



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:53 pm BST

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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

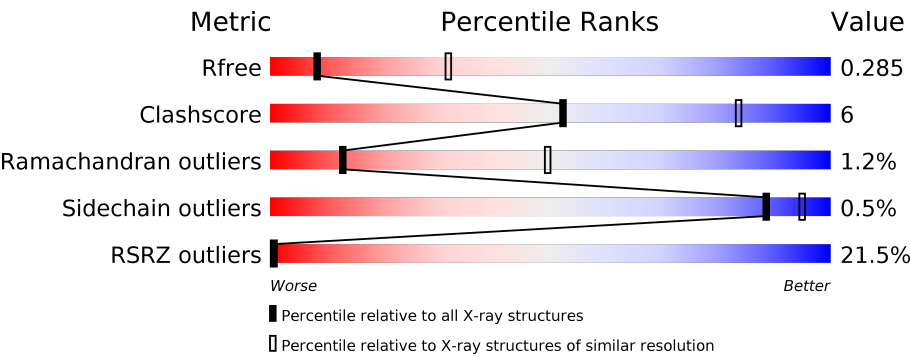
1 Overall quality at a glance i

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	450	<div><div>12%</div><div>81%10%8%</div></div>
1	B	450	<div><div>24%</div><div>82%10%8%</div></div>
1	C	450	<div><div>12%</div><div>82%9%8%</div></div>
1	D	450	<div><div>18%</div><div>79%12%8%</div></div>
1	E	450	<div><div>12%</div><div>78%13%8%</div></div>
1	F	450	<div><div>12%</div><div>76%15%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div>22%</div><div><div></div><div>80%</div><div>12%</div><div>8%</div></div></div>
1	H	450	<div><div>32%</div><div><div></div><div>79%</div><div>12%</div><div>8%</div></div></div>
1	I	450	<div><div>40%</div><div><div></div><div>82%</div><div>10%</div><div>8%</div></div></div>
1	J	450	<div><div>14%</div><div><div></div><div>80%</div><div>12%</div><div>8%</div></div></div>

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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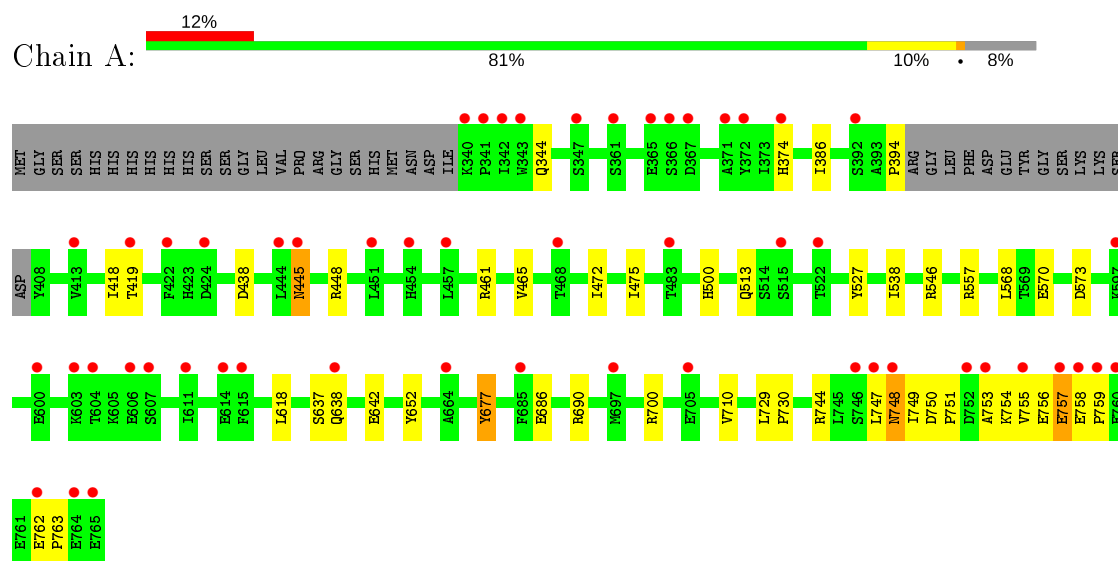
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Chain	Residue	Modelled	Actual	Comment	Reference
I	333	GLY	-	EXPRESSION TAG	UNP P41148
I	334	SER	-	EXPRESSION TAG	UNP P41148
I	335	HIS	-	EXPRESSION TAG	UNP P41148
J	316	MET	-	EXPRESSION TAG	UNP P41148
J	317	GLY	-	EXPRESSION TAG	UNP P41148
J	318	SER	-	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

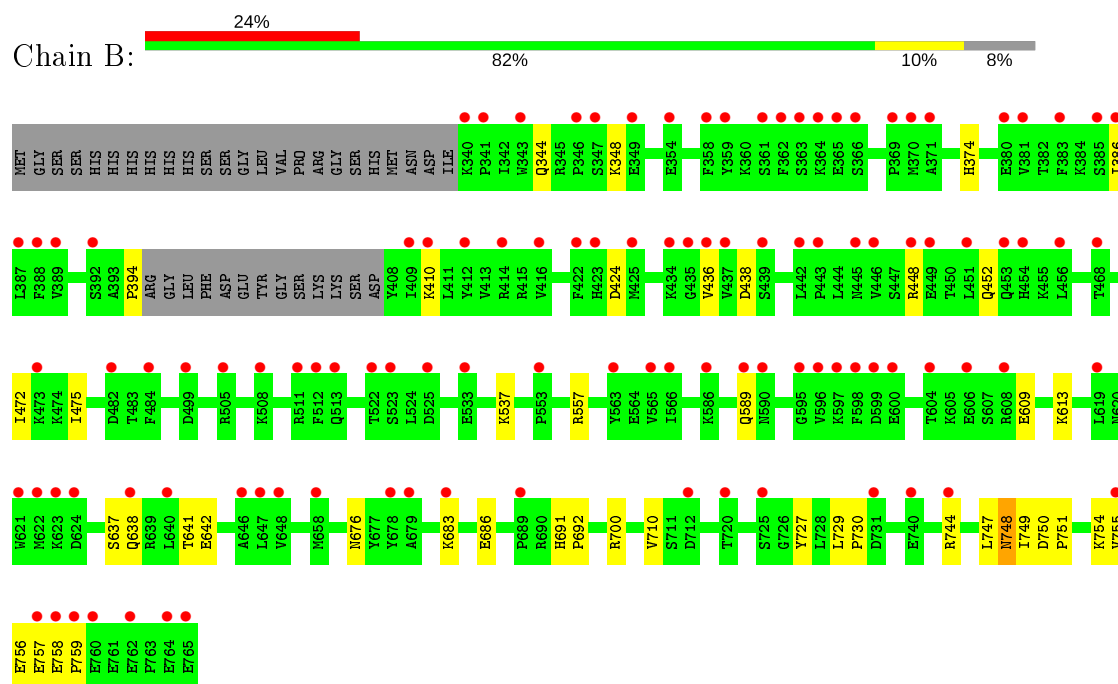
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

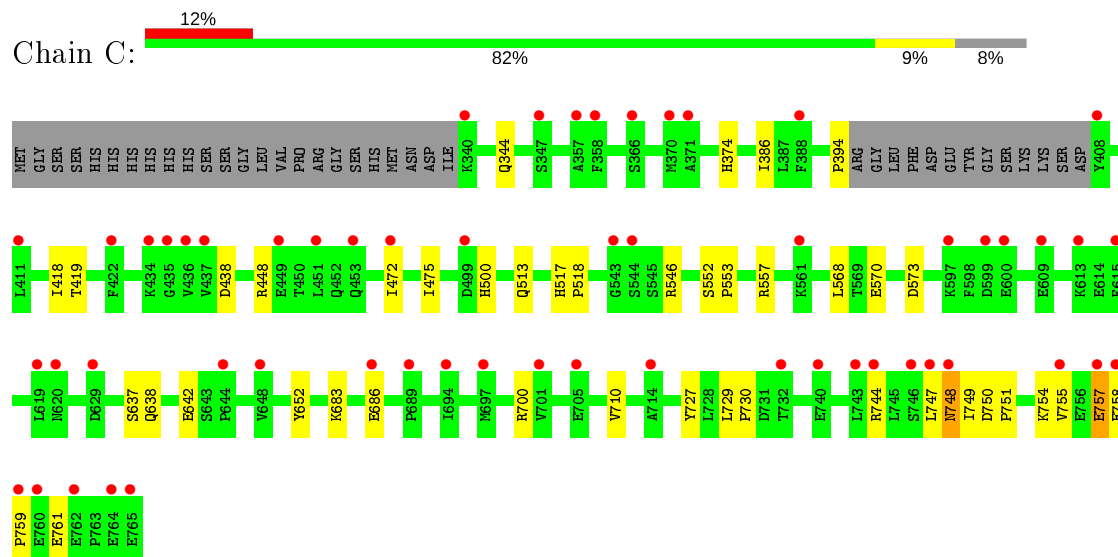
• Molecule 1: Endoplasmin



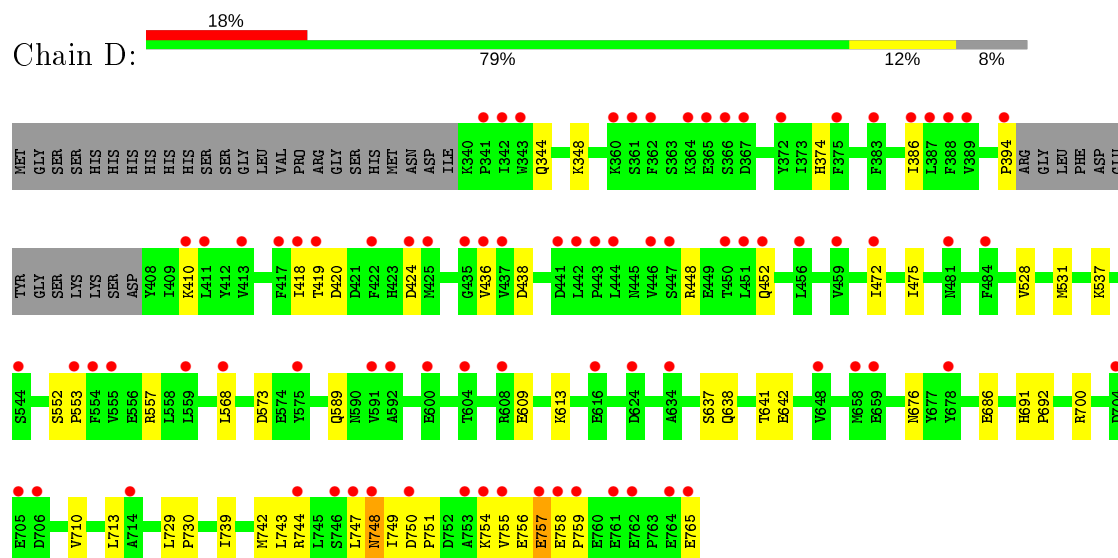
• Molecule 1: Endoplasmin



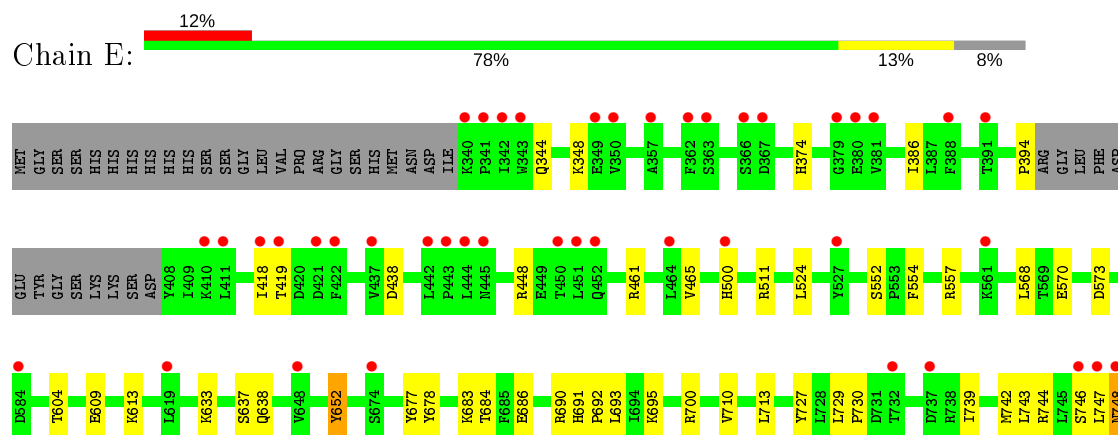
- Molecule 1: Endoplasmic

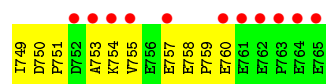


- Molecule 1: Endoplasmic

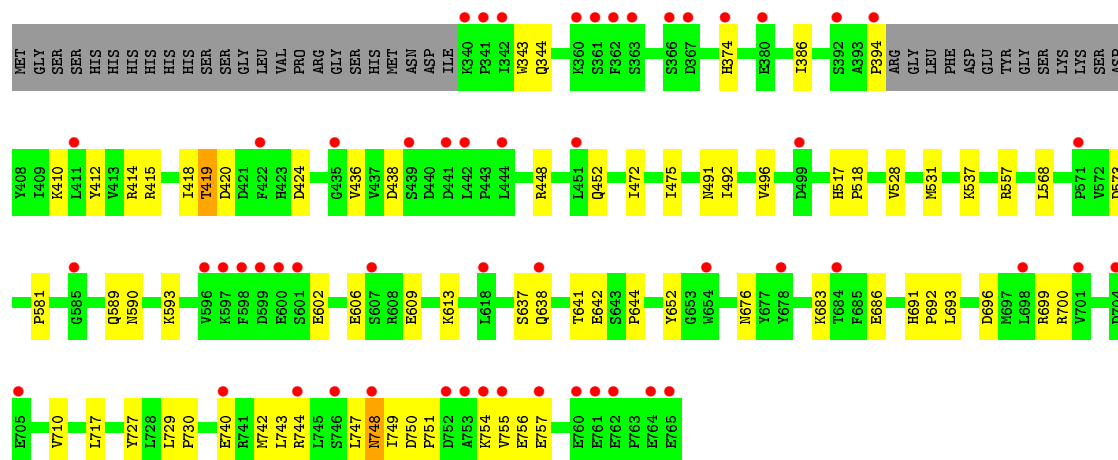
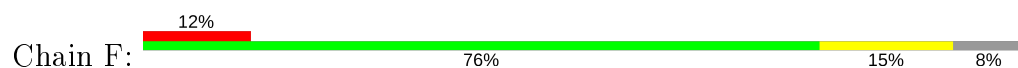


- Molecule 1: Endoplasmic

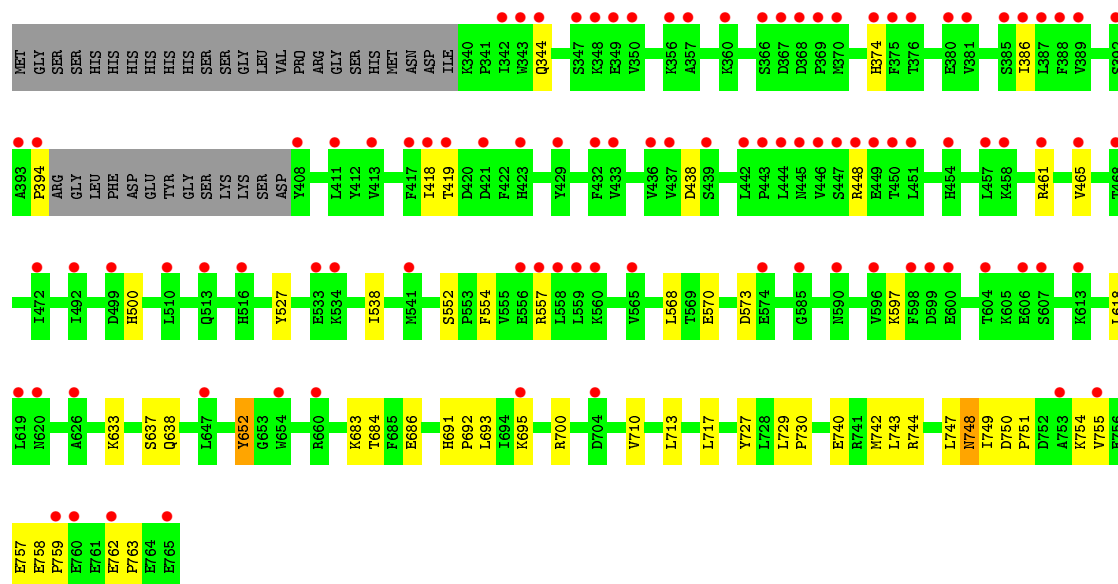
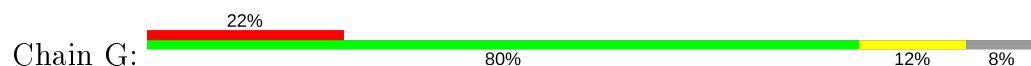




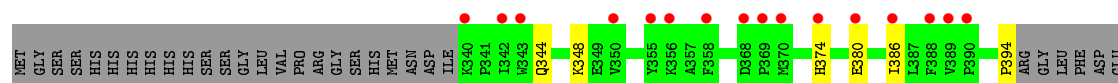
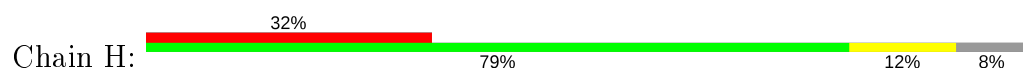
• Molecule 1: Endoplasmic

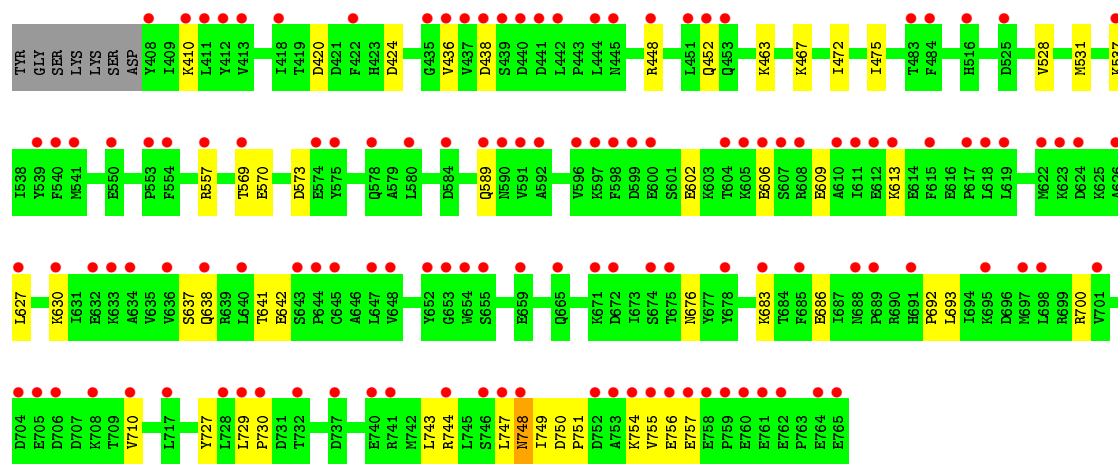


• Molecule 1: Endoplasmic

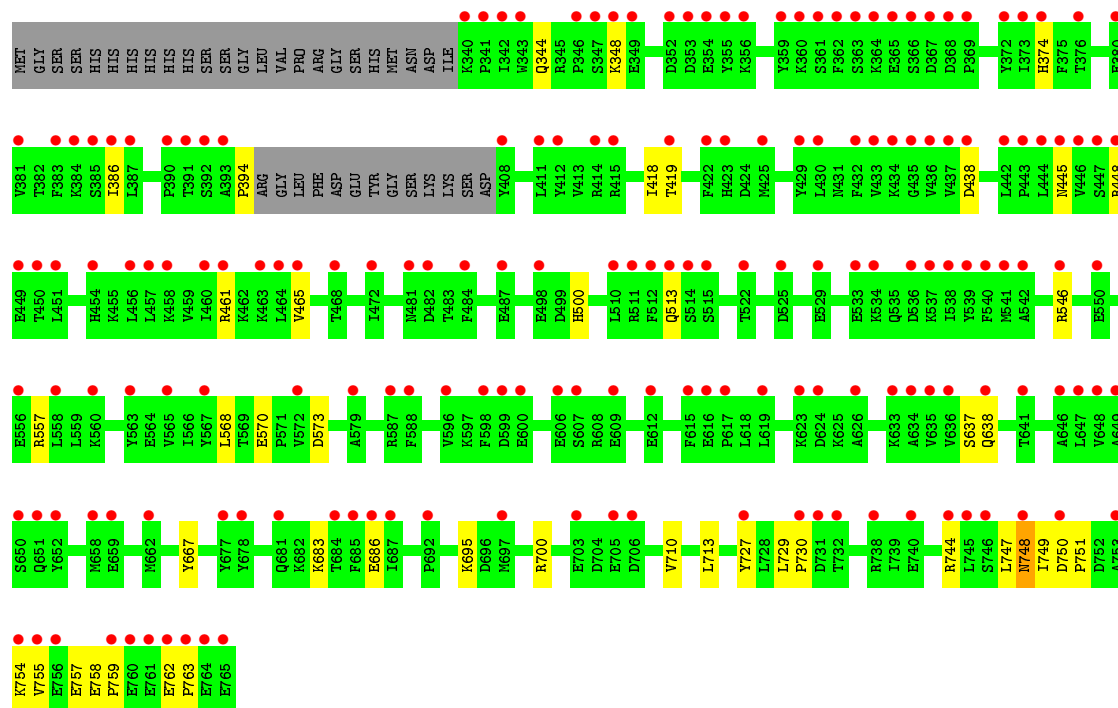
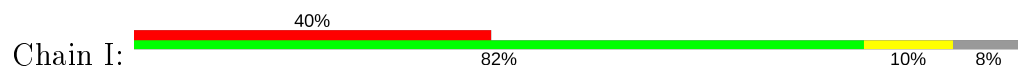


• Molecule 1: Endoplasmic

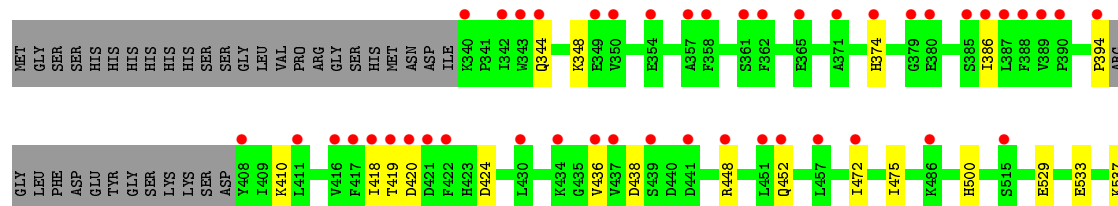
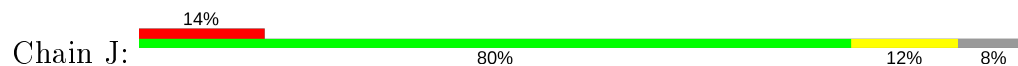


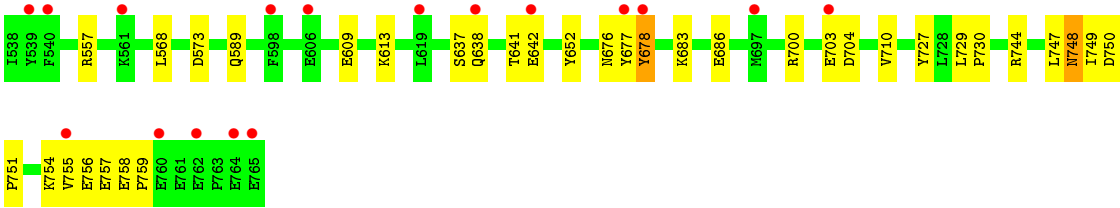


- Molecule 1: Endoplasmin



- Molecule 1: Endoplasmin





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 0.273 , 0.285	Depositor DCC
R_{free} test set	5021 reflections (5.00%)	wwPDB-VP
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 , 163.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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	0.54	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:D:750:ASP:HB3	1:D:754:LYS:HG2	1.75	0.68
1:E:750:ASP:O	1:E:754:LYS:HB2	1.93	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:D:742:MET:CE	1:E:742:MET:HE3	2.26	0.65
1:F:740:GLU:OE2	1:G:691:HIS:NE2	2.28	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:D:713:LEU:HG	1:E:743:LEU:HD22	1.81	0.63
1:F:652:TYR:CE2	1:J:756:GLU:OE2	2.50	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:A:700:ARG:HD2	1:A:710:VAL:HG22	1.84	0.60
1:D:744:ARG:NH2	1:D:755:VAL:HB	2.16	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:A:729:LEU:HD12	1:A:730:PRO:HD2	1.85	0.59
1:F:652:TYR:HE2	1:J:756:GLU:OE2	1.84	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:B:374:HIS:HD2	1:B:386:ILE:HG12	1.67	0.58
1:H:374:HIS:HD2	1:H:386:ILE:HG12	1.68	0.58
1:C:700:ARG:HD2	1:C:710:VAL:HG22	1.84	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: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:D:374:HIS:HD2	1:D:386:ILE:HG12	1.70	0.57
1:I:729:LEU:HD12	1:I:730:PRO:HD2	1.85	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:D:557:ARG:HD3	1:D:638:GLN:O	2.05	0.56
1:D:750:ASP:HB3	1:D:754:LYS:CG	2.36	0.56
1:E:750:ASP:HB3	1:E:754:LYS:HG2	1.88	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:E:729:LEU:HD12	1:E:730:PRO:HD2	1.88	0.55
1:F:742:MET:HE3	1:G:742:MET:CE	2.37	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:H:744:ARG:NH2	1:H:755:VAL:HB	2.23	0.54
1:F:652:TYR:CZ	1:J:756:GLU:HG2	2.43	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:F:750:ASP:HB3	1:F:754:LYS:HG2	1.88	0.53
1:H:693:LEU:HD13	1:I:744:ARG:HG2	1.91	0.53
1:A:344:GLN:NE2	1:A:438:ASP:OD2	2.38	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: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:C:729:LEU:HD12	1:C:730:PRO:HD2	1.92	0.52
1:D:750:ASP:O	1:D:754:LYS:HB2	2.10	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:A:570:GLU:HB2	1:A:573:ASP:CG	2.30	0.52
1:H:467:LYS:HD3	1:J:529:GLU:OE2	2.10	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:570:GLU:HB2	1:E:573:ASP:CG	2.30	0.52
1:E:744:ARG:NH2	1:E:755:VAL:HB	2.25	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:D:742:MET:HE3	1:E:742:MET:HE3	1.92	0.52
1:I:374:HIS:HD2	1:I:386:ILE:HG12	1.75	0.51
1:J:750:ASP:HB3	1:J:754:LYS:HG2	1.93	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:A:750:ASP:HB2	1:E:652:TYR:HB2	1.92	0.51
1:D:759:PRO:HG3	1:E:692:PRO:HD2	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:A:500:HIS:H	1:A:500:HIS:CD2	2.28	0.50
1:I:744:ARG:NH2	1:I:755:VAL:HB	2.27	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:F:414:ARG:O	1:F:415:ARG:HB2	2.12	0.50
1:I:557:ARG:HD3	1:I:638:GLN:O	2.11	0.50
1:C:557:ARG:HD3	1:C:638:GLN:O	2.11	0.49
1:E:374:HIS:HD2	1:E:386:ILE:HG12	1.77	0.49
1:F:700:ARG:HD2	1:F:710:VAL:HG22	1.94	0.49
1:H:380:GLU:CD	1:J:533:GLU:HB2	2.33	0.49
1:C:744:ARG:NH2	1:C:755:VAL:HB	2.26	0.49
1:G:570:GLU:HB2	1:G:573:ASP:CG	2.32	0.49
1:H:692:PRO:HB3	1:I:754:LYS:CE	2.40	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:C:418:ILE:HG22	1:C:419:THR:HG22	1.95	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: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:B:344:GLN:NE2	1:B:438:ASP:OD2	2.41	0.48
1:E:418:ILE:HG22	1:E:419:THR:HG22	1.94	0.48
1:F:691:HIS:CE1	1:G:744:ARG:HD3	2.47	0.48
1:H:743:LEU:HD22	1:I:713:LEU:HG	1.94	0.48
1:C:757:GLU:HG2	1:J:677:TYR:CA	2.44	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:J:754:LYS:C	1:J:756:GLU:H	2.16	0.48
1:D:472:ILE:O	1:D:475:ILE:HG12	2.14	0.48
1:D:742:MET:CE	1:E:742:MET:CE	2.91	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:E:552:SER:OG	1:E:554:PHE:HD1	1.97	0.47
1:G:418:ILE:HG22	1:G:419:THR:HG22	1.96	0.47
1:H:750:ASP:HB3	1:H:754:LYS:CG	2.44	0.47
1:C:700:ARG:HD2	1:C:710:VAL:CG2	2.43	0.47
1:D:759:PRO:CD	1:E:692:PRO:HD3	2.27	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:A:744:ARG:NH2	1:A:755:VAL:HB	2.30	0.47
1:C:747:LEU:O	1:C:748:ASN:CB	2.62	0.47
1:E:461:ARG:O	1:E:465:VAL:HG23	2.15	0.47
1:I:500:HIS:H	1:I:500:HIS:CD2	2.32	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:E:700:ARG:HD2	1:E:710:VAL:CG2	2.45	0.47
1:F:644:PRO:HD3	1:G:740:GLU:OE2	2.14	0.47
1:E:557:ARG:HD3	1:E:638:GLN:O	2.15	0.47
1:J:472:ILE:O	1:J:475:ILE:HG12	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:B:683:LYS:HE3	1:B:727:TYR:CE1	2.51	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:700:ARG:HD2	1:B:710:VAL:HG22	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:H:692:PRO:HD3	1:I:758:GLU:HB2	1.97	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:472:ILE:O	1:H:475:ILE:HG12	2.16	0.45
1:H:700:ARG:HD2	1:H:710:VAL:HG22	1.98	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:A:557:ARG:HD3	1:A:638:GLN:O	2.17	0.45
1:C:748:ASN:O	1:J:652:TYR:CD1	2.70	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:F:410:LYS:HB2	1:F:436:VAL:HG12	1.99	0.45
1:F:609:GLU:O	1:F:613:LYS:HD3	2.17	0.45
1:J:424:ASP:CG	1:J:452:GLN:HE21	2.20	0.45
1:E:747:LEU:O	1:E:748:ASN:CB	2.64	0.45
1:B:700:ARG:HD2	1:B:710:VAL:CG2	2.47	0.45
1:D:754:LYS:C	1:D:756:GLU:H	2.19	0.45
1:C:754:LYS:CE	1:J:678:TYR:HE2	2.30	0.45
1:D:759:PRO:HG3	1:E:691:HIS:HA	1.98	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:F:528:VAL:HA	1:F:531:MET:SD	2.57	0.44
1:H:537:LYS:HE2	1:H:589:GLN:HB2	1.99	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:528:VAL:HA	1:H:531:MET:SD	2.57	0.44
1:H:700:ARG:HD2	1:H:710:VAL:CG2	2.48	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:D:348:LYS:HE3	1:D:348:LYS:HB2	1.71	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: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:B:472:ILE:O	1:B:475:ILE:HG12	2.18	0.43
1:E:374:HIS:CD2	1:E:386:ILE:HG12	2.53	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:B:537:LYS:HE2	1:B:589:GLN:HB2	2.01	0.43
1:D:424:ASP:CG	1:D:452:GLN:HE21	2.22	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:B:348:LYS:HB2	1:B:348:LYS:HE3	1.76	0.43
1:C:517:HIS:HA	1:C:518:PRO:HD2	1.78	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:J:609:GLU:O	1:J:613:LYS:HD3	2.19	0.43
1:B:410:LYS:HB2	1:B:436:VAL:HG12	1.99	0.43
1:D:729:LEU:HA	1:D:730:PRO:HD2	1.85	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:C:472:ILE:O	1:C:475:ILE:HG12	2.20	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:D:410:LYS:HB2	1:D:436:VAL:HG12	2.01	0.42
1:D:418:ILE:HG22	1:D:419:THR:HG22	2.01	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:G:500:HIS:H	1:G:500:HIS:CD2	2.36	0.42
1:H:463:LYS:NZ	1:J:529:GLU:O	2.53	0.42
1:A:568:LEU:HB3	1:A:573:ASP:HB3	2.00	0.42
1:A:729:LEU:HA	1:A:730:PRO:HD2	1.81	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:C:552:SER:HA	1:C:553:PRO:HD3	1.94	0.42
1:G:633:LYS:HG3	1:G:684:THR:HG23	2.01	0.42
1:H:410:LYS:HB2	1:H:436:VAL:HG12	2.02	0.42
1:A:527:TYR:CE2	1:A:538:ILE:HG23	2.54	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:C:374:HIS:CD2	1:C:386:ILE:HG12	2.55	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:A:642:GLU:HG2	1:J:759:PRO:HB3	1.99	0.42
1:E:758:GLU:N	1:E:759:PRO:CD	2.83	0.42
1:F:517:HIS:HA	1:F:518:PRO:HD2	1.87	0.42
1:I:348:LYS:HB2	1:I:348:LYS:HE3	1.90	0.42
1:J:418:ILE:HG22	1:J:419:THR:HG22	2.01	0.42
1:A:747:LEU:O	1:A:748:ASN:CB	2.68	0.42
1:F:747:LEU:O	1:F:748:ASN:CB	2.67	0.42
1:C:754:LYS:HZ3	1:J:678:TYR:HE2	1.62	0.41
1:E:633:LYS:HG3	1:E:684:THR:HG23	2.02	0.41
1:F:692:PRO:HG3	1:G:754:LYS:HB3	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:A:513:GLN:HB3	1:A:546:ARG:NH1	2.35	0.41
1:D:641:THR:HG22	1:D:642:GLU:HG3	2.02	0.41
1:G:695:LYS:HE2	1:G:695:LYS:HB3	1.88	0.41
1:I:758:GLU:N	1:I:759:PRO:CD	2.83	0.41
1:A:754:LYS:C	1:A:756:GLU:N	2.74	0.41
1:G:527:TYR:CE2	1:G:538:ILE:HG23	2.55	0.41
1:J:700:ARG:HD2	1:J:710:VAL:HG22	2.02	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: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:B:758:GLU:N	1:B:759:PRO:CD	2.84	0.41
1:D:759:PRO:CA	1:E:690:ARG:O	2.68	0.41
1:A:570:GLU:HB2	1:A:573:ASP:OD2	2.21	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:642:GLU:HA	1:G:759:PRO:HB3	2.03	0.41
1:D:537:LYS:HE2	1:D:589:GLN:HB2	2.01	0.41
1:G:552:SER:OG	1:G:554:PHE:HD1	2.04	0.41
1:F:744:ARG:CD	1:G:693:LEU:HB2	2.50	0.41
1:H:747:LEU:O	1:H:748:ASN:CB	2.68	0.41
1:B:747:LEU:O	1:B:748:ASN:CB	2.68	0.41
1:E:511:ARG:HA	1:E:511:ARG:HD3	1.97	0.41
1:E:524:LEU:HD23	1:E:524:LEU:HA	1.87	0.41
1:G:597:LYS:HE3	1:G:597:LYS:HB2	1.94	0.41
1:I:762:GLU:N	1:I:763:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:568:LEU:HB3	1:J:573:ASP:HB3	2.03	0.41
1:E:348:LYS:HB2	1:E:348:LYS:HE3	1.91	0.41
1:G:762:GLU:N	1:G:763:PRO:CD	2.84	0.41
1:H:683:LYS:HE3	1:H:727:TYR:CE1	2.55	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:E:609:GLU:O	1:E:613:LYS:HD3	2.22	0.40
1:E:729:LEU:HA	1:E:730:PRO:HD2	1.79	0.40
1:F:602:GLU:O	1:F:606:GLU:HG3	2.21	0.40
1:F:691:HIS:NE2	1:G:740:GLU:OE2	2.54	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:D:609:GLU:O	1:D:613:LYS:HD3	2.21	0.40
1:D:700:ARG:HD2	1:D:710:VAL:HG22	2.02	0.40
1:D:747:LEU:O	1:D:748:ASN:CB	2.70	0.40
1:E:500:HIS:CD2	1:E:500:HIS:N	2.85	0.40
1:I:513:GLN:HB3	1:I:546:ARG:NH1	2.36	0.40
1:E:500:HIS:ND1	1:J:704:ASP:HB2	2.28	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%)	15	54
1	B	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	13	49
1	C	409/450 (91%)	365 (89%)	40 (10%)	4 (1%)	15	54
1	D	409/450 (91%)	368 (90%)	35 (9%)	6 (2%)	10	44
1	E	409/450 (91%)	357 (87%)	47 (12%)	5 (1%)	13	49
1	F	409/450 (91%)	365 (89%)	36 (9%)	8 (2%)	7	38
1	G	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	15	54
1	H	409/450 (91%)	367 (90%)	36 (9%)	6 (2%)	10	44
1	I	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	15	54
1	J	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	13	49
All	All	4090/4500 (91%)	3637 (89%)	402 (10%)	51 (1%)	13	49

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%)	78	91
1	B	352/410 (86%)	351 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	352/410 (86%)	350 (99%)	2 (1%)	86	94
1	D	352/410 (86%)	351 (100%)	1 (0%)	92	96
1	E	352/410 (86%)	349 (99%)	3 (1%)	78	91
1	F	352/410 (86%)	350 (99%)	2 (1%)	86	94
1	G	352/410 (86%)	350 (99%)	2 (1%)	86	94
1	H	352/410 (86%)	351 (100%)	1 (0%)	92	96
1	I	352/410 (86%)	351 (100%)	1 (0%)	92	96
1	J	352/410 (86%)	350 (99%)	2 (1%)	86	94
All	All	3520/4100 (86%)	3502 (100%)	18 (0%)	88	95

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%)	0.88	53 (12%) 3 2	129, 151, 152, 165	0
1	B	413/450 (91%)	1.52	109 (26%) 0 0	129, 151, 152, 165	0
1	C	413/450 (91%)	0.94	56 (13%) 3 2	129, 151, 152, 165	0
1	D	413/450 (91%)	1.21	82 (19%) 1 1	129, 151, 152, 165	0
1	E	413/450 (91%)	1.01	54 (13%) 3 2	129, 151, 152, 165	0
1	F	413/450 (91%)	0.88	54 (13%) 3 2	129, 151, 152, 165	0
1	G	413/450 (91%)	1.50	98 (23%) 0 0	129, 151, 152, 165	0
1	H	413/450 (91%)	1.82	144 (34%) 0 0	129, 151, 152, 165	0
1	I	413/450 (91%)	2.63	178 (43%) 0 0	129, 151, 152, 165	0
1	J	413/450 (91%)	0.88	62 (15%) 2 1	129, 151, 152, 165	0
All	All	4130/4500 (91%)	1.33	890 (21%) 0 1	129, 151, 153, 165	0

All (890) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	443	PRO	20.1
1	I	437	VAL	19.2
1	I	443	PRO	18.9
1	I	363	SER	17.4
1	D	765	GLU	17.1
1	I	392	SER	16.7
1	E	753	ALA	16.3
1	I	651	GLN	15.5
1	I	364	LYS	15.2
1	I	444	LEU	15.0
1	I	386	ILE	14.7
1	G	347	SER	14.0
1	A	758	GLU	13.9

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Mol	Chain	Res	Type	RSRZ
1	C	755	VAL	13.7
1	I	387	LEU	13.7
1	I	755	VAL	13.7
1	I	765	GLU	12.6
1	I	349	GLU	12.5
1	D	366	SER	12.1
1	E	342	ILE	12.0
1	B	759	PRO	11.9
1	I	436	VAL	11.9
1	G	375	PHE	11.6
1	H	697	MET	11.6
1	H	757	GLU	11.6
1	A	765	GLU	11.5
1	D	755	VAL	11.5
1	I	764	GLU	11.4
1	I	447	SER	11.4
1	G	600	GLU	11.3
1	H	753	ALA	11.2
1	I	446	VAL	10.9
1	D	762	GLU	10.9
1	G	448	ARG	10.8
1	B	388	PHE	10.3
1	I	449	GLU	10.1
1	I	457	LEU	10.0
1	I	634	ALA	9.9
1	B	599	ASP	9.9
1	I	442	LEU	9.7
1	G	381	VAL	9.5
1	B	435	GLY	9.4
1	B	755	VAL	9.4
1	H	598	PHE	9.4
1	B	600	GLU	9.3
1	H	761	GLU	9.2
1	I	445	ASN	9.1
1	H	760	GLU	9.1
1	D	411	LEU	9.1
1	E	452	GLN	8.9
1	D	753	ALA	8.8
1	I	366	SER	8.8
1	H	619	LEU	8.8
1	G	388	PHE	8.7
1	I	763	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
1	I	746	SER	8.5
1	H	638	GLN	8.5
1	B	762	GLU	8.5
1	A	759	PRO	8.4
1	I	677	TYR	8.4
1	D	443	PRO	8.3
1	B	765	GLU	8.3
1	I	468	THR	8.3
1	J	765	GLU	8.2
1	H	758	GLU	8.1
1	E	757	GLU	8.0
1	I	450	THR	8.0
1	B	760	GLU	8.0
1	I	646	ALA	8.0
1	H	436	VAL	7.9
1	C	435	GLY	7.8
1	F	754	LYS	7.8
1	H	704	ASP	7.8
1	H	617	PRO	7.8
1	G	446	VAL	7.7
1	I	635	VAL	7.7
1	A	341	PRO	7.7
1	G	433	VAL	7.6
1	G	451	LEU	7.6
1	D	754	LYS	7.6
1	H	597	LYS	7.6
1	D	388	PHE	7.5
1	E	380	GLU	7.5
1	I	600	GLU	7.5
1	J	390	PRO	7.5
1	G	604	THR	7.4
1	G	454	HIS	7.4
1	E	366	SER	7.4
1	G	765	GLU	7.3
1	H	765	GLU	7.3
1	I	373	ILE	7.3
1	D	437	VAL	7.1
1	B	436	VAL	7.1
1	E	754	LYS	7.1
1	B	646	ALA	7.1
1	A	764	GLU	7.0
1	H	678	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	G	368	ASP	7.0
1	J	451	LEU	7.0
1	D	342	ILE	7.0
1	B	359	TYR	6.9
1	H	730	PRO	6.9
1	G	444	LEU	6.8
1	H	358	PHE	6.8
1	B	363	SER	6.8
1	H	613	LYS	6.8
1	A	340	LYS	6.8
1	H	622	MET	6.8
1	I	754	LYS	6.7
1	G	442	LEU	6.7
1	B	437	VAL	6.7
1	I	411	LEU	6.6
1	B	608	ARG	6.6
1	D	367	ASP	6.6
1	F	761	GLU	6.6
1	E	763	PRO	6.6
1	D	678	TYR	6.6
1	I	759	PRO	6.6
1	F	599	ASP	6.5
1	G	370	MET	6.5
1	H	752	ASP	6.5
1	I	456	LEU	6.4
1	I	391	THR	6.4
1	I	385	SER	6.4
1	F	435	GLY	6.4
1	I	340	LYS	6.3
1	I	341	PRO	6.3
1	I	464	LEU	6.2
1	C	765	GLU	6.2
1	I	448	ARG	6.2
1	I	362	PHE	6.2
1	G	596	VAL	6.1
1	G	380	GLU	6.1
1	E	451	LEU	6.1
1	F	753	ALA	6.0
1	I	454	HIS	6.0
1	G	356	LYS	5.9
1	F	451	LEU	5.9
1	I	624	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	679	ALA	5.9
1	C	388	PHE	5.9
1	B	386	ILE	5.9
1	G	458	LYS	5.8
1	G	755	VAL	5.8
1	I	352	ASP	5.8
1	I	451	LEU	5.8
1	C	764	GLU	5.8
1	I	342	ILE	5.8
1	D	600	GLU	5.8
1	I	619	LEU	5.8
1	I	658	MET	5.8
1	C	714	ALA	5.7
1	I	393	ALA	5.7
1	F	760	GLU	5.7
1	I	356	LYS	5.7
1	F	765	GLU	5.7
1	H	606	GLU	5.6
1	I	433	VAL	5.6
1	F	757	GLU	5.6
1	I	354	GLU	5.6
1	J	762	GLU	5.6
1	J	760	GLU	5.6
1	I	510	LEU	5.6
1	I	414	ARG	5.6
1	J	358	PHE	5.5
1	J	418	ILE	5.5
1	C	434	LYS	5.5
1	F	755	VAL	5.5
1	D	447	SER	5.5
1	D	451	LEU	5.5
1	B	451	LEU	5.4
1	G	374	HIS	5.4
1	G	421	ASP	5.4
1	J	380	GLU	5.4
1	H	645	CYS	5.4
1	A	342	ILE	5.4
1	C	760	GLU	5.4
1	C	697	MET	5.4
1	I	684	THR	5.4
1	H	554	PHE	5.4
1	B	423	HIS	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	675	THR	5.4
1	E	350	VAL	5.3
1	E	764	GLU	5.3
1	B	442	LEU	5.3
1	I	355	TYR	5.3
1	I	408	TYR	5.3
1	B	725	SER	5.3
1	A	422	PHE	5.2
1	I	422	PHE	5.2
1	D	758	GLU	5.2
1	G	598	PHE	5.2
1	B	364	LYS	5.2
1	H	422	PHE	5.2
1	H	688	ASN	5.2
1	J	606	GLU	5.1
1	H	516	HIS	5.1
1	G	411	LEU	5.1
1	I	514	SER	5.1
1	I	687	ILE	5.1
1	D	436	VAL	5.1
1	B	422	PHE	5.1
1	H	615	PHE	5.1
1	G	376	THR	5.1
1	E	367	ASP	5.1
1	F	361	SER	5.1
1	B	369	PRO	5.0
1	E	762	GLU	5.0
1	G	366	SER	5.0
1	H	589	GLN	5.0
1	B	340	LYS	5.0
1	B	757	GLU	5.0
1	G	445	ASN	5.0
1	I	419	THR	5.0
1	E	341	PRO	5.0
1	I	762	GLU	5.0
1	H	612	GLU	5.0
1	F	422	PHE	5.0
1	H	648	VAL	5.0
1	F	764	GLU	4.9
1	D	422	PHE	4.9
1	H	762	GLU	4.9
1	I	435	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	553	PRO	4.9
1	I	612	GLU	4.9
1	E	379	GLY	4.9
1	F	342	ILE	4.9
1	I	745	LEU	4.9
1	C	762	GLU	4.9
1	F	762	GLU	4.9
1	H	632	GLU	4.8
1	C	694	ILE	4.8
1	J	452	GLN	4.8
1	B	647	LEU	4.8
1	I	659	GLU	4.8
1	F	678	TYR	4.7
1	I	686	GLU	4.7
1	A	600	GLU	4.7
1	E	746	SER	4.7
1	F	752	ASP	4.7
1	H	604	THR	4.7
1	D	365	GLU	4.7
1	I	598	PHE	4.7
1	I	705	GLU	4.7
1	H	537	LYS	4.6
1	J	437	VAL	4.6
1	I	372	TYR	4.6
1	A	444	LEU	4.6
1	E	340	LYS	4.6
1	G	360	LYS	4.6
1	A	760	GLU	4.6
1	H	764	GLU	4.6
1	H	592	ALA	4.6
1	A	445	ASN	4.5
1	I	617	PRO	4.5
1	B	712	ASP	4.5
1	D	757	GLU	4.5
1	G	447	SER	4.5
1	I	461	ARG	4.5
1	H	413	VAL	4.5
1	G	492	ILE	4.5
1	B	744	ARG	4.5
1	I	560	LYS	4.5
1	I	511	ARG	4.5
1	F	600	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	634	ALA	4.5
1	B	358	PHE	4.5
1	H	672	ASP	4.5
1	B	758	GLU	4.5
1	I	412	TYR	4.5
1	H	374	HIS	4.4
1	I	750	ASP	4.4
1	B	365	GLU	4.4
1	G	342	ILE	4.4
1	A	753	ALA	4.4
1	C	599	ASP	4.4
1	I	367	ASP	4.4
1	G	344	GLN	4.4
1	I	541	MET	4.4
1	G	559	LEU	4.4
1	G	599	ASP	4.4
1	A	604	THR	4.4
1	A	607	SER	4.3
1	G	343	TRP	4.3
1	H	759	PRO	4.3
1	I	498	GLU	4.3
1	F	340	LYS	4.3
1	D	764	GLU	4.3
1	I	458	LYS	4.3
1	B	366	SER	4.3
1	I	374	HIS	4.3
1	J	764	GLU	4.3
1	G	349	GLU	4.3
1	H	740	GLU	4.3
1	J	408	TYR	4.3
1	I	730	PRO	4.3
1	I	648	VAL	4.3
1	H	654	TRP	4.2
1	B	389	VAL	4.2
1	G	533	GLU	4.2
1	I	678	TYR	4.2
1	J	349	GLU	4.2
1	I	633	LYS	4.2
1	J	638	GLN	4.2
1	G	419	THR	4.2
1	H	540	PHE	4.2
1	B	453	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	386	ILE	4.2
1	H	630	LYS	4.2
1	D	419	THR	4.2
1	J	374	HIS	4.2
1	G	606	GLU	4.2
1	I	761	GLU	4.2
1	B	678	TYR	4.2
1	D	575	TYR	4.2
1	F	654	TRP	4.1
1	D	446	VAL	4.1
1	B	624	ASP	4.1
1	H	695	LYS	4.1
1	I	425	MET	4.1
1	H	691	HIS	4.1
1	G	389	VAL	4.1
1	B	380	GLU	4.1
1	J	357	ALA	4.1
1	B	604	THR	4.1
1	E	362	PHE	4.1
1	I	607	SER	4.1
1	B	589	GLN	4.1
1	E	388	PHE	4.0
1	I	360	LYS	4.0
1	J	342	ILE	4.0
1	I	460	ILE	4.0
1	I	538	ILE	4.0
1	E	444	LEU	4.0
1	I	361	SER	4.0
1	E	755	VAL	4.0
1	I	347	SER	4.0
1	H	705	GLU	4.0
1	I	662	MET	3.9
1	G	450	THR	3.9
1	I	515	SER	3.9
1	A	392	SER	3.9
1	F	366	SER	3.9
1	B	354	GLU	3.9
1	F	701	VAL	3.9
1	C	453	GLN	3.9
1	C	746	SER	3.9
1	I	383	PHE	3.9
1	I	415	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	384	LYS	3.9
1	J	439	SER	3.9
1	I	579	ALA	3.9
1	J	421	ASP	3.9
1	D	361	SER	3.8
1	B	606	GLU	3.8
1	A	697	MET	3.8
1	I	567	TYR	3.8
1	C	366	SER	3.8
1	G	449	GLU	3.8
1	I	434	LYS	3.8
1	C	543	GLY	3.8
1	B	448	ARG	3.8
1	I	606	GLU	3.8
1	C	757	GLU	3.8
1	B	764	GLU	3.8
1	I	756	GLU	3.8
1	H	689	PRO	3.8
1	J	379	GLY	3.7
1	H	644	PRO	3.7
1	I	641	THR	3.7
1	C	747	LEU	3.7
1	B	370	MET	3.7
1	J	350	VAL	3.7
1	F	394	PRO	3.7
1	H	451	LEU	3.7
1	H	683	LYS	3.7
1	F	607	SER	3.7
1	H	350	VAL	3.7
1	F	442	LEU	3.6
1	H	729	LEU	3.6
1	C	437	VAL	3.6
1	I	556	GLU	3.6
1	B	381	VAL	3.6
1	H	659	GLU	3.6
1	J	385	SER	3.6
1	J	419	THR	3.6
1	F	380	GLU	3.6
1	I	432	PHE	3.6
1	G	357	ALA	3.6
1	H	484	PHE	3.6
1	G	418	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	614	GLU	3.6
1	A	757	GLU	3.6
1	H	483	THR	3.6
1	H	643	SER	3.6
1	H	569	THR	3.5
1	I	522	THR	3.5
1	G	541	MET	3.5
1	H	370	MET	3.5
1	H	737	ASP	3.5
1	E	391	THR	3.5
1	E	674	SER	3.5
1	H	623	LYS	3.5
1	J	344	GLN	3.5
1	F	367	ASP	3.5
1	I	638	GLN	3.5
1	I	359	TYR	3.5
1	H	591	VAL	3.5
1	C	629	ASP	3.5
1	E	422	PHE	3.5
1	B	434	LYS	3.5
1	H	380	GLU	3.5
1	B	449	GLU	3.4
1	F	704	ASP	3.4
1	H	600	GLU	3.4
1	B	563	TYR	3.4
1	A	755	VAL	3.4
1	I	539	TYR	3.4
1	J	340	LYS	3.4
1	H	698	LEU	3.4
1	A	483	THR	3.4
1	G	585	GLY	3.4
1	C	613	LYS	3.4
1	H	386	ILE	3.4
1	I	438	ASP	3.4
1	H	550	GLU	3.4
1	H	701	VAL	3.4
1	H	728	LEU	3.4
1	G	385	SER	3.4
1	H	596	VAL	3.4
1	J	678	TYR	3.4
1	A	366	SER	3.4
1	I	685	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	701	VAL	3.4
1	I	343	TRP	3.4
1	H	410	LYS	3.4
1	H	627	LEU	3.4
1	D	343	TRP	3.4
1	G	432	PHE	3.4
1	C	600	GLU	3.4
1	D	706	ASP	3.3
1	D	387	LEU	3.3
1	G	613	LYS	3.3
1	A	451	LEU	3.3
1	D	714	ALA	3.3
1	G	557	ARG	3.3
1	D	444	LEU	3.3
1	H	755	VAL	3.3
1	D	472	ILE	3.3
1	D	705	GLU	3.3
1	E	765	GLU	3.3
1	A	367	ASP	3.3
1	H	418	ILE	3.3
1	H	575	TYR	3.3
1	J	343	TRP	3.3
1	I	423	HIS	3.3
1	E	464	LEU	3.3
1	D	591	VAL	3.3
1	H	607	SER	3.3
1	G	348	LYS	3.3
1	I	558	LEU	3.3
1	I	647	LEU	3.3
1	H	746	SER	3.3
1	H	754	LYS	3.3
1	I	681	GLN	3.3
1	F	597	LYS	3.3
1	J	388	PHE	3.3
1	I	525	ASP	3.2
1	H	388	PHE	3.2
1	I	381	VAL	3.2
1	J	703	GLU	3.2
1	F	601	SER	3.2
1	H	634	ALA	3.2
1	B	392	SER	3.2
1	I	465	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	748	ASN	3.2
1	B	598	PHE	3.2
1	I	540	PHE	3.2
1	A	424	ASP	3.2
1	H	599	ASP	3.2
1	A	468	THR	3.2
1	I	753	ALA	3.2
1	B	565	VAL	3.2
1	H	652	TYR	3.2
1	E	761	GLU	3.2
1	E	349	GLU	3.2
1	H	441	ASP	3.2
1	B	343	TRP	3.1
1	C	340	LYS	3.1
1	B	482	ASP	3.1
1	I	599	ASP	3.1
1	E	418	ILE	3.1
1	D	341	PRO	3.1
1	H	744	ARG	3.1
1	D	383	PHE	3.1
1	I	703	GLU	3.1
1	J	697	MET	3.1
1	I	484	PHE	3.1
1	C	648	VAL	3.1
1	H	343	TRP	3.1
1	B	349	GLU	3.1
1	D	386	ILE	3.1
1	F	705	GLU	3.1
1	H	732	THR	3.1
1	J	515	SER	3.1
1	B	341	PRO	3.0
1	A	606	GLU	3.0
1	A	374	HIS	3.0
1	D	592	ALA	3.0
1	D	616	GLU	3.0
1	B	622	MET	3.0
1	G	461	ARG	3.0
1	I	760	GLU	3.0
1	J	394	PRO	3.0
1	H	655	SER	3.0
1	B	371	ALA	3.0
1	G	394	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	348	LYS	3.0
1	C	422	PHE	3.0
1	I	542	ALA	3.0
1	D	648	VAL	3.0
1	H	442	LEU	3.0
1	G	759	PRO	3.0
1	J	389	VAL	3.0
1	G	369	PRO	3.0
1	B	412	TYR	3.0
1	H	408	TYR	3.0
1	C	358	PHE	3.0
1	B	443	PRO	3.0
1	G	436	VAL	3.0
1	F	362	PHE	3.0
1	E	411	LEU	2.9
1	D	750	ASP	2.9
1	B	638	GLN	2.9
1	B	658	MET	2.9
1	I	546	ARG	2.9
1	I	609	GLU	2.9
1	J	755	VAL	2.9
1	C	615	PHE	2.9
1	J	354	GLU	2.9
1	I	732	THR	2.9
1	E	619	LEU	2.9
1	H	647	LEU	2.9
1	J	362	PHE	2.9
1	B	553	PRO	2.9
1	B	619	LEU	2.9
1	I	537	LYS	2.9
1	E	752	ASP	2.9
1	J	411	LEU	2.9
1	D	746	SER	2.9
1	H	671	LYS	2.9
1	A	343	TRP	2.9
1	J	642	GLU	2.9
1	C	472	ILE	2.9
1	F	744	ARG	2.9
1	E	561	LYS	2.9
1	F	638	GLN	2.9
1	H	440	ASP	2.9
1	C	759	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	341	PRO	2.9
1	C	436	VAL	2.9
1	F	698	LEU	2.9
1	H	708	LYS	2.9
1	I	636	VAL	2.9
1	F	684	THR	2.9
1	B	346	PRO	2.9
1	B	596	VAL	2.8
1	G	468	THR	2.8
1	A	762	GLU	2.8
1	B	522	THR	2.8
1	I	513	GLN	2.8
1	C	744	ARG	2.8
1	F	746	SER	2.8
1	F	618	LEU	2.8
1	C	561	LYS	2.8
1	I	697	MET	2.8
1	I	365	GLU	2.8
1	G	626	ALA	2.8
1	D	568	LEU	2.8
1	D	747	LEU	2.8
1	H	636	VAL	2.8
1	A	752	ASP	2.8
1	C	743	LEU	2.8
1	H	610	ALA	2.8
1	A	748	ASN	2.8
1	A	664	ALA	2.8
1	D	424	ASP	2.8
1	G	753	ALA	2.8
1	F	374	HIS	2.8
1	D	362	PHE	2.8
1	F	585	GLY	2.8
1	B	383	PHE	2.8
1	H	368	ASP	2.8
1	G	499	ASP	2.7
1	D	364	LYS	2.7
1	A	361	SER	2.7
1	B	454	HIS	2.7
1	I	587	ARG	2.7
1	A	615	PHE	2.7
1	D	459	VAL	2.7
1	I	652	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	439	SER	2.7
1	D	410	LYS	2.7
1	E	500	HIS	2.7
1	B	512	PHE	2.7
1	E	648	VAL	2.7
1	J	434	LYS	2.7
1	H	390	PRO	2.7
1	G	417	PHE	2.7
1	A	419	THR	2.7
1	C	357	ALA	2.7
1	D	442	LEU	2.7
1	H	444	LEU	2.7
1	B	566	ILE	2.7
1	J	598	PHE	2.7
1	H	706	ASP	2.7
1	I	623	LYS	2.7
1	G	660	ARG	2.7
1	E	443	PRO	2.7
1	B	347	SER	2.6
1	D	394	PRO	2.6
1	H	439	SER	2.6
1	H	580	LEU	2.6
1	C	620	ASN	2.6
1	G	558	LEU	2.6
1	H	717	LEU	2.6
1	H	608	ARG	2.6
1	J	371	ALA	2.6
1	G	654	TRP	2.6
1	C	449	GLU	2.6
1	F	441	ASP	2.6
1	F	596	VAL	2.6
1	H	685	PHE	2.6
1	B	499	ASP	2.6
1	H	741	ARG	2.6
1	I	346	PRO	2.6
1	I	738	ARG	2.6
1	I	533	GLU	2.6
1	A	638	GLN	2.6
1	F	363	SER	2.6
1	G	560	LYS	2.6
1	B	689	PRO	2.6
1	E	437	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	410	LYS	2.6
1	D	748	ASN	2.6
1	B	740	GLU	2.6
1	E	419	THR	2.6
1	E	381	VAL	2.6
1	G	457	LEU	2.6
1	I	534	LYS	2.6
1	E	527	TYR	2.6
1	G	387	LEU	2.6
1	G	647	LEU	2.6
1	C	705	GLU	2.5
1	B	586	LYS	2.5
1	I	588	PHE	2.5
1	I	615	PHE	2.5
1	I	380	GLU	2.5
1	A	611	ILE	2.5
1	E	363	SER	2.5
1	E	737	ASP	2.5
1	H	574	GLU	2.5
1	H	448	ARG	2.5
1	A	371	ALA	2.5
1	G	534	LYS	2.5
1	D	608	ARG	2.5
1	H	342	ILE	2.5
1	C	499	ASP	2.5
1	D	372	TYR	2.5
1	D	759	PRO	2.5
1	C	370	MET	2.5
1	A	372	TYR	2.5
1	H	438	ASP	2.5
1	I	429	TYR	2.5
1	A	522	THR	2.5
1	J	416	VAL	2.5
1	B	361	SER	2.5
1	B	445	ASN	2.5
1	E	747	LEU	2.5
1	C	544	SER	2.5
1	I	565	VAL	2.5
1	G	704	ASP	2.5
1	A	515	SER	2.5
1	D	544	SER	2.5
1	D	624	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	704	ASP	2.4
1	D	658	MET	2.4
1	G	439	SER	2.4
1	G	437	VAL	2.4
1	G	762	GLU	2.4
1	A	347	SER	2.4
1	B	385	SER	2.4
1	C	451	LEU	2.4
1	B	484	PHE	2.4
1	I	744	ARG	2.4
1	C	732	THR	2.4
1	G	516	HIS	2.4
1	F	598	PHE	2.4
1	H	541	MET	2.4
1	E	343	TRP	2.4
1	C	619	LEU	2.4
1	F	444	LEU	2.4
1	G	350	VAL	2.4
1	B	525	ASP	2.4
1	C	371	ALA	2.4
1	H	611	ILE	2.4
1	B	513	GLN	2.4
1	E	450	THR	2.4
1	E	732	THR	2.4
1	I	463	LYS	2.4
1	I	487	GLU	2.4
1	J	448	ARG	2.4
1	C	748	ASN	2.4
1	G	423	HIS	2.4
1	H	452	GLN	2.4
1	J	430	LEU	2.4
1	B	473	LYS	2.4
1	J	619	LEU	2.4
1	D	484	PHE	2.3
1	D	604	THR	2.3
1	G	413	VAL	2.3
1	A	365	GLU	2.3
1	D	452	GLN	2.3
1	A	413	VAL	2.3
1	D	425	MET	2.3
1	H	539	TYR	2.3
1	J	387	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	472	ILE	2.3
1	D	553	PRO	2.3
1	H	435	GLY	2.3
1	B	387	LEU	2.3
1	I	529	GLU	2.3
1	B	409	ILE	2.3
1	B	456	LEU	2.3
1	H	525	ASP	2.3
1	I	706	ASP	2.3
1	C	689	PRO	2.3
1	I	626	ALA	2.3
1	I	649	ALA	2.3
1	H	665	GLN	2.3
1	E	357	ALA	2.3
1	I	748	ASN	2.3
1	J	386	ILE	2.3
1	A	746	SER	2.3
1	B	621	TRP	2.3
1	C	408	TYR	2.3
1	D	481	ASN	2.3
1	H	557	ARG	2.3
1	H	584	ASP	2.3
1	A	685	PHE	2.3
1	I	376	THR	2.3
1	B	425	MET	2.3
1	H	369	PRO	2.3
1	G	513	GLN	2.3
1	H	453	GLN	2.3
1	D	360	LYS	2.3
1	H	633	LYS	2.3
1	B	595	GLY	2.3
1	I	482	ASP	2.3
1	I	536	ASP	2.3
1	I	390	PRO	2.3
1	D	375	PHE	2.3
1	F	439	SER	2.3
1	G	607	SER	2.3
1	D	761	GLU	2.2
1	B	683	LYS	2.2
1	J	677	TYR	2.2
1	C	740	GLU	2.2
1	B	640	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	421	ASP	2.2
1	I	731	ASP	2.2
1	J	422	PHE	2.2
1	H	578	GLN	2.2
1	J	361	SER	2.2
1	G	695	LYS	2.2
1	B	414	ARG	2.2
1	C	686	GLU	2.2
1	A	603	LYS	2.2
1	B	623	LYS	2.2
1	F	411	LEU	2.2
1	G	472	ILE	2.2
1	G	760	GLU	2.2
1	H	445	ASN	2.2
1	C	597	LYS	2.2
1	H	756	GLU	2.2
1	I	550	GLU	2.2
1	C	758	GLU	2.2
1	I	369	PRO	2.2
1	I	512	PHE	2.2
1	B	446	VAL	2.2
1	D	555	VAL	2.2
1	J	561	LYS	2.2
1	D	659	GLU	2.2
1	F	740	GLU	2.2
1	E	442	LEU	2.2
1	F	748	ASN	2.2
1	G	620	ASN	2.2
1	I	692	PRO	2.2
1	G	574	GLU	2.2
1	H	710	VAL	2.2
1	G	429	TYR	2.2
1	C	609	GLU	2.2
1	I	650	SER	2.2
1	B	511	ARG	2.2
1	F	360	LYS	2.2
1	E	445	ASN	2.2
1	I	481	ASN	2.2
1	H	340	LYS	2.2
1	J	457	LEU	2.2
1	I	353	ASP	2.2
1	J	540	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	437	VAL	2.2
1	H	653	GLY	2.2
1	C	644	PRO	2.2
1	I	368	ASP	2.2
1	I	740	GLU	2.2
1	B	590	ASN	2.2
1	C	411	LEU	2.1
1	G	619	LEU	2.1
1	F	571	PRO	2.1
1	B	505	ARG	2.1
1	B	731	ASP	2.1
1	G	367	ASP	2.1
1	A	454	HIS	2.1
1	H	626	ALA	2.1
1	C	347	SER	2.1
1	G	465	VAL	2.1
1	G	565	VAL	2.1
1	I	472	ILE	2.1
1	D	435	GLY	2.1
1	A	747	LEU	2.1
1	D	441	ASP	2.1
1	E	584	ASP	2.1
1	I	563	TYR	2.1
1	B	410	LYS	2.1
1	B	533	GLU	2.1
1	G	590	ASN	2.1
1	I	572	VAL	2.1
1	I	596	VAL	2.1
1	D	744	ARG	2.1
1	H	605	LYS	2.1
1	J	486	LYS	2.1
1	B	362	PHE	2.1
1	J	539	TYR	2.1
1	A	457	LEU	2.1
1	H	748	ASN	2.1
1	F	392	SER	2.1
1	G	392	SER	2.1
1	G	393	ALA	2.1
1	H	412	TYR	2.1
1	D	417	PHE	2.1
1	G	408	TYR	2.1
1	H	355	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	597	LYS	2.1
1	B	648	VAL	2.1
1	H	624	ASP	2.1
1	D	554	PHE	2.1
1	I	616	GLU	2.1
1	J	365	GLU	2.1
1	B	416	VAL	2.1
1	D	389	VAL	2.1
1	B	523	SER	2.1
1	F	499	ASP	2.1
1	H	640	LEU	2.1
1	J	436	VAL	2.1
1	J	420	ASP	2.1
1	B	508	LYS	2.0
1	H	747	LEU	2.0
1	I	430	LEU	2.0
1	J	441	ASP	2.0
1	D	413	VAL	2.0
1	D	418	ILE	2.0
1	D	450	THR	2.0
1	G	510	LEU	2.0
1	H	356	LYS	2.0
1	I	727	TYR	2.0
1	J	417	PHE	2.0
1	A	705	GLU	2.0
1	G	556	GLU	2.0
1	H	674	SER	2.0
1	H	389	VAL	2.0
1	H	411	LEU	2.0
1	H	618	LEU	2.0
1	E	760	GLU	2.0
1	A	597	LYS	2.0
1	D	456	LEU	2.0
1	B	468	THR	2.0
1	B	720	THR	2.0
1	H	590	ASN	2.0
1	D	559	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.