B	34	GLN
1	B	91	GLN
1	B	104	GLN
1	B	170	HIS
1	B	172	ASN
1	B	238	ASN
1	B	245	GLN
1	B	264	ASN
1	B	282	HIS
1	B	291	ASN
1	B	314	GLN
1	B	378	GLN
1	B	406	ASN
1	C	30	GLN
1	C	34	GLN
1	C	49	HIS
1	C	91	GLN
1	C	104	GLN
1	C	134	ASN
1	C	137	GLN
1	C	238	ASN

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Mol	Chain	Res	Type
1	C	254	ASN
1	C	264	ASN
1	C	267	ASN
1	C	277	ASN
1	C	307	GLN
1	C	347	GLN
1	C	381	ASN
1	D	34	GLN
1	D	155	ASN
1	D	193	ASN
1	D	238	ASN
1	D	264	ASN
1	D	277	ASN
1	D	291	ASN
1	D	294	ASN
1	D	307	GLN
1	D	378	GLN
1	E	34	GLN
1	E	49	HIS
1	E	50	ASN
1	E	91	GLN
1	E	104	GLN
1	E	141	ASN
1	E	165	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	307	GLN
1	E	313	GLN
1	E	347	GLN
1	E	378	GLN
1	F	34	GLN
1	F	91	GLN
1	F	94	ASN
1	F	104	GLN
1	F	113	ASN
1	F	254	ASN
1	F	270	ASN
1	F	291	ASN

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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	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	224	ASN
1	H	226	GLN
1	H	245	GLN
1	H	270	ASN
1	H	291	ASN
1	H	294	ASN
1	H	313	GLN
1	H	347	GLN
1	H	378	GLN
1	I	34	GLN
1	I	48	ASN
1	I	91	GLN
1	I	104	GLN
1	I	111	GLN
1	I	113	ASN
1	I	145	HIS
1	I	193	ASN
1	I	233	GLN
1	I	270	ASN
1	I	291	ASN
1	I	313	GLN
1	I	314	GLN
1	I	347	GLN

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Mol	Chain	Res	Type
1	I	378	GLN
1	I	383	ASN
1	J	34	GLN
1	J	104	GLN
1	J	134	ASN
1	J	155	ASN
1	J	170	HIS
1	J	193	ASN
1	J	226	GLN
1	J	233	GLN
1	J	254	ASN
1	J	270	ASN
1	J	277	ASN
1	J	291	ASN
1	J	307	GLN
1	J	347	GLN
1	K	30	GLN
1	K	34	GLN
1	K	104	GLN
1	K	172	ASN
1	K	193	ASN
1	K	210	ASN
1	K	313	GLN
1	K	347	GLN
1	K	378	GLN
1	K	406	ASN
1	L	34	GLN
1	L	91	GLN
1	L	104	GLN
1	L	137	GLN
1	L	141	ASN
1	L	165	ASN
1	L	193	ASN
1	L	224	ASN
1	L	233	GLN
1	L	270	ASN
1	L	313	GLN
1	L	347	GLN
1	L	378	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	356/397 (89%)	-1.52	0 100 100	24, 38, 62, 90	0
1	B	355/397 (89%)	-1.51	0 100 100	27, 43, 65, 90	0
1	C	354/397 (89%)	-1.55	0 100 100	18, 36, 58, 98	0
1	D	355/397 (89%)	-1.49	0 100 100	21, 41, 66, 94	0
1	E	356/397 (89%)	-1.53	0 100 100	23, 40, 65, 87	0
1	F	353/397 (88%)	-1.53	0 100 100	32, 45, 65, 89	0
1	G	357/397 (89%)	-1.51	0 100 100	24, 43, 63, 85	0
1	H	357/397 (89%)	-1.48	0 100 100	24, 46, 69, 95	0
1	I	356/397 (89%)	-1.50	0 100 100	24, 43, 69, 84	0
1	J	355/397 (89%)	-1.52	0 100 100	23, 42, 66, 88	0
1	K	356/397 (89%)	-1.48	0 100 100	26, 43, 75, 96	0
1	L	356/397 (89%)	-1.54	0 100 100	24, 40, 56, 83	0
All	All	4266/4764 (89%)	-1.51	0 100 100	18, 42, 66, 98	0

There are no RSRZ outliers to report.

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.