



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 AM GMT

PDB ID : 2O1T
Title : Structure of Middle plus C-terminal domains (M+C) of GRP94
Authors : Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on : 2006-11-29
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

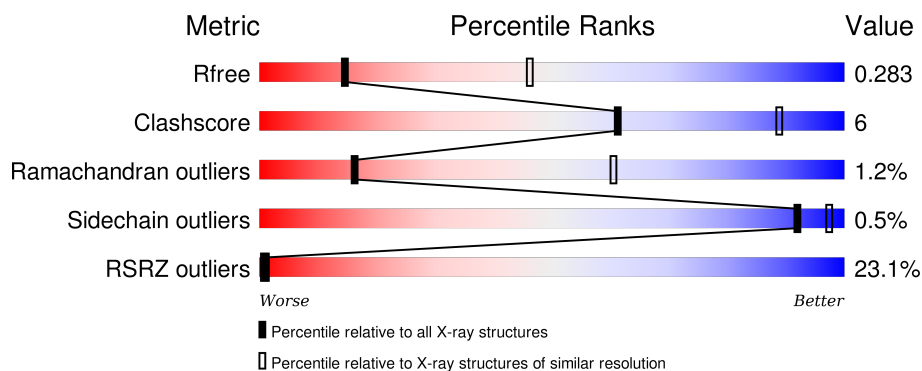
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	450	<div> <div>12%</div> <div>81%</div> <div>10%</div> <div>8%</div> </div>
1	B	450	<div> <div>25%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	C	450	<div> <div>14%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	D	450	<div> <div>21%</div> <div>79%</div> <div>12%</div> <div>8%</div> </div>
1	E	450	<div> <div>13%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	450	
1	G	450	
1	H	450	
1	I	450	
1	J	450	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33009 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	B	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	C	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	D	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	E	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	F	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	G	413	Total	C	N	O	S	0	0	0
			3300	2101	548	638	13			
1	H	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	I	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	J	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	MET	-	EXPRESSION TAG	UNP P41148
A	317	GLY	-	EXPRESSION TAG	UNP P41148
A	318	SER	-	EXPRESSION TAG	UNP P41148
A	319	SER	-	EXPRESSION TAG	UNP P41148
A	320	HIS	-	EXPRESSION TAG	UNP P41148
A	321	HIS	-	EXPRESSION TAG	UNP P41148
A	322	HIS	-	EXPRESSION TAG	UNP P41148
A	323	HIS	-	EXPRESSION TAG	UNP P41148
A	324	HIS	-	EXPRESSION TAG	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	-	EXPRESSION TAG	UNP P41148
A	326	SER	-	EXPRESSION TAG	UNP P41148
A	327	SER	-	EXPRESSION TAG	UNP P41148
A	328	GLY	-	EXPRESSION TAG	UNP P41148
A	329	LEU	-	EXPRESSION TAG	UNP P41148
A	330	VAL	-	EXPRESSION TAG	UNP P41148
A	331	PRO	-	EXPRESSION TAG	UNP P41148
A	332	ARG	-	EXPRESSION TAG	UNP P41148
A	333	GLY	-	EXPRESSION TAG	UNP P41148
A	334	SER	-	EXPRESSION TAG	UNP P41148
A	335	HIS	-	EXPRESSION TAG	UNP P41148
B	316	MET	-	EXPRESSION TAG	UNP P41148
B	317	GLY	-	EXPRESSION TAG	UNP P41148
B	318	SER	-	EXPRESSION TAG	UNP P41148
B	319	SER	-	EXPRESSION TAG	UNP P41148
B	320	HIS	-	EXPRESSION TAG	UNP P41148
B	321	HIS	-	EXPRESSION TAG	UNP P41148
B	322	HIS	-	EXPRESSION TAG	UNP P41148
B	323	HIS	-	EXPRESSION TAG	UNP P41148
B	324	HIS	-	EXPRESSION TAG	UNP P41148
B	325	HIS	-	EXPRESSION TAG	UNP P41148
B	326	SER	-	EXPRESSION TAG	UNP P41148
B	327	SER	-	EXPRESSION TAG	UNP P41148
B	328	GLY	-	EXPRESSION TAG	UNP P41148
B	329	LEU	-	EXPRESSION TAG	UNP P41148
B	330	VAL	-	EXPRESSION TAG	UNP P41148
B	331	PRO	-	EXPRESSION TAG	UNP P41148
B	332	ARG	-	EXPRESSION TAG	UNP P41148
B	333	GLY	-	EXPRESSION TAG	UNP P41148
B	334	SER	-	EXPRESSION TAG	UNP P41148
B	335	HIS	-	EXPRESSION TAG	UNP P41148
C	316	MET	-	EXPRESSION TAG	UNP P41148
C	317	GLY	-	EXPRESSION TAG	UNP P41148
C	318	SER	-	EXPRESSION TAG	UNP P41148
C	319	SER	-	EXPRESSION TAG	UNP P41148
C	320	HIS	-	EXPRESSION TAG	UNP P41148
C	321	HIS	-	EXPRESSION TAG	UNP P41148
C	322	HIS	-	EXPRESSION TAG	UNP P41148
C	323	HIS	-	EXPRESSION TAG	UNP P41148
C	324	HIS	-	EXPRESSION TAG	UNP P41148
C	325	HIS	-	EXPRESSION TAG	UNP P41148
C	326	SER	-	EXPRESSION TAG	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
C	327	SER	-	EXPRESSION TAG	UNP P41148
C	328	GLY	-	EXPRESSION TAG	UNP P41148
C	329	LEU	-	EXPRESSION TAG	UNP P41148
C	330	VAL	-	EXPRESSION TAG	UNP P41148
C	331	PRO	-	EXPRESSION TAG	UNP P41148
C	332	ARG	-	EXPRESSION TAG	UNP P41148
C	333	GLY	-	EXPRESSION TAG	UNP P41148
C	334	SER	-	EXPRESSION TAG	UNP P41148
C	335	HIS	-	EXPRESSION TAG	UNP P41148
D	316	MET	-	EXPRESSION TAG	UNP P41148
D	317	GLY	-	EXPRESSION TAG	UNP P41148
D	318	SER	-	EXPRESSION TAG	UNP P41148
D	319	SER	-	EXPRESSION TAG	UNP P41148
D	320	HIS	-	EXPRESSION TAG	UNP P41148
D	321	HIS	-	EXPRESSION TAG	UNP P41148
D	322	HIS	-	EXPRESSION TAG	UNP P41148
D	323	HIS	-	EXPRESSION TAG	UNP P41148
D	324	HIS	-	EXPRESSION TAG	UNP P41148
D	325	HIS	-	EXPRESSION TAG	UNP P41148
D	326	SER	-	EXPRESSION TAG	UNP P41148
D	327	SER	-	EXPRESSION TAG	UNP P41148
D	328	GLY	-	EXPRESSION TAG	UNP P41148
D	329	LEU	-	EXPRESSION TAG	UNP P41148
D	330	VAL	-	EXPRESSION TAG	UNP P41148
D	331	PRO	-	EXPRESSION TAG	UNP P41148
D	332	ARG	-	EXPRESSION TAG	UNP P41148
D	333	GLY	-	EXPRESSION TAG	UNP P41148
D	334	SER	-	EXPRESSION TAG	UNP P41148
D	335	HIS	-	EXPRESSION TAG	UNP P41148
E	316	MET	-	EXPRESSION TAG	UNP P41148
E	317	GLY	-	EXPRESSION TAG	UNP P41148
E	318	SER	-	EXPRESSION TAG	UNP P41148
E	319	SER	-	EXPRESSION TAG	UNP P41148
E	320	HIS	-	EXPRESSION TAG	UNP P41148
E	321	HIS	-	EXPRESSION TAG	UNP P41148
E	322	HIS	-	EXPRESSION TAG	UNP P41148
E	323	HIS	-	EXPRESSION TAG	UNP P41148
E	324	HIS	-	EXPRESSION TAG	UNP P41148
E	325	HIS	-	EXPRESSION TAG	UNP P41148
E	326	SER	-	EXPRESSION TAG	UNP P41148
E	327	SER	-	EXPRESSION TAG	UNP P41148
E	328	GLY	-	EXPRESSION TAG	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
E	329	LEU	-	EXPRESSION TAG	UNP P41148
E	330	VAL	-	EXPRESSION TAG	UNP P41148
E	331	PRO	-	EXPRESSION TAG	UNP P41148
E	332	ARG	-	EXPRESSION TAG	UNP P41148
E	333	GLY	-	EXPRESSION TAG	UNP P41148
E	334	SER	-	EXPRESSION TAG	UNP P41148
E	335	HIS	-	EXPRESSION TAG	UNP P41148
F	316	MET	-	EXPRESSION TAG	UNP P41148
F	317	GLY	-	EXPRESSION TAG	UNP P41148
F	318	SER	-	EXPRESSION TAG	UNP P41148
F	319	SER	-	EXPRESSION TAG	UNP P41148
F	320	HIS	-	EXPRESSION TAG	UNP P41148
F	321	HIS	-	EXPRESSION TAG	UNP P41148
F	322	HIS	-	EXPRESSION TAG	UNP P41148
F	323	HIS	-	EXPRESSION TAG	UNP P41148
F	324	HIS	-	EXPRESSION TAG	UNP P41148
F	325	HIS	-	EXPRESSION TAG	UNP P41148
F	326	SER	-	EXPRESSION TAG	UNP P41148
F	327	SER	-	EXPRESSION TAG	UNP P41148
F	328	GLY	-	EXPRESSION TAG	UNP P41148
F	329	LEU	-	EXPRESSION TAG	UNP P41148
F	330	VAL	-	EXPRESSION TAG	UNP P41148
F	331	PRO	-	EXPRESSION TAG	UNP P41148
F	332	ARG	-	EXPRESSION TAG	UNP P41148
F	333	GLY	-	EXPRESSION TAG	UNP P41148
F	334	SER	-	EXPRESSION TAG	UNP P41148
F	335	HIS	-	EXPRESSION TAG	UNP P41148
G	316	MET	-	EXPRESSION TAG	UNP P41148
G	317	GLY	-	EXPRESSION TAG	UNP P41148
G	318	SER	-	EXPRESSION TAG	UNP P41148
G	319	SER	-	EXPRESSION TAG	UNP P41148
G	320	HIS	-	EXPRESSION TAG	UNP P41148
G	321	HIS	-	EXPRESSION TAG	UNP P41148
G	322	HIS	-	EXPRESSION TAG	UNP P41148
G	323	HIS	-	EXPRESSION TAG	UNP P41148
G	324	HIS	-	EXPRESSION TAG	UNP P41148
G	325	HIS	-	EXPRESSION TAG	UNP P41148
G	326	SER	-	EXPRESSION TAG	UNP P41148
G	327	SER	-	EXPRESSION TAG	UNP P41148
G	328	GLY	-	EXPRESSION TAG	UNP P41148
G	329	LEU	-	EXPRESSION TAG	UNP P41148
G	330	VAL	-	EXPRESSION TAG	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
G	331	PRO	-	EXPRESSION TAG	UNP P41148
G	332	ARG	-	EXPRESSION TAG	UNP P41148
G	333	GLY	-	EXPRESSION TAG	UNP P41148
G	334	SER	-	EXPRESSION TAG	UNP P41148
G	335	HIS	-	EXPRESSION TAG	UNP P41148
H	316	MET	-	EXPRESSION TAG	UNP P41148
H	317	GLY	-	EXPRESSION TAG	UNP P41148
H	318	SER	-	EXPRESSION TAG	UNP P41148
H	319	SER	-	EXPRESSION TAG	UNP P41148
H	320	HIS	-	EXPRESSION TAG	UNP P41148
H	321	HIS	-	EXPRESSION TAG	UNP P41148
H	322	HIS	-	EXPRESSION TAG	UNP P41148
H	323	HIS	-	EXPRESSION TAG	UNP P41148
H	324	HIS	-	EXPRESSION TAG	UNP P41148
H	325	HIS	-	EXPRESSION TAG	UNP P41148
H	326	SER	-	EXPRESSION TAG	UNP P41148
H	327	SER	-	EXPRESSION TAG	UNP P41148
H	328	GLY	-	EXPRESSION TAG	UNP P41148
H	329	LEU	-	EXPRESSION TAG	UNP P41148
H	330	VAL	-	EXPRESSION TAG	UNP P41148
H	331	PRO	-	EXPRESSION TAG	UNP P41148
H	332	ARG	-	EXPRESSION TAG	UNP P41148
H	333	GLY	-	EXPRESSION TAG	UNP P41148
H	334	SER	-	EXPRESSION TAG	UNP P41148
H	335	HIS	-	EXPRESSION TAG	UNP P41148
I	316	MET	-	EXPRESSION TAG	UNP P41148
I	317	GLY	-	EXPRESSION TAG	UNP P41148
I	318	SER	-	EXPRESSION TAG	UNP P41148
I	319	SER	-	EXPRESSION TAG	UNP P41148
I	320	HIS	-	EXPRESSION TAG	UNP P41148
I	321	HIS	-	EXPRESSION TAG	UNP P41148
I	322	HIS	-	EXPRESSION TAG	UNP P41148
I	323	HIS	-	EXPRESSION TAG	UNP P41148
I	324	HIS	-	EXPRESSION TAG	UNP P41148
I	325	HIS	-	EXPRESSION TAG	UNP P41148
I	326	SER	-	EXPRESSION TAG	UNP P41148
I	327	SER	-	EXPRESSION TAG	UNP P41148
I	328	GLY	-	EXPRESSION TAG	UNP P41148
I	329	LEU	-	EXPRESSION TAG	UNP P41148
I	330	VAL	-	EXPRESSION TAG	UNP P41148
I	331	PRO	-	EXPRESSION TAG	UNP P41148
I	332	ARG	-	EXPRESSION TAG	UNP P41148

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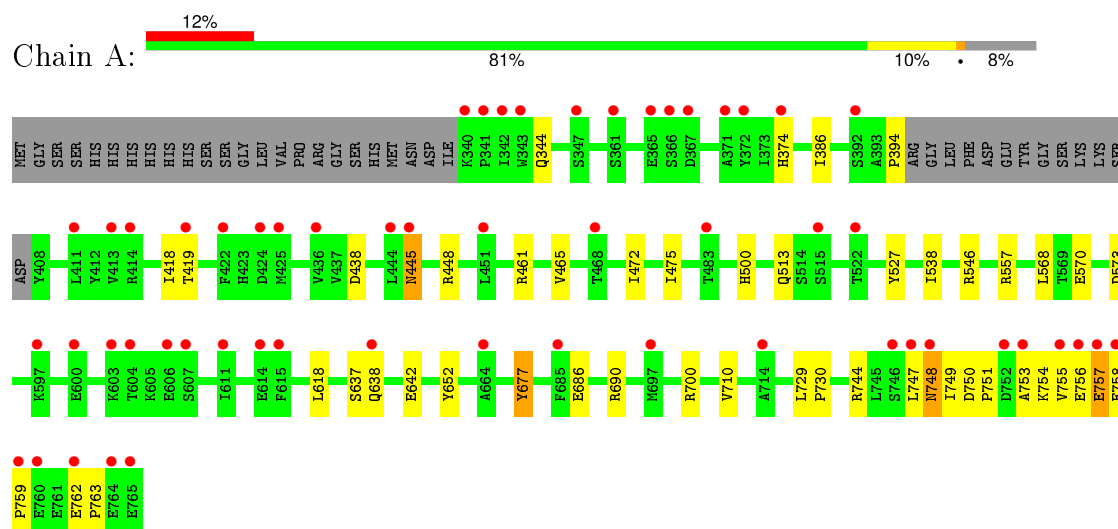
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Chain	Residue	Modelled	Actual	Comment	Reference
I	333	GLY	-	EXPRESSION TAG	UNP P41148
I	334	SER	-	EXPRESSION TAG	UNP P41148
I	335	HIS	-	EXPRESSION TAG	UNP P41148
J	316	MET	-	EXPRESSION TAG	UNP P41148
J	317	GLY	-	EXPRESSION TAG	UNP P41148
J	318	SER	-	EXPRESSION TAG	UNP P41148
J	319	SER	-	EXPRESSION TAG	UNP P41148
J	320	HIS	-	EXPRESSION TAG	UNP P41148
J	321	HIS	-	EXPRESSION TAG	UNP P41148
J	322	HIS	-	EXPRESSION TAG	UNP P41148
J	323	HIS	-	EXPRESSION TAG	UNP P41148
J	324	HIS	-	EXPRESSION TAG	UNP P41148
J	325	HIS	-	EXPRESSION TAG	UNP P41148
J	326	SER	-	EXPRESSION TAG	UNP P41148
J	327	SER	-	EXPRESSION TAG	UNP P41148
J	328	GLY	-	EXPRESSION TAG	UNP P41148
J	329	LEU	-	EXPRESSION TAG	UNP P41148
J	330	VAL	-	EXPRESSION TAG	UNP P41148
J	331	PRO	-	EXPRESSION TAG	UNP P41148
J	332	ARG	-	EXPRESSION TAG	UNP P41148
J	333	GLY	-	EXPRESSION TAG	UNP P41148
J	334	SER	-	EXPRESSION TAG	UNP P41148
J	335	HIS	-	EXPRESSION TAG	UNP P41148

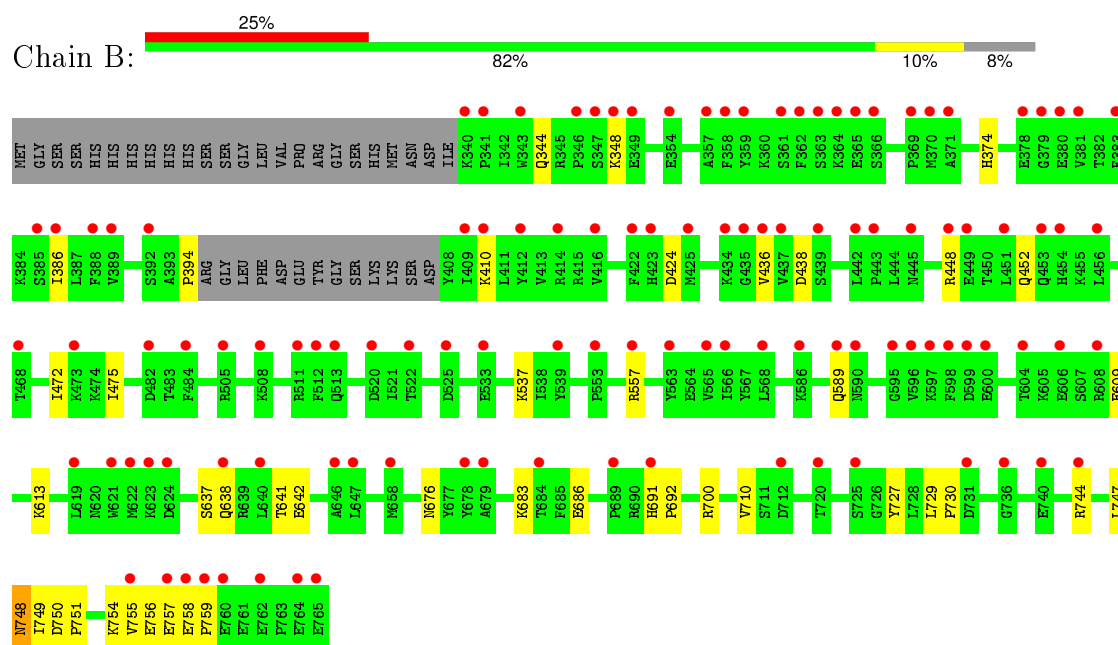
3 Residue-property plots

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.

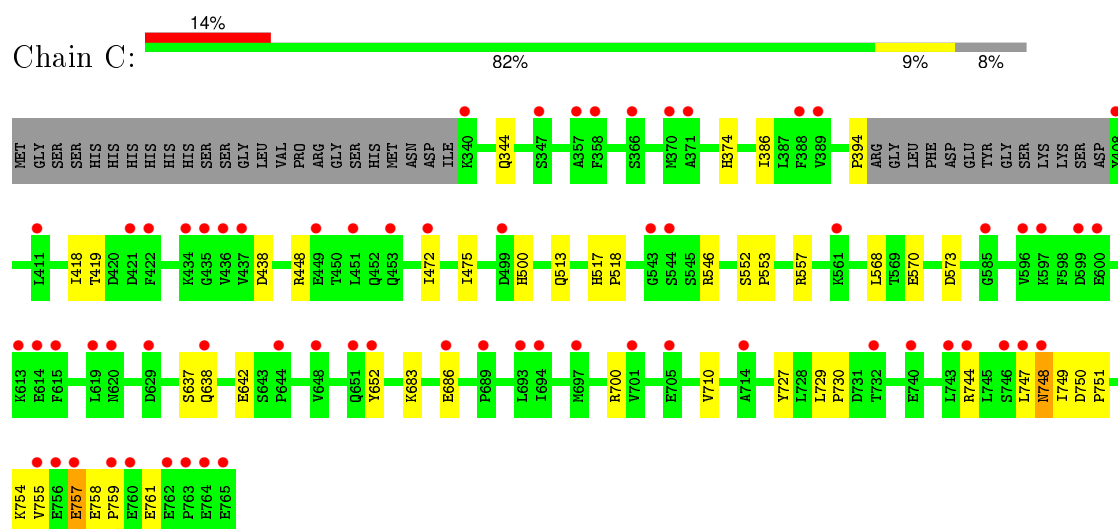
• Molecule 1: Endoplasmin



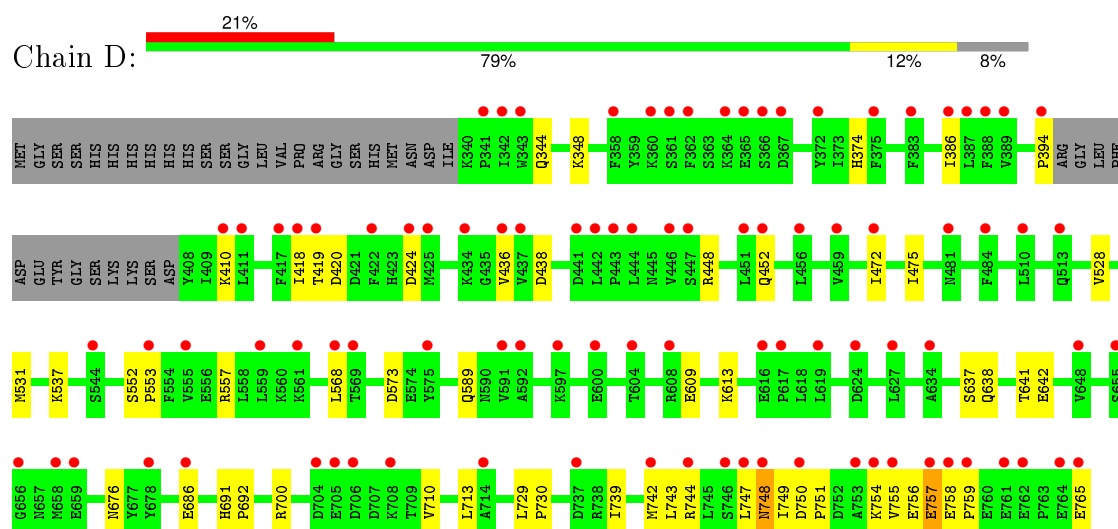
• Molecule 1: Endoplasmin



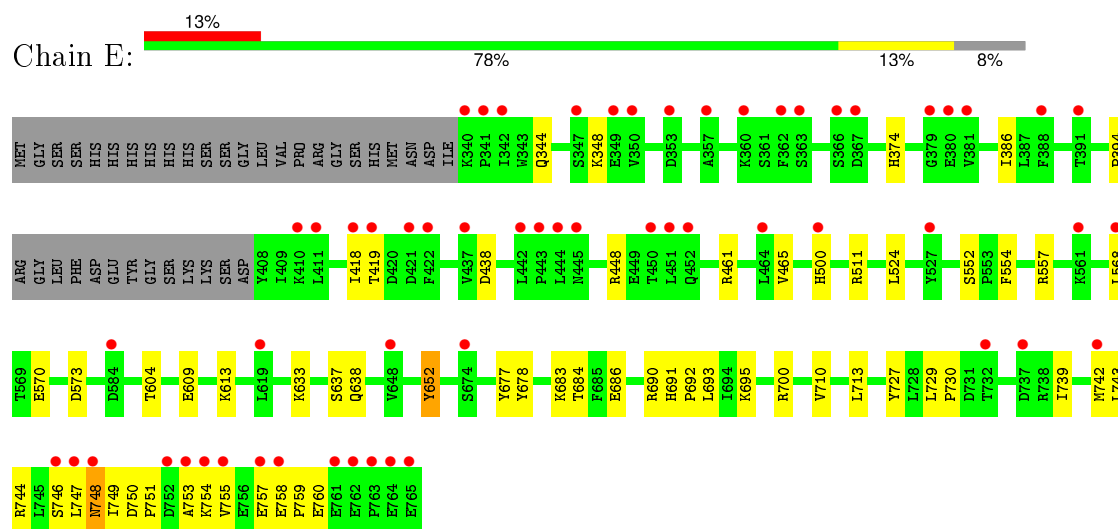
• Molecule 1: Endoplasmin



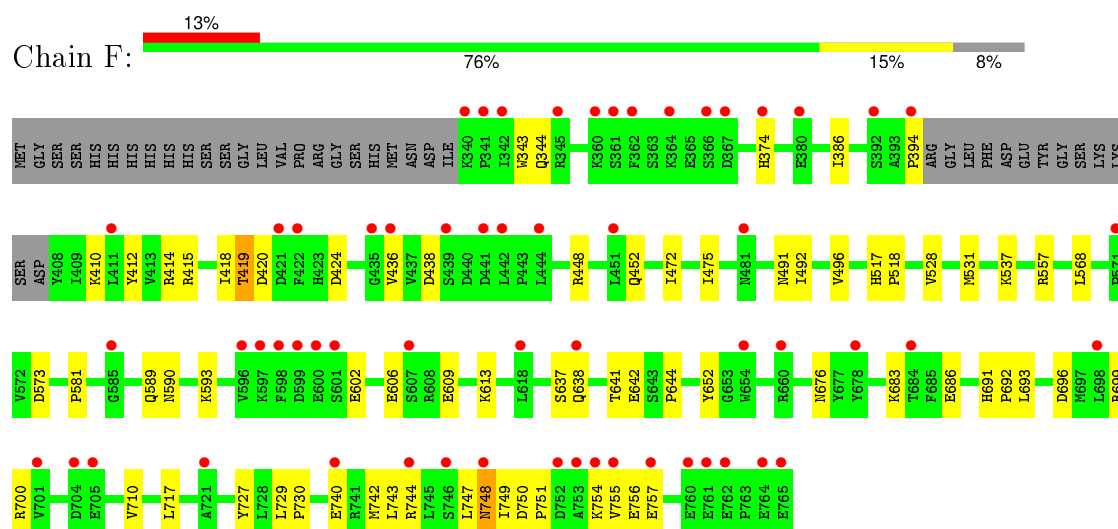
• Molecule 1: Endoplasmic reticulum



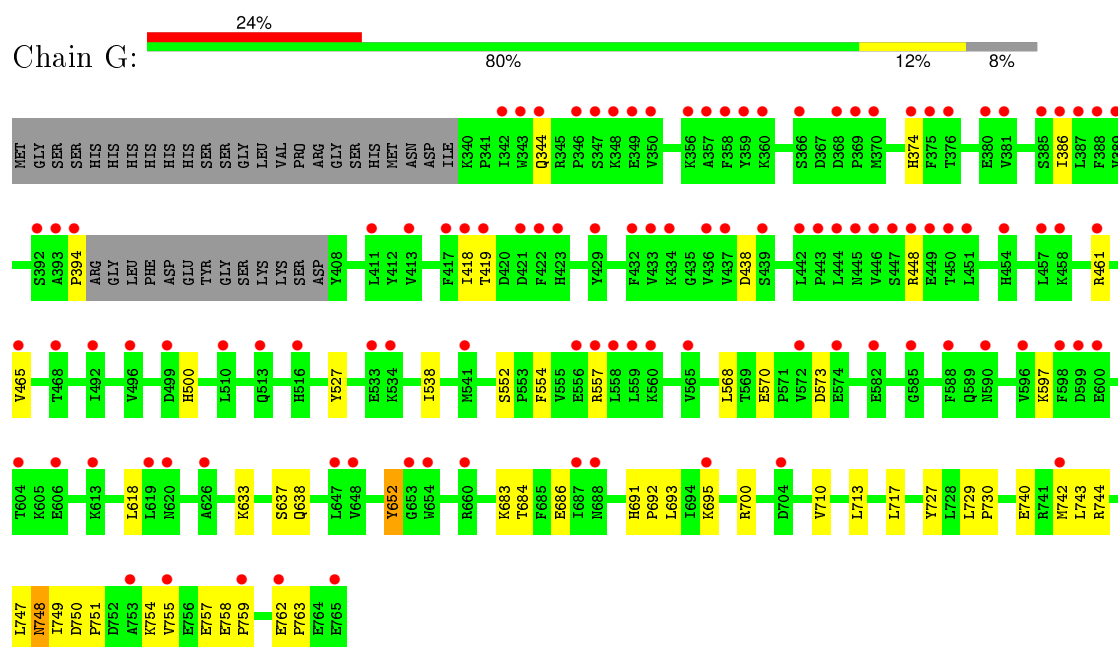
• Molecule 1: Endoplasmic reticulum



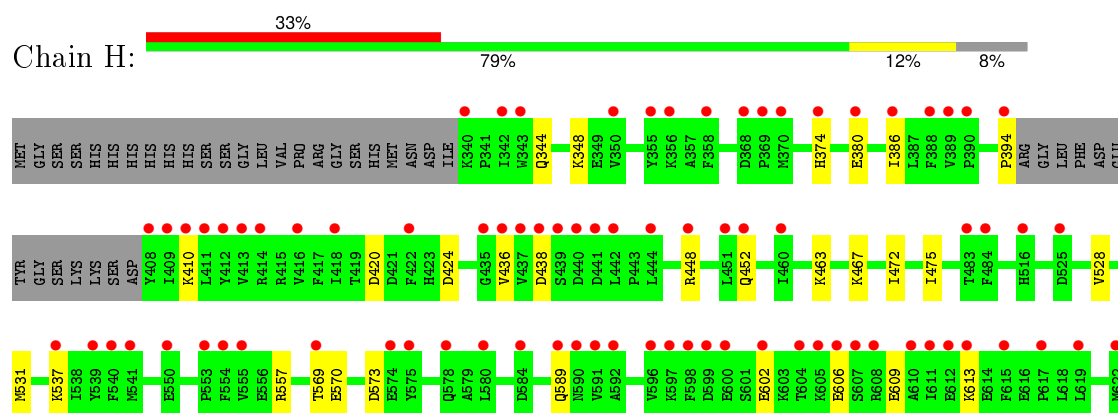
• Molecule 1: Endoplasmic reticulum

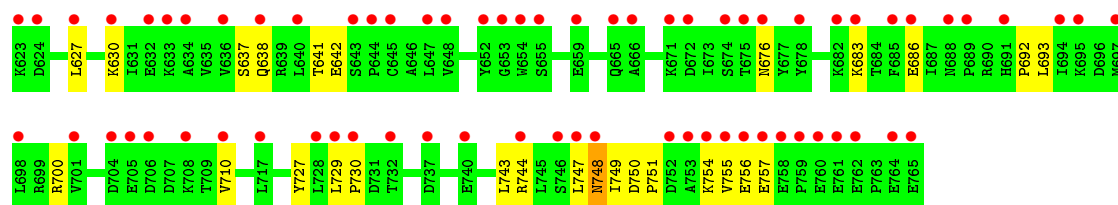


• Molecule 1: Endoplasmic

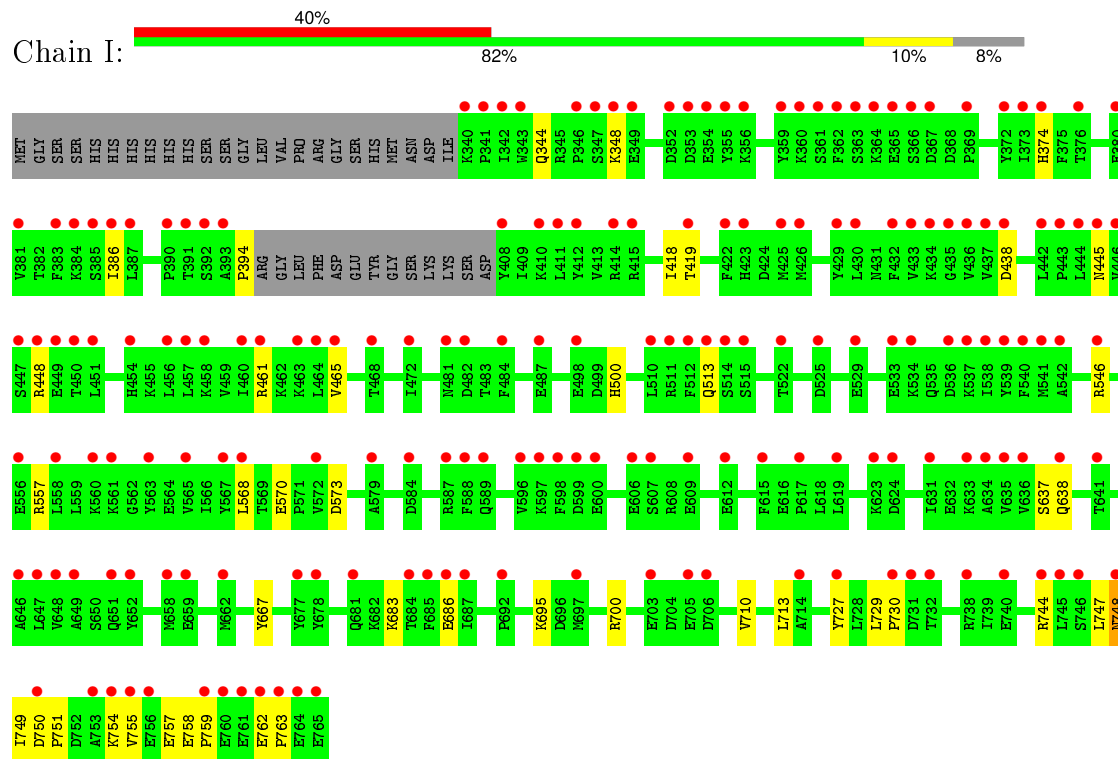


• Molecule 1: Endoplasmic

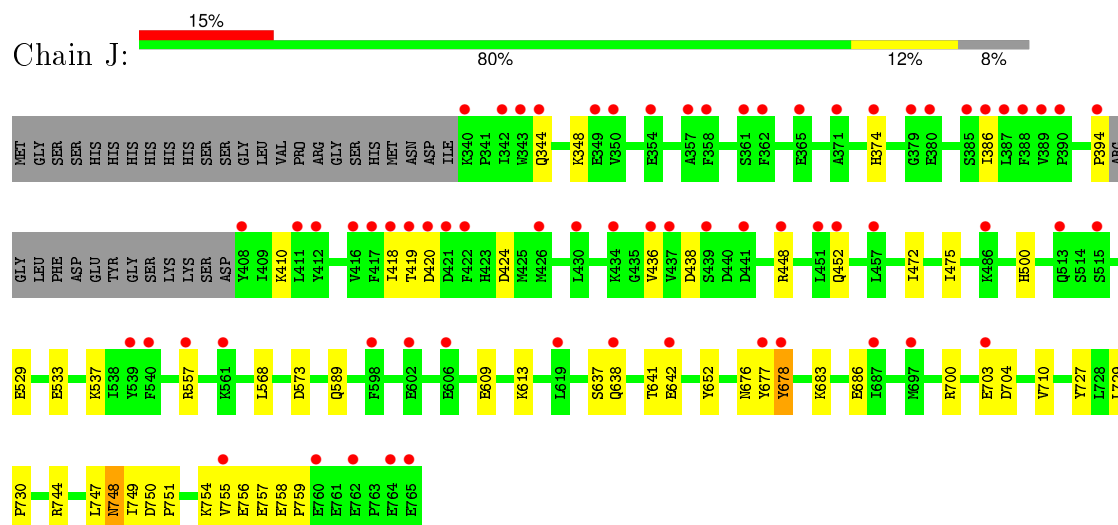




• Molecule 1: Endoplasmic



• Molecule 1: Endoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.30Å 129.54Å 184.78Å 90.00° 99.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 45.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.20) 99.6 (45.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.284 , 0.294 0.270 , 0.283	Depositor DCC
R_{free} test set	5004 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	109.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 163.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	2 of 100402 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33009	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	1/3368 (0.0%)	0.68	2/4543 (0.0%)
1	B	0.37	0/3368	0.61	1/4543 (0.0%)
1	C	0.42	0/3368	0.64	1/4543 (0.0%)
1	D	0.43	0/3368	0.64	1/4543 (0.0%)
1	E	0.53	0/3368	0.68	1/4543 (0.0%)
1	F	0.51	0/3368	0.66	1/4543 (0.0%)
1	G	0.43	0/3366	0.65	2/4540 (0.0%)
1	H	0.36	0/3368	0.61	1/4543 (0.0%)
1	I	0.35	0/3368	0.62	1/4543 (0.0%)
1	J	0.48	0/3368	0.65	1/4543 (0.0%)
All	All	0.45	1/33678 (0.0%)	0.64	12/45427 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	TYR	CA-CB	-6.37	1.40	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	394	PRO	N-CA-CB	7.79	112.64	103.30
1	B	394	PRO	N-CA-CB	7.39	112.16	103.30
1	E	394	PRO	N-CA-CB	7.35	112.12	103.30
1	A	394	PRO	N-CA-CB	7.34	112.11	103.30
1	J	394	PRO	N-CA-CB	7.33	112.10	103.30
1	G	394	PRO	N-CA-CB	7.29	112.05	103.30
1	C	394	PRO	N-CA-CB	7.24	111.99	103.30
1	H	394	PRO	N-CA-CB	7.23	111.98	103.30
1	D	394	PRO	N-CA-CB	7.11	111.83	103.30
1	I	394	PRO	N-CA-CB	7.01	111.72	103.30
1	G	618	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	618	LEU	CA-CB-CG	5.03	126.87	115.30

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	3301	0	3196	44	4
1	B	3301	0	3196	25	0
1	C	3301	0	3196	40	0
1	D	3301	0	3196	51	1
1	E	3301	0	3196	69	1
1	F	3301	0	3196	59	5
1	G	3300	0	3194	47	1
1	H	3301	0	3196	36	0
1	I	3301	0	3196	29	2
1	J	3301	0	3196	62	0
All	All	33009	0	31958	360	7

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 6.

All (360) 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:C:757:GLU:OE2	1:J:677:TYR:HA	1.21	1.31
1:E:500:HIS:CE1	1:J:704:ASP:HB2	1.80	1.16
1:D:759:PRO:HD3	1:E:692:PRO:HD3	1.38	1.05
1:A:754:LYS:HD3	1:E:678:TYR:OH	1.61	1.00
1:C:757:GLU:OE2	1:J:677:TYR:CA	2.11	0.98
1:A:750:ASP:CG	1:E:652:TYR:HB2	1.84	0.97
1:F:652:TYR:CE2	1:J:756:GLU:CD	2.40	0.95
1:E:500:HIS:NE2	1:J:703:GLU:HB3	1.83	0.93
1:D:743:LEU:HD22	1:E:713:LEU:HG	1.52	0.91
1:C:757:GLU:CD	1:J:677:TYR:HA	1.91	0.90
1:E:500:HIS:HE1	1:J:704:ASP:HB2	1.39	0.87
1:C:754:LYS:HD3	1:J:678:TYR:CD2	2.10	0.85
1:H:692:PRO:HB3	1:I:754:LYS:HE3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:743:LEU:HD22	1:G:713:LEU:HG	1.66	0.78
1:D:637:SER:HB2	1:D:686:GLU:HB3	1.66	0.78
1:F:637:SER:HB2	1:F:686:GLU:HB3	1.64	0.77
1:C:754:LYS:HD3	1:J:678:TYR:HD2	1.49	0.76
1:A:637:SER:HB2	1:A:686:GLU:HB3	1.68	0.75
1:I:637:SER:HB2	1:I:686:GLU:HB3	1.68	0.75
1:E:637:SER:HB2	1:E:686:GLU:HB3	1.68	0.75
1:H:637:SER:HB2	1:H:686:GLU:HB3	1.69	0.75
1:J:637:SER:HB2	1:J:686:GLU:HB3	1.69	0.74
1:B:637:SER:HB2	1:B:686:GLU:HB3	1.69	0.74
1:A:753:ALA:O	1:E:678:TYR:CE2	2.40	0.74
1:C:637:SER:HB2	1:C:686:GLU:HB3	1.69	0.73
1:D:758:GLU:HG3	1:E:695:LYS:HD3	1.73	0.71
1:A:642:GLU:HA	1:J:759:PRO:HB3	1.73	0.70
1:A:750:ASP:O	1:A:754:LYS:HB2	1.92	0.70
1:G:637:SER:HB2	1:G:686:GLU:HB3	1.74	0.69
1:C:750:ASP:O	1:C:754:LYS:HB2	1.92	0.69
1:E:750:ASP:O	1:E:754:LYS:HB2	1.93	0.68
1:D:750:ASP:HB3	1:D:754:LYS:HG2	1.75	0.68
1:A:750:ASP:CB	1:E:652:TYR:HB2	2.24	0.68
1:A:750:ASP:OD1	1:E:652:TYR:HB2	1.93	0.68
1:E:500:HIS:CD2	1:J:703:GLU:HB3	2.29	0.67
1:D:744:ARG:HG2	1:E:693:LEU:HD13	1.77	0.66
1:D:759:PRO:HD3	1:E:692:PRO:CD	2.22	0.65
1:F:740:GLU:OE2	1:G:691:HIS:NE2	2.28	0.65
1:D:742:MET:CE	1:E:742:MET:HE3	2.26	0.65
1:D:729:LEU:HD12	1:D:730:PRO:HD2	1.79	0.65
1:I:750:ASP:O	1:I:754:LYS:HB2	1.95	0.65
1:F:744:ARG:HD3	1:G:693:LEU:HB2	1.80	0.64
1:D:744:ARG:HD3	1:E:693:LEU:HB2	1.79	0.64
1:F:729:LEU:HD12	1:F:730:PRO:HD2	1.79	0.64
1:F:652:TYR:CE2	1:J:756:GLU:OE2	2.50	0.63
1:D:713:LEU:HG	1:E:743:LEU:HD22	1.81	0.63
1:F:717:LEU:HD13	1:G:743:LEU:HD13	1.81	0.63
1:A:753:ALA:O	1:E:678:TYR:CD2	2.52	0.62
1:C:748:ASN:O	1:J:652:TYR:CE1	2.52	0.62
1:J:729:LEU:HD12	1:J:730:PRO:HD2	1.79	0.62
1:B:729:LEU:HD12	1:B:730:PRO:HD2	1.83	0.61
1:C:757:GLU:CG	1:J:677:TYR:HA	2.30	0.61
1:A:690:ARG:O	1:J:758:GLU:HB3	2.00	0.61
1:H:750:ASP:HB3	1:H:754:LYS:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:750:ASP:O	1:G:754:LYS:HB2	2.00	0.61
1:A:750:ASP:HB3	1:A:754:LYS:HG2	1.82	0.61
1:F:374:HIS:HD2	1:F:386:ILE:HG12	1.65	0.61
1:H:729:LEU:HD12	1:H:730:PRO:HD2	1.83	0.61
1:C:750:ASP:HB3	1:C:754:LYS:HG2	1.83	0.60
1:D:744:ARG:NH2	1:D:755:VAL:HB	2.16	0.60
1:A:700:ARG:HD2	1:A:710:VAL:HG22	1.84	0.60
1:C:754:LYS:HD3	1:J:678:TYR:CE2	2.37	0.59
1:H:569:THR:O	1:I:667:TYR:OH	2.18	0.59
1:F:652:TYR:HE2	1:J:756:GLU:OE2	1.84	0.59
1:A:729:LEU:HD12	1:A:730:PRO:HD2	1.85	0.59
1:F:743:LEU:CD2	1:G:713:LEU:HG	2.32	0.59
1:A:642:GLU:HG2	1:J:759:PRO:HB2	1.85	0.58
1:H:374:HIS:HD2	1:H:386:ILE:HG12	1.68	0.58
1:B:374:HIS:HD2	1:B:386:ILE:HG12	1.67	0.58
1:E:500:HIS:CD2	1:E:500:HIS:H	2.20	0.58
1:F:691:HIS:HE1	1:G:744:ARG:HD3	1.67	0.58
1:C:700:ARG:HD2	1:C:710:VAL:HG22	1.84	0.58
1:D:692:PRO:HD3	1:E:758:GLU:HB2	1.86	0.58
1:F:742:MET:CE	1:G:742:MET:HE3	2.34	0.58
1:I:700:ARG:HD2	1:I:710:VAL:HG22	1.86	0.58
1:A:642:GLU:HG2	1:J:759:PRO:CB	2.33	0.57
1:G:683:LYS:HE3	1:G:727:TYR:CE1	2.38	0.57
1:A:418:ILE:HG22	1:A:419:THR:HG22	1.86	0.57
1:H:557:ARG:HD3	1:H:638:GLN:O	2.04	0.57
1:B:744:ARG:NH2	1:B:755:VAL:HB	2.20	0.57
1:I:729:LEU:HD12	1:I:730:PRO:HD2	1.85	0.57
1:D:374:HIS:HD2	1:D:386:ILE:HG12	1.70	0.57
1:F:557:ARG:HD3	1:F:638:GLN:O	2.05	0.56
1:G:700:ARG:HD2	1:G:710:VAL:HG22	1.88	0.56
1:G:729:LEU:HD12	1:G:730:PRO:HD2	1.88	0.56
1:C:344:GLN:NE2	1:C:438:ASP:OD2	2.37	0.56
1:I:750:ASP:HB3	1:I:754:LYS:HG2	1.87	0.56
1:J:744:ARG:NH2	1:J:755:VAL:HB	2.21	0.56
1:E:750:ASP:HB3	1:E:754:LYS:HG2	1.88	0.56
1:D:750:ASP:HB3	1:D:754:LYS:CG	2.36	0.56
1:D:557:ARG:HD3	1:D:638:GLN:O	2.05	0.56
1:C:757:GLU:OE2	1:J:676:ASN:O	2.25	0.55
1:J:374:HIS:HD2	1:J:386:ILE:HG12	1.69	0.55
1:B:557:ARG:HD3	1:B:638:GLN:O	2.06	0.55
1:F:743:LEU:HD13	1:G:717:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:344:GLN:NE2	1:I:438:ASP:OD2	2.38	0.55
1:G:750:ASP:HB3	1:G:754:LYS:HG2	1.89	0.55
1:F:742:MET:HE3	1:G:742:MET:CE	2.37	0.55
1:E:729:LEU:HD12	1:E:730:PRO:HD2	1.88	0.55
1:E:700:ARG:HD2	1:E:710:VAL:HG22	1.89	0.55
1:F:652:TYR:CD2	1:J:756:GLU:OE1	2.60	0.54
1:A:754:LYS:HD3	1:E:678:TYR:HH	1.68	0.54
1:F:652:TYR:CZ	1:J:756:GLU:HG2	2.43	0.54
1:H:744:ARG:NH2	1:H:755:VAL:HB	2.23	0.54
1:B:750:ASP:HB3	1:B:754:LYS:HG2	1.90	0.54
1:J:557:ARG:HD3	1:J:638:GLN:O	2.08	0.53
1:F:744:ARG:HG2	1:G:693:LEU:HD13	1.91	0.53
1:H:693:LEU:HD13	1:I:744:ARG:HG2	1.91	0.53
1:F:750:ASP:HB3	1:F:754:LYS:HG2	1.88	0.53
1:D:759:PRO:HA	1:E:690:ARG:O	2.08	0.53
1:F:742:MET:HE3	1:G:742:MET:HE1	1.91	0.53
1:A:344:GLN:NE2	1:A:438:ASP:OD2	2.38	0.53
1:D:742:MET:HE2	1:E:742:MET:CE	2.39	0.53
1:A:754:LYS:HD3	1:E:678:TYR:CZ	2.43	0.53
1:D:750:ASP:O	1:D:754:LYS:HB2	2.10	0.52
1:C:729:LEU:HD12	1:C:730:PRO:HD2	1.92	0.52
1:G:344:GLN:NE2	1:G:438:ASP:OD2	2.41	0.52
1:J:344:GLN:NE2	1:J:438:ASP:OD2	2.39	0.52
1:G:744:ARG:NH2	1:G:755:VAL:HB	2.24	0.52
1:H:467:LYS:HD3	1:J:529:GLU:OE2	2.10	0.52
1:A:570:GLU:HB2	1:A:573:ASP:CG	2.30	0.52
1:C:761:GLU:OE2	1:J:676:ASN:O	2.28	0.52
1:A:374:HIS:HD2	1:A:386:ILE:HG12	1.73	0.52
1:E:744:ARG:NH2	1:E:755:VAL:HB	2.25	0.52
1:E:570:GLU:HB2	1:E:573:ASP:CG	2.30	0.52
1:D:742:MET:HE3	1:E:742:MET:HE3	1.92	0.52
1:E:344:GLN:NE2	1:E:438:ASP:OD2	2.40	0.52
1:E:683:LYS:HE3	1:E:727:TYR:CE1	2.45	0.52
1:J:750:ASP:HB3	1:J:754:LYS:HG2	1.93	0.51
1:I:374:HIS:HD2	1:I:386:ILE:HG12	1.75	0.51
1:D:528:VAL:HA	1:D:531:MET:SD	2.50	0.51
1:C:500:HIS:CD2	1:C:500:HIS:H	2.29	0.51
1:D:759:PRO:HG3	1:E:692:PRO:HD2	1.92	0.51
1:A:750:ASP:HB2	1:E:652:TYR:HB2	1.92	0.51
1:F:374:HIS:CD2	1:F:386:ILE:HG12	2.46	0.50
1:F:744:ARG:NH2	1:F:755:VAL:HB	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:742:MET:HE1	1:G:742:MET:HE3	1.92	0.50
1:I:570:GLU:HB2	1:I:573:ASP:CG	2.31	0.50
1:F:424:ASP:CG	1:F:452:GLN:HE21	2.15	0.50
1:I:744:ARG:NH2	1:I:755:VAL:HB	2.27	0.50
1:A:500:HIS:H	1:A:500:HIS:CD2	2.28	0.50
1:G:374:HIS:HD2	1:G:386:ILE:HG12	1.77	0.50
1:D:742:MET:HE2	1:E:742:MET:HE3	1.92	0.50
1:H:374:HIS:CD2	1:H:386:ILE:HG12	2.47	0.50
1:I:557:ARG:HD3	1:I:638:GLN:O	2.11	0.50
1:F:414:ARG:O	1:F:415:ARG:HB2	2.12	0.50
1:C:557:ARG:HD3	1:C:638:GLN:O	2.11	0.49
1:H:380:GLU:CD	1:J:533:GLU:HB2	2.33	0.49
1:F:700:ARG:HD2	1:F:710:VAL:HG22	1.94	0.49
1:E:374:HIS:HD2	1:E:386:ILE:HG12	1.77	0.49
1:C:744:ARG:NH2	1:C:755:VAL:HB	2.26	0.49
1:H:692:PRO:HB3	1:I:754:LYS:CE	2.40	0.49
1:G:570:GLU:HB2	1:G:573:ASP:CG	2.32	0.49
1:H:750:ASP:O	1:H:754:LYS:HB2	2.12	0.49
1:F:472:ILE:O	1:F:475:ILE:HG12	2.13	0.49
1:F:652:TYR:CD2	1:J:756:GLU:CD	2.86	0.49
1:F:742:MET:CE	1:G:742:MET:CE	2.90	0.49
1:C:418:ILE:HG22	1:C:419:THR:HG22	1.95	0.49
1:H:344:GLN:NE2	1:H:438:ASP:OD2	2.43	0.49
1:F:683:LYS:HE3	1:F:727:TYR:CE1	2.48	0.48
1:A:750:ASP:HB2	1:E:652:TYR:CB	2.44	0.48
1:C:374:HIS:HD2	1:C:386:ILE:HG12	1.78	0.48
1:C:757:GLU:HG2	1:J:677:TYR:CA	2.44	0.48
1:F:691:HIS:CE1	1:G:744:ARG:HD3	2.47	0.48
1:B:344:GLN:NE2	1:B:438:ASP:OD2	2.41	0.48
1:H:743:LEU:HD22	1:I:713:LEU:HG	1.94	0.48
1:E:418:ILE:HG22	1:E:419:THR:HG22	1.94	0.48
1:J:754:LYS:C	1:J:756:GLU:H	2.16	0.48
1:F:652:TYR:CE2	1:J:756:GLU:CG	2.97	0.48
1:G:557:ARG:HD3	1:G:638:GLN:O	2.13	0.48
1:D:742:MET:CE	1:E:742:MET:CE	2.91	0.48
1:D:472:ILE:O	1:D:475:ILE:HG12	2.14	0.48
1:F:537:LYS:HE2	1:F:589:GLN:HB2	1.96	0.48
1:F:700:ARG:HD2	1:F:710:VAL:CG2	2.44	0.48
1:I:418:ILE:HG22	1:I:419:THR:HG22	1.95	0.48
1:D:739:ILE:HD12	1:E:739:ILE:HD12	1.96	0.48
1:F:750:ASP:O	1:F:754:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:750:ASP:HB3	1:H:754:LYS:CG	2.44	0.47
1:G:418:ILE:HG22	1:G:419:THR:HG22	1.96	0.47
1:E:552:SER:OG	1:E:554:PHE:HD1	1.97	0.47
1:D:759:PRO:CD	1:E:692:PRO:HD3	2.27	0.47
1:C:700:ARG:HD2	1:C:710:VAL:CG2	2.43	0.47
1:I:700:ARG:HD2	1:I:710:VAL:CG2	2.44	0.47
1:A:700:ARG:HD2	1:A:710:VAL:CG2	2.44	0.47
1:C:747:LEU:O	1:C:748:ASN:CB	2.62	0.47
1:A:744:ARG:NH2	1:A:755:VAL:HB	2.30	0.47
1:I:500:HIS:H	1:I:500:HIS:CD2	2.32	0.47
1:E:461:ARG:O	1:E:465:VAL:HG23	2.15	0.47
1:F:644:PRO:HD3	1:G:740:GLU:OE2	2.14	0.47
1:E:700:ARG:HD2	1:E:710:VAL:CG2	2.45	0.47
1:B:750:ASP:O	1:B:754:LYS:HB2	2.15	0.47
1:D:344:GLN:NE2	1:D:438:ASP:OD2	2.41	0.47
1:J:472:ILE:O	1:J:475:ILE:HG12	2.15	0.47
1:E:557:ARG:HD3	1:E:638:GLN:O	2.15	0.47
1:A:461:ARG:O	1:A:465:VAL:HG23	2.15	0.47
1:I:461:ARG:O	1:I:465:VAL:HG23	2.15	0.47
1:B:759:PRO:HB3	1:C:642:GLU:HA	1.97	0.46
1:B:374:HIS:CD2	1:B:386:ILE:HG12	2.48	0.46
1:F:693:LEU:HD13	1:G:744:ARG:HG2	1.97	0.46
1:H:424:ASP:CG	1:H:452:GLN:HE21	2.19	0.46
1:C:570:GLU:HB2	1:C:573:ASP:CG	2.35	0.46
1:E:500:HIS:CD2	1:J:703:GLU:OE1	2.68	0.46
1:G:700:ARG:HD2	1:G:710:VAL:CG2	2.46	0.46
1:J:641:THR:HG22	1:J:642:GLU:HG3	1.97	0.46
1:B:683:LYS:HE3	1:B:727:TYR:CE1	2.51	0.46
1:B:700:ARG:HD2	1:B:710:VAL:HG22	1.97	0.46
1:H:692:PRO:HD3	1:I:758:GLU:HB2	1.97	0.46
1:B:609:GLU:O	1:B:613:LYS:HD3	2.15	0.46
1:G:461:ARG:O	1:G:465:VAL:HG23	2.16	0.46
1:F:754:LYS:C	1:F:756:GLU:H	2.18	0.46
1:C:757:GLU:HG2	1:J:677:TYR:CB	2.46	0.46
1:H:700:ARG:HD2	1:H:710:VAL:HG22	1.98	0.45
1:H:472:ILE:O	1:H:475:ILE:HG12	2.16	0.45
1:J:348:LYS:HB2	1:J:348:LYS:HE3	1.73	0.45
1:C:568:LEU:HB3	1:C:573:ASP:HB3	1.98	0.45
1:F:344:GLN:NE2	1:F:438:ASP:OD2	2.43	0.45
1:C:748:ASN:O	1:J:652:TYR:CD1	2.70	0.45
1:A:557:ARG:HD3	1:A:638:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:GLU:N	1:C:759:PRO:CD	2.80	0.45
1:H:609:GLU:O	1:H:613:LYS:HD3	2.17	0.45
1:I:683:LYS:HE3	1:I:727:TYR:CE1	2.51	0.45
1:C:683:LYS:HE3	1:C:727:TYR:CE1	2.51	0.45
1:J:424:ASP:CG	1:J:452:GLN:HE21	2.20	0.45
1:F:609:GLU:O	1:F:613:LYS:HD3	2.17	0.45
1:F:410:LYS:HB2	1:F:436:VAL:HG12	1.99	0.45
1:E:747:LEU:O	1:E:748:ASN:CB	2.64	0.45
1:D:754:LYS:C	1:D:756:GLU:H	2.19	0.45
1:B:700:ARG:HD2	1:B:710:VAL:CG2	2.47	0.45
1:D:759:PRO:HG3	1:E:691:HIS:HA	1.98	0.45
1:C:754:LYS:CE	1:J:678:TYR:HE2	2.30	0.45
1:I:568:LEU:HB3	1:I:573:ASP:HB3	1.98	0.45
1:A:374:HIS:CD2	1:A:386:ILE:HG12	2.51	0.45
1:A:758:GLU:N	1:A:759:PRO:CD	2.80	0.45
1:E:695:LYS:HE2	1:E:695:LYS:HB3	1.79	0.44
1:H:537:LYS:HE2	1:H:589:GLN:HB2	1.99	0.44
1:F:528:VAL:HA	1:F:531:MET:SD	2.57	0.44
1:A:750:ASP:OD1	1:A:753:ALA:HB3	2.17	0.44
1:G:568:LEU:HB3	1:G:573:ASP:HB3	2.00	0.44
1:H:641:THR:HG22	1:H:642:GLU:HG3	1.99	0.44
1:D:568:LEU:HB3	1:D:573:ASP:HB3	1.99	0.44
1:D:374:HIS:CD2	1:D:386:ILE:HG12	2.50	0.44
1:F:568:LEU:HB3	1:F:573:ASP:HB3	2.00	0.44
1:G:758:GLU:N	1:G:759:PRO:CD	2.81	0.44
1:F:754:LYS:HB3	1:G:692:PRO:HB3	1.99	0.44
1:H:700:ARG:HD2	1:H:710:VAL:CG2	2.48	0.44
1:H:528:VAL:HA	1:H:531:MET:SD	2.57	0.44
1:B:754:LYS:C	1:B:756:GLU:H	2.21	0.44
1:F:641:THR:HG22	1:F:642:GLU:HG3	2.00	0.44
1:F:691:HIS:HA	1:F:692:PRO:HD2	1.78	0.44
1:J:374:HIS:CD2	1:J:386:ILE:HG12	2.50	0.44
1:D:348:LYS:HE3	1:D:348:LYS:HB2	1.71	0.44
1:F:750:ASP:HB3	1:F:754:LYS:CG	2.48	0.43
1:H:348:LYS:HE3	1:H:348:LYS:HB2	1.74	0.43
1:F:418:ILE:HG22	1:F:419:THR:HG22	2.00	0.43
1:D:759:PRO:CG	1:E:692:PRO:HD2	2.48	0.43
1:J:410:LYS:HB2	1:J:436:VAL:HG12	2.00	0.43
1:J:537:LYS:HE2	1:J:589:GLN:HB2	2.00	0.43
1:I:747:LEU:O	1:I:748:ASN:CB	2.66	0.43
1:B:641:THR:HG22	1:B:642:GLU:HG3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:GLN:HB3	1:C:546:ARG:NH1	2.33	0.43
1:E:374:HIS:CD2	1:E:386:ILE:HG12	2.53	0.43
1:B:472:ILE:O	1:B:475:ILE:HG12	2.18	0.43
1:A:757:GLU:HB2	1:E:677:TYR:CB	2.49	0.43
1:B:691:HIS:HA	1:B:692:PRO:HD2	1.80	0.43
1:D:691:HIS:HA	1:D:692:PRO:HD2	1.79	0.43
1:H:380:GLU:OE1	1:J:533:GLU:HB2	2.19	0.43
1:D:424:ASP:CG	1:D:452:GLN:HE21	2.22	0.43
1:B:537:LYS:HE2	1:B:589:GLN:HB2	2.01	0.43
1:H:754:LYS:C	1:H:756:GLU:H	2.21	0.43
1:I:374:HIS:CD2	1:I:386:ILE:HG12	2.53	0.43
1:C:517:HIS:HA	1:C:518:PRO:HD2	1.78	0.43
1:J:609:GLU:O	1:J:613:LYS:HD3	2.19	0.43
1:B:348:LYS:HB2	1:B:348:LYS:HE3	1.76	0.43
1:D:729:LEU:HA	1:D:730:PRO:HD2	1.85	0.43
1:B:410:LYS:HB2	1:B:436:VAL:HG12	1.99	0.43
1:H:602:GLU:O	1:H:606:GLU:HG3	2.19	0.43
1:J:500:HIS:CD2	1:J:500:HIS:H	2.37	0.42
1:D:758:GLU:N	1:D:759:PRO:CD	2.82	0.42
1:F:492:ILE:O	1:F:496:VAL:HG23	2.19	0.42
1:C:472:ILE:O	1:C:475:ILE:HG12	2.20	0.42
1:D:755:VAL:HA	1:E:692:PRO:HG3	2.00	0.42
1:F:693:LEU:HB2	1:G:744:ARG:HD3	1.99	0.42
1:H:463:LYS:NZ	1:J:529:GLU:O	2.53	0.42
1:D:418:ILE:HG22	1:D:419:THR:HG22	2.01	0.42
1:D:410:LYS:HB2	1:D:436:VAL:HG12	2.01	0.42
1:G:500:HIS:H	1:G:500:HIS:CD2	2.36	0.42
1:A:729:LEU:HA	1:A:730:PRO:HD2	1.81	0.42
1:A:568:LEU:HB3	1:A:573:ASP:HB3	2.00	0.42
1:E:568:LEU:HB3	1:E:573:ASP:HB3	2.01	0.42
1:G:374:HIS:CD2	1:G:386:ILE:HG12	2.55	0.42
1:C:729:LEU:HA	1:C:730:PRO:HD2	1.80	0.42
1:J:683:LYS:HE3	1:J:727:TYR:CE1	2.54	0.42
1:B:750:ASP:HB3	1:B:754:LYS:CG	2.50	0.42
1:H:410:LYS:HB2	1:H:436:VAL:HG12	2.02	0.42
1:G:633:LYS:HG3	1:G:684:THR:HG23	2.01	0.42
1:C:552:SER:HA	1:C:553:PRO:HD3	1.94	0.42
1:A:750:ASP:HB3	1:A:754:LYS:CG	2.49	0.42
1:J:747:LEU:O	1:J:748:ASN:CB	2.68	0.42
1:A:527:TYR:CE2	1:A:538:ILE:HG23	2.54	0.42
1:A:642:GLU:HG2	1:J:759:PRO:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:MET:SD	1:E:743:LEU:HD23	2.60	0.42
1:C:374:HIS:CD2	1:C:386:ILE:HG12	2.55	0.42
1:E:758:GLU:N	1:E:759:PRO:CD	2.83	0.42
1:J:418:ILE:HG22	1:J:419:THR:HG22	2.01	0.42
1:I:348:LYS:HE3	1:I:348:LYS:HB2	1.90	0.42
1:F:517:HIS:HA	1:F:518:PRO:HD2	1.87	0.42
1:F:747:LEU:O	1:F:748:ASN:CB	2.67	0.42
1:A:747:LEU:O	1:A:748:ASN:CB	2.68	0.42
1:C:754:LYS:HZ3	1:J:678:TYR:HE2	1.62	0.41
1:F:692:PRO:HG3	1:G:754:LYS:HB3	2.02	0.41
1:E:633:LYS:HG3	1:E:684:THR:HG23	2.02	0.41
1:B:424:ASP:CG	1:B:452:GLN:HE21	2.23	0.41
1:F:590:ASN:HD22	1:F:593:LYS:HE3	1.85	0.41
1:C:757:GLU:CG	1:J:677:TYR:CA	2.98	0.41
1:G:747:LEU:O	1:G:748:ASN:CB	2.67	0.41
1:I:758:GLU:N	1:I:759:PRO:CD	2.83	0.41
1:A:513:GLN:HB3	1:A:546:ARG:NH1	2.35	0.41
1:G:695:LYS:HE2	1:G:695:LYS:HB3	1.88	0.41
1:D:641:THR:HG22	1:D:642:GLU:HG3	2.02	0.41
1:A:754:LYS:C	1:A:756:GLU:N	2.74	0.41
1:J:750:ASP:O	1:J:754:LYS:HB2	2.20	0.41
1:J:758:GLU:N	1:J:759:PRO:CD	2.82	0.41
1:J:700:ARG:HD2	1:J:710:VAL:HG22	2.02	0.41
1:G:527:TYR:CE2	1:G:538:ILE:HG23	2.55	0.41
1:D:759:PRO:CA	1:E:690:ARG:O	2.68	0.41
1:B:758:GLU:N	1:B:759:PRO:CD	2.84	0.41
1:A:472:ILE:O	1:A:475:ILE:HG12	2.20	0.41
1:A:762:GLU:N	1:A:763:PRO:CD	2.84	0.41
1:A:570:GLU:HB2	1:A:573:ASP:OD2	2.21	0.41
1:F:642:GLU:HA	1:G:759:PRO:HB3	2.03	0.41
1:D:700:ARG:HD2	1:D:710:VAL:CG2	2.50	0.41
1:D:765:GLU:O	1:E:604:THR:HG23	2.21	0.41
1:F:744:ARG:CD	1:G:693:LEU:HB2	2.50	0.41
1:G:552:SER:OG	1:G:554:PHE:HD1	2.04	0.41
1:H:747:LEU:O	1:H:748:ASN:CB	2.68	0.41
1:D:537:LYS:HE2	1:D:589:GLN:HB2	2.01	0.41
1:B:747:LEU:O	1:B:748:ASN:CB	2.68	0.41
1:G:597:LYS:HE3	1:G:597:LYS:HB2	1.94	0.41
1:E:524:LEU:HD23	1:E:524:LEU:HA	1.87	0.41
1:E:511:ARG:HA	1:E:511:ARG:HD3	1.97	0.41
1:J:568:LEU:HB3	1:J:573:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:762:GLU:N	1:I:763:PRO:CD	2.84	0.41
1:H:683:LYS:HE3	1:H:727:TYR:CE1	2.55	0.41
1:G:762:GLU:N	1:G:763:PRO:CD	2.84	0.41
1:E:348:LYS:HB2	1:E:348:LYS:HE3	1.91	0.41
1:A:750:ASP:CB	1:E:652:TYR:CB	2.95	0.41
1:I:695:LYS:HE2	1:I:695:LYS:HB3	1.87	0.40
1:F:691:HIS:NE2	1:G:740:GLU:OE2	2.54	0.40
1:E:729:LEU:HA	1:E:730:PRO:HD2	1.79	0.40
1:E:609:GLU:O	1:E:613:LYS:HD3	2.22	0.40
1:F:602:GLU:O	1:F:606:GLU:HG3	2.21	0.40
1:H:570:GLU:HB2	1:H:573:ASP:CG	2.41	0.40
1:H:627:LEU:HB3	1:H:630:LYS:HB2	2.03	0.40
1:D:552:SER:HA	1:D:553:PRO:HD3	1.96	0.40
1:E:500:HIS:N	1:E:500:HIS:CD2	2.85	0.40
1:E:500:HIS:ND1	1:J:704:ASP:HB2	2.28	0.40
1:D:700:ARG:HD2	1:D:710:VAL:HG22	2.02	0.40
1:I:513:GLN:HB3	1:I:546:ARG:NH1	2.36	0.40
1:D:609:GLU:O	1:D:613:LYS:HD3	2.21	0.40
1:D:747:LEU:O	1:D:748:ASN:CB	2.70	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:753:ALA:O	1:G:652:TYR:OH[1_455]	1.62	0.58
1:A:677:TYR:CB	1:D:757:GLU:OE1[2_655]	1.73	0.47
1:F:699:ARG:NH2	1:I:445:ASN:O[1_655]	1.74	0.46
1:A:445:ASN:ND2	1:F:412:TYR:CD1[1_565]	1.91	0.29
1:F:696:ASP:OD2	1:I:445:ASN:ND2[1_655]	2.03	0.17
1:A:445:ASN:O	1:F:415:ARG:O[1_565]	2.07	0.13
1:A:445:ASN:OD1	1:F:343:TRP:CZ2[1_565]	2.17	0.03

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	409/450 (91%)	361 (88%)	44 (11%)	4 (1%)	19	65
1	B	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	16	60
1	C	409/450 (91%)	365 (89%)	40 (10%)	4 (1%)	19	65
1	D	409/450 (91%)	368 (90%)	35 (9%)	6 (2%)	13	55
1	E	409/450 (91%)	357 (87%)	47 (12%)	5 (1%)	16	60
1	F	409/450 (91%)	365 (89%)	36 (9%)	8 (2%)	9	48
1	G	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	19	65
1	H	409/450 (91%)	367 (90%)	36 (9%)	6 (2%)	13	55
1	I	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	19	65
1	J	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	16	60
All	All	4090/4500 (91%)	3637 (89%)	402 (10%)	51 (1%)	16	60

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	ILE
1	C	749	ILE
1	D	757	GLU
1	E	749	ILE
1	I	749	ILE
1	A	748	ASN
1	B	748	ASN
1	B	749	ILE
1	B	757	GLU
1	C	748	ASN
1	D	748	ASN
1	D	749	ILE
1	E	748	ASN
1	E	757	GLU
1	F	748	ASN
1	F	749	ILE
1	F	757	GLU
1	G	748	ASN
1	G	749	ILE
1	G	757	GLU
1	H	748	ASN
1	H	749	ILE

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Mol	Chain	Res	Type
1	H	757	GLU
1	I	748	ASN
1	I	757	GLU
1	J	748	ASN
1	J	749	ILE
1	J	757	GLU
1	A	751	PRO
1	A	757	GLU
1	C	751	PRO
1	C	757	GLU
1	E	751	PRO
1	G	751	PRO
1	I	751	PRO
1	F	420	ASP
1	J	420	ASP
1	B	676	ASN
1	D	420	ASP
1	D	751	PRO
1	E	746	SER
1	F	419	THR
1	F	676	ASN
1	F	751	PRO
1	H	420	ASP
1	H	676	ASN
1	B	751	PRO
1	D	676	ASN
1	H	751	PRO
1	J	751	PRO
1	F	581	PRO

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	352/410 (86%)	349 (99%)	3 (1%)	84	95
1	B	352/410 (86%)	351 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	352/410 (86%)	350 (99%)	2 (1%)	90	97
1	D	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	E	352/410 (86%)	349 (99%)	3 (1%)	84	95
1	F	352/410 (86%)	350 (99%)	2 (1%)	90	97
1	G	352/410 (86%)	350 (99%)	2 (1%)	90	97
1	H	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	I	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	J	352/410 (86%)	350 (99%)	2 (1%)	90	97
All	All	3520/4100 (86%)	3502 (100%)	18 (0%)	92	97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	448	ARG
1	A	652	TYR
1	B	448	ARG
1	C	448	ARG
1	C	652	TYR
1	D	448	ARG
1	E	448	ARG
1	E	652	TYR
1	E	760	GLU
1	F	448	ARG
1	F	491	ASN
1	G	448	ARG
1	G	652	TYR
1	H	448	ARG
1	I	448	ARG
1	J	448	ARG
1	J	678	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	452	GLN
1	D	452	GLN
1	E	500	HIS

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Mol	Chain	Res	Type
1	F	452	GLN
1	H	452	GLN
1	J	452	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	413/450 (91%)	0.92	56 (13%) 4 2	129, 151, 152, 165	0
1	B	413/450 (91%)	1.59	114 (27%) 1 0	129, 151, 152, 165	0
1	C	413/450 (91%)	0.99	65 (15%) 3 2	129, 151, 152, 165	0
1	D	413/450 (91%)	1.27	94 (22%) 1 1	129, 151, 152, 165	0
1	E	413/450 (91%)	1.07	58 (14%) 4 2	129, 151, 152, 165	0
1	F	413/450 (91%)	0.92	59 (14%) 4 2	129, 151, 152, 165	0
1	G	413/450 (91%)	1.58	107 (25%) 1 0	129, 151, 152, 165	0
1	H	413/450 (91%)	1.86	150 (36%) 0 0	129, 151, 152, 165	0
1	I	413/450 (91%)	2.74	182 (44%) 0 0	129, 151, 152, 165	0
1	J	413/450 (91%)	0.93	67 (16%) 3 2	129, 151, 152, 165	0
All	All	4130/4500 (91%)	1.39	952 (23%) 1 1	129, 151, 153, 165	0

All (952) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	443	PRO	23.3
1	I	443	PRO	22.2
1	I	437	VAL	19.2
1	I	392	SER	18.2
1	D	765	GLU	17.5
1	I	363	SER	16.3
1	I	364	LYS	16.1
1	E	753	ALA	15.3
1	I	444	LEU	14.8
1	I	386	ILE	14.7
1	G	347	SER	14.4
1	I	651	GLN	14.3
1	I	387	LEU	14.1

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Mol	Chain	Res	Type	RSRZ
1	I	755	VAL	13.5
1	A	758	GLU	13.5
1	D	366	SER	13.0
1	I	447	SER	12.9
1	I	436	VAL	12.7
1	I	449	GLU	12.4
1	C	755	VAL	12.4
1	G	600	GLU	12.3
1	I	457	LEU	12.2
1	I	349	GLU	12.1
1	H	697	MET	12.1
1	B	759	PRO	11.8
1	I	765	GLU	11.7
1	I	442	LEU	11.6
1	I	634	ALA	11.5
1	E	342	ILE	11.5
1	G	448	ARG	11.2
1	I	446	VAL	11.2
1	I	764	GLU	11.1
1	G	381	VAL	11.1
1	D	755	VAL	11.0
1	B	599	ASP	10.8
1	G	375	PHE	10.7
1	D	762	GLU	10.7
1	A	765	GLU	10.2
1	H	757	GLU	10.2
1	H	760	GLU	9.9
1	G	388	PHE	9.9
1	H	761	GLU	9.9
1	H	753	ALA	9.9
1	D	411	LEU	9.9
1	B	388	PHE	9.8
1	H	598	PHE	9.7
1	D	443	PRO	9.7
1	E	452	GLN	9.7
1	H	638	GLN	9.6
1	I	677	TYR	9.5
1	I	450	THR	9.5
1	H	436	VAL	9.4
1	I	468	THR	9.0
1	B	436	VAL	9.0
1	I	635	VAL	9.0

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Mol	Chain	Res	Type	RSRZ
1	I	763	PRO	8.9
1	A	759	PRO	8.9
1	B	435	GLY	8.8
1	B	755	VAL	8.8
1	B	600	GLU	8.7
1	G	433	VAL	8.5
1	H	619	LEU	8.5
1	E	757	GLU	8.5
1	E	763	PRO	8.5
1	I	445	ASN	8.4
1	A	341	PRO	8.4
1	B	762	GLU	8.3
1	C	435	GLY	8.3
1	D	437	VAL	8.2
1	I	746	SER	8.2
1	D	388	PHE	8.2
1	G	451	LEU	8.1
1	D	753	ALA	8.1
1	E	366	SER	8.1
1	H	597	LYS	8.0
1	J	765	GLU	8.0
1	I	600	GLU	7.8
1	I	366	SER	7.8
1	G	446	VAL	7.8
1	E	380	GLU	7.7
1	B	765	GLU	7.7
1	F	754	LYS	7.7
1	G	370	MET	7.6
1	H	622	MET	7.6
1	J	390	PRO	7.6
1	B	760	GLU	7.6
1	F	753	ALA	7.5
1	H	758	GLU	7.5
1	J	451	LEU	7.5
1	G	368	ASP	7.4
1	G	444	LEU	7.4
1	H	358	PHE	7.3
1	I	385	SER	7.2
1	H	617	PRO	7.2
1	I	373	ILE	7.2
1	D	678	TYR	7.2
1	D	367	ASP	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	437	VAL	7.1
1	H	678	TYR	7.0
1	B	608	ARG	7.0
1	A	340	LYS	7.0
1	G	604	THR	7.0
1	G	454	HIS	7.0
1	I	646	ALA	7.0
1	G	442	LEU	7.0
1	D	754	LYS	7.0
1	H	704	ASP	6.9
1	H	765	GLU	6.8
1	B	646	ALA	6.8
1	C	388	PHE	6.8
1	C	765	GLU	6.8
1	I	510	LEU	6.8
1	B	363	SER	6.8
1	B	359	TYR	6.6
1	G	765	GLU	6.6
1	I	411	LEU	6.5
1	G	411	LEU	6.5
1	B	386	ILE	6.5
1	C	714	ALA	6.4
1	H	675	THR	6.4
1	I	456	LEU	6.4
1	E	754	LYS	6.4
1	I	341	PRO	6.4
1	I	464	LEU	6.4
1	E	451	LEU	6.4
1	I	754	LYS	6.4
1	E	341	PRO	6.3
1	B	423	HIS	6.3
1	I	362	PHE	6.3
1	F	760	GLU	6.3
1	J	760	GLU	6.3
1	I	759	PRO	6.3
1	C	760	GLU	6.3
1	I	448	ARG	6.2
1	I	356	LYS	6.2
1	H	613	LYS	6.2
1	I	342	ILE	6.2
1	G	421	ASP	6.2
1	F	761	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	I	451	LEU	6.1
1	I	391	THR	6.1
1	B	679	ALA	6.1
1	C	764	GLU	6.1
1	F	599	ASP	6.1
1	F	435	GLY	6.1
1	A	764	GLU	6.1
1	I	414	ARG	6.1
1	H	730	PRO	6.0
1	G	374	HIS	6.0
1	H	606	GLU	6.0
1	B	442	LEU	6.0
1	F	451	LEU	6.0
1	I	624	ASP	6.0
1	G	458	LYS	5.9
1	G	380	GLU	5.9
1	A	444	LEU	5.9
1	H	615	PHE	5.9
1	D	451	LEU	5.8
1	I	684	THR	5.8
1	I	433	VAL	5.8
1	I	393	ALA	5.8
1	I	619	LEU	5.8
1	D	342	ILE	5.8
1	G	356	LYS	5.8
1	F	764	GLU	5.8
1	H	645	CYS	5.7
1	E	762	GLU	5.7
1	D	758	GLU	5.7
1	I	454	HIS	5.7
1	I	352	ASP	5.6
1	D	447	SER	5.6
1	B	725	SER	5.6
1	D	436	VAL	5.6
1	G	596	VAL	5.6
1	B	451	LEU	5.6
1	I	355	TYR	5.6
1	I	422	PHE	5.6
1	I	658	MET	5.5
1	I	340	LYS	5.5
1	B	364	LYS	5.5
1	F	757	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	H	592	ALA	5.5
1	H	553	PRO	5.4
1	E	764	GLU	5.4
1	H	612	GLU	5.4
1	G	366	SER	5.4
1	C	697	MET	5.4
1	J	358	PHE	5.4
1	C	434	LYS	5.4
1	H	589	GLN	5.3
1	I	745	LEU	5.3
1	A	342	ILE	5.3
1	A	760	GLU	5.3
1	C	762	GLU	5.3
1	D	600	GLU	5.3
1	I	435	GLY	5.3
1	C	599	ASP	5.3
1	H	648	VAL	5.3
1	I	687	ILE	5.2
1	I	514	SER	5.2
1	F	765	GLU	5.2
1	J	380	GLU	5.2
1	H	752	ASP	5.2
1	A	600	GLU	5.2
1	I	761	GLU	5.1
1	H	654	TRP	5.1
1	H	688	ASN	5.1
1	C	694	ILE	5.1
1	G	606	GLU	5.1
1	B	369	PRO	5.1
1	I	360	LYS	5.1
1	G	389	VAL	5.1
1	H	604	THR	5.1
1	J	437	VAL	5.1
1	G	419	THR	5.0
1	I	408	TYR	5.0
1	B	389	VAL	5.0
1	F	755	VAL	5.0
1	D	422	PHE	5.0
1	I	612	GLU	5.0
1	I	354	GLU	5.0
1	J	606	GLU	5.0
1	A	422	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	755	VAL	5.0
1	E	367	ASP	4.9
1	F	678	TYR	4.9
1	I	419	THR	4.9
1	G	492	ILE	4.9
1	I	686	GLU	4.9
1	B	358	PHE	4.9
1	H	759	PRO	4.9
1	H	413	VAL	4.9
1	B	340	LYS	4.9
1	B	422	PHE	4.9
1	F	340	LYS	4.9
1	I	347	SER	4.9
1	I	460	ILE	4.9
1	H	516	HIS	4.9
1	I	560	LYS	4.9
1	J	762	GLU	4.8
1	J	418	ILE	4.8
1	G	450	THR	4.8
1	E	746	SER	4.8
1	D	361	SER	4.8
1	H	632	GLU	4.8
1	H	691	HIS	4.7
1	B	757	GLU	4.7
1	G	598	PHE	4.7
1	G	376	THR	4.7
1	E	350	VAL	4.7
1	F	361	SER	4.7
1	I	659	GLU	4.7
1	I	648	VAL	4.7
1	A	445	ASN	4.7
1	I	434	LYS	4.7
1	F	342	ILE	4.7
1	F	422	PHE	4.7
1	G	599	ASP	4.7
1	A	753	ALA	4.7
1	I	458	LYS	4.7
1	G	447	SER	4.6
1	F	394	PRO	4.6
1	J	408	TYR	4.6
1	E	444	LEU	4.6
1	I	730	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	340	LYS	4.6
1	A	604	THR	4.6
1	J	349	GLU	4.6
1	G	360	LYS	4.6
1	H	762	GLU	4.6
1	H	422	PHE	4.6
1	I	541	MET	4.5
1	I	461	ARG	4.5
1	I	384	LYS	4.5
1	F	600	GLU	4.5
1	I	498	GLU	4.5
1	I	617	PRO	4.5
1	F	752	ASP	4.5
1	G	533	GLU	4.5
1	G	559	LEU	4.5
1	I	372	TYR	4.5
1	H	554	PHE	4.5
1	B	758	GLU	4.5
1	I	374	HIS	4.5
1	H	540	PHE	4.5
1	I	415	ARG	4.5
1	H	764	GLU	4.4
1	G	386	ILE	4.4
1	B	589	GLN	4.4
1	D	764	GLU	4.4
1	G	385	SER	4.4
1	I	762	GLU	4.4
1	I	511	ARG	4.4
1	I	598	PHE	4.4
1	H	683	LYS	4.4
1	B	380	GLU	4.4
1	I	538	ILE	4.4
1	D	634	ALA	4.4
1	H	591	VAL	4.4
1	E	388	PHE	4.4
1	A	392	SER	4.4
1	I	705	GLU	4.4
1	J	357	ALA	4.4
1	H	672	ASP	4.4
1	I	756	GLU	4.4
1	F	607	SER	4.4
1	A	697	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	750	ASP	4.3
1	H	374	HIS	4.3
1	B	365	GLU	4.3
1	E	674	SER	4.3
1	D	446	VAL	4.3
1	B	604	THR	4.3
1	I	348	LYS	4.3
1	A	366	SER	4.3
1	I	678	TYR	4.3
1	B	712	ASP	4.3
1	F	762	GLU	4.3
1	H	689	PRO	4.2
1	C	629	ASP	4.2
1	H	623	LYS	4.2
1	I	607	SER	4.2
1	F	654	TRP	4.2
1	C	437	VAL	4.2
1	A	607	SER	4.2
1	G	445	ASN	4.2
1	D	757	GLU	4.2
1	E	765	GLU	4.2
1	H	410	LYS	4.2
1	B	448	ARG	4.2
1	B	647	LEU	4.2
1	J	764	GLU	4.2
1	H	698	LEU	4.2
1	J	374	HIS	4.2
1	H	740	GLU	4.2
1	I	367	ASP	4.2
1	B	563	TYR	4.1
1	B	366	SER	4.1
1	B	764	GLU	4.1
1	B	381	VAL	4.1
1	E	379	GLY	4.1
1	F	601	SER	4.1
1	B	453	GLN	4.1
1	I	425	MET	4.1
1	C	453	GLN	4.0
1	D	419	THR	4.0
1	E	362	PHE	4.0
1	B	744	ARG	4.0
1	B	606	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	344	GLN	3.9
1	F	380	GLU	3.9
1	I	662	MET	3.9
1	I	515	SER	3.9
1	H	647	LEU	3.9
1	B	370	MET	3.9
1	H	418	ILE	3.9
1	I	685	PHE	3.9
1	C	746	SER	3.9
1	I	361	SER	3.9
1	J	439	SER	3.9
1	E	391	THR	3.9
1	H	659	GLU	3.9
1	H	484	PHE	3.9
1	H	630	LYS	3.9
1	C	543	GLY	3.9
1	H	483	THR	3.9
1	I	412	TYR	3.9
1	F	366	SER	3.9
1	C	747	LEU	3.8
1	D	575	TYR	3.8
1	D	387	LEU	3.8
1	B	598	PHE	3.8
1	G	349	GLU	3.8
1	H	380	GLU	3.8
1	I	432	PHE	3.8
1	H	451	LEU	3.8
1	H	627	LEU	3.8
1	C	366	SER	3.8
1	D	444	LEU	3.8
1	F	442	LEU	3.8
1	I	633	LYS	3.8
1	H	729	LEU	3.8
1	B	678	TYR	3.8
1	C	757	GLU	3.8
1	H	701	VAL	3.7
1	I	638	GLN	3.7
1	H	370	MET	3.7
1	I	540	PHE	3.7
1	D	365	GLU	3.7
1	B	443	PRO	3.7
1	H	599	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	423	HIS	3.7
1	H	737	ASP	3.7
1	B	449	GLU	3.7
1	F	597	LYS	3.7
1	I	567	TYR	3.7
1	E	422	PHE	3.6
1	I	383	PHE	3.6
1	J	452	GLN	3.6
1	H	644	PRO	3.6
1	D	591	VAL	3.6
1	H	537	LYS	3.6
1	J	421	ASP	3.6
1	G	418	ILE	3.6
1	G	449	GLU	3.6
1	C	701	VAL	3.6
1	I	542	ALA	3.6
1	J	350	VAL	3.6
1	J	385	SER	3.6
1	H	575	TYR	3.6
1	I	703	GLU	3.6
1	I	599	ASP	3.6
1	G	585	GLY	3.6
1	H	569	THR	3.6
1	G	342	ILE	3.5
1	H	728	LEU	3.5
1	B	624	ASP	3.5
1	J	388	PHE	3.5
1	C	600	GLU	3.5
1	H	643	SER	3.5
1	J	703	GLU	3.5
1	B	341	PRO	3.5
1	G	461	ARG	3.5
1	B	511	ARG	3.5
1	H	746	SER	3.5
1	A	451	LEU	3.5
1	I	753	ALA	3.5
1	J	419	THR	3.5
1	D	568	LEU	3.5
1	E	761	GLU	3.5
1	A	614	GLU	3.5
1	G	557	ARG	3.5
1	I	525	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	606	GLU	3.5
1	D	472	ILE	3.5
1	H	388	PHE	3.5
1	H	744	ARG	3.5
1	B	371	ALA	3.4
1	I	558	LEU	3.4
1	J	342	ILE	3.4
1	G	343	TRP	3.4
1	D	706	ASP	3.4
1	E	464	LEU	3.4
1	H	600	GLU	3.4
1	J	379	GLY	3.4
1	H	705	GLU	3.4
1	A	424	ASP	3.4
1	I	522	THR	3.4
1	F	367	ASP	3.4
1	B	638	GLN	3.4
1	J	697	MET	3.4
1	H	695	LYS	3.4
1	F	701	VAL	3.4
1	E	418	ILE	3.4
1	A	367	ASP	3.3
1	J	411	LEU	3.3
1	B	622	MET	3.3
1	D	714	ALA	3.3
1	A	419	THR	3.3
1	I	381	VAL	3.3
1	H	408	TYR	3.3
1	I	513	GLN	3.3
1	G	348	LYS	3.3
1	G	613	LYS	3.3
1	F	684	THR	3.3
1	F	341	PRO	3.3
1	D	410	LYS	3.3
1	I	539	TYR	3.3
1	H	596	VAL	3.3
1	H	755	VAL	3.3
1	G	457	LEU	3.3
1	C	340	LYS	3.3
1	J	362	PHE	3.3
1	E	411	LEU	3.3
1	I	681	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	705	GLU	3.3
1	A	361	SER	3.3
1	H	607	SER	3.3
1	B	434	LYS	3.2
1	J	638	GLN	3.2
1	D	705	GLU	3.2
1	H	550	GLU	3.2
1	D	750	ASP	3.2
1	H	386	ILE	3.2
1	B	619	LEU	3.2
1	G	369	PRO	3.2
1	J	340	LYS	3.2
1	H	368	ASP	3.2
1	A	468	THR	3.2
1	I	760	GLU	3.2
1	B	482	ASP	3.2
1	H	634	ALA	3.2
1	J	642	GLU	3.2
1	G	357	ALA	3.2
1	I	465	VAL	3.2
1	I	546	ARG	3.2
1	G	413	VAL	3.2
1	C	422	PHE	3.2
1	I	609	GLU	3.2
1	C	436	VAL	3.2
1	G	436	VAL	3.2
1	E	419	THR	3.2
1	H	754	LYS	3.2
1	E	619	LEU	3.2
1	A	374	HIS	3.1
1	J	389	VAL	3.1
1	H	717	LEU	3.1
1	D	383	PHE	3.1
1	B	566	ILE	3.1
1	I	641	THR	3.1
1	C	648	VAL	3.1
1	I	744	ARG	3.1
1	B	357	ALA	3.1
1	B	354	GLU	3.1
1	H	732	THR	3.1
1	B	553	PRO	3.1
1	F	441	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	613	LYS	3.1
1	I	587	ARG	3.1
1	B	565	VAL	3.1
1	B	383	PHE	3.1
1	G	423	HIS	3.1
1	G	560	LYS	3.1
1	H	685	PHE	3.1
1	B	416	VAL	3.1
1	I	438	ASP	3.1
1	A	606	GLU	3.0
1	J	755	VAL	3.0
1	I	579	ALA	3.0
1	G	387	LEU	3.0
1	I	597	LYS	3.0
1	F	704	ASP	3.0
1	C	561	LYS	3.0
1	E	748	ASN	3.0
1	I	346	PRO	3.0
1	A	483	THR	3.0
1	H	350	VAL	3.0
1	H	633	LYS	3.0
1	B	658	MET	3.0
1	C	357	ALA	3.0
1	G	753	ALA	3.0
1	E	755	VAL	3.0
1	G	468	THR	3.0
1	A	343	TRP	3.0
1	H	708	LYS	3.0
1	I	732	THR	3.0
1	I	623	LYS	3.0
1	H	652	TYR	3.0
1	E	410	LYS	3.0
1	C	743	LEU	3.0
1	H	452	GLN	3.0
1	B	392	SER	3.0
1	J	416	VAL	3.0
1	D	759	PRO	3.0
1	J	678	TYR	3.0
1	E	381	VAL	3.0
1	H	655	SER	3.0
1	G	394	PRO	3.0
1	E	752	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	620	ASN	3.0
1	B	410	LYS	3.0
1	I	652	TYR	2.9
1	C	358	PHE	2.9
1	D	616	GLU	2.9
1	I	636	VAL	2.9
1	G	541	MET	2.9
1	G	432	PHE	2.9
1	A	755	VAL	2.9
1	F	746	SER	2.9
1	G	437	VAL	2.9
1	E	561	LYS	2.9
1	D	343	TRP	2.9
1	E	437	VAL	2.9
1	J	354	GLU	2.9
1	D	747	LEU	2.9
1	B	590	ASN	2.9
1	D	746	SER	2.9
1	G	417	PHE	2.9
1	D	592	ALA	2.9
1	D	658	MET	2.9
1	I	343	TRP	2.9
1	J	344	GLN	2.9
1	D	648	VAL	2.9
1	F	744	ARG	2.9
1	C	759	PRO	2.8
1	E	443	PRO	2.8
1	J	515	SER	2.8
1	I	390	PRO	2.8
1	I	359	TYR	2.8
1	C	597	LYS	2.8
1	E	527	TYR	2.8
1	C	615	PHE	2.8
1	I	487	GLU	2.8
1	B	343	TRP	2.8
1	F	618	LEU	2.8
1	F	698	LEU	2.8
1	B	347	SER	2.8
1	I	556	GLU	2.8
1	J	598	PHE	2.8
1	D	341	PRO	2.8
1	H	390	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	343	TRP	2.8
1	E	500	HIS	2.8
1	I	484	PHE	2.8
1	G	626	ALA	2.8
1	H	437	VAL	2.8
1	B	586	LYS	2.8
1	B	484	PHE	2.8
1	G	558	LEU	2.8
1	D	604	THR	2.8
1	E	737	ASP	2.8
1	G	660	ARG	2.8
1	I	738	ARG	2.8
1	B	361	SER	2.8
1	H	682	LYS	2.8
1	B	512	PHE	2.8
1	F	362	PHE	2.8
1	H	441	ASP	2.8
1	D	748	ASN	2.7
1	I	697	MET	2.7
1	D	484	PHE	2.7
1	H	435	GLY	2.7
1	D	394	PRO	2.7
1	A	748	ASN	2.7
1	D	386	ILE	2.7
1	H	590	ASN	2.7
1	I	647	LEU	2.7
1	A	522	THR	2.7
1	G	534	LYS	2.7
1	A	615	PHE	2.7
1	C	449	GLU	2.7
1	I	563	TYR	2.7
1	H	706	ASP	2.7
1	I	482	ASP	2.7
1	I	536	ASP	2.7
1	I	748	ASN	2.7
1	I	376	THR	2.7
1	J	457	LEU	2.7
1	B	740	GLU	2.7
1	F	585	GLY	2.7
1	H	653	GLY	2.7
1	G	654	TRP	2.7
1	D	364	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	374	HIS	2.7
1	H	610	ALA	2.7
1	A	752	ASP	2.7
1	B	522	THR	2.7
1	B	596	VAL	2.7
1	B	513	GLN	2.7
1	G	392	SER	2.7
1	G	759	PRO	2.7
1	H	636	VAL	2.7
1	B	623	LYS	2.6
1	A	371	ALA	2.6
1	B	412	TYR	2.6
1	J	371	ALA	2.6
1	G	687	ILE	2.6
1	C	748	ASN	2.6
1	D	459	VAL	2.6
1	C	644	PRO	2.6
1	D	424	ASP	2.6
1	C	472	ILE	2.6
1	A	347	SER	2.6
1	B	346	PRO	2.6
1	E	442	LEU	2.6
1	F	598	PHE	2.6
1	H	608	ARG	2.6
1	J	361	SER	2.6
1	I	533	GLU	2.6
1	H	389	VAL	2.6
1	E	363	SER	2.6
1	H	671	LYS	2.6
1	I	537	LYS	2.6
1	C	370	MET	2.6
1	A	685	PHE	2.6
1	D	362	PHE	2.6
1	D	375	PHE	2.6
1	J	486	LYS	2.6
1	D	418	ILE	2.6
1	A	756	GLU	2.6
1	A	757	GLU	2.6
1	D	761	GLU	2.6
1	I	568	LEU	2.6
1	G	346	PRO	2.6
1	B	425	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	544	SER	2.6
1	E	732	THR	2.6
1	G	647	LEU	2.6
1	A	638	GLN	2.6
1	D	608	ARG	2.5
1	I	615	PHE	2.6
1	H	748	ASN	2.5
1	D	417	PHE	2.5
1	H	442	LEU	2.5
1	B	597	LYS	2.5
1	J	434	LYS	2.5
1	H	440	ASP	2.5
1	I	365	GLU	2.5
1	J	619	LEU	2.5
1	G	350	VAL	2.5
1	I	596	VAL	2.5
1	C	732	THR	2.5
1	D	360	LYS	2.5
1	G	556	GLU	2.5
1	H	438	ASP	2.5
1	F	444	LEU	2.5
1	J	394	PRO	2.5
1	E	349	GLU	2.5
1	E	357	ALA	2.5
1	F	638	GLN	2.5
1	J	540	PHE	2.5
1	C	744	ARG	2.5
1	I	740	GLU	2.5
1	C	408	TYR	2.5
1	E	747	LEU	2.5
1	B	362	PHE	2.5
1	G	516	HIS	2.5
1	B	445	ASN	2.5
1	B	439	SER	2.5
1	A	762	GLU	2.5
1	D	659	GLU	2.5
1	A	664	ALA	2.5
1	I	534	LYS	2.5
1	D	372	TYR	2.5
1	B	689	PRO	2.4
1	C	689	PRO	2.4
1	I	429	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	421	ASP	2.4
1	H	574	GLU	2.4
1	H	416	VAL	2.4
1	B	349	GLU	2.4
1	B	505	ARG	2.4
1	D	624	ASP	2.4
1	F	421	ASP	2.4
1	I	588	PHE	2.4
1	J	448	ARG	2.4
1	F	740	GLU	2.4
1	G	574	GLU	2.4
1	H	605	LYS	2.4
1	A	413	VAL	2.4
1	D	442	LEU	2.4
1	F	436	VAL	2.4
1	J	422	PHE	2.4
1	F	411	LEU	2.4
1	I	353	ASP	2.4
1	D	744	ARG	2.4
1	H	665	GLN	2.4
1	G	393	ALA	2.4
1	H	584	ASP	2.4
1	B	378	GLU	2.4
1	H	580	LEU	2.4
1	H	356	LYS	2.4
1	C	347	SER	2.4
1	I	731	ASP	2.4
1	B	473	LYS	2.4
1	I	426	MET	2.4
1	C	421	ASP	2.4
1	H	686	GLU	2.4
1	H	578	GLN	2.4
1	G	429	TYR	2.4
1	H	342	ILE	2.4
1	A	411	LEU	2.4
1	I	463	LYS	2.4
1	E	648	VAL	2.4
1	H	640	LEU	2.4
1	H	710	VAL	2.4
1	I	430	LEU	2.4
1	J	430	LEU	2.4
1	E	568	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	444	LEU	2.4
1	H	411	LEU	2.3
1	A	597	LYS	2.3
1	D	559	LEU	2.3
1	E	347	SER	2.3
1	H	674	SER	2.3
1	B	456	LEU	2.3
1	B	691	HIS	2.3
1	B	414	ARG	2.3
1	B	379	GLY	2.3
1	I	706	ASP	2.3
1	A	611	ILE	2.3
1	B	640	LEU	2.3
1	G	510	LEU	2.3
1	H	448	ARG	2.3
1	B	539	TYR	2.3
1	I	380	GLU	2.3
1	H	611	ILE	2.3
1	A	746	SER	2.3
1	G	620	ASN	2.3
1	E	758	GLU	2.3
1	G	704	ASP	2.3
1	C	740	GLU	2.3
1	J	602	GLU	2.3
1	B	557	ARG	2.3
1	J	687	ILE	2.3
1	B	525	ASP	2.3
1	H	539	TYR	2.3
1	G	513	GLN	2.3
1	G	590	ASN	2.3
1	D	555	VAL	2.3
1	B	731	ASP	2.3
1	E	584	ASP	2.3
1	G	499	ASP	2.3
1	F	360	LYS	2.3
1	C	652	TYR	2.3
1	E	360	LYS	2.3
1	A	365	GLU	2.3
1	B	621	TRP	2.3
1	D	425	MET	2.3
1	D	389	VAL	2.3
1	J	386	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	553	PRO	2.3
1	B	409	ILE	2.3
1	G	496	VAL	2.3
1	J	677	TYR	2.2
1	H	541	MET	2.2
1	E	450	THR	2.2
1	C	619	LEU	2.2
1	G	359	TYR	2.2
1	G	695	LYS	2.2
1	H	355	TYR	2.2
1	C	756	GLU	2.2
1	D	569	THR	2.2
1	I	410	LYS	2.2
1	I	565	VAL	2.2
1	I	631	ILE	2.2
1	J	557	ARG	2.2
1	J	365	GLU	2.2
1	F	364	LYS	2.2
1	J	513	GLN	2.2
1	C	411	LEU	2.2
1	D	456	LEU	2.2
1	D	704	ASP	2.2
1	B	454	HIS	2.2
1	C	585	GLY	2.2
1	G	588	PHE	2.2
1	B	348	LYS	2.2
1	D	597	LYS	2.2
1	J	436	VAL	2.2
1	I	481	ASN	2.2
1	A	414	ARG	2.2
1	A	372	TYR	2.2
1	B	385	SER	2.2
1	C	763	PRO	2.2
1	G	422	PHE	2.2
1	A	603	LYS	2.2
1	C	596	VAL	2.2
1	F	660	ARG	2.2
1	H	439	SER	2.2
1	I	529	GLU	2.2
1	B	684	THR	2.2
1	D	510	LEU	2.2
1	E	445	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	737	ASP	2.2
1	F	596	VAL	2.2
1	H	343	TRP	2.2
1	H	414	ARG	2.2
1	D	544	SER	2.2
1	F	392	SER	2.2
1	G	619	LEU	2.2
1	I	649	ALA	2.2
1	J	387	LEU	2.2
1	H	676	ASN	2.2
1	A	436	VAL	2.2
1	H	460	ILE	2.2
1	H	525	ASP	2.2
1	B	533	GLU	2.1
1	B	595	GLY	2.1
1	F	439	SER	2.1
1	G	439	SER	2.1
1	G	565	VAL	2.1
1	H	555	VAL	2.1
1	I	512	PHE	2.1
1	G	572	VAL	2.1
1	H	694	ILE	2.1
1	J	561	LYS	2.1
1	C	499	ASP	2.1
1	A	714	ALA	2.1
1	C	451	LEU	2.1
1	D	452	GLN	2.1
1	G	582	GLU	2.1
1	G	648	VAL	2.1
1	B	520	ASP	2.1
1	E	353	ASP	2.1
1	G	688	ASN	2.1
1	D	656	GLY	2.1
1	D	627	LEU	2.1
1	J	426	MET	2.1
1	C	371	ALA	2.1
1	D	513	GLN	2.1
1	G	762	GLU	2.1
1	A	425	MET	2.1
1	F	748	ASN	2.1
1	B	508	LYS	2.1
1	D	655	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	624	ASP	2.1
1	I	472	ILE	2.1
1	D	708	LYS	2.1
1	I	561	LYS	2.1
1	C	693	LEU	2.1
1	I	727	TYR	2.1
1	B	468	THR	2.1
1	B	720	THR	2.1
1	C	614	GLU	2.1
1	D	441	ASP	2.1
1	I	572	VAL	2.1
1	J	420	ASP	2.1
1	D	617	PRO	2.1
1	D	742	MET	2.1
1	D	358	PHE	2.1
1	C	686	GLU	2.1
1	H	369	PRO	2.1
1	H	756	GLU	2.1
1	C	638	GLN	2.1
1	C	651	GLN	2.1
1	H	409	ILE	2.1
1	A	747	LEU	2.1
1	D	481	ASN	2.1
1	A	515	SER	2.0
1	I	584	ASP	2.0
1	B	736	GLY	2.0
1	C	389	VAL	2.0
1	E	742	MET	2.0
1	G	465	VAL	2.0
1	G	742	MET	2.0
1	H	394	PRO	2.0
1	I	714	ALA	2.0
1	F	345	ARG	2.0
1	I	589	GLN	2.0
1	F	481	ASN	2.0
1	H	602	GLU	2.0
1	I	692	PRO	2.0
1	H	747	LEU	2.0
1	G	653	GLY	2.0
1	H	666	ALA	2.0
1	D	561	LYS	2.0
1	J	417	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	705	GLU	2.0
1	G	434	LYS	2.0
1	H	340	LYS	2.0
1	B	568	LEU	2.0
1	D	619	LEU	2.0
1	F	571	PRO	2.0
1	G	358	PHE	2.0
1	I	369	PRO	2.0
1	D	686	GLU	2.0
1	D	434	LYS	2.0
1	H	412	TYR	2.0
1	J	412	TYR	2.0
1	J	441	ASP	2.0
1	J	539	TYR	2.0
1	F	721	ALA	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 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.