



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 2O1T / pdb_00002o1t
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

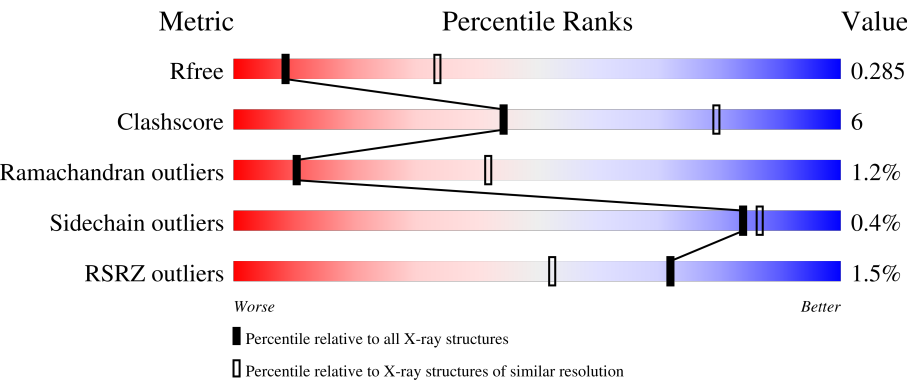
1 Overall quality at a glance i

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.



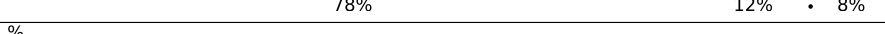
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 80% 11% 8%
1	B	450	2% 80% 11% 8%
1	C	450	% 81% 9% 8%
1	D	450	% 78% 13% 8%
1	E	450	% 77% 14% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	450	 74% 16% • 8%
1	G	450	 2% 78% 12% • 8%
1	H	450	 % 78% 14% 8%
1	I	450	 4% 80% 10% • 8%
1	J	450	 78% 14% 8%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

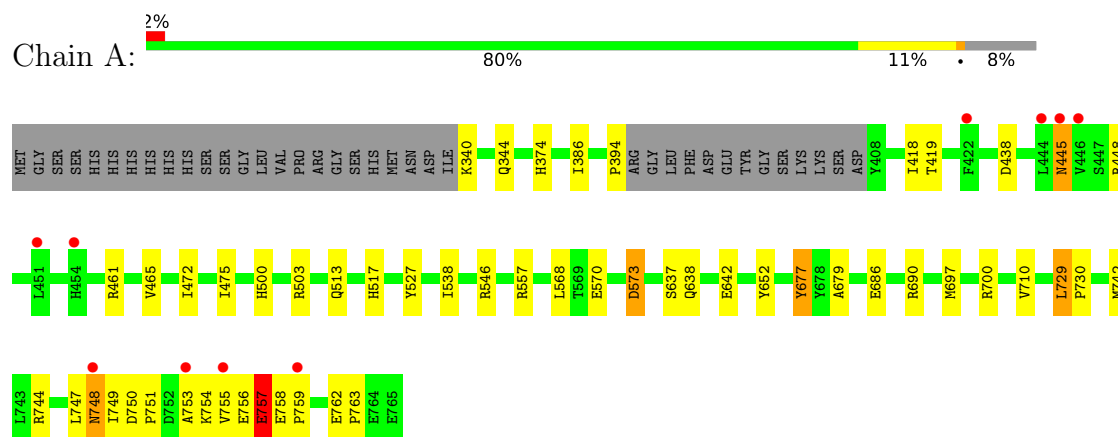
Continued from previous page...

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

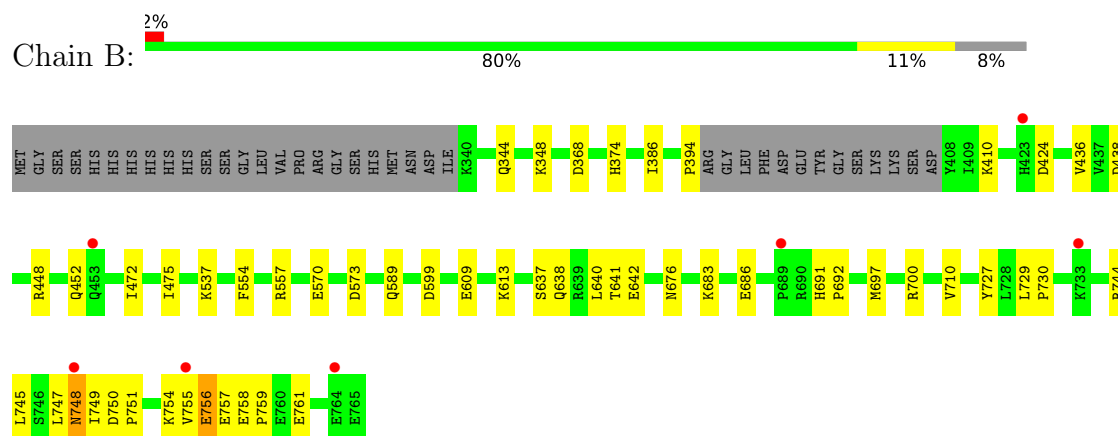
3 Residue-property plots [i](#)

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

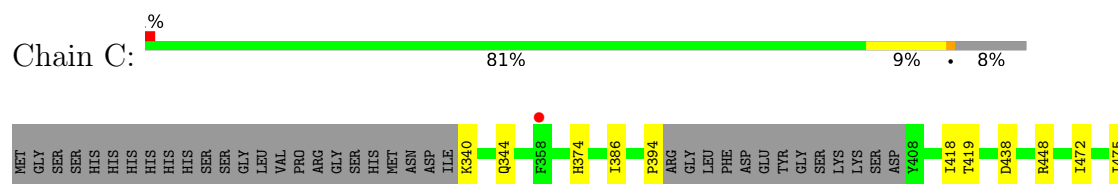
• Molecule 1: Endoplasmin



• Molecule 1: Endoplasmin

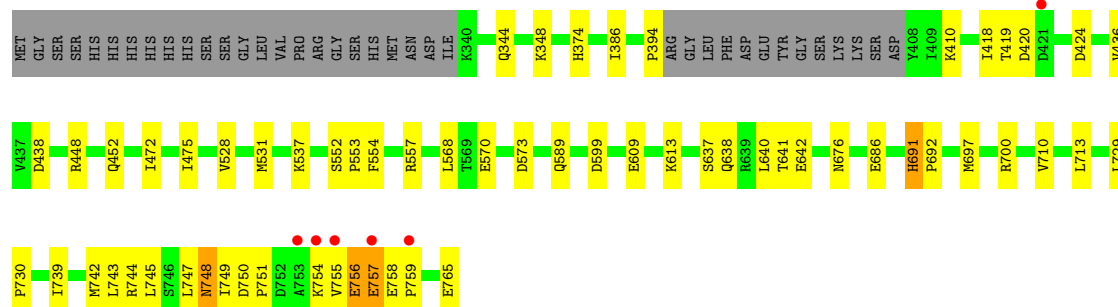
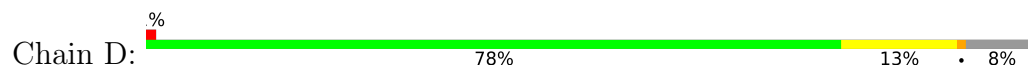


• Molecule 1: Endoplasmin

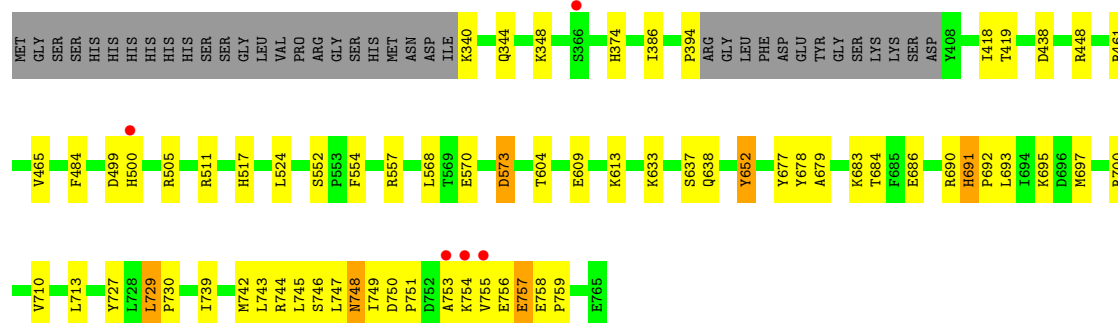
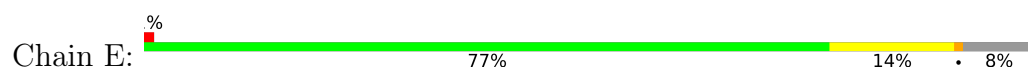




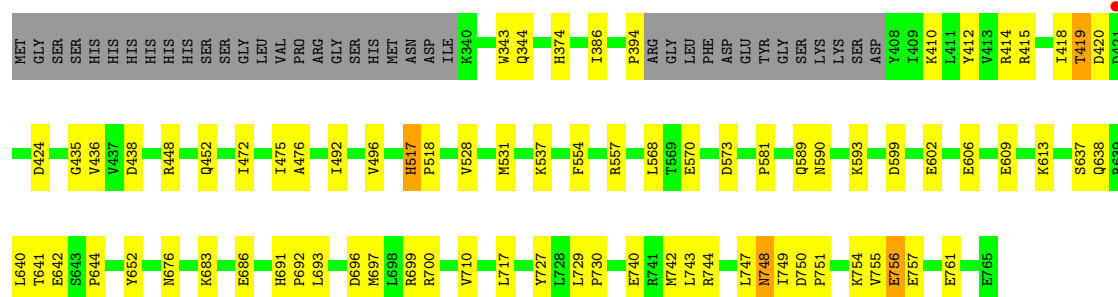
• Molecule 1: Endoplasmic



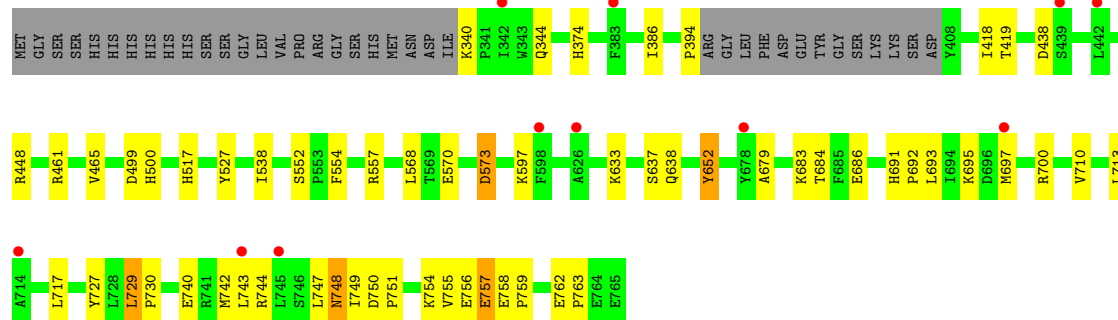
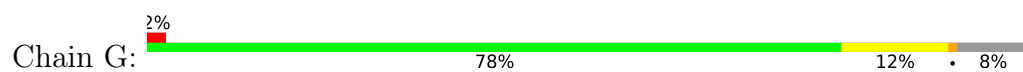
• Molecule 1: Endoplasmic



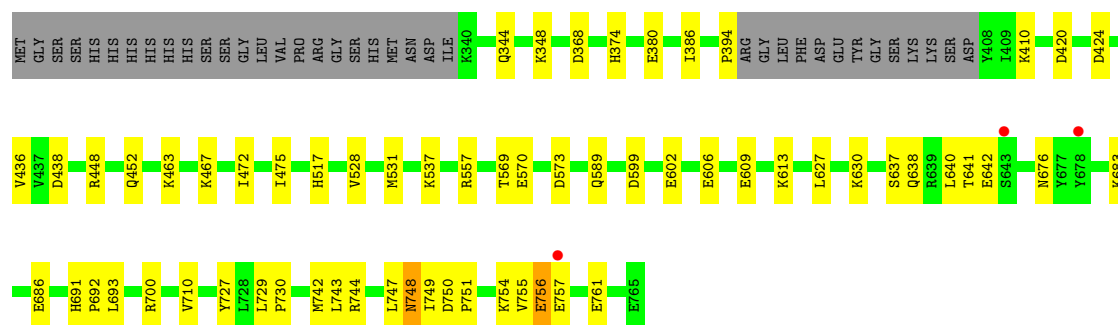
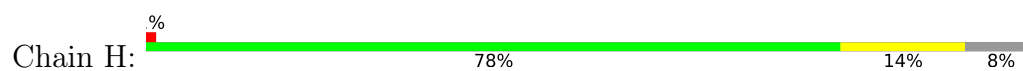
• Molecule 1: Endoplasmic



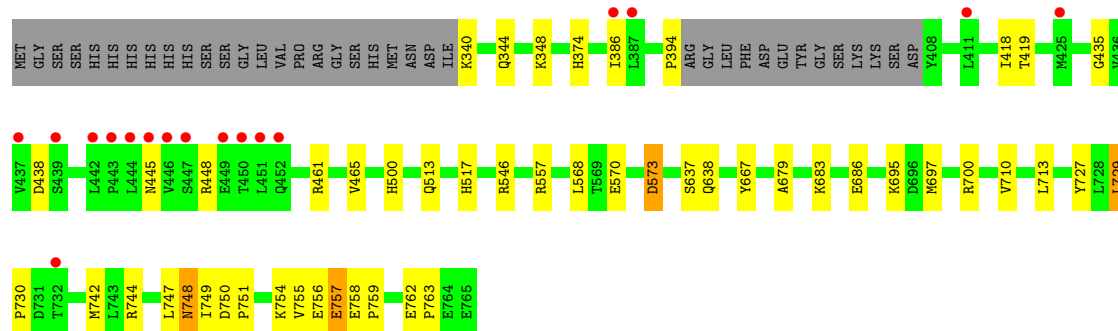
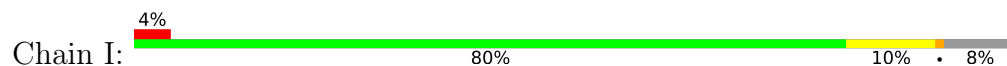
• Molecule 1: Endoplasmic



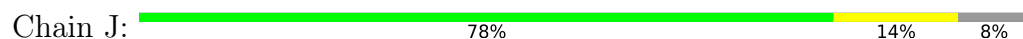
• Molecule 1: Endoplasmic

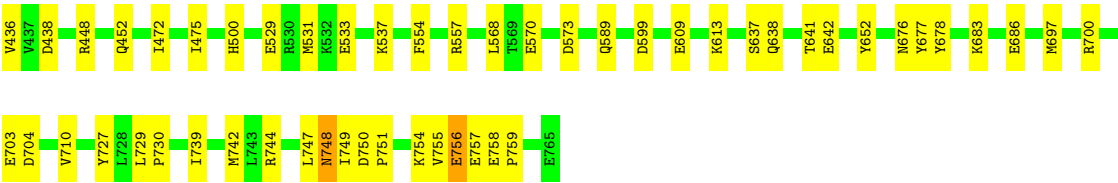


• Molecule 1: Endoplasmic



• Molecule 1: 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 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.20) 99.3 (20.00-3.20)	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 (4.98%)	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 , 163.2	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	0.92	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	0.67	2/3368 (0.1%)	1.02	11/4543 (0.2%)
1	B	0.48	0/3368	0.95	7/4543 (0.2%)
1	C	0.53	1/3368 (0.0%)	0.98	10/4543 (0.2%)
1	D	0.53	0/3368	0.96	7/4543 (0.2%)
1	E	0.65	0/3368	1.02	15/4543 (0.3%)
1	F	0.62	0/3368	0.98	9/4543 (0.2%)
1	G	0.55	0/3366	0.98	11/4540 (0.2%)
1	H	0.46	0/3368	0.95	10/4543 (0.2%)
1	I	0.45	0/3368	0.97	11/4543 (0.2%)
1	J	0.59	0/3368	0.98	7/4543 (0.2%)
All	All	0.56	3/33678 (0.0%)	0.98	98/45427 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	TYR	CA-CB	-8.01	1.40	1.53
1	C	677	TYR	CA-CB	-5.40	1.44	1.53
1	A	677	TYR	CA-C	-5.06	1.46	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	394	PRO	N-CA-CB	8.77	112.64	103.00
1	B	394	PRO	N-CA-CB	8.33	112.16	103.00
1	E	394	PRO	N-CA-CB	8.29	112.12	103.00
1	A	394	PRO	N-CA-CB	8.28	112.11	103.00
1	J	394	PRO	N-CA-CB	8.27	112.10	103.00
1	G	394	PRO	N-CA-CB	8.22	112.05	103.00
1	C	394	PRO	N-CA-CB	8.17	111.99	103.00
1	H	394	PRO	N-CA-CB	8.16	111.98	103.00
1	D	394	PRO	N-CA-CB	8.02	111.83	103.00
1	I	394	PRO	N-CA-CB	7.92	111.72	103.00
1	A	729	LEU	CA-C-N	7.36	126.62	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	LEU	C-N-CA	7.36	126.62	118.97
1	A	573	ASP	N-CA-C	7.32	119.89	111.11
1	D	756	GLU	N-CA-C	-7.05	103.55	112.93
1	E	517	HIS	CA-C-N	6.96	128.54	119.84
1	E	517	HIS	C-N-CA	6.96	128.54	119.84
1	I	340	LYS	CA-C-N	6.61	126.64	119.89
1	I	340	LYS	C-N-CA	6.61	126.64	119.89
1	C	729	LEU	CA-C-N	6.61	126.11	119.24
1	C	729	LEU	C-N-CA	6.61	126.11	119.24
1	E	573	ASP	N-CA-C	6.60	119.03	111.11
1	A	679	ALA	N-CA-C	-6.59	104.88	113.12
1	I	517	HIS	CA-C-N	6.57	128.05	119.84
1	I	517	HIS	C-N-CA	6.57	128.05	119.84
1	A	517	HIS	CA-C-N	6.54	128.02	119.84
1	A	517	HIS	C-N-CA	6.54	128.02	119.84
1	I	729	LEU	CA-C-N	6.51	126.02	119.24
1	I	729	LEU	C-N-CA	6.51	126.02	119.24
1	E	729	LEU	CA-C-N	6.51	126.01	119.24
1	E	729	LEU	C-N-CA	6.51	126.01	119.24
1	A	340	LYS	CA-C-N	6.51	126.53	119.89
1	A	340	LYS	C-N-CA	6.51	126.53	119.89
1	G	517	HIS	CA-C-N	6.50	127.97	119.84
1	G	517	HIS	C-N-CA	6.50	127.97	119.84
1	C	573	ASP	N-CA-C	6.46	118.86	111.11
1	D	554	PHE	N-CA-C	6.41	119.08	111.71
1	C	679	ALA	N-CA-C	-6.37	105.16	113.12
1	G	573	ASP	N-CA-C	6.35	118.72	111.11
1	I	573	ASP	N-CA-C	6.32	118.69	111.11
1	G	729	LEU	CA-C-N	6.27	125.76	119.24
1	G	729	LEU	C-N-CA	6.27	125.76	119.24
1	C	517	HIS	CA-C-N	6.24	127.64	119.84
1	C	517	HIS	C-N-CA	6.24	127.64	119.84
1	J	599	ASP	N-CA-C	6.19	118.54	111.11
1	J	756	GLU	N-CA-C	-6.18	103.66	112.13
1	D	599	ASP	N-CA-C	6.08	118.41	111.11
1	F	756	GLU	N-CA-C	-5.98	103.94	112.13
1	B	756	GLU	N-CA-C	-5.93	104.01	112.13
1	G	679	ALA	N-CA-C	-5.91	105.74	113.12
1	I	679	ALA	N-CA-C	-5.89	105.75	113.12
1	B	599	ASP	N-CA-C	5.84	118.12	111.11
1	E	505	ARG	N-CA-C	-5.80	104.55	111.69
1	H	599	ASP	N-CA-C	5.68	117.93	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	757	GLU	N-CA-C	5.64	122.81	110.80
1	J	554	PHE	N-CA-C	5.59	118.14	111.71
1	A	757	GLU	N-CA-C	5.58	122.67	110.80
1	J	368	ASP	N-CA-C	5.57	117.58	109.84
1	H	756	GLU	N-CA-C	-5.56	104.12	111.96
1	D	640	LEU	N-CA-C	5.55	118.28	109.24
1	F	599	ASP	N-CA-C	5.46	117.67	111.11
1	H	368	ASP	N-CA-C	5.45	117.41	109.84
1	B	554	PHE	N-CA-C	5.44	117.96	111.71
1	C	757	GLU	N-CA-C	5.39	122.28	110.80
1	J	531	MET	N-CA-C	5.36	117.21	110.24
1	B	640	LEU	N-CA-C	5.29	117.86	109.24
1	G	340	LYS	CA-C-N	5.29	126.45	119.84
1	G	340	LYS	C-N-CA	5.29	126.45	119.84
1	E	484	PHE	N-CA-C	5.28	117.45	111.11
1	D	691	HIS	CA-C-N	5.28	126.44	119.84
1	D	691	HIS	C-N-CA	5.28	126.44	119.84
1	E	679	ALA	N-CA-C	-5.26	106.54	113.12
1	F	761	GLU	N-CA-C	-5.26	106.54	113.17
1	E	340	LYS	CA-C-N	5.25	126.41	119.84
1	E	340	LYS	C-N-CA	5.25	126.41	119.84
1	F	640	LEU	N-CA-C	5.24	117.78	109.24
1	H	640	LEU	N-CA-C	5.21	117.74	109.24
1	E	691	HIS	CA-C-N	5.21	125.26	119.32
1	E	691	HIS	C-N-CA	5.21	125.26	119.32
1	J	739	ILE	N-CA-C	-5.20	105.33	111.00
1	C	340	LYS	CA-C-N	5.19	126.33	119.84
1	C	340	LYS	C-N-CA	5.19	126.33	119.84
1	G	757	GLU	N-CA-C	5.18	121.83	110.80
1	F	517	HIS	CA-C-N	5.17	126.31	119.84
1	F	517	HIS	C-N-CA	5.17	126.31	119.84
1	I	757	GLU	N-CA-C	5.17	121.80	110.80
1	F	435	GLY	N-CA-C	5.16	118.01	110.63
1	H	761	GLU	N-CA-C	-5.16	106.67	113.17
1	B	761	GLU	N-CA-C	-5.15	106.68	113.17
1	I	435	GLY	N-CA-C	5.05	117.41	110.69
1	F	554	PHE	N-CA-C	5.05	117.52	111.71
1	B	368	ASP	N-CA-C	5.03	116.84	109.84
1	G	499	ASP	N-CA-C	5.03	117.32	108.56
1	H	517	HIS	CA-C-N	5.02	125.30	119.47
1	H	517	HIS	C-N-CA	5.02	125.30	119.47
1	H	691	HIS	CA-C-N	5.02	126.11	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	691	HIS	C-N-CA	5.02	126.11	119.84
1	E	499	ASP	N-CA-C	5.01	117.28	108.56
1	A	503	ARG	N-CA-C	5.00	116.42	111.07

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	47	4
1	B	3301	0	3196	28	0
1	C	3301	0	3196	42	0
1	D	3301	0	3196	52	1
1	E	3301	0	3196	69	1
1	F	3301	0	3196	61	5
1	G	3300	0	3194	49	1
1	H	3301	0	3196	38	0
1	I	3301	0	3196	33	2
1	J	3301	0	3196	67	0
All	All	33009	0	31958	387	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 (387) 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:F:742:MET:HE3	1:G:742:MET:HE3	1.18	1.09
1:D:742:MET:HE3	1:E:742:MET:HE3	1.34	1.06
1:D:759:PRO:HD3	1:E:692:PRO:HD3	1.38	1.05
1:A:750:ASP:CG	1:E:652:TYR:HB2	1.84	1.02
1:A:754:LYS:HD3	1:E:678:TYR:OH	1.61	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:652:TYR:CE2	1:J:756:GLU:CD	2.40	0.99
1:C:757:GLU:OE2	1:J:677:TYR:CA	2.11	0.98
1:C:757:GLU:CD	1:J:677:TYR:HA	1.91	0.95
1:D:742:MET:HE3	1:E:742:MET:CE	1.96	0.94
1:E:500:HIS:NE2	1:J:703:GLU:HB3	1.83	0.93
1:F:742:MET:HE3	1:G:742:MET:CE	1.99	0.91
1:D:743:LEU:HD22	1:E:713:LEU:HG	1.52	0.91
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:742:MET:HE3	1:I:742:MET:HE3	1.57	0.84
1:H:692:PRO:HB3	1:I:754:LYS:HE3	1.63	0.81
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:F:742:MET:CE	1:G:742:MET:HE3	2.10	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:690:ARG:O	1:J:758:GLU:HB3	2.00	0.61
1:C:757:GLU:CG	1:J:677:TYR:HA	2.30	0.61
1:H:750:ASP:HB3	1:H:754:LYS:HG2	1.83	0.61
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: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:A:742:MET:HE3	1:J:742:MET:HE3	1.87	0.57
1:A:570:GLU:HB2	1:A:573:ASP:CG	2.30	0.56
1:F:557:ARG:HD3	1:F:638:GLN:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:GLU:HB2	1:E:573:ASP:CG	2.30	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
1:I:344:GLN:NE2	1:I:438:ASP:OD2	2.38	0.55
1:F:424:ASP:CG	1:F:452:GLN:HE21	2.15	0.55
1:I:570:GLU:HB2	1:I:573:ASP:CG	2.31	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: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:H:380:GLU:CD	1:J:533:GLU:HB2	2.33	0.54
1:F:652:TYR:CZ	1:J:756:GLU:HG2	2.43	0.54
1:G:570:GLU:HB2	1:G:573:ASP:CG	2.32	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:F:652:TYR:CD2	1:J:756:GLU:CD	2.86	0.53
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:A:754:LYS:HD3	1:E:678:TYR:CZ	2.43	0.53
1:J:754:LYS:C	1:J:756:GLU:H	2.16	0.52
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H	1:C:500:HIS:CD2	2.29	0.51
1:A:750:ASP:HB2	1:E:652:TYR:HB2	1.92	0.51
1:C:570:GLU:HB2	1:C:573:ASP:CG	2.35	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
1:A:500:HIS:CD2	1:A:500:HIS:H	2.28	0.50
1:F:754:LYS:C	1:F:756:GLU:H	2.18	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:H:424:ASP:CG	1:H:452:GLN:HE21	2.19	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:J:424:ASP:CG	1:J:452:GLN:HE21	2.20	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:C:744:ARG:NH2	1:C:755:VAL:HB	2.26	0.49
1:D:754:LYS:C	1:D:756:GLU:H	2.19	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:B:754:LYS:C	1:B:756:GLU:H	2.21	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: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:C:757:GLU:HG2	1:J:677:TYR:CA	2.44	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:424:ASP:CG	1:D:452:GLN:HE21	2.22	0.47
1:F:750:ASP:O	1:F:754:LYS:HB2	2.14	0.47
1:H:754:LYS:C	1:H:756:GLU:H	2.21	0.47
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:CD2	1:I:500:HIS:H	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: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:C:757:GLU:HG2	1:J:677:TYR:CB	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:J:348:LYS:HB2	1.73	0.45
1:A:697:MET:HE3	1:A:697:MET:HB2	1.87	0.45
1:A:742:MET:CE	1:J:742:MET:HE3	2.46	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
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:H:570:GLU:HB2	1:H:573:ASP:CG	2.41	0.45
1:I:683:LYS:HE3	1:I:727:TYR:CE1	2.51	0.45
1:B:570:GLU:HB2	1:B:573:ASP:CG	2.42	0.45
1:C:683:LYS:HE3	1:C:727:TYR:CE1	2.51	0.45
1:B:424:ASP:CG	1:B:452:GLN:HE21	2.23	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:697:MET:HE3	1:J:697:MET:HB2	1.79	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: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:G:754:LYS:C	1:G:756:GLU:H	2.25	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:G:754:LYS:C	1:G:756:GLU:N	2.74	0.44
1:H:641:THR:HG22	1:H:642:GLU:HG3	1.99	0.44
1:B:697:MET:HE3	1:B:697:MET:HB2	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:700:ARG:HD2	1:H:710:VAL:CG2	2.48	0.44
1:F:641:THR:HG22	1:F:642:GLU:HG3	2.00	0.44
1:D:348:LYS:HB2	1:D:348:LYS:HE3	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:F:754:LYS:C	1:F:756:GLU:N	2.75	0.43
1:A:754:LYS:C	1:A:756:GLU:H	2.25	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:E:697:MET:HE3	1:E:697:MET:HB2	1.86	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
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:754:LYS:C	1:A:756:GLU:N	2.74	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:E:754:LYS:C	1:E:756:GLU:N	2.76	0.43
1:G:713:LEU:HD23	1:G:713:LEU:C	2.44	0.43
1:B:537:LYS:HE2	1:B:589:GLN:HB2	2.01	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:HE3	1:B:348:LYS:HB2	1.76	0.43
1:C:517:HIS:HA	1:C:518:PRO:HD2	1.78	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:J:754:LYS:C	1:J:756:GLU:N	2.76	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:C:754:LYS:C	1:C:756:GLU:N	2.76	0.42
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:697:MET:HE3	1:D:697:MET:HB2	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:754:LYS:NZ	1:J:678:TYR:CE2	2.86	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:CD2	1:G:500:HIS:H	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:D:754:LYS:C	1:D:756:GLU:N	2.77	0.42
1:E:568:LEU:HB3	1:E:573:ASP:HB3	2.01	0.42
1:F:570:GLU:HB2	1:F:573:ASP:CG	2.44	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:C:754:LYS:C	1:C:756:GLU:H	2.26	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:A:642:GLU:HG2	1:J:759:PRO:HB3	1.99	0.42
1:C:374:HIS:CD2	1:C:386:ILE:HG12	2.55	0.42
1:D:742:MET:SD	1:E:743:LEU:HD23	2.60	0.42
1:E:745:LEU:C	1:E:747:LEU:H	2.27	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:HE3	1:I:348:LYS:HB2	1.90	0.42
1:J:418:ILE:HG22	1:J:419:THR:HG22	2.01	0.42
1:F:747:LEU:O	1:F:748:ASN:CB	2.67	0.42
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:F:590:ASN:HD22	1:F:593:LYS:HE3	1.85	0.41
1:I:697:MET:HE3	1:I:697:MET:HB2	1.86	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:570:GLU:HB2	1:D:573:ASP:CG	2.45	0.41
1:D:641:THR:HG22	1:D:642:GLU:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:754:LYS:C	1:E:756:GLU:H	2.27	0.41
1:G:695:LYS:HB3	1:G:695:LYS:HE2	1.88	0.41
1:I:754:LYS:C	1:I:756:GLU:N	2.77	0.41
1:I:758:GLU:N	1:I:759:PRO:CD	2.83	0.41
1:J:570:GLU:HB2	1:J:573:ASP:CG	2.45	0.41
1:G:527:TYR:CE2	1:G:538:ILE:HG23	2.55	0.41
1:G:697:MET:HE3	1:G:697:MET:HB2	1.84	0.41
1:H:754:LYS:C	1:H:756:GLU:N	2.78	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:F:697:MET:HE3	1:F:697:MET:HB2	1.79	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:B:745:LEU:C	1:B:747:LEU:H	2.29	0.41
1:B:747:LEU:O	1:B:748:ASN:CB	2.68	0.41
1:D:745:LEU:C	1:D:747:LEU:H	2.29	0.41
1:E:348:LYS:HB2	1:E:348:LYS:HE3	1.91	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: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:I:762:GLU:N	1:I:763:PRO:CD	2.84	0.41
1:J:568:LEU:HB3	1:J:573:ASP:HB3	2.03	0.41
1:A:750:ASP:CB	1:E:652:TYR:CB	2.95	0.41
1:I:754:LYS:C	1:I:756:GLU:H	2.28	0.41
1:I:695:LYS:HB3	1:I:695:LYS:HE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:691:HIS:NE2	1:G:740:GLU:OE2	2.54	0.40
1:A:747:LEU:O	1:A:748:ASN:CB	2.68	0.40
1:F:475:ILE:O	1:F:476:ALA:C	2.64	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:E:500:HIS:ND1	1:J:704:ASP:HB2	2.28	0.40
1:I:513:GLN:HB3	1:I:546:ARG:NH1	2.36	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/450 (91%)	361 (88%)	44 (11%)	4 (1%)	12	45
1	B	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	10	42
1	C	409/450 (91%)	365 (89%)	40 (10%)	4 (1%)	12	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	409/450 (91%)	368 (90%)	35 (9%)	6 (2%)	8	37
1	E	409/450 (91%)	357 (87%)	47 (12%)	5 (1%)	10	42
1	F	409/450 (91%)	365 (89%)	36 (9%)	8 (2%)	6	31
1	G	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	12	45
1	H	409/450 (91%)	367 (90%)	36 (9%)	6 (2%)	8	37
1	I	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	12	45
1	J	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	10	42
All	All	4090/4500 (91%)	3637 (89%)	402 (10%)	51 (1%)	10	42

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
1	H	757	GLU
1	I	748	ASN
1	I	757	GLU
1	J	748	ASN
1	J	749	ILE
1	J	757	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	70	81
1	B	352/410 (86%)	351 (100%)	1 (0%)	86	88
1	C	352/410 (86%)	351 (100%)	1 (0%)	86	88
1	D	352/410 (86%)	351 (100%)	1 (0%)	86	88
1	E	352/410 (86%)	350 (99%)	2 (1%)	78	84
1	F	352/410 (86%)	351 (100%)	1 (0%)	86	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	352/410 (86%)	350 (99%)	2 (1%)	78	84
1	H	352/410 (86%)	351 (100%)	1 (0%)	86	88
1	I	352/410 (86%)	351 (100%)	1 (0%)	86	88
1	J	352/410 (86%)	351 (100%)	1 (0%)	86	88
All	All	3520/4100 (86%)	3506 (100%)	14 (0%)	84	86

All (14) 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	D	448	ARG
1	E	448	ARG
1	E	652	TYR
1	F	448	ARG
1	G	448	ARG
1	G	652	TYR
1	H	448	ARG
1	I	448	ARG
1	J	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	GLN
1	A	651	GLN
1	B	452	GLN
1	C	651	GLN
1	D	423	HIS
1	D	452	GLN
1	E	500	HIS
1	E	513	GLN
1	F	452	GLN
1	F	651	GLN
1	G	651	GLN
1	H	452	GLN
1	I	651	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	423	HIS
1	J	452	GLN
1	J	651	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.03	10 (2%) 59 40	129, 151, 152, 165	0
1	B	413/450 (91%)	-0.08	7 (1%) 69 49	129, 151, 152, 165	0
1	C	413/450 (91%)	-0.15	4 (0%) 79 63	129, 151, 152, 165	0
1	D	413/450 (91%)	-0.21	6 (1%) 72 52	129, 151, 152, 165	0
1	E	413/450 (91%)	-0.08	5 (1%) 76 58	129, 151, 152, 165	0
1	F	413/450 (91%)	-0.17	1 (0%) 91 85	129, 151, 152, 165	0
1	G	413/450 (91%)	0.21	11 (2%) 56 36	129, 151, 152, 165	0
1	H	413/450 (91%)	-0.32	3 (0%) 84 69	129, 151, 152, 165	0
1	I	413/450 (91%)	-0.04	17 (4%) 41 25	129, 151, 152, 165	0
1	J	413/450 (91%)	-0.16	0 100 100	129, 151, 152, 165	0
All	All	4130/4500 (91%)	-0.10	64 (1%) 72 52	129, 151, 153, 165	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	ASN	6.4
1	I	386	ILE	4.4
1	I	446	VAL	4.3
1	E	753	ALA	4.0
1	H	757	GLU	4.0
1	I	451	LEU	3.9
1	E	754	LYS	3.8
1	D	757	GLU	3.6
1	E	755	VAL	3.6
1	A	446	VAL	3.4
1	A	451	LEU	3.4
1	I	443	PRO	3.4
1	D	753	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	442	LEU	3.2
1	G	743	LEU	2.8
1	I	442	LEU	2.8
1	A	444	LEU	2.8
1	C	358	PHE	2.8
1	I	450	THR	2.7
1	I	445	ASN	2.7
1	B	453	GLN	2.6
1	I	452	GLN	2.6
1	H	643	SER	2.6
1	B	733	LYS	2.6
1	A	755	VAL	2.5
1	G	678	TYR	2.5
1	G	714	ALA	2.4
1	I	444	LEU	2.4
1	B	423	HIS	2.4
1	E	500	HIS	2.4
1	E	366	SER	2.4
1	G	439	SER	2.4
1	D	759	PRO	2.4
1	B	755	VAL	2.3
1	C	689	PRO	2.3
1	G	383	PHE	2.3
1	D	755	VAL	2.3
1	G	626	ALA	2.3
1	B	764	GLU	2.3
1	I	437	VAL	2.3
1	A	748	ASN	2.2
1	A	422	PHE	2.2
1	G	342	ILE	2.2
1	I	425	MET	2.2
1	A	454	HIS	2.2
1	C	701	VAL	2.1
1	C	757	GLU	2.1
1	I	439	SER	2.1
1	I	387	LEU	2.1
1	I	411	LEU	2.1
1	I	447	SER	2.1
1	D	421	ASP	2.1
1	G	697	MET	2.1
1	H	678	TYR	2.1
1	I	732	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	689	PRO	2.1
1	G	598	PHE	2.1
1	D	754	LYS	2.0
1	B	748	ASN	2.0
1	G	745	LEU	2.0
1	F	421	ASP	2.0
1	I	449	GLU	2.0
1	A	753	ALA	2.0
1	A	759	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.