



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:17 PM UTC

PDB ID : 7Y1I / pdb_00007y1i
Title : Crystal Structure of TTR-G67R
Authors : Luan, X.D.; Chen, B.X.; Zhang, S.Y.
Deposited on : 2022-06-08
Resolution : 2.79 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

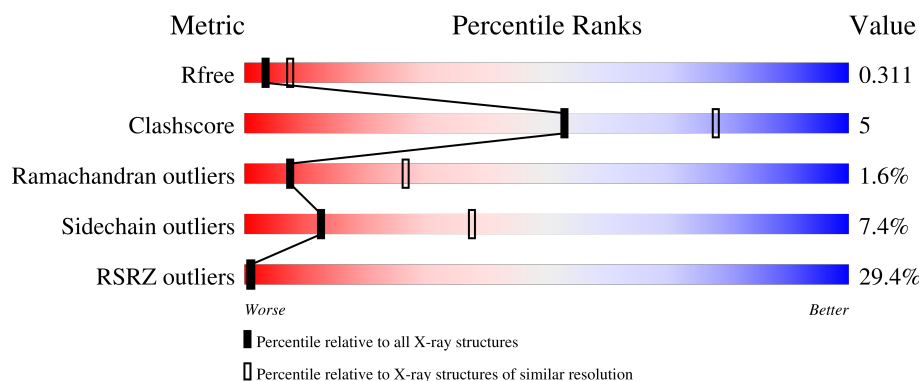
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	147	16% 65% 14% • 20%
1	B	147	35% 69% 11% • 16%
1	C	147	14% 65% 14% • 20%
1	D	147	27% 63% 20% • 16%
1	E	147	27% 65% 13% • 20%

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Mol	Chain	Length	Quality of chain
1	F	147	
1	G	147	
1	H	147	
1	I	147	
1	J	147	
1	K	147	
1	L	147	
1	M	147	
1	N	147	
1	O	147	
1	P	147	
1	Q	147	
1	R	147	
1	S	147	
1	T	147	
1	U	147	
1	V	147	
1	W	147	
1	X	147	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22028 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 Transthyretin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	B	124	Total	C	N	O	S	0	0	0
			947	602	155	187	3			
1	C	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	D	124	Total	C	N	O	S	0	0	0
			947	602	155	187	3			
1	E	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	F	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			
1	G	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	H	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			
1	I	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	J	124	Total	C	N	O	S	0	0	0
			947	602	155	187	3			
1	K	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	L	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			
1	M	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	N	124	Total	C	N	O	S	0	0	0
			947	602	155	187	3			
1	O	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	P	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	R	124	Total	C	N	O	S	0	0	0
			947	602	155	187	3			
1	S	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	T	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			
1	U	118	Total	C	N	O	S	0	0	0
			911	582	150	176	3			
1	V	123	Total	C	N	O	S	0	0	0
			943	599	155	186	3			
1	W	117	Total	C	N	O	S	0	0	0
			902	576	148	175	3			
1	X	118	Total	C	N	O	S	0	0	0
			912	582	150	177	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	VAL	variant	UNP P02766
B	30	MET	VAL	variant	UNP P02766
C	30	MET	VAL	variant	UNP P02766
D	30	MET	VAL	variant	UNP P02766
E	30	MET	VAL	variant	UNP P02766
F	30	MET	VAL	variant	UNP P02766
G	30	MET	VAL	variant	UNP P02766
H	30	MET	VAL	variant	UNP P02766
I	30	MET	VAL	variant	UNP P02766
J	30	MET	VAL	variant	UNP P02766
K	30	MET	VAL	variant	UNP P02766
L	30	MET	VAL	variant	UNP P02766
M	30	MET	VAL	variant	UNP P02766
N	30	MET	VAL	variant	UNP P02766
O	30	MET	VAL	variant	UNP P02766
P	30	MET	VAL	variant	UNP P02766
Q	30	MET	VAL	variant	UNP P02766
R	30	MET	VAL	variant	UNP P02766
S	30	MET	VAL	variant	UNP P02766
T	30	MET	VAL	variant	UNP P02766
U	30	MET	VAL	variant	UNP P02766
V	30	MET	VAL	variant	UNP P02766
W	30	MET	VAL	variant	UNP P02766

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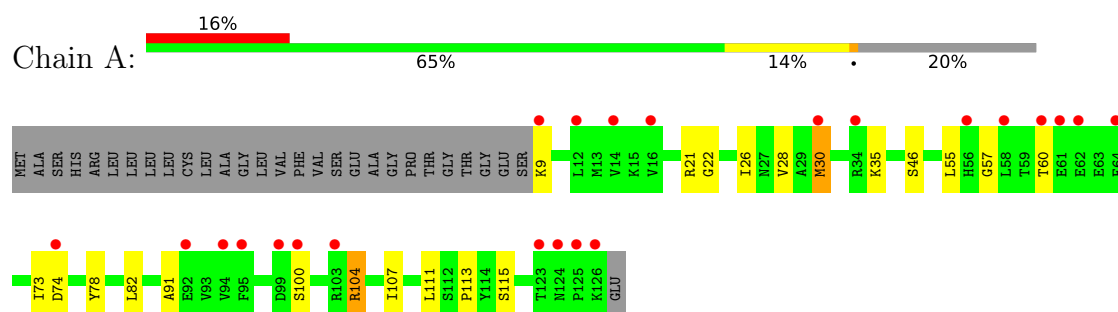
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Chain	Residue	Modelled	Actual	Comment	Reference
X	30	MET	VAL	variant	UNP P02766

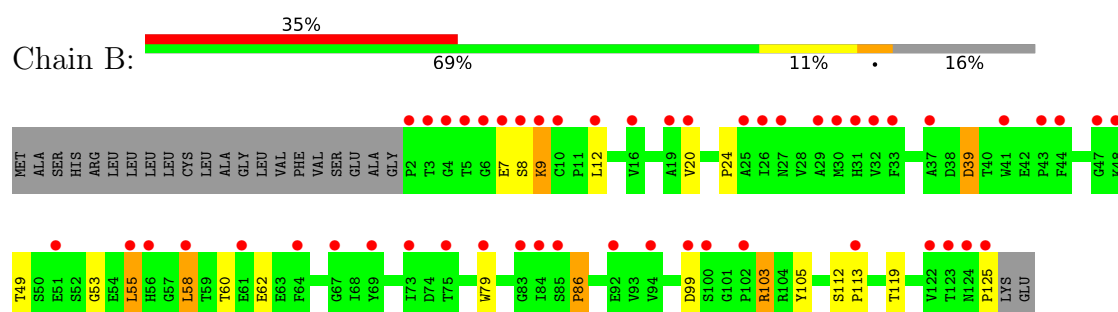
3 Residue-property plots [i](#)

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.

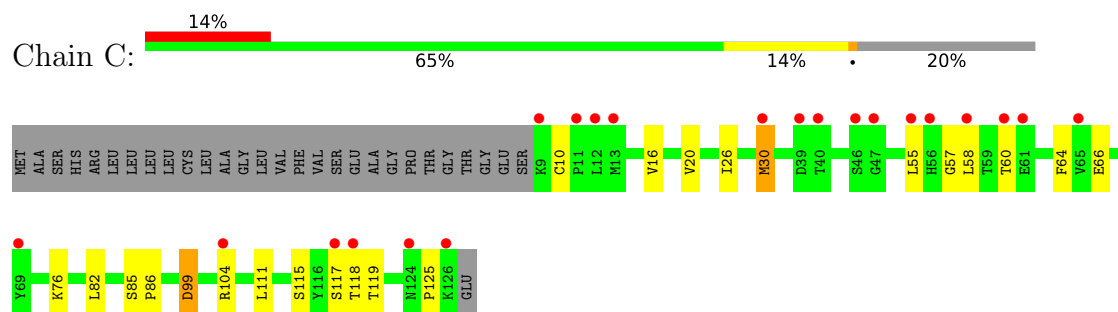
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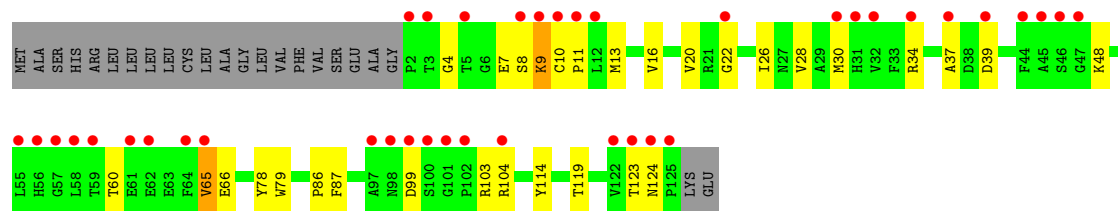


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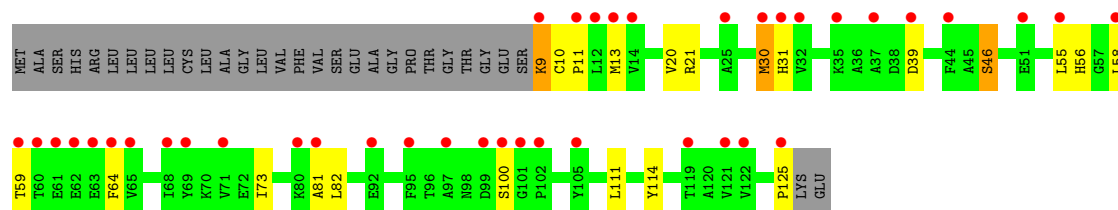


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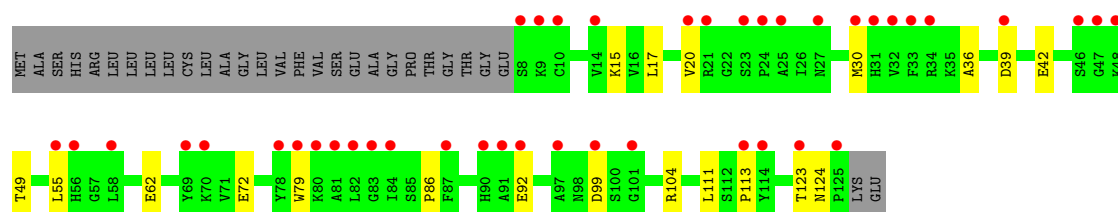




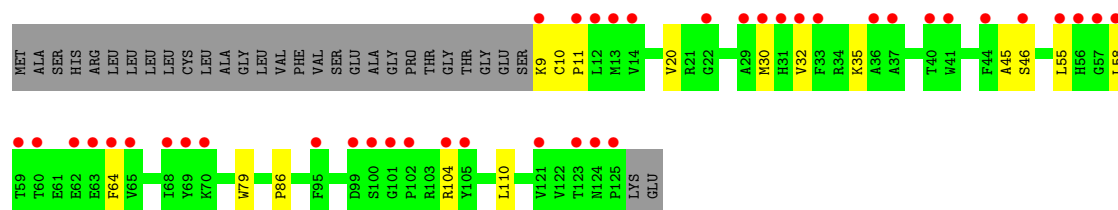
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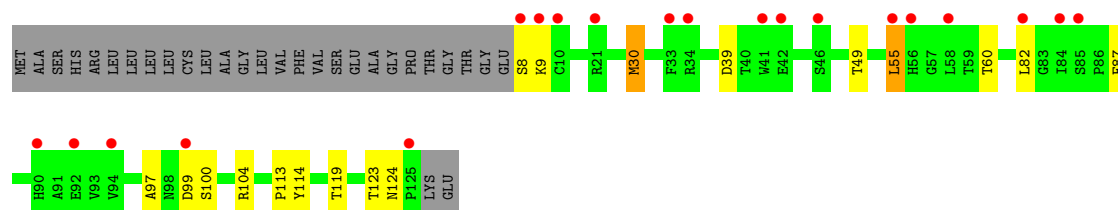
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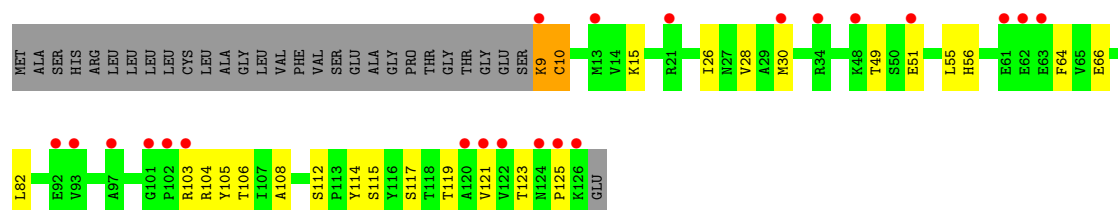
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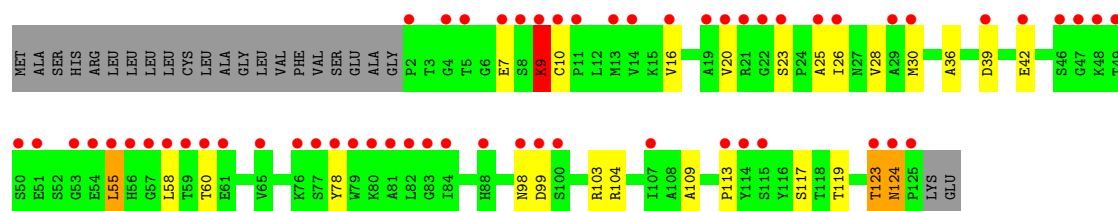
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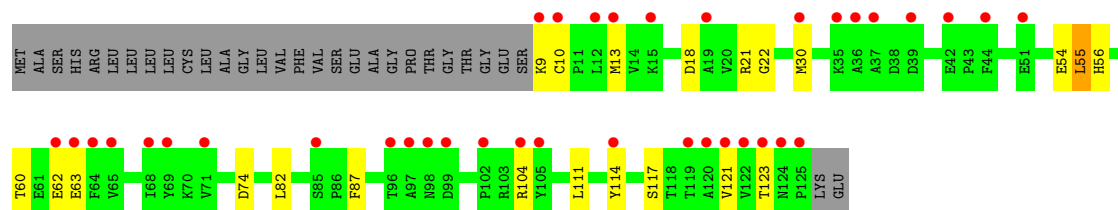
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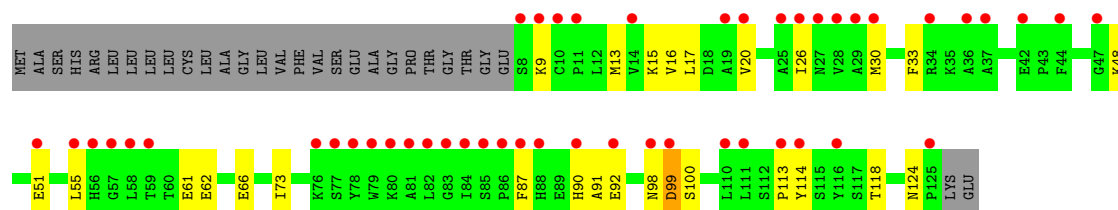
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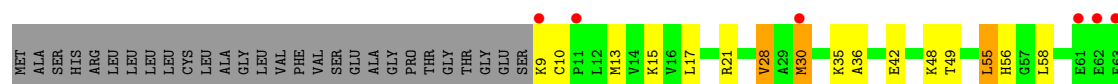
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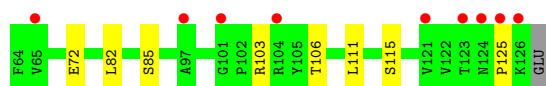


- Molecule 1: Transthyretin

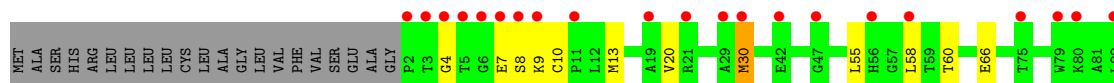


- Molecule 1: Transthyretin





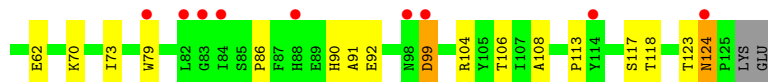
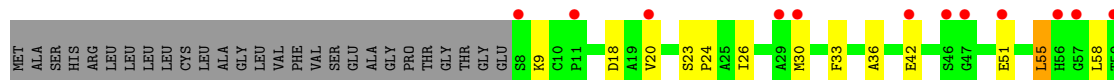
• Molecule 1: Transthyretin



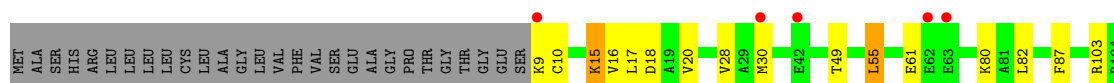
• Molecule 1: Transthyretin



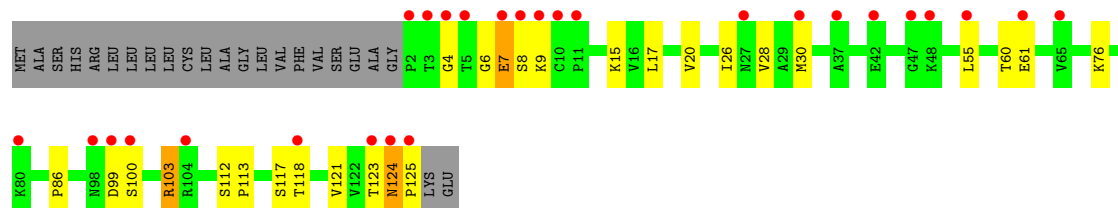
• Molecule 1: Transthyretin



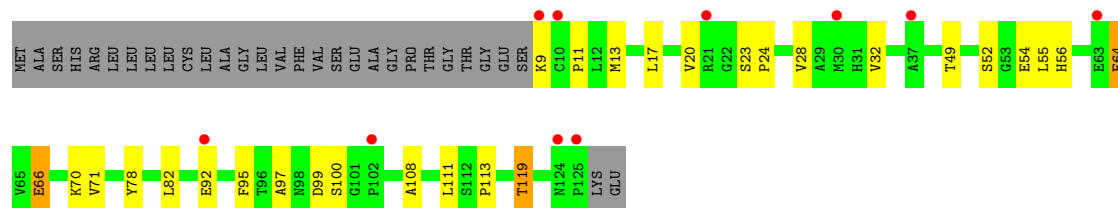
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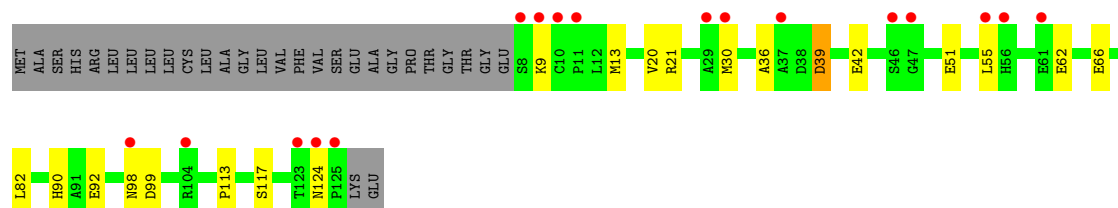
• Molecule 1: Transthyretin



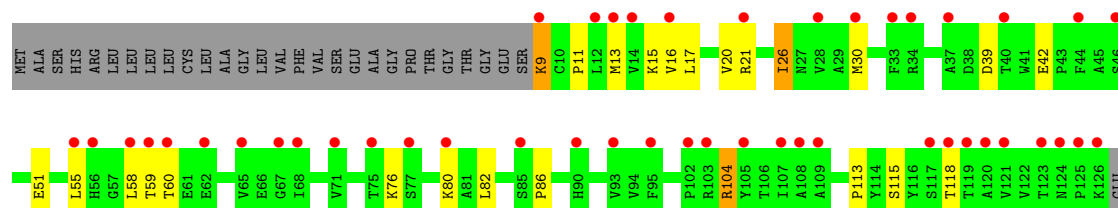
• Molecule 1: Transthyretin



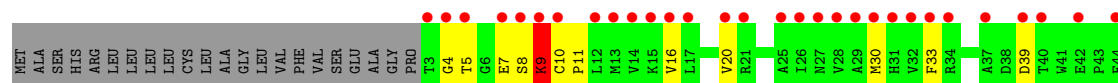
• Molecule 1: Transthyretin

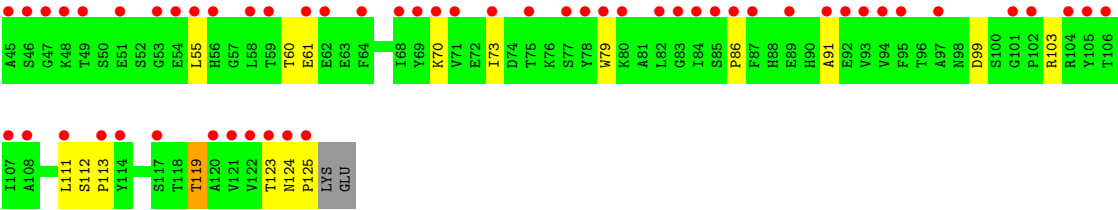


• Molecule 1: Transthyretin

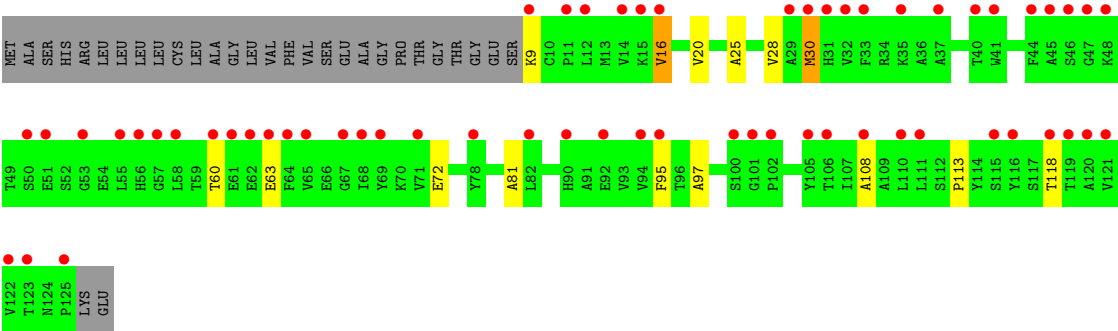


• Molecule 1: Transthyretin

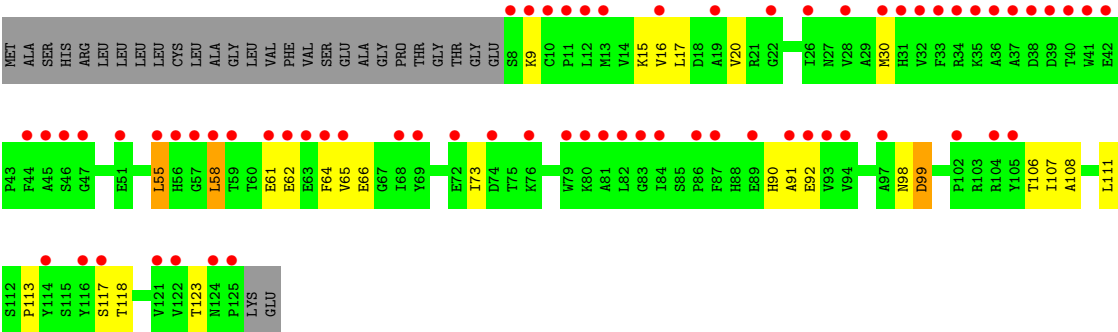




● Molecule 1: Transthyretin



● Molecule 1: Transthyretin



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	140.98Å 140.98Å 165.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.79 46.15 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.15-2.79) 99.9 (46.15-2.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.272 , 0.314 0.272 , 0.311	Depositor DCC
R_{free} test set	4615 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.026 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22028	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 53.81 % 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 3.9976e-05. 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	0.80	0/935	1.22	2/1274 (0.2%)
1	B	0.79	0/969	1.24	0/1318
1	C	0.77	0/935	1.21	1/1274 (0.1%)
1	D	0.82	0/969	1.24	2/1318 (0.2%)
1	E	0.74	0/926	1.17	0/1263
1	F	0.72	0/936	1.17	0/1275
1	G	0.81	0/926	1.21	0/1263
1	H	0.78	0/936	1.20	2/1275 (0.2%)
1	I	0.87	1/935 (0.1%)	1.22	1/1274 (0.1%)
1	J	0.82	0/969	1.22	2/1318 (0.2%)
1	K	0.87	0/926	1.26	3/1263 (0.2%)
1	L	0.78	0/936	1.18	1/1275 (0.1%)
1	M	0.82	0/935	1.20	1/1274 (0.1%)
1	N	0.75	0/969	1.17	2/1318 (0.2%)
1	O	0.75	0/926	1.14	0/1263
1	P	0.75	0/936	1.19	3/1275 (0.2%)
1	Q	0.92	1/935 (0.1%)	1.33	7/1274 (0.5%)
1	R	0.80	0/969	1.24	4/1318 (0.3%)
1	S	0.86	0/926	1.23	2/1263 (0.2%)
1	T	0.85	0/936	1.22	1/1275 (0.1%)
1	U	0.83	0/935	1.22	2/1274 (0.2%)
1	V	0.82	0/967	1.20	1/1317 (0.1%)
1	W	0.88	0/926	1.23	0/1263
1	X	0.84	0/936	1.23	1/1275 (0.1%)
All	All	0.81	2/22594 (0.0%)	1.22	38/30779 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	112	SER	CA-C	6.34	1.58	1.52
1	Q	112	SER	CA-C	5.12	1.57	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	64	PHE	CA-CB-CG	7.09	120.89	113.80
1	P	124	ASN	CA-CB-CG	5.97	118.57	112.60
1	M	111	LEU	N-CA-C	5.93	118.61	109.07
1	I	64	PHE	CA-CB-CG	5.88	119.67	113.80
1	D	26	ILE	CA-C-N	5.83	130.41	122.19
1	D	26	ILE	C-N-CA	5.83	130.41	122.19
1	P	99	ASP	CA-CB-CG	5.75	118.35	112.60
1	K	74	ASP	CA-C-N	5.71	128.39	120.29
1	K	74	ASP	C-N-CA	5.71	128.39	120.29
1	Q	125	PRO	CA-C-N	5.69	131.94	121.70
1	Q	125	PRO	C-N-CA	5.69	131.94	121.70
1	T	124	ASN	CA-CB-CG	5.62	118.22	112.60
1	J	26	ILE	CA-C-N	5.54	130.22	122.36
1	J	26	ILE	C-N-CA	5.54	130.22	122.36
1	A	26	ILE	CA-C-N	5.53	130.02	122.34
1	A	26	ILE	C-N-CA	5.53	130.02	122.34
1	Q	28	VAL	N-CA-CB	5.40	116.61	110.72
1	R	124	ASN	CA-CB-CG	5.39	117.99	112.60
1	S	111	LEU	N-CA-C	5.34	117.67	109.07
1	Q	61	GLU	CA-C-N	5.32	127.86	120.63
1	Q	61	GLU	C-N-CA	5.32	127.86	120.63
1	Q	18	ASP	CA-CB-CG	5.29	117.89	112.60
1	S	64	PHE	CA-CB-CG	5.27	119.07	113.80
1	N	99	ASP	CA-C-N	5.25	127.32	120.28
1	N	99	ASP	C-N-CA	5.25	127.32	120.28
1	P	18	ASP	CA-CB-CG	5.21	117.81	112.60
1	R	28	VAL	N-CA-C	-5.21	102.01	108.89
1	V	112	SER	N-CA-C	-5.20	101.11	109.58
1	U	26	ILE	CA-C-N	5.13	129.43	122.19
1	U	26	ILE	C-N-CA	5.13	129.43	122.19
1	Q	111	LEU	N-CA-C	5.13	117.59	109.24
1	L	33	PHE	CA-CB-CG	5.11	118.91	113.80
1	H	97	ALA	CA-C-N	5.08	131.23	121.54
1	H	97	ALA	C-N-CA	5.08	131.23	121.54
1	R	26	ILE	CA-C-N	5.07	129.56	122.36
1	R	26	ILE	C-N-CA	5.07	129.56	122.36
1	K	63	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	64	PHE	CA-CB-CG	5.02	118.82	113.80

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	911	0	884	10	0
1	B	947	0	915	10	0
1	C	911	0	884	8	0
1	D	947	0	915	12	0
1	E	902	0	871	12	0
1	F	912	0	887	9	0
1	G	902	0	871	6	0
1	H	912	0	887	7	0
1	I	911	0	884	10	0
1	J	947	0	915	13	0
1	K	902	0	871	11	0
1	L	912	0	887	11	0
1	M	911	0	884	10	0
1	N	947	0	915	10	0
1	O	902	0	871	13	0
1	P	912	0	887	13	0
1	Q	911	0	884	8	0
1	R	947	0	915	12	0
1	S	902	0	871	18	0
1	T	912	0	887	5	0
1	U	911	0	884	13	0
1	V	943	0	913	12	0
1	W	902	0	871	8	0
1	X	912	0	887	11	0
All	All	22028	0	21340	217	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 (217) 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:A:30:MET:HG3	1:A:55:LEU:HD22	1.48	0.96
1:H:30:MET:HE1	1:H:49:THR:HG23	1.56	0.84
1:A:30:MET:HG3	1:A:55:LEU:CD2	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:MET:SD	1:O:55:LEU:HD22	2.22	0.79
1:H:30:MET:SD	1:H:55:LEU:HD13	2.28	0.74
1:F:30:MET:HE1	1:F:49:THR:HG23	1.71	0.72
1:X:73:ILE:HB	1:X:91:ALA:HB3	1.73	0.70
1:F:104:ARG:HB3	1:F:123:THR:HB	1.74	0.69
1:J:55:LEU:HB3	1:J:58:LEU:HD11	1.72	0.69
1:V:113:PRO:HD2	1:X:20:VAL:HA	1.76	0.67
1:B:20:VAL:HA	1:F:113:PRO:HD2	1.80	0.64
1:S:108:ALA:HB3	1:S:119:THR:HG22	1.79	0.64
1:N:7:GLU:H	1:N:60:THR:HG23	1.63	0.63
1:L:73:ILE:HB	1:L:91:ALA:HB3	1.80	0.62
1:J:7:GLU:H	1:J:60:THR:HG23	1.64	0.61
1:D:4:GLY:H	1:D:60:THR:HG21	1.65	0.60
1:U:115:SER:HB2	1:V:119:THR:HG23	1.83	0.60
1:N:113:PRO:HD2	1:P:20:VAL:HA	1.84	0.60
1:V:7:GLU:H	1:V:60:THR:HG23	1.66	0.60
1:G:55:LEU:HD23	1:G:58:LEU:HD11	1.84	0.59
1:H:104:ARG:HB3	1:H:123:THR:HB	1.83	0.59
1:H:8:SER:HA	1:H:60:THR:HG22	1.84	0.59
1:X:16:VAL:HG21	1:X:30:MET:HE1	1.84	0.59
1:A:100:SER:HA	1:O:100:SER:HA	1.85	0.58
1:Q:15:LYS:HE2	1:Q:17:LEU:HD21	1.84	0.58
1:I:108:ALA:HB3	1:I:119:THR:HG22	1.84	0.58
1:D:20:VAL:HA	1:H:113:PRO:HD2	1.85	0.58
1:A:115:SER:HB2	1:B:119:THR:HG23	1.86	0.58
1:T:21:ARG:HE	1:T:82:LEU:HD21	1.68	0.57
1:C:115:SER:HB2	1:D:119:THR:HG23	1.85	0.57
1:J:113:PRO:HD2	1:L:20:VAL:HA	1.85	0.57
1:V:9:LYS:HG2	1:V:61:GLU:HB2	1.86	0.57
1:D:7:GLU:H	1:D:60:THR:HG23	1.70	0.56
1:M:115:SER:HB2	1:N:119:THR:HG23	1.86	0.56
1:U:9:LYS:HD2	1:U:104:ARG:HH11	1.70	0.56
1:P:90:HIS:CD2	1:P:92:GLU:HG2	2.41	0.56
1:V:79:TRP:HB2	1:V:86:PRO:HG3	1.88	0.55
1:U:11:PRO:HG2	1:U:59:THR:HG23	1.89	0.55
1:R:6:GLY:O	1:R:7:GLU:HB2	2.07	0.55
1:I:49:THR:HA	1:I:55:LEU:HD13	1.88	0.54
1:S:95:PHE:CE2	1:S:97:ALA:HB2	2.43	0.54
1:X:55:LEU:HD13	1:X:58:LEU:HD21	1.90	0.54
1:R:4:GLY:H	1:R:60:THR:HG21	1.73	0.54
1:I:106:THR:HB	1:I:121:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:33:PHE:HB2	1:P:70:LYS:HB3	1.90	0.54
1:S:17:LEU:HD23	1:S:24:PRO:HA	1.89	0.54
1:U:113:PRO:HD2	1:W:20:VAL:HA	1.89	0.54
1:E:30:MET:HG3	1:E:55:LEU:HD22	1.90	0.53
1:B:55:LEU:HB3	1:B:58:LEU:HD11	1.90	0.53
1:M:13:MET:HG2	1:M:56:HIS:HD2	1.73	0.53
1:U:15:LYS:HE2	1:U:17:LEU:HD21	1.91	0.53
1:G:79:TRP:HB2	1:G:86:PRO:HG3	1.91	0.53
1:N:55:LEU:HD13	1:N:58:LEU:HD21	1.90	0.53
1:P:55:LEU:HD23	1:P:58:LEU:HD21	1.91	0.53
1:A:113:PRO:HD2	1:E:20:VAL:HA	1.90	0.53
1:E:30:MET:HE1	1:E:73:ILE:HG23	1.91	0.53
1:S:28:VAL:HG22	1:S:78:TYR:CD1	2.43	0.53
1:X:9:LYS:HG2	1:X:61:GLU:HB2	1.91	0.52
1:B:7:GLU:H	1:B:60:THR:HG23	1.74	0.52
1:X:15:LYS:HE3	1:X:17:LEU:HD21	1.89	0.52
1:C:20:VAL:HG22	1:G:20:VAL:HG22	1.92	0.52
1:V:33:PHE:HB2	1:V:70:LYS:HB3	1.92	0.52
1:E:100:SER:HB3	1:M:103:ARG:HH12	1.74	0.52
1:U:16:VAL:HG21	1:U:30:MET:HE1	1.92	0.52
1:S:11:PRO:HB2	1:S:64:PHE:HD2	1.74	0.51
1:C:99:ASP:O	1:S:100:SER:HA	2.10	0.51
1:D:87:PHE:HB2	1:D:114:TYR:CD2	2.45	0.51
1:O:28:VAL:HG22	1:O:78:TYR:CD1	2.46	0.51
1:L:87:PHE:HB2	1:L:114:TYR:CD2	2.45	0.51
1:K:60:THR:HG22	1:K:62:GLU:H	1.74	0.51
1:R:123:THR:C	1:R:125:PRO:HD3	2.36	0.51
1:L:66:GLU:HG3	1:L:99:ASP:H	1.76	0.50
1:N:30:MET:HG3	1:N:55:LEU:HD11	1.92	0.50
1:A:28:VAL:HG22	1:A:78:TYR:CD1	2.46	0.50
1:L:16:VAL:HG21	1:L:30:MET:HE1	1.94	0.50
1:M:9:LYS:HE3	1:M:125:PRO:HB3	1.94	0.50
1:N:20:VAL:HA	1:P:113:PRO:HD2	1.94	0.50
1:F:30:MET:SD	1:F:55:LEU:HD12	2.52	0.49
1:L:9:LYS:HG2	1:L:61:GLU:HB2	1.95	0.49
1:L:15:LYS:HE3	1:L:17:LEU:HD21	1.93	0.49
1:O:55:LEU:HD23	1:O:58:LEU:HD11	1.94	0.49
1:O:30:MET:SD	1:O:55:LEU:CD2	2.99	0.49
1:P:73:ILE:HB	1:P:91:ALA:HB3	1.95	0.49
1:R:113:PRO:HD2	1:T:20:VAL:HA	1.95	0.49
1:S:49:THR:HA	1:S:55:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:16:VAL:HG21	1:W:30:MET:HE1	1.94	0.49
1:A:22:GLY:HA3	1:E:114:TYR:CD2	2.48	0.49
1:N:103:ARG:HG3	1:N:125:PRO:HD2	1.94	0.49
1:X:66:GLU:HG3	1:X:99:ASP:H	1.77	0.49
1:O:15:LYS:HE2	1:O:17:LEU:HD21	1.94	0.48
1:R:121:VAL:HG13	1:S:23:SER:HA	1.96	0.48
1:I:114:TYR:CD2	1:K:22:GLY:HA3	2.48	0.48
1:U:21:ARG:HH11	1:U:82:LEU:HD21	1.78	0.48
1:I:26:ILE:HG12	1:I:51:GLU:HA	1.95	0.48
1:R:7:GLU:H	1:R:60:THR:HG23	1.79	0.48
1:O:11:PRO:HA	1:O:104:ARG:HG3	1.96	0.48
1:F:72:GLU:HG3	1:F:92:GLU:HG2	1.95	0.48
1:L:90:HIS:CD2	1:L:92:GLU:HG3	2.48	0.47
1:W:30:MET:HA	1:W:72:GLU:O	2.14	0.47
1:J:16:VAL:HG21	1:J:30:MET:HE1	1.95	0.47
1:U:76:LYS:HA	1:U:86:PRO:HG3	1.96	0.47
1:Q:49:THR:HA	1:Q:55:LEU:HD13	1.95	0.47
1:S:70:LYS:HD2	1:S:92:GLU:CD	2.39	0.47
1:B:103:ARG:HA	1:B:125:PRO:HD2	1.95	0.47
1:E:55:LEU:HD23	1:E:58:LEU:HD11	1.95	0.47
1:S:66:GLU:CG	1:S:99:ASP:HA	2.44	0.47
1:F:36:ALA:HB2	1:F:42:GLU:HG2	1.96	0.47
1:O:13:MET:HB2	1:O:106:THR:HG23	1.96	0.47
1:M:36:ALA:HB2	1:M:42:GLU:HG3	1.97	0.47
1:E:9:LYS:HE3	1:E:125:PRO:HG3	1.97	0.46
1:J:123:THR:HG22	1:J:124:ASN:H	1.80	0.46
1:W:25:ALA:HB1	1:W:28:VAL:HG21	1.96	0.46
1:O:30:MET:HE1	1:O:49:THR:HG23	1.97	0.46
1:V:16:VAL:HG21	1:V:30:MET:HE1	1.97	0.46
1:G:32:VAL:HB	1:G:45:ALA:HB3	1.98	0.46
1:V:73:ILE:HB	1:V:91:ALA:HB3	1.98	0.46
1:K:87:PHE:HB2	1:K:114:TYR:CD2	2.51	0.46
1:R:20:VAL:HA	1:T:113:PRO:HD2	1.98	0.46
1:E:13:MET:HG2	1:E:56:HIS:HD2	1.81	0.46
1:M:49:THR:HA	1:M:55:LEU:HD13	1.98	0.46
1:Q:108:ALA:O	1:Q:118:THR:HA	2.16	0.46
1:V:124:ASN:N	1:V:125:PRO:HD3	2.31	0.46
1:J:36:ALA:HB2	1:J:42:GLU:HG2	1.97	0.45
1:K:54:GLU:HB3	1:K:56:HIS:CE1	2.52	0.45
1:C:30:MET:HG3	1:C:55:LEU:CD2	2.46	0.45
1:P:30:MET:HE2	1:P:30:MET:HB3	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:82:LEU:HG	1:W:81:ALA:HB1	1.98	0.45
1:D:79:TRP:HB2	1:D:86:PRO:HG3	1.97	0.45
1:N:30:MET:HB3	1:N:30:MET:HE2	1.73	0.45
1:M:30:MET:HE2	1:M:30:MET:HB3	1.87	0.45
1:D:10:CYS:N	1:D:11:PRO:HD3	2.32	0.45
1:P:79:TRP:CD1	1:P:86:PRO:HB3	2.52	0.45
1:A:30:MET:CE	1:A:73:ILE:HG23	2.47	0.45
1:B:79:TRP:HB2	1:B:86:PRO:HG3	1.99	0.45
1:D:16:VAL:HG21	1:D:30:MET:HE1	1.98	0.45
1:D:28:VAL:HG22	1:D:78:TYR:CD1	2.52	0.45
1:E:30:MET:CE	1:E:73:ILE:HG23	2.47	0.45
1:T:90:HIS:CD2	1:T:92:GLU:HG2	2.52	0.45
1:I:9:LYS:HE3	1:I:125:PRO:HB3	1.99	0.44
1:P:23:SER:HB2	1:P:24:PRO:HD2	2.00	0.44
1:V:20:VAL:HA	1:X:113:PRO:HD2	1.98	0.44
1:I:115:SER:HB2	1:J:119:THR:HG23	1.98	0.44
1:S:52:SER:C	1:S:54:GLU:H	2.26	0.44
1:W:95:PHE:CE2	1:W:97:ALA:HB2	2.52	0.44
1:B:24:PRO:HB2	1:B:53:GLY:HA3	1.99	0.44
1:C:55:LEU:HD21	1:C:58:LEU:HD21	1.99	0.44
1:O:11:PRO:HB2	1:O:64:PHE:HD2	1.83	0.44
1:O:66:GLU:CG	1:O:99:ASP:HA	2.47	0.44
1:D:119:THR:HG21	1:G:110:LEU:HD11	1.99	0.44
1:B:12:LEU:HD12	1:B:105:TYR:HB2	1.99	0.44
1:F:79:TRP:HB2	1:F:86:PRO:HG3	1.99	0.44
1:A:9:LYS:HE2	1:A:104:ARG:HD2	2.00	0.44
1:Q:20:VAL:HA	1:S:113:PRO:HD2	2.00	0.44
1:C:104:ARG:HH11	1:C:125:PRO:HA	1.83	0.44
1:J:9:LYS:CB	1:J:60:THR:HA	2.48	0.43
1:J:20:VAL:HA	1:L:113:PRO:HD2	2.00	0.43
1:D:34:ARG:HH21	1:D:65:VAL:HG23	1.83	0.43
1:R:100:SER:HA	1:X:99:ASP:HB3	2.00	0.43
1:B:60:THR:C	1:B:62:GLU:H	2.26	0.43
1:C:30:MET:HG3	1:C:55:LEU:HD22	2.00	0.43
1:P:108:ALA:O	1:P:118:THR:HA	2.18	0.43
1:U:76:LYS:HE2	1:U:80:LYS:HE2	2.01	0.43
1:K:9:LYS:HB2	1:K:104:ARG:HH11	1.83	0.43
1:B:113:PRO:HD2	1:F:20:VAL:HA	2.01	0.43
1:E:31:HIS:CE1	1:E:46:SER:HB3	2.54	0.43
1:G:11:PRO:HB2	1:G:64:PHE:CD2	2.54	0.43
1:J:16:VAL:HG12	1:J:25:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:76:LYS:HA	1:R:86:PRO:HG3	1.99	0.43
1:M:28:VAL:O	1:M:48:LYS:HA	2.18	0.43
1:D:22:GLY:HA3	1:H:114:TYR:CG	2.54	0.43
1:J:16:VAL:HG22	1:J:109:ALA:HB3	2.01	0.43
1:R:30:MET:HE2	1:R:30:MET:HB3	1.82	0.42
1:E:11:PRO:HG2	1:E:59:THR:HG23	2.01	0.42
1:L:30:MET:HE2	1:L:30:MET:HB3	1.81	0.42
1:L:26:ILE:HG12	1:L:51:GLU:HA	2.00	0.42
1:E:81:ALA:HB1	1:I:82:LEU:HG	2.01	0.42
1:A:73:ILE:HB	1:A:91:ALA:HB3	2.01	0.42
1:F:15:LYS:HE3	1:F:17:LEU:HD21	2.02	0.42
1:T:36:ALA:HB2	1:T:42:GLU:HG2	2.00	0.42
1:U:26:ILE:HG12	1:U:51:GLU:HA	2.02	0.42
1:P:26:ILE:HG12	1:P:51:GLU:HA	2.02	0.42
1:U:55:LEU:HD23	1:U:58:LEU:HD11	2.01	0.42
1:M:30:MET:HA	1:M:72:GLU:O	2.20	0.42
1:R:103:ARG:HA	1:R:125:PRO:HD2	2.02	0.42
1:U:20:VAL:HA	1:W:113:PRO:HD2	2.02	0.42
1:J:28:VAL:HG22	1:J:78:TYR:CD1	2.54	0.42
1:N:4:GLY:H	1:N:60:THR:HG21	1.84	0.42
1:P:36:ALA:HB2	1:P:42:GLU:HG2	2.02	0.42
1:H:87:PHE:HB2	1:H:114:TYR:CD2	2.55	0.41
1:V:4:GLY:H	1:V:60:THR:HG21	1.84	0.41
1:I:10:CYS:SG	1:I:56:HIS:HB3	2.61	0.41
1:S:32:VAL:HG22	1:S:71:VAL:HG22	2.03	0.41
1:K:18:ASP:OD2	1:K:21:ARG:HD3	2.20	0.41
1:K:104:ARG:HB3	1:K:123:THR:HB	2.01	0.41
1:M:15:LYS:HE3	1:M:17:LEU:HD21	2.02	0.41
1:R:15:LYS:HE3	1:R:17:LEU:HD21	2.02	0.41
1:X:108:ALA:O	1:X:118:THR:HA	2.20	0.41
1:J:23:SER:HA	1:K:121:VAL:HG13	2.02	0.41
1:Q:87:PHE:HB2	1:Q:114:TYR:CD2	2.56	0.41
1:K:13:MET:HG2	1:K:56:HIS:HD2	1.85	0.41
1:K:30:MET:SD	1:K:55:LEU:HD22	2.61	0.41
1:Q:103:ARG:HB2	1:Q:105:TYR:CE2	2.56	0.41
1:S:66:GLU:HG2	1:S:99:ASP:HA	2.03	0.41
1:V:10:CYS:N	1:V:11:PRO:HD3	2.36	0.41
1:X:90:HIS:CD2	1:X:92:GLU:HG2	2.56	0.41
1:Q:20:VAL:HG22	1:S:20:VAL:HG22	2.02	0.41
1:S:95:PHE:HE2	1:S:97:ALA:HB2	1.85	0.41
1:W:108:ALA:O	1:W:118:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:103:ARG:HB2	1:I:105:TYR:CE2	2.56	0.41
1:P:104:ARG:HB3	1:P:123:THR:HB	2.03	0.41
1:O:95:PHE:CE2	1:O:97:ALA:HB2	2.57	0.40
1:S:13:MET:HG2	1:S:56:HIS:CD2	2.56	0.40
1:U:21:ARG:NH1	1:U:82:LEU:HD21	2.36	0.40
1:C:76:LYS:HA	1:C:86:PRO:HG3	2.03	0.40
1:K:30:MET:HE2	1:K:30:MET:HB3	1.85	0.40
1:Q:16:VAL:HG21	1:Q:30:MET:HE1	2.03	0.40
1:N:119:THR:HG21	1:O:110:LEU:HD11	2.04	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	116/147 (79%)	109 (94%)	6 (5%)	1 (1%)	14	41
1	B	121/147 (82%)	104 (86%)	12 (10%)	5 (4%)	2	8
1	C	116/147 (79%)	110 (95%)	4 (3%)	2 (2%)	7	25
1	D	121/147 (82%)	105 (87%)	10 (8%)	6 (5%)	1	5
1	E	115/147 (78%)	107 (93%)	8 (7%)	0	100	100
1	F	116/147 (79%)	108 (93%)	7 (6%)	1 (1%)	14	41
1	G	115/147 (78%)	109 (95%)	5 (4%)	1 (1%)	14	41
1	H	116/147 (79%)	112 (97%)	3 (3%)	1 (1%)	14	41
1	I	116/147 (79%)	107 (92%)	9 (8%)	0	100	100
1	J	121/147 (82%)	106 (88%)	11 (9%)	4 (3%)	3	11
1	K	115/147 (78%)	104 (90%)	10 (9%)	1 (1%)	14	41
1	L	116/147 (79%)	110 (95%)	4 (3%)	2 (2%)	7	25
1	M	116/147 (79%)	110 (95%)	5 (4%)	1 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	121/147 (82%)	106 (88%)	11 (9%)	4 (3%)	3	11
1	O	115/147 (78%)	108 (94%)	6 (5%)	1 (1%)	14	41
1	P	116/147 (79%)	109 (94%)	6 (5%)	1 (1%)	14	41
1	Q	116/147 (79%)	109 (94%)	7 (6%)	0	100	100
1	R	121/147 (82%)	107 (88%)	9 (7%)	5 (4%)	2	8
1	S	115/147 (78%)	109 (95%)	6 (5%)	0	100	100
1	T	116/147 (79%)	107 (92%)	5 (4%)	4 (3%)	3	11
1	U	116/147 (79%)	110 (95%)	6 (5%)	0	100	100
1	V	121/147 (82%)	105 (87%)	13 (11%)	3 (2%)	4	16
1	W	115/147 (78%)	106 (92%)	9 (8%)	0	100	100
1	X	116/147 (79%)	108 (93%)	6 (5%)	2 (2%)	7	25
All	All	2808/3528 (80%)	2585 (92%)	178 (6%)	45 (2%)	7	27

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	LYS
1	R	7	GLU
1	R	9	LYS
1	V	9	LYS
1	A	57	GLY
1	B	9	LYS
1	B	99	ASP
1	D	99	ASP
1	H	99	ASP
1	J	9	LYS
1	J	99	ASP
1	N	99	ASP
1	P	99	ASP
1	R	99	ASP
1	T	99	ASP
1	V	99	ASP
1	C	57	GLY
1	N	9	LYS
1	O	64	PHE
1	T	9	LYS
1	B	39	ASP
1	B	86	PRO

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Mol	Chain	Res	Type
1	D	8	SER
1	D	37	ALA
1	D	66	GLU
1	L	98	ASN
1	R	8	SER
1	T	98	ASN
1	V	8	SER
1	X	98	ASN
1	X	99	ASP
1	B	8	SER
1	D	124	ASN
1	F	99	ASP
1	J	98	ASN
1	K	10	CYS
1	N	8	SER
1	R	124	ASN
1	G	10	CYS
1	L	99	ASP
1	M	10	CYS
1	T	39	ASP
1	C	10	CYS
1	N	10	CYS
1	J	10	CYS

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	98/121 (81%)	88 (90%)	10 (10%)	7	23
1	B	102/121 (84%)	95 (93%)	7 (7%)	14	41
1	C	98/121 (81%)	86 (88%)	12 (12%)	5	16
1	D	102/121 (84%)	94 (92%)	8 (8%)	11	35
1	E	97/121 (80%)	88 (91%)	9 (9%)	8	27
1	F	99/121 (82%)	95 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	97/121 (80%)	92 (95%)	5 (5%)	21	53
1	H	99/121 (82%)	91 (92%)	8 (8%)	11	33
1	I	98/121 (81%)	89 (91%)	9 (9%)	8	27
1	J	102/121 (84%)	94 (92%)	8 (8%)	11	35
1	K	97/121 (80%)	93 (96%)	4 (4%)	27	62
1	L	99/121 (82%)	92 (93%)	7 (7%)	13	39
1	M	98/121 (81%)	89 (91%)	9 (9%)	8	27
1	N	102/121 (84%)	94 (92%)	8 (8%)	11	35
1	O	97/121 (80%)	88 (91%)	9 (9%)	8	27
1	P	99/121 (82%)	93 (94%)	6 (6%)	17	46
1	Q	98/121 (81%)	91 (93%)	7 (7%)	13	39
1	R	102/121 (84%)	96 (94%)	6 (6%)	18	48
1	S	97/121 (80%)	94 (97%)	3 (3%)	35	70
1	T	99/121 (82%)	91 (92%)	8 (8%)	11	33
1	U	98/121 (81%)	91 (93%)	7 (7%)	13	39
1	V	102/121 (84%)	94 (92%)	8 (8%)	11	35
1	W	97/121 (80%)	92 (95%)	5 (5%)	21	53
1	X	99/121 (82%)	90 (91%)	9 (9%)	9	28
All	All	2376/2904 (82%)	2200 (93%)	176 (7%)	13	37

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	30	MET
1	A	35	LYS
1	A	46	SER
1	A	60	THR
1	A	74	ASP
1	A	82	LEU
1	A	104	ARG
1	A	107	ILE
1	A	111	LEU
1	B	9	LYS
1	B	39	ASP
1	B	49	THR

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Mol	Chain	Res	Type
1	B	55	LEU
1	B	58	LEU
1	B	103	ARG
1	B	112	SER
1	C	16	VAL
1	C	26	ILE
1	C	30	MET
1	C	60	THR
1	C	66	GLU
1	C	82	LEU
1	C	85	SER
1	C	99	ASP
1	C	111	LEU
1	C	117	SER
1	C	118	THR
1	C	119	THR
1	D	9	LYS
1	D	13	MET
1	D	39	ASP
1	D	48	LYS
1	D	65	VAL
1	D	103	ARG
1	D	104	ARG
1	D	123	THR
1	E	9	LYS
1	E	10	CYS
1	E	21	ARG
1	E	30	MET
1	E	39	ASP
1	E	46	SER
1	E	64	PHE
1	E	82	LEU
1	E	111	LEU
1	F	39	ASP
1	F	62	GLU
1	F	111	LEU
1	F	124	ASN
1	G	9	LYS
1	G	30	MET
1	G	35	LYS
1	G	46	SER
1	G	104	ARG

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Mol	Chain	Res	Type
1	H	9	LYS
1	H	30	MET
1	H	39	ASP
1	H	55	LEU
1	H	82	LEU
1	H	100	SER
1	H	119	THR
1	H	124	ASN
1	I	9	LYS
1	I	10	CYS
1	I	15	LYS
1	I	28	VAL
1	I	30	MET
1	I	66	GLU
1	I	104	ARG
1	I	117	SER
1	I	123	THR
1	J	9	LYS
1	J	39	ASP
1	J	55	LEU
1	J	103	ARG
1	J	104	ARG
1	J	117	SER
1	J	123	THR
1	J	124	ASN
1	K	55	LEU
1	K	82	LEU
1	K	111	LEU
1	K	117	SER
1	L	13	MET
1	L	48	LYS
1	L	55	LEU
1	L	62	GLU
1	L	100	SER
1	L	118	THR
1	L	124	ASN
1	M	21	ARG
1	M	28	VAL
1	M	30	MET
1	M	35	LYS
1	M	55	LEU
1	M	58	LEU

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Mol	Chain	Res	Type
1	M	82	LEU
1	M	85	SER
1	M	106	THR
1	N	13	MET
1	N	30	MET
1	N	66	GLU
1	N	92	GLU
1	N	103	ARG
1	N	104	ARG
1	N	112	SER
1	N	123	THR
1	O	35	LYS
1	O	55	LEU
1	O	60	THR
1	O	66	GLU
1	O	100	SER
1	O	106	THR
1	O	107	ILE
1	O	117	SER
1	O	119	THR
1	P	9	LYS
1	P	55	LEU
1	P	62	GLU
1	P	106	THR
1	P	117	SER
1	P	124	ASN
1	Q	9	LYS
1	Q	10	CYS
1	Q	15	LYS
1	Q	55	LEU
1	Q	80	LYS
1	Q	82	LEU
1	Q	117	SER
1	R	55	LEU
1	R	61	GLU
1	R	103	ARG
1	R	112	SER
1	R	117	SER
1	R	118	THR
1	S	9	LYS
1	S	66	GLU
1	S	119	THR

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Mol	Chain	Res	Type
1	T	13	MET
1	T	30	MET
1	T	39	ASP
1	T	51	GLU
1	T	55	LEU
1	T	62	GLU
1	T	66	GLU
1	T	117	SER
1	U	9	LYS
1	U	13	MET
1	U	39	ASP
1	U	42	GLU
1	U	60	THR
1	U	104	ARG
1	U	118	THR
1	V	5	THR
1	V	9	LYS
1	V	39	ASP
1	V	55	LEU
1	V	103	ARG
1	V	111	LEU
1	V	119	THR
1	V	123	THR
1	W	9	LYS
1	W	16	VAL
1	W	30	MET
1	W	60	THR
1	W	63	GLU
1	X	55	LEU
1	X	58	LEU
1	X	62	GLU
1	X	65	VAL
1	X	106	THR
1	X	107	ILE
1	X	111	LEU
1	X	117	SER
1	X	123	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN

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Mol	Chain	Res	Type
1	E	56	HIS
1	F	90	HIS
1	H	88	HIS
1	H	90	HIS
1	I	56	HIS
1	J	31	HIS
1	J	90	HIS
1	K	56	HIS
1	K	124	ASN
1	L	124	ASN
1	M	27	ASN
1	M	56	HIS
1	N	124	ASN
1	O	56	HIS
1	O	90	HIS
1	P	56	HIS
1	P	88	HIS
1	P	90	HIS
1	P	124	ASN
1	Q	27	ASN
1	Q	56	HIS
1	S	27	ASN
1	S	31	HIS
1	S	56	HIS
1	U	27	ASN
1	V	124	ASN
1	W	27	ASN
1	X	90	HIS
1	X	98	ASN

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 oligosaccharides 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, 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	118/147 (80%)	1.27	23 (19%) 3 2	27, 59, 108, 177	0
1	B	124/147 (84%)	1.87	51 (41%) 0 0	42, 73, 147, 184	0
1	C	118/147 (80%)	1.08	21 (17%) 4 3	29, 54, 108, 176	0
1	D	124/147 (84%)	1.62	39 (31%) 1 1	36, 68, 151, 188	0
1	E	117/147 (79%)	1.56	40 (34%) 1 1	30, 61, 116, 139	0
1	F	118/147 (80%)	1.86	42 (35%) 1 0	39, 72, 106, 131	0
1	G	117/147 (79%)	1.68	41 (35%) 1 0	26, 61, 110, 125	0
1	H	118/147 (80%)	1.22	20 (16%) 4 3	34, 60, 98, 124	0
1	I	118/147 (80%)	1.06	22 (18%) 3 2	25, 44, 100, 160	0
1	J	124/147 (84%)	2.13	58 (46%) 0 0	37, 77, 140, 176	0
1	K	117/147 (79%)	1.44	37 (31%) 1 1	26, 49, 95, 119	0
1	L	118/147 (80%)	1.98	48 (40%) 0 0	31, 67, 100, 123	0
1	M	118/147 (80%)	0.81	15 (12%) 8 6	16, 32, 91, 157	0
1	N	124/147 (84%)	1.46	30 (24%) 2 1	23, 57, 114, 164	0
1	O	117/147 (79%)	0.85	14 (11%) 9 6	14, 34, 87, 115	0
1	P	118/147 (80%)	1.24	21 (17%) 4 3	21, 49, 86, 111	0
1	Q	118/147 (80%)	0.73	6 (5%) 33 25	18, 36, 76, 143	0
1	R	124/147 (84%)	1.10	27 (21%) 2 2	25, 51, 122, 179	0
1	S	117/147 (79%)	0.66	10 (8%) 16 12	20, 36, 80, 111	0
1	T	118/147 (80%)	0.99	17 (14%) 6 5	22, 47, 97, 129	0
1	U	118/147 (80%)	1.81	46 (38%) 1 0	39, 72, 123, 167	0
1	V	123/147 (83%)	2.61	85 (69%) 0 0	51, 96, 152, 190	0
1	W	117/147 (79%)	2.10	60 (51%) 0 0	37, 69, 110, 122	0
1	X	118/147 (80%)	2.31	68 (57%) 0 0	52, 83, 134, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2861/3528 (81%)	1.48	841 (29%) 1 1	14, 59, 119, 190	0

All (841) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	2	PRO	6.7
1	B	2	PRO	6.4
1	D	8	SER	6.1
1	E	30	MET	6.0
1	W	69	TYR	6.0
1	V	121	VAL	5.8
1	N	8	SER	5.7
1	L	85	SER	5.4
1	L	84	ILE	5.4
1	J	2	PRO	5.3
1	U	30	MET	5.2
1	J	125	PRO	5.2
1	F	91	ALA	5.0
1	J	82	LEU	5.0
1	B	8	SER	5.0
1	L	83	GLY	5.0
1	W	64	PHE	4.9
1	F	8	SER	4.9
1	V	12	LEU	4.9
1	X	114	TYR	4.8
1	X	55	LEU	4.8
1	A	30	MET	4.8
1	U	109	ALA	4.8
1	O	63	GLU	4.8
1	R	4	GLY	4.7
1	V	3	THR	4.7
1	V	123	THR	4.7
1	V	125	PRO	4.7
1	C	126	LYS	4.7
1	U	126	LYS	4.7
1	K	63	GLU	4.7
1	J	113	PRO	4.6
1	V	47	GLY	4.6
1	V	55	LEU	4.6
1	D	58	LEU	4.6
1	V	30	MET	4.6
1	K	30	MET	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	21	ARG	4.5
1	L	113	PRO	4.5
1	J	30	MET	4.5
1	S	125	PRO	4.5
1	F	30	MET	4.4
1	U	119	THR	4.4
1	L	79	TRP	4.4
1	G	32	VAL	4.4
1	E	69	TYR	4.4
1	G	69	TYR	4.4
1	B	44	PHE	4.4
1	M	123	THR	4.4
1	X	33	PHE	4.4
1	V	4	GLY	4.3
1	G	64	PHE	4.3
1	Q	126	LYS	4.3
1	V	14	VAL	4.3
1	O	9	LYS	4.3
1	N	30	MET	4.3
1	N	100	SER	4.3
1	K	123	THR	4.3
1	W	55	LEU	4.2
1	J	56	HIS	4.2
1	G	12	LEU	4.2
1	V	79	TRP	4.2
1	N	2	PRO	4.2
1	R	3	THR	4.2
1	L	114	TYR	4.1
1	N	29	ALA	4.1
1	P	47	GLY	4.1
1	J	55	LEU	4.1
1	J	9	LYS	4.1
1	J	8	SER	4.1
1	X	58	LEU	4.1
1	L	20	VAL	4.1
1	L	82	LEU	4.1
1	W	121	VAL	4.1
1	D	30	MET	4.0
1	P	30	MET	4.0
1	A	126	LYS	4.0
1	V	45	ALA	4.0
1	W	105	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	U	46	SER	4.0
1	J	13	MET	4.0
1	J	21	ARG	4.0
1	L	81	ALA	4.0
1	G	99	ASP	4.0
1	V	15	LYS	4.0
1	D	65	VAL	4.0
1	R	5	THR	3.9
1	L	55	LEU	3.9
1	B	83	GLY	3.9
1	J	123	THR	3.9
1	W	68	ILE	3.9
1	J	47	GLY	3.9
1	G	11	PRO	3.9
1	M	104	ARG	3.9
1	X	92	GLU	3.9
1	C	30	MET	3.9
1	X	40	THR	3.8
1	V	77	SER	3.8
1	F	55	LEU	3.8
1	J	26	ILE	3.8
1	G	36	ALA	3.8
1	V	44	PHE	3.8
1	X	30	MET	3.8
1	V	120	ALA	3.8
1	V	59	THR	3.8
1	G	13	MET	3.8
1	U	120	ALA	3.8
1	K	125	PRO	3.8
1	N	3	THR	3.8
1	V	61	GLU	3.8
1	F	31	HIS	3.8
1	V	58	LEU	3.8
1	J	84	ILE	3.8
1	R	9	LYS	3.8
1	E	60	THR	3.7
1	J	98	ASN	3.7
1	V	124	ASN	3.7
1	L	30	MET	3.7
1	B	58	LEU	3.7
1	H	55	LEU	3.7
1	J	19	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	W	125	PRO	3.7
1	F	78	TYR	3.7
1	V	69	TYR	3.7
1	F	81	ALA	3.7
1	T	9	LYS	3.7
1	K	39	ASP	3.7
1	L	8	SER	3.7
1	D	3	THR	3.7
1	X	47	GLY	3.7
1	X	65	VAL	3.7
1	M	61	GLU	3.7
1	M	63	GLU	3.7
1	G	59	THR	3.6
1	X	68	ILE	3.6
1	M	124	ASN	3.6
1	B	30	MET	3.6
1	O	125	PRO	3.6
1	B	55	LEU	3.6
1	G	68	ILE	3.6
1	X	41	TRP	3.6
1	N	4	GLY	3.6
1	M	30	MET	3.6
1	V	122	VAL	3.6
1	M	126	LYS	3.6
1	T	124	ASN	3.6
1	J	81	ALA	3.6
1	W	48	LYS	3.6
1	F	47	GLY	3.6
1	H	33	PHE	3.6
1	Q	30	MET	3.5
1	U	125	PRO	3.5
1	J	20	VAL	3.5
1	L	88	HIS	3.5
1	V	84	ILE	3.5
1	V	80	LYS	3.5
1	L	58	LEU	3.5
1	O	100	SER	3.5
1	U	60	THR	3.5
1	I	61	GLU	3.5
1	E	64	PHE	3.5
1	G	55	LEU	3.5
1	B	31	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	84	ILE	3.5
1	X	8	SER	3.5
1	L	47	GLY	3.5
1	T	125	PRO	3.5
1	P	82	LEU	3.5
1	D	125	PRO	3.4
1	N	125	PRO	3.4
1	A	58	LEU	3.4
1	L	110	LEU	3.4
1	X	26	ILE	3.4
1	E	58	LEU	3.4
1	F	20	VAL	3.4
1	V	26	ILE	3.4
1	V	105	TYR	3.4
1	X	46	SER	3.4
1	O	123	THR	3.4
1	E	37	ALA	3.4
1	F	97	ALA	3.4
1	R	125	PRO	3.4
1	V	51	GLU	3.4
1	W	51	GLU	3.4
1	X	37	ALA	3.4
1	X	83	GLY	3.4
1	W	58	LEU	3.4
1	N	9	LYS	3.4
1	F	82	LEU	3.4
1	M	101	GLY	3.4
1	F	114	TYR	3.3
1	N	83	GLY	3.3
1	X	19	ALA	3.3
1	J	23	SER	3.3
1	W	123	THR	3.3
1	L	51	GLU	3.3
1	O	61	GLU	3.3
1	U	103	ARG	3.3
1	X	102	PRO	3.3
1	D	100	SER	3.3
1	F	46	SER	3.3
1	X	28	VAL	3.3
1	D	2	PRO	3.3
1	T	30	MET	3.3
1	W	44	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	12	LEU	3.2
1	Q	63	GLU	3.2
1	J	80	LYS	3.2
1	B	47	GLY	3.2
1	V	37	ALA	3.2
1	K	44	PHE	3.2
1	X	94	VAL	3.2
1	J	39	ASP	3.2
1	V	10	CYS	3.2
1	F	58	LEU	3.2
1	I	9	LYS	3.2
1	V	8	SER	3.2
1	V	83	GLY	3.2
1	K	105	TYR	3.2
1	L	78	TYR	3.2
1	V	29	ALA	3.2
1	I	126	LYS	3.2
1	W	30	MET	3.2
1	D	61	GLU	3.2
1	E	12	LEU	3.2
1	L	86	PRO	3.2
1	W	90	HIS	3.2
1	J	46	SER	3.2
1	T	8	SER	3.2
1	D	9	LYS	3.2
1	M	9	LYS	3.2
1	L	92	GLU	3.2
1	X	81	ALA	3.2
1	E	55	LEU	3.1
1	D	31	HIS	3.1
1	J	10	CYS	3.1
1	U	123	THR	3.1
1	N	79	TRP	3.1
1	W	115	SER	3.1
1	W	94	VAL	3.1
1	X	86	PRO	3.1
1	X	34	ARG	3.1
1	D	98	ASN	3.1
1	K	12	LEU	3.1
1	U	55	LEU	3.1
1	X	82	LEU	3.1
1	D	62	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	3	THR	3.1
1	B	25	ALA	3.1
1	V	91	ALA	3.1
1	U	65	VAL	3.1
1	V	33	PHE	3.1
1	V	64	PHE	3.1
1	V	93	VAL	3.1
1	G	30	MET	3.1
1	V	13	MET	3.1
1	X	124	ASN	3.1
1	A	62	GLU	3.1
1	I	62	GLU	3.1
1	I	63	GLU	3.1
1	P	51	GLU	3.1
1	G	125	PRO	3.1
1	V	49	THR	3.1
1	L	80	LYS	3.1
1	V	107	ILE	3.1
1	X	84	ILE	3.1
1	F	79	TRP	3.1
1	K	122	VAL	3.1
1	L	87	PHE	3.1
1	E	31	HIS	3.0
1	S	63	GLU	3.0
1	U	62	GLU	3.0
1	V	92	GLU	3.0
1	B	125	PRO	3.0
1	L	11	PRO	3.0
1	G	9	LYS	3.0
1	K	9	LYS	3.0
1	W	60	THR	3.0
1	E	95	PHE	3.0
1	U	16	VAL	3.0
1	H	85	SER	3.0
1	U	77	SER	3.0
1	N	7	GLU	3.0
1	V	62	GLU	3.0
1	W	31	HIS	3.0
1	B	27	ASN	3.0
1	J	58	LEU	3.0
1	X	56	HIS	3.0
1	D	124	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	V	9	LYS	3.0
1	O	34	ARG	3.0
1	J	49	THR	3.0
1	J	79	TRP	3.0
1	V	117	SER	3.0
1	H	10	CYS	3.0
1	I	125	PRO	3.0
1	R	48	LYS	3.0
1	S	9	LYS	3.0
1	W	9	LYS	3.0
1	A	60	THR	3.0
1	F	33	PHE	3.0
1	W	95	PHE	3.0
1	G	70	LYS	2.9
1	F	10	CYS	2.9
1	X	116	TYR	2.9
1	F	84	ILE	2.9
1	B	4	GLY	2.9
1	J	57	GLY	2.9
1	A	94	VAL	2.9
1	N	58	LEU	2.9
1	E	9	LYS	2.9
1	A	99	ASP	2.9
1	L	37	ALA	2.9
1	G	121	VAL	2.9
1	D	55	LEU	2.9
1	A	100	SER	2.9
1	J	100	SER	2.9
1	V	73	ILE	2.9
1	X	69	TYR	2.9
1	E	59	THR	2.9
1	V	5	THR	2.9
1	U	108	ALA	2.9
1	V	97	ALA	2.9
1	G	58	LEU	2.9
1	P	20	VAL	2.9
1	J	48	LYS	2.9
1	V	111	LEU	2.9
1	X	44	PHE	2.9
1	E	92	GLU	2.9
1	L	56	HIS	2.9
1	J	77	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	W	46	SER	2.9
1	T	98	ASN	2.9
1	J	5	THR	2.9
1	C	9	LYS	2.9
1	X	9	LYS	2.9
1	X	36	ALA	2.9
1	V	32	VAL	2.9
1	A	124	ASN	2.8
1	J	124	ASN	2.8
1	X	39	ASP	2.8
1	F	69	TYR	2.8
1	J	29	ALA	2.8
1	V	40	THR	2.8
1	V	108	ALA	2.8
1	X	91	ALA	2.8
1	B	16	VAL	2.8
1	B	20	VAL	2.8
1	T	56	HIS	2.8
1	W	71	VAL	2.8
1	J	61	GLU	2.8
1	I	13	MET	2.8
1	G	102	PRO	2.8
1	N	11	PRO	2.8
1	D	46	SER	2.8
1	R	8	SER	2.8
1	C	124	ASN	2.8
1	B	9	LYS	2.8
1	P	83	GLY	2.8
1	A	12	LEU	2.8
1	U	58	LEU	2.8
1	F	87	PHE	2.8
1	W	63	GLU	2.8
1	B	79	TRP	2.8
1	B	6	GLY	2.8
1	G	22	GLY	2.8
1	G	31	HIS	2.8
1	L	36	ALA	2.8
1	L	59	THR	2.8
1	T	37	ALA	2.8
1	L	44	PHE	2.8
1	M	11	PRO	2.8
1	P	79	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	99	ASP	2.8
1	P	56	HIS	2.8
1	V	31	HIS	2.8
1	X	38	ASP	2.8
1	B	61	GLU	2.8
1	K	102	PRO	2.7
1	L	125	PRO	2.7
1	W	100	SER	2.7
1	D	39	ASP	2.7
1	G	14	VAL	2.7
1	P	29	ALA	2.7
1	W	14	VAL	2.7
1	X	72	GLU	2.7
1	J	11	PRO	2.7
1	T	11	PRO	2.7
1	U	9	LYS	2.7
1	X	35	LYS	2.7
1	W	82	LEU	2.7
1	H	8	SER	2.7
1	J	115	SER	2.7
1	R	100	SER	2.7
1	B	56	HIS	2.7
1	V	27	ASN	2.7
1	X	51	GLU	2.7
1	E	71	VAL	2.7
1	U	44	PHE	2.7
1	X	80	LYS	2.7
1	T	10	CYS	2.7
1	B	7	GLU	2.7
1	D	44	PHE	2.7
1	D	123	THR	2.7
1	E	65	VAL	2.7
1	F	123	THR	2.7
1	K	71	VAL	2.7
1	K	96	THR	2.7
1	K	97	ALA	2.7
1	U	37	ALA	2.7
1	X	87	PHE	2.7
1	W	102	PRO	2.7
1	G	105	TYR	2.7
1	H	90	HIS	2.7
1	G	46	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	46	SER	2.7
1	K	124	ASN	2.7
1	M	62	GLU	2.7
1	U	124	ASN	2.7
1	V	46	SER	2.7
1	X	89	GLU	2.7
1	B	5	THR	2.7
1	D	5	THR	2.7
1	K	120	ALA	2.7
1	L	29	ALA	2.7
1	U	95	PHE	2.7
1	X	64	PHE	2.7
1	F	125	PRO	2.7
1	J	99	ASP	2.7
1	F	80	LYS	2.6
1	L	27	ASN	2.6
1	U	80	LYS	2.6
1	L	19	ALA	2.6
1	V	20	VAL	2.6
1	D	11	PRO	2.6
1	N	5	THR	2.6
1	V	78	TYR	2.6
1	S	30	MET	2.6
1	V	82	LEU	2.6
1	X	12	LEU	2.6
1	V	21	ARG	2.6
1	X	10	CYS	2.6
1	I	48	LYS	2.6
1	J	42	GLU	2.6
1	V	53	GLY	2.6
1	W	35	LYS	2.6
1	C	46	SER	2.6
1	C	117	SER	2.6
1	D	45	ALA	2.6
1	G	37	ALA	2.6
1	K	37	ALA	2.6
1	K	85	SER	2.6
1	C	60	THR	2.6
1	D	102	PRO	2.6
1	M	97	ALA	2.6
1	G	40	THR	2.6
1	W	41	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	30	MET	2.6
1	G	56	HIS	2.6
1	N	104	ARG	2.6
1	X	104	ARG	2.6
1	D	10	CYS	2.6
1	X	42	GLU	2.6
1	E	101	GLY	2.6
1	D	32	VAL	2.6
1	E	102	PRO	2.6
1	R	124	ASN	2.6
1	U	102	PRO	2.6
1	W	29	ALA	2.6
1	G	60	THR	2.6
1	R	123	THR	2.6
1	U	117	SER	2.6
1	W	50	SER	2.6
1	U	68	ILE	2.6
1	W	56	HIS	2.6
1	X	76	LYS	2.6
1	W	92	GLU	2.6
1	F	83	GLY	2.6
1	U	121	VAL	2.6
1	W	37	ALA	2.6
1	X	125	PRO	2.6
1	G	95	PHE	2.6
1	J	50	SER	2.5
1	E	39	ASP	2.5
1	L	26	ILE	2.5
1	O	103	ARG	2.5
1	K	69	TYR	2.5
1	W	61	GLU	2.5
1	G	101	GLY	2.5
1	E	121	VAL	2.5
1	F	32	VAL	2.5
1	W	32	VAL	2.5
1	X	93	VAL	2.5
1	G	29	ALA	2.5
1	O	124	ASN	2.5
1	K	35	LYS	2.5
1	A	92	GLU	2.5
1	E	51	GLU	2.5
1	V	7	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	6	GLY	2.5
1	M	121	VAL	2.5
1	D	97	ALA	2.5
1	D	59	THR	2.5
1	G	123	THR	2.5
1	L	98	ASN	2.5
1	W	40	THR	2.5
1	W	106	THR	2.5
1	X	59	THR	2.5
1	X	117	SER	2.5
1	X	79	TRP	2.5
1	I	103	ARG	2.5
1	X	74	ASP	2.5
1	D	56	HIS	2.5
1	H	56	HIS	2.5
1	A	61	GLU	2.5
1	J	7	GLU	2.5
1	K	42	GLU	2.5
1	L	28	VAL	2.5
1	W	122	VAL	2.5
1	X	32	VAL	2.5
1	E	25	ALA	2.5
1	K	64	PHE	2.5
1	C	118	THR	2.5
1	D	34	ARG	2.5
1	H	58	LEU	2.5
1	F	56	HIS	2.5
1	B	51	GLU	2.5
1	P	42	GLU	2.5
1	R	61	GLU	2.5
1	J	83	GLY	2.5
1	X	13	MET	2.5
1	V	94	VAL	2.5
1	O	97	ALA	2.5
1	V	87	PHE	2.5
1	F	48	LYS	2.4
1	V	75	THR	2.4
1	I	124	ASN	2.4
1	C	12	LEU	2.4
1	V	17	LEU	2.4
1	P	8	SER	2.4
1	P	88	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	102	PRO	2.4
1	J	78	TYR	2.4
1	C	65	VAL	2.4
1	A	95	PHE	2.4
1	J	76	LYS	2.4
1	R	80	LYS	2.4
1	U	93	VAL	2.4
1	O	37	ALA	2.4
1	I	34	ARG	2.4
1	B	12	LEU	2.4
1	L	111	LEU	2.4
1	U	56	HIS	2.4
1	B	10	CYS	2.4
1	N	99	ASP	2.4
1	D	47	GLY	2.4
1	F	101	GLY	2.4
1	L	57	GLY	2.4
1	O	102	PRO	2.4
1	Q	9	LYS	2.4
1	V	70	LYS	2.4
1	W	116	TYR	2.4
1	B	19	ALA	2.4
1	K	36	ALA	2.4
1	E	100	SER	2.4
1	G	41	TRP	2.4
1	H	42	GLU	2.4
1	J	51	GLU	2.4
1	K	62	GLU	2.4
1	K	99	ASP	2.4
1	V	39	ASP	2.4
1	L	10	CYS	2.4
1	A	125	PRO	2.4
1	H	125	PRO	2.4
1	W	15	LYS	2.4
1	N	47	GLY	2.4
1	V	71	VAL	2.4
1	K	114	TYR	2.4
1	W	33	PHE	2.4
1	U	40	THR	2.4
1	U	75	THR	2.4
1	U	118	THR	2.4
1	V	68	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	98	ASN	2.4
1	E	62	GLU	2.4
1	G	100	SER	2.4
1	H	92	GLU	2.4
1	I	92	GLU	2.4
1	W	62	GLU	2.4
1	D	99	ASP	2.4
1	K	10	CYS	2.4
1	B	102	PRO	2.4
1	E	125	PRO	2.4
1	W	11	PRO	2.4
1	J	53	GLY	2.4
1	W	57	GLY	2.4
1	A	34	ARG	2.4
1	L	14	VAL	2.4
1	L	25	ALA	2.4
1	X	45	ALA	2.4
1	K	68	ILE	2.3
1	E	119	THR	2.3
1	E	61	GLU	2.3
1	V	54	GLU	2.3
1	I	30	MET	2.3
1	R	99	ASP	2.3
1	N	113	PRO	2.3
1	J	4	GLY	2.3
1	D	122	VAL	2.3
1	G	65	VAL	2.3
1	J	16	VAL	2.3
1	U	14	VAL	2.3
1	U	71	VAL	2.3
1	D	37	ALA	2.3
1	T	29	ALA	2.3
1	W	110	LEU	2.3
1	B	26	ILE	2.3
1	T	123	THR	2.3
1	E	13	MET	2.3
1	K	15	LYS	2.3
1	X	61	GLU	2.3
1	E	99	ASP	2.3
1	W	53	GLY	2.3
1	W	65	VAL	2.3
1	C	58	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	44	PHE	2.3
1	R	55	LEU	2.3
1	V	25	ALA	2.3
1	P	84	ILE	2.3
1	L	116	TYR	2.3
1	W	118	THR	2.3
1	G	62	GLU	2.3
1	A	103	ARG	2.3
1	H	41	TRP	2.3
1	G	57	GLY	2.3
1	F	14	VAL	2.3
1	N	82	LEU	2.3
1	U	12	LEU	2.3
1	F	25	ALA	2.3
1	C	56	HIS	2.3
1	V	56	HIS	2.3
1	B	123	THR	2.3
1	K	13	MET	2.3
1	V	106	THR	2.3
1	B	69	TYR	2.3
1	V	42	GLU	2.3
1	P	124	ASN	2.3
1	C	39	ASP	2.3
1	G	104	ARG	2.3
1	K	104	ARG	2.3
1	M	125	PRO	2.3
1	V	85	SER	2.3
1	I	101	GLY	2.3
1	P	57	GLY	2.3
1	I	122	VAL	2.3
1	K	65	VAL	2.3
1	W	111	LEU	2.3
1	X	121	VAL	2.3
1	B	64	PHE	2.3
1	B	48	LYS	2.2
1	U	59	THR	2.2
1	C	61	GLU	2.2
1	Q	62	GLU	2.2
1	C	69	TYR	2.2
1	F	24	PRO	2.2
1	F	113	PRO	2.2
1	X	22	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	65	VAL	2.2
1	K	121	VAL	2.2
1	I	120	ALA	2.2
1	K	19	ALA	2.2
1	U	107	ILE	2.2
1	T	61	GLU	2.2
1	W	119	THR	2.2
1	X	105	TYR	2.2
1	F	27	ASN	2.2
1	G	124	ASN	2.2
1	N	21	ARG	2.2
1	P	98	ASN	2.2
1	B	85	SER	2.2
1	B	100	SER	2.2
1	R	47	GLY	2.2
1	H	82	LEU	2.2
1	B	122	VAL	2.2
1	E	32	VAL	2.2
1	L	76	LYS	2.2
1	V	28	VAL	2.2
1	W	16	VAL	2.2
1	U	90	HIS	2.2
1	I	97	ALA	2.2
1	R	37	ALA	2.2
1	G	63	GLU	2.2
1	J	54	GLU	2.2
1	P	59	THR	2.2
1	R	7	GLU	2.2
1	R	10	CYS	2.2
1	V	89	GLU	2.2
1	X	62	GLU	2.2
1	R	11	PRO	2.2
1	A	74	ASP	2.2
1	B	67	GLY	2.2
1	C	47	GLY	2.2
1	F	23	SER	2.2
1	F	70	LYS	2.2
1	L	9	LYS	2.2
1	W	67	GLY	2.2
1	B	94	VAL	2.2
1	E	122	VAL	2.2
1	M	65	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	13	MET	2.2
1	V	16	VAL	2.2
1	A	64	PHE	2.2
1	B	33	PHE	2.2
1	G	33	PHE	2.2
1	B	92	GLU	2.2
1	R	42	GLU	2.2
1	C	40	THR	2.2
1	F	34	ARG	2.2
1	S	10	CYS	2.2
1	V	34	ARG	2.2
1	V	104	ARG	2.2
1	B	124	ASN	2.2
1	J	114	TYR	2.2
1	K	98	ASN	2.2
1	P	114	TYR	2.2
1	A	9	LYS	2.2
1	E	80	LYS	2.2
1	F	9	LYS	2.2
1	N	80	LYS	2.2
1	T	47	GLY	2.2
1	T	55	LEU	2.2
1	O	99	ASP	2.2
1	A	14	VAL	2.2
1	H	94	VAL	2.2
1	U	28	VAL	2.2
1	V	95	PHE	2.2
1	B	29	ALA	2.1
1	W	45	ALA	2.1
1	X	97	ALA	2.1
1	E	63	GLU	2.1
1	F	92	GLU	2.1
1	Q	42	GLU	2.1
1	S	21	ARG	2.1
1	B	43	PRO	2.1
1	U	105	TYR	2.1
1	U	67	GLY	2.1
1	A	16	VAL	2.1
1	J	88	HIS	2.1
1	J	107	ILE	2.1
1	L	99	ASP	2.1
1	L	77	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	122	VAL	2.1
1	R	65	VAL	2.1
1	T	46	SER	2.1
1	E	44	PHE	2.1
1	J	25	ALA	2.1
1	N	19	ALA	2.1
1	L	42	GLU	2.1
1	H	34	ARG	2.1
1	I	21	ARG	2.1
1	U	21	ARG	2.1
1	J	59	THR	2.1
1	H	9	LYS	2.1
1	P	11	PRO	2.1
1	S	102	PRO	2.1
1	V	86	PRO	2.1
1	E	105	TYR	2.1
1	X	57	GLY	2.1
1	B	73	ILE	2.1
1	P	99	ASP	2.1
1	X	16	VAL	2.1
1	P	46	SER	2.1
1	B	37	ALA	2.1
1	W	120	ALA	2.1
1	K	51	GLU	2.1
1	S	92	GLU	2.1
1	D	104	ARG	2.1
1	T	104	ARG	2.1
1	U	34	ARG	2.1
1	J	60	THR	2.1
1	E	35	LYS	2.1
1	V	48	LYS	2.1
1	V	102	PRO	2.1
1	X	11	PRO	2.1
1	C	13	MET	2.1
1	C	55	LEU	2.1
1	W	12	LEU	2.1
1	D	57	GLY	2.1
1	F	90	HIS	2.1
1	W	78	TYR	2.1
1	B	32	VAL	2.1
1	I	121	VAL	2.1
1	B	99	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	99	ASP	2.1
1	U	33	PHE	2.1
1	C	104	ARG	2.1
1	E	81	ALA	2.1
1	N	42	GLU	2.1
1	N	92	GLU	2.1
1	B	75	THR	2.1
1	K	119	THR	2.1
1	B	113	PRO	2.1
1	C	11	PRO	2.1
1	V	113	PRO	2.1
1	A	56	HIS	2.1
1	D	22	GLY	2.1
1	J	22	GLY	2.1
1	N	56	HIS	2.1
1	V	101	GLY	2.1
1	W	47	GLY	2.1
1	E	68	ILE	2.1
1	H	84	ILE	2.1
1	V	114	TYR	2.1
1	E	14	VAL	2.1
1	I	93	VAL	2.1
1	D	64	PHE	2.1
1	S	37	ALA	2.0
1	A	123	THR	2.0
1	R	118	THR	2.0
1	L	90	HIS	2.0
1	N	84	ILE	2.0
1	W	101	GLY	2.0
1	J	14	VAL	2.0
1	L	34	ARG	2.0
1	I	51	GLU	2.0
1	E	97	ALA	2.0
1	F	39	ASP	2.0
1	X	63	GLU	2.0
1	W	108	ALA	2.0
1	U	85	SER	2.0
1	B	41	TRP	2.0
1	E	11	PRO	2.0
1	N	75	THR	2.0
1	X	31	HIS	2.0
1	D	101	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	98	ASN	2.0
1	R	27	ASN	2.0
1	S	124	ASN	2.0
1	H	21	ARG	2.0
1	R	104	ARG	2.0
1	X	122	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.