



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O1W
Title : Structure of N-terminal plus middle domains (N+M) of GRP94
Authors : Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on : 2006-11-29
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

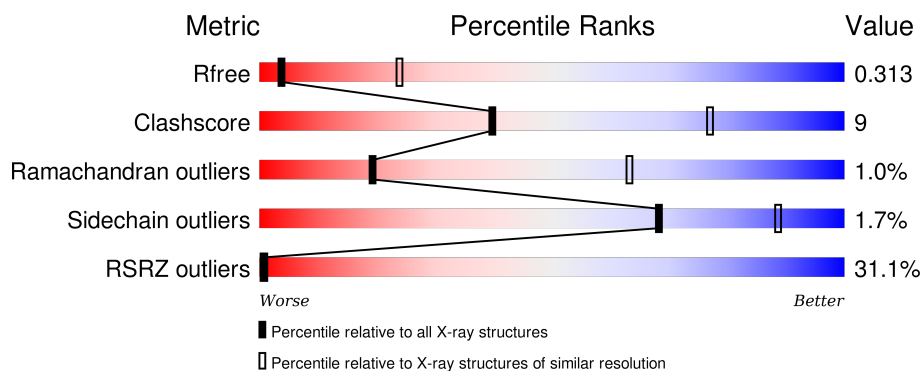
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	506	<div> <div>24%</div> <div>66%</div> <div>15%</div> <div>•</div> <div>18%</div> </div>
1	B	506	<div> <div>19%</div> <div>68%</div> <div>23%</div> <div>•</div> <div>7%</div> </div>
1	C	506	<div> <div>22%</div> <div>65%</div> <div>17%</div> <div>18%</div> </div>
1	D	506	<div> <div>27%</div> <div>67%</div> <div>15%</div> <div>18%</div> </div>
1	E	506	<div> <div>40%</div> <div>69%</div> <div>14%</div> <div>18%</div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17042 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	416	Total	C	N	O	S	0	1	0
			3333	2133	552	638	10			
1	B	469	Total	C	N	O	S	0	0	0
			3710	2373	615	709	13			
1	C	416	Total	C	N	O	S	0	0	0
			3333	2133	552	638	10			
1	D	416	Total	C	N	O	S	0	0	0
			3333	2133	552	638	10			
1	E	416	Total	C	N	O	S	0	0	0
			3333	2133	552	638	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	EXPRESSION TAG	UNP P41148
A	53	GLY	-	EXPRESSION TAG	UNP P41148
A	54	SER	-	EXPRESSION TAG	UNP P41148
A	55	SER	-	EXPRESSION TAG	UNP P41148
A	56	HIS	-	EXPRESSION TAG	UNP P41148
A	57	HIS	-	EXPRESSION TAG	UNP P41148
A	58	HIS	-	EXPRESSION TAG	UNP P41148
A	59	HIS	-	EXPRESSION TAG	UNP P41148
A	60	HIS	-	EXPRESSION TAG	UNP P41148
A	61	HIS	-	EXPRESSION TAG	UNP P41148
A	62	SER	-	EXPRESSION TAG	UNP P41148
A	63	SER	-	EXPRESSION TAG	UNP P41148
A	64	GLY	-	EXPRESSION TAG	UNP P41148
A	65	LEU	-	EXPRESSION TAG	UNP P41148
A	66	VAL	-	EXPRESSION TAG	UNP P41148
A	67	PRO	-	EXPRESSION TAG	UNP P41148
A	68	ARG	-	EXPRESSION TAG	UNP P41148
A	69	GLY	-	EXPRESSION TAG	UNP P41148
A	70	SER	-	EXPRESSION TAG	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	HIS	-	EXPRESSION TAG	UNP P41148
A	72	MET	-	EXPRESSION TAG	UNP P41148
A	287	GLY	-	see remark 999	UNP P41148
A	288	GLY	-	see remark 999	UNP P41148
A	289	GLY	-	see remark 999	UNP P41148
A	290	GLY	-	see remark 999	UNP P41148
B	52	MET	-	EXPRESSION TAG	UNP P41148
B	53	GLY	-	EXPRESSION TAG	UNP P41148
B	54	SER	-	EXPRESSION TAG	UNP P41148
B	55	SER	-	EXPRESSION TAG	UNP P41148
B	56	HIS	-	EXPRESSION TAG	UNP P41148
B	57	HIS	-	EXPRESSION TAG	UNP P41148
B	58	HIS	-	EXPRESSION TAG	UNP P41148
B	59	HIS	-	EXPRESSION TAG	UNP P41148
B	60	HIS	-	EXPRESSION TAG	UNP P41148
B	61	HIS	-	EXPRESSION TAG	UNP P41148
B	62	SER	-	EXPRESSION TAG	UNP P41148
B	63	SER	-	EXPRESSION TAG	UNP P41148
B	64	GLY	-	EXPRESSION TAG	UNP P41148
B	65	LEU	-	EXPRESSION TAG	UNP P41148
B	66	VAL	-	EXPRESSION TAG	UNP P41148
B	67	PRO	-	EXPRESSION TAG	UNP P41148
B	68	ARG	-	EXPRESSION TAG	UNP P41148
B	69	GLY	-	EXPRESSION TAG	UNP P41148
B	70	SER	-	EXPRESSION TAG	UNP P41148
B	71	HIS	-	EXPRESSION TAG	UNP P41148
B	72	MET	-	EXPRESSION TAG	UNP P41148
B	287	GLY	-	see remark 999	UNP P41148
B	288	GLY	-	see remark 999	UNP P41148
B	289	GLY	-	see remark 999	UNP P41148
B	290	GLY	-	see remark 999	UNP P41148
C	52	MET	-	EXPRESSION TAG	UNP P41148
C	53	GLY	-	EXPRESSION TAG	UNP P41148
C	54	SER	-	EXPRESSION TAG	UNP P41148
C	55	SER	-	EXPRESSION TAG	UNP P41148
C	56	HIS	-	EXPRESSION TAG	UNP P41148
C	57	HIS	-	EXPRESSION TAG	UNP P41148
C	58	HIS	-	EXPRESSION TAG	UNP P41148
C	59	HIS	-	EXPRESSION TAG	UNP P41148
C	60	HIS	-	EXPRESSION TAG	UNP P41148
C	61	HIS	-	EXPRESSION TAG	UNP P41148
C	62	SER	-	EXPRESSION TAG	UNP P41148

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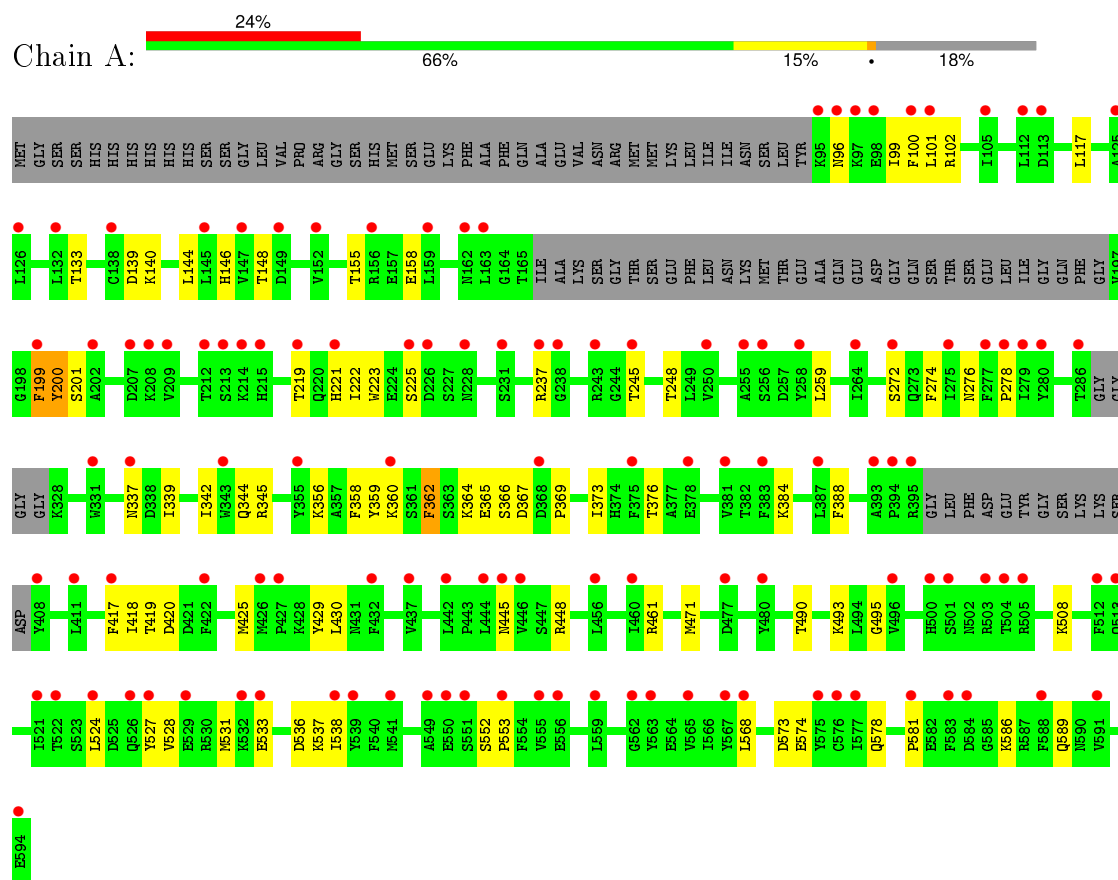
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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	SER	-	EXPRESSION TAG	UNP P41148
C	64	GLY	-	EXPRESSION TAG	UNP P41148
C	65	LEU	-	EXPRESSION TAG	UNP P41148
C	66	VAL	-	EXPRESSION TAG	UNP P41148
C	67	PRO	-	EXPRESSION TAG	UNP P41148
C	68	ARG	-	EXPRESSION TAG	UNP P41148
C	69	GLY	-	EXPRESSION TAG	UNP P41148
C	70	SER	-	EXPRESSION TAG	UNP P41148
C	71	HIS	-	EXPRESSION TAG	UNP P41148
C	72	MET	-	EXPRESSION TAG	UNP P41148
C	287	GLY	-	see remark 999	UNP P41148
C	288	GLY	-	see remark 999	UNP P41148
C	289	GLY	-	see remark 999	UNP P41148
C	290	GLY	-	see remark 999	UNP P41148
D	52	MET	-	EXPRESSION TAG	UNP P41148
D	53	GLY	-	EXPRESSION TAG	UNP P41148
D	54	SER	-	EXPRESSION TAG	UNP P41148
D	55	SER	-	EXPRESSION TAG	UNP P41148
D	56	HIS	-	EXPRESSION TAG	UNP P41148
D	57	HIS	-	EXPRESSION TAG	UNP P41148
D	58	HIS	-	EXPRESSION TAG	UNP P41148
D	59	HIS	-	EXPRESSION TAG	UNP P41148
D	60	HIS	-	EXPRESSION TAG	UNP P41148
D	61	HIS	-	EXPRESSION TAG	UNP P41148
D	62	SER	-	EXPRESSION TAG	UNP P41148
D	63	SER	-	EXPRESSION TAG	UNP P41148
D	64	GLY	-	EXPRESSION TAG	UNP P41148
D	65	LEU	-	EXPRESSION TAG	UNP P41148
D	66	VAL	-	EXPRESSION TAG	UNP P41148
D	67	PRO	-	EXPRESSION TAG	UNP P41148
D	68	ARG	-	EXPRESSION TAG	UNP P41148
D	69	GLY	-	EXPRESSION TAG	UNP P41148
D	70	SER	-	EXPRESSION TAG	UNP P41148
D	71	HIS	-	EXPRESSION TAG	UNP P41148
D	72	MET	-	EXPRESSION TAG	UNP P41148
D	287	GLY	-	see remark 999	UNP P41148
D	288	GLY	-	see remark 999	UNP P41148
D	289	GLY	-	see remark 999	UNP P41148
D	290	GLY	-	see remark 999	UNP P41148

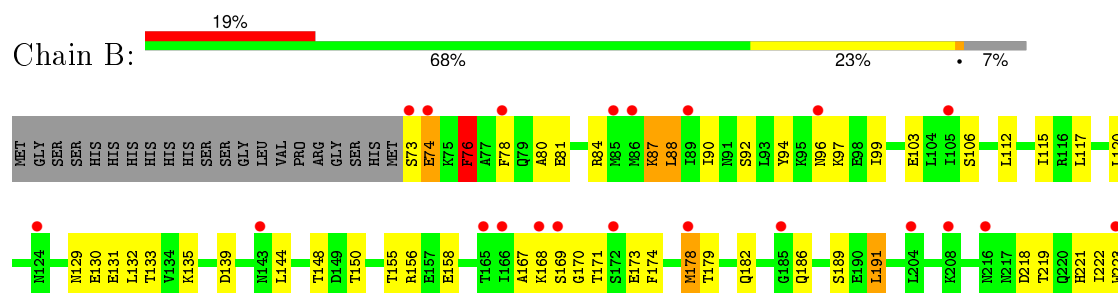
3 Residue-property plots [i](#)

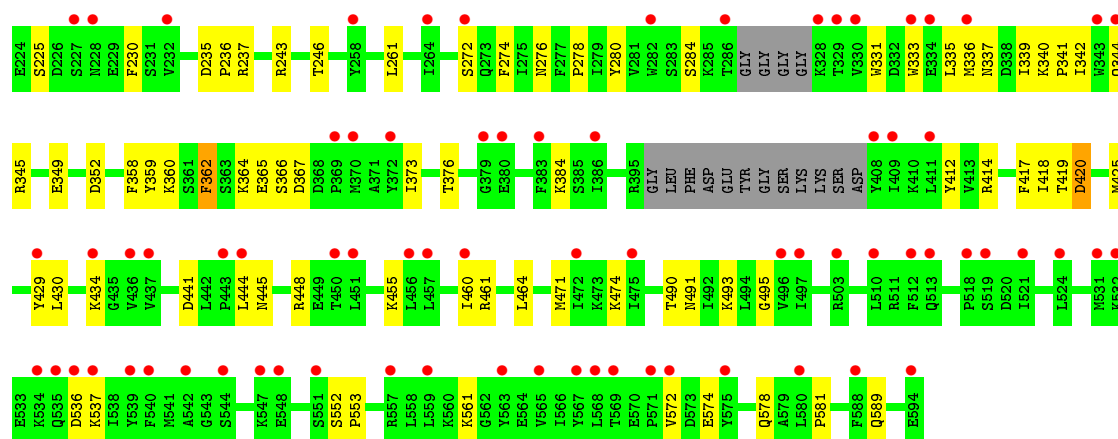
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Endoplasmic

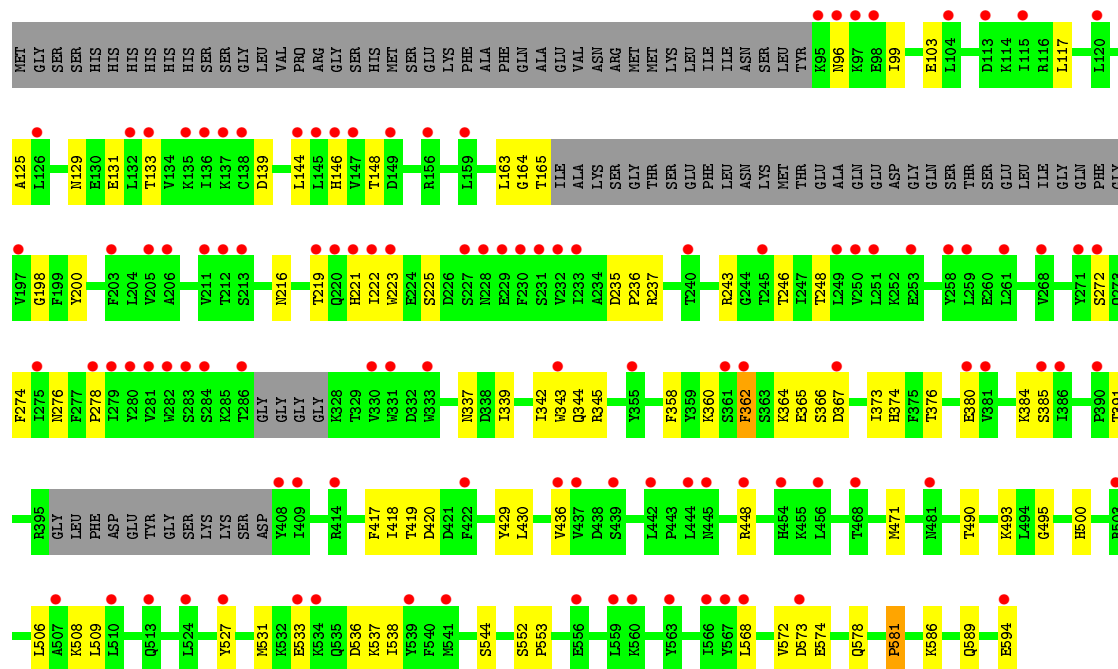


• Molecule 1: Endoplasmic

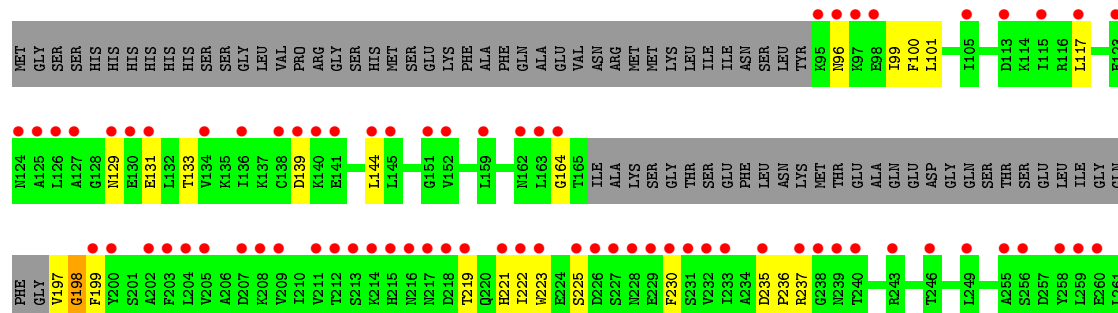


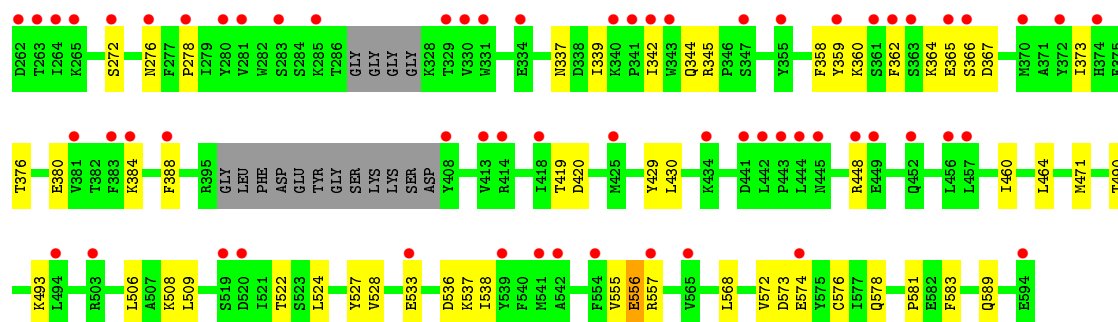


• Molecule 1: Endoplasmic

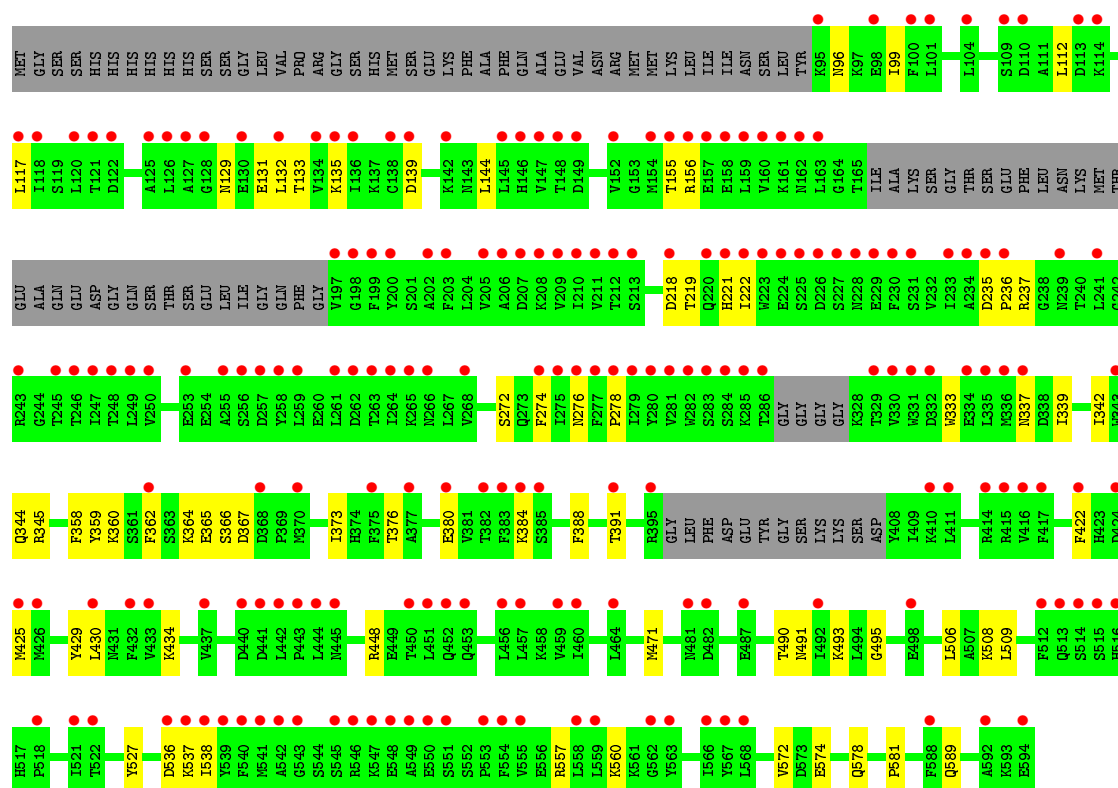
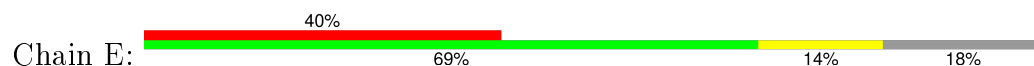


• Molecule 1: Endoplasmic





• Molecule 1: Endoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.33Å 137.50Å 133.15Å 90.00° 124.10° 90.00°	Depositor
Resolution (Å)	47.30 – 3.40 47.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.30-3.40) 98.1 (47.73-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.314 , 0.332 0.294 , 0.313	Depositor DCC
R_{free} test set	2122 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	148.6	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 247.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	3 of 42416 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å ²)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/3400	0.56	0/4599
1	B	0.83	9/3783 (0.2%)	0.71	3/5117 (0.1%)
1	C	0.57	3/3400 (0.1%)	0.56	0/4599
1	D	0.53	1/3400 (0.0%)	0.58	1/4599 (0.0%)
1	E	0.37	0/3400	0.52	0/4599
All	All	0.58	13/17383 (0.1%)	0.59	4/23513 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	LYS	CE-NZ	18.68	1.95	1.49
1	C	164	GLY	C-N	12.88	1.63	1.34
1	B	87	LYS	CD-CE	10.94	1.78	1.51
1	B	87	LYS	CG-CD	10.16	1.86	1.52
1	C	165	THR	CB-OG1	8.56	1.60	1.43
1	C	165	THR	C-O	7.99	1.38	1.23
1	B	81	GLU	CD-OE1	7.93	1.34	1.25
1	B	76	PHE	CE2-CZ	6.58	1.49	1.37
1	D	576	CYS	CB-SG	-6.52	1.71	1.82
1	B	81	GLU	CD-OE2	6.52	1.32	1.25
1	B	74	GLU	CG-CD	5.94	1.60	1.51
1	B	76	PHE	CG-CD2	5.87	1.47	1.38
1	B	76	PHE	CG-CD1	5.26	1.46	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	LYS	CD-CE-NZ	-10.41	87.76	111.70
1	B	76	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	B	87	LYS	CG-CD-CE	-5.73	94.70	111.90
1	D	557	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	3333	0	3257	52	1
1	B	3710	0	3611	111	5
1	C	3333	0	3258	82	1
1	D	3333	0	3258	48	0
1	E	3333	0	3258	47	3
All	All	17042	0	16642	297	5

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 9.

All (297) 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:B:87:LYS:CE	1:B:87:LYS:CD	1.78	1.61
1:B:87:LYS:CG	1:B:87:LYS:CD	1.87	1.49
1:B:455:LYS:CB	1:C:594:GLU:HB2	1.45	1.44
1:B:414:ARG:NH2	1:C:578:GLN:HG2	1.38	1.36
1:B:414:ARG:NH2	1:C:578:GLN:CG	1.89	1.34
1:B:87:LYS:CE	1:B:87:LYS:NZ	1.95	1.28
1:D:366:SER:O	1:E:366:SER:O	1.56	1.18
1:B:414:ARG:HH21	1:C:578:GLN:CB	1.64	1.10
1:B:445:ASN:HB3	1:C:581:PRO:CB	1.82	1.09
1:B:445:ASN:HB3	1:C:581:PRO:HB3	1.24	1.09
1:B:445:ASN:CB	1:C:581:PRO:HG3	1.81	1.09
1:B:445:ASN:CB	1:C:581:PRO:HB3	1.84	1.06
1:B:445:ASN:CB	1:C:581:PRO:CB	2.34	1.05
1:B:278:PRO:HD3	1:B:339:ILE:HD12	1.45	0.99
1:B:414:ARG:HH21	1:C:578:GLN:HB3	1.22	0.99
1:B:414:ARG:HH21	1:C:578:GLN:CG	1.62	0.99
1:B:455:LYS:CB	1:C:594:GLU:CB	2.42	0.98
1:B:445:ASN:CB	1:C:581:PRO:CG	2.41	0.97
1:B:445:ASN:HB3	1:C:581:PRO:CG	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:GLU:OE1	1:D:533:GLU:HB2	1.67	0.94
1:B:414:ARG:HH22	1:C:578:GLN:HG2	0.85	0.93
1:E:278:PRO:HD3	1:E:339:ILE:HD12	1.50	0.91
1:B:445:ASN:CG	1:C:581:PRO:HG3	1.89	0.90
1:B:445:ASN:HB3	1:C:581:PRO:HG3	1.54	0.89
1:B:222:ILE:HD11	1:B:237:ARG:HH21	1.36	0.88
1:D:278:PRO:HD3	1:D:339:ILE:HD12	1.56	0.88
1:A:278:PRO:HD3	1:A:339:ILE:HD12	1.53	0.88
1:C:278:PRO:HD3	1:C:339:ILE:HD12	1.54	0.87
1:B:445:ASN:HB2	1:C:581:PRO:CB	2.04	0.86
1:B:364:LYS:C	1:B:366:SER:H	1.79	0.85
1:B:414:ARG:HH22	1:C:578:GLN:CG	1.65	0.84
1:A:533:GLU:HB2	1:E:380:GLU:OE1	1.78	0.83
1:B:445:ASN:HB2	1:C:581:PRO:CA	2.07	0.83
1:C:364:LYS:C	1:C:366:SER:H	1.82	0.83
1:E:364:LYS:C	1:E:366:SER:H	1.81	0.82
1:B:222:ILE:HD11	1:B:237:ARG:NH2	1.94	0.81
1:B:441:ASP:HA	1:C:578:GLN:HE22	1.46	0.79
1:B:78:PHE:HZ	1:B:225:SER:HG	1.31	0.79
1:A:364:LYS:C	1:A:366:SER:H	1.83	0.79
1:B:414:ARG:NH2	1:C:578:GLN:CD	2.34	0.78
1:D:364:LYS:C	1:D:366:SER:H	1.85	0.78
1:A:222:ILE:HD11	1:A:237:ARG:HH21	1.49	0.78
1:D:222:ILE:HD11	1:D:237:ARG:HH21	1.53	0.74
1:B:344:GLN:OE1	1:B:384:LYS:HD2	1.87	0.74
1:E:222:ILE:HD11	1:E:237:ARG:HH21	1.52	0.74
1:C:222:ILE:HD11	1:C:237:ARG:HH21	1.54	0.72
1:B:441:ASP:HA	1:C:578:GLN:NE2	2.04	0.72
1:B:414:ARG:NH2	1:C:578:GLN:HB3	2.02	0.71
1:B:414:ARG:NH2	1:C:578:GLN:CB	2.35	0.71
1:E:272:SER:HB3	1:E:337:ASN:HB3	1.72	0.71
1:B:87:LYS:CG	1:B:87:LYS:CE	2.68	0.71
1:B:99:ILE:HD12	1:B:189:SER:HB2	1.72	0.71
1:A:272:SER:HB3	1:A:337:ASN:HB3	1.73	0.70
1:B:272:SER:HB3	1:B:337:ASN:HB3	1.74	0.69
1:C:272:SER:HB3	1:C:337:ASN:HB3	1.73	0.69
1:B:364:LYS:O	1:B:366:SER:N	2.22	0.69
1:A:508:LYS:NZ	1:E:508:LYS:NZ	2.42	0.68
1:B:87:LYS:CB	1:B:87:LYS:CD	2.72	0.67
1:A:508:LYS:NZ	1:E:508:LYS:HZ3	1.92	0.67
1:D:272:SER:HB3	1:D:337:ASN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:LYS:O	1:E:366:SER:N	2.25	0.66
1:C:103:GLU:HB3	1:C:198:GLY:O	1.94	0.66
1:B:167:ALA:O	1:B:169:SER:N	2.27	0.66
1:B:87:LYS:CD	1:B:87:LYS:NZ	2.59	0.66
1:C:373:ILE:HB	1:C:471:MET:HB2	1.79	0.65
1:A:508:LYS:HZ1	1:E:508:LYS:HZ3	1.44	0.65
1:E:342:ILE:HA	1:E:345:ARG:HD3	1.78	0.64
1:B:76:PHE:N	1:B:76:PHE:CD1	2.64	0.64
1:A:342:ILE:HA	1:A:345:ARG:HD3	1.79	0.64
1:D:344:GLN:OE1	1:D:384:LYS:HD2	1.98	0.64
1:C:537:LYS:HE2	1:C:589:GLN:HB2	1.78	0.63
1:A:364:LYS:O	1:A:366:SER:N	2.30	0.63
1:A:508:LYS:HZ1	1:E:508:LYS:NZ	1.97	0.63
1:D:373:ILE:HB	1:D:471:MET:HB2	1.81	0.62
1:D:527:TYR:CE2	1:D:538:ILE:HG23	2.35	0.62
1:B:373:ILE:HB	1:B:471:MET:HB2	1.81	0.62
1:B:445:ASN:O	1:C:581:PRO:HB3	1.99	0.62
1:A:222:ILE:HD11	1:A:237:ARG:NH2	2.15	0.62
1:E:364:LYS:C	1:E:366:SER:N	2.53	0.62
1:A:537:LYS:HE2	1:A:589:GLN:HB2	1.82	0.62
1:B:276:ASN:O	1:B:339:ILE:HG13	1.99	0.62
1:C:342:ILE:HA	1:C:345:ARG:HD3	1.81	0.61
1:B:445:ASN:HB2	1:C:581:PRO:CG	2.27	0.61
1:B:364:LYS:C	1:B:366:SER:N	2.52	0.61
1:E:537:LYS:HE2	1:E:589:GLN:HB2	1.82	0.61
1:B:537:LYS:HE2	1:B:589:GLN:HB2	1.83	0.61
1:B:342:ILE:HA	1:B:345:ARG:HD3	1.82	0.61
1:E:373:ILE:HB	1:E:471:MET:HB2	1.83	0.61
1:D:574:GLU:O	1:D:578:GLN:HB2	2.01	0.61
1:B:96:ASN:O	1:B:99:ILE:HG22	2.00	0.60
1:D:342:ILE:HA	1:D:345:ARG:HD3	1.84	0.60
1:B:88:LEU:HB3	1:B:178:MET:HE3	1.84	0.60
1:B:445:ASN:HB2	1:C:581:PRO:HA	1.82	0.60
1:C:364:LYS:C	1:C:366:SER:N	2.54	0.60
1:A:360:LYS:HG2	1:A:366:SER:HA	1.83	0.60
1:A:364:LYS:C	1:A:366:SER:N	2.55	0.60
1:E:222:ILE:HD11	1:E:237:ARG:NH2	2.16	0.59
1:A:425:MET:O	1:A:461:ARG:HD2	2.01	0.59
1:D:537:LYS:HE2	1:D:589:GLN:HB2	1.84	0.59
1:C:222:ILE:HD11	1:C:237:ARG:NH2	2.17	0.59
1:A:429:TYR:CE1	1:A:430:LEU:HG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:HB	1:A:471:MET:HB2	1.84	0.59
1:D:222:ILE:HD11	1:D:237:ARG:NH2	2.18	0.59
1:D:364:LYS:O	1:D:366:SER:N	2.32	0.59
1:E:574:GLU:O	1:E:578:GLN:HB2	2.03	0.58
1:A:574:GLU:O	1:A:578:GLN:HB2	2.03	0.58
1:C:364:LYS:O	1:C:366:SER:N	2.29	0.58
1:C:574:GLU:O	1:C:578:GLN:HB2	2.04	0.58
1:A:276:ASN:O	1:A:339:ILE:HG13	2.04	0.57
1:B:360:LYS:HG2	1:B:366:SER:HA	1.85	0.57
1:D:364:LYS:C	1:D:366:SER:N	2.57	0.57
1:B:78:PHE:HZ	1:B:225:SER:OG	1.86	0.57
1:B:76:PHE:HB2	1:B:230:PHE:CZ	2.40	0.57
1:B:574:GLU:O	1:B:578:GLN:HB2	2.05	0.57
1:C:360:LYS:HG2	1:C:366:SER:HA	1.87	0.56
1:D:197:VAL:HG23	1:D:198:GLY:H	1.70	0.56
1:B:445:ASN:ND2	1:C:581:PRO:HG3	2.20	0.56
1:A:199:PHE:CD2	1:A:200:TYR:N	2.74	0.56
1:B:429:TYR:CE1	1:B:430:LEU:HG	2.41	0.56
1:E:276:ASN:O	1:E:339:ILE:HG13	2.07	0.55
1:C:429:TYR:CE1	1:C:430:LEU:HG	2.42	0.55
1:E:155:THR:HG22	1:E:218:ASP:HB2	1.89	0.54
1:B:92:SER:HB3	1:B:182:GLN:NE2	2.22	0.54
1:B:274:PHE:CE1	1:B:358:PHE:HB2	2.42	0.54
1:D:429:TYR:CE1	1:D:430:LEU:HG	2.42	0.54
1:E:344:GLN:OE1	1:E:384:LYS:HD2	2.09	0.53
1:E:429:TYR:CE1	1:E:430:LEU:HG	2.44	0.52
1:B:135:LYS:HB3	1:B:333:TRP:CH2	2.45	0.52
1:D:524:LEU:O	1:D:528:VAL:HG23	2.11	0.51
1:A:96:ASN:O	1:A:99:ILE:HG22	2.09	0.51
1:B:112:LEU:HD22	1:B:132:LEU:HB3	1.93	0.51
1:E:360:LYS:HG2	1:E:366:SER:HA	1.91	0.51
1:C:362:PHE:O	1:C:362:PHE:HD2	1.94	0.51
1:B:80:ALA:O	1:B:84:ARG:NH1	2.43	0.51
1:A:418:ILE:HG22	1:A:419:THR:HG22	1.93	0.51
1:B:139:ASP:HB3	1:B:144:LEU:HB2	1.92	0.50
1:B:219:THR:O	1:B:221:HIS:ND1	2.42	0.50
1:B:129:ASN:OD1	1:B:131:GLU:HG2	2.12	0.50
1:A:199:PHE:O	1:A:201:SER:N	2.45	0.50
1:D:360:LYS:HG2	1:D:366:SER:HA	1.94	0.50
1:D:133:THR:HG22	1:D:278:PRO:HG2	1.93	0.50
1:B:429:TYR:CD2	1:B:495:GLY:HA2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:221:HIS:ND1	2.45	0.50
1:C:536:ASP:OD2	1:C:537:LYS:HG2	2.12	0.49
1:C:358:PHE:CE1	1:C:362:PHE:HE1	2.31	0.49
1:D:568:LEU:HD22	1:D:573:ASP:HB3	1.94	0.49
1:D:276:ASN:O	1:D:339:ILE:HG13	2.12	0.49
1:B:536:ASP:OD2	1:B:537:LYS:HG2	2.13	0.49
1:B:76:PHE:HD1	1:B:76:PHE:N	2.10	0.48
1:B:148:THR:HG23	1:B:246:THR:OG1	2.12	0.48
1:B:133:THR:HG22	1:B:278:PRO:HG2	1.95	0.48
1:B:155:THR:OG1	1:B:158:GLU:HG3	2.13	0.48
1:A:344:GLN:OE1	1:A:384:LYS:HD2	2.13	0.48
1:E:96:ASN:O	1:E:99:ILE:HG22	2.13	0.48
1:C:96:ASN:O	1:C:99:ILE:HG22	2.13	0.48
1:D:96:ASN:O	1:D:99:ILE:HG22	2.13	0.48
1:E:536:ASP:OD2	1:E:537:LYS:HG2	2.14	0.48
1:C:276:ASN:O	1:C:339:ILE:HG13	2.14	0.48
1:D:536:ASP:OD2	1:D:537:LYS:HG2	2.13	0.48
1:B:429:TYR:O	1:B:491:ASN:HB3	2.14	0.48
1:C:133:THR:HG22	1:C:278:PRO:HG2	1.96	0.47
1:C:274:PHE:CE1	1:C:358:PHE:HB2	2.49	0.47
1:B:490:THR:HA	1:B:493:LYS:HE3	1.96	0.47
1:B:417:PHE:O	1:B:418:ILE:HD13	2.14	0.47
1:C:344:GLN:OE1	1:C:384:LYS:HD2	2.13	0.47
1:C:367:ASP:OD1	1:C:367:ASP:N	2.47	0.47
1:B:223:TRP:NE1	1:B:230:PHE:CD1	2.83	0.47
1:B:76:PHE:HB2	1:B:230:PHE:CE2	2.50	0.47
1:A:536:ASP:OD2	1:A:537:LYS:HG2	2.15	0.47
1:A:417:PHE:O	1:A:418:ILE:HD13	2.15	0.47
1:C:223:TRP:CH2	1:C:225:SER:HB3	2.50	0.47
1:D:129:ASN:OD1	1:D:131:GLU:HG2	2.15	0.47
1:B:150:THR:O	1:B:243:ARG:NH2	2.45	0.47
1:C:506:LEU:HA	1:C:509:LEU:HD12	1.97	0.47
1:A:140:LYS:HA	1:A:259:LEU:HD22	1.97	0.46
1:A:155:THR:OG1	1:A:158:GLU:HG3	2.16	0.46
1:D:358:PHE:CE1	1:D:362:PHE:HE1	2.33	0.46
1:B:135:LYS:HD3	1:B:333:TRP:CZ2	2.51	0.46
1:C:508:LYS:HZ1	1:D:508:LYS:HZ1	1.62	0.46
1:C:235:ASP:HA	1:C:236:PRO:HD2	1.84	0.46
1:C:219:THR:O	1:C:221:HIS:ND1	2.48	0.46
1:D:555:VAL:O	1:D:556:GLU:C	2.53	0.46
1:A:133:THR:HG22	1:A:278:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:LEU:HB3	1:D:583:PHE:CE2	2.51	0.46
1:B:335:LEU:HD12	1:B:336:MET:H	1.80	0.46
1:B:155:THR:HG22	1:B:218:ASP:HB2	1.97	0.46
1:E:362:PHE:HD2	1:E:362:PHE:O	1.99	0.46
1:C:429:TYR:CD2	1:C:495:GLY:HA2	2.51	0.46
1:E:490:THR:HA	1:E:493:LYS:HE3	1.97	0.45
1:B:460:ILE:O	1:B:464:LEU:HG	2.17	0.45
1:E:133:THR:HG22	1:E:278:PRO:HG2	1.98	0.45
1:A:99:ILE:HD11	1:A:102:ARG:NH2	2.31	0.45
1:C:129:ASN:OD1	1:C:131:GLU:HG2	2.17	0.45
1:C:380:GLU:OE1	1:D:533:GLU:CB	2.51	0.45
1:C:533:GLU:HB2	1:D:380:GLU:OE1	2.16	0.45
1:C:163:LEU:HA	1:C:200:TYR:OH	2.16	0.45
1:B:167:ALA:C	1:B:169:SER:H	2.17	0.45
1:C:417:PHE:O	1:C:418:ILE:HD13	2.16	0.45
1:A:490:THR:HA	1:A:493:LYS:HE3	1.98	0.45
1:A:359:TYR:HB2	1:A:388:PHE:CE1	2.52	0.45
1:B:425:MET:O	1:B:461:ARG:HD2	2.16	0.45
1:B:359:TYR:HE1	1:B:434:LYS:HD2	1.82	0.45
1:B:235:ASP:HA	1:B:236:PRO:HD2	1.81	0.45
1:A:367:ASP:N	1:A:367:ASP:OD1	2.47	0.44
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.17	0.44
1:D:367:ASP:OD1	1:D:367:ASP:N	2.50	0.44
1:E:358:PHE:CE1	1:E:362:PHE:HE1	2.36	0.44
1:E:235:ASP:HA	1:E:236:PRO:HD2	1.85	0.44
1:A:199:PHE:HD2	1:A:200:TYR:N	2.15	0.44
1:B:218:ASP:OD1	1:B:219:THR:N	2.48	0.44
1:A:362:PHE:O	1:A:362:PHE:HD2	2.01	0.44
1:E:367:ASP:N	1:E:367:ASP:OD1	2.51	0.44
1:D:359:TYR:HB2	1:D:388:PHE:CE1	2.53	0.44
1:A:146:HIS:CE1	1:A:248:THR:HG23	2.53	0.44
1:D:490:THR:HG23	1:D:572:VAL:HG11	2.00	0.44
1:C:343:TRP:CD2	1:C:436:VAL:HG21	2.53	0.43
1:D:366:SER:HB3	1:E:366:SER:HB3	2.01	0.43
1:C:362:PHE:CD2	1:C:362:PHE:O	2.71	0.43
1:B:243:ARG:CZ	1:B:243:ARG:HB3	2.49	0.43
1:B:278:PRO:HB2	1:B:280:TYR:CE2	2.53	0.43
1:B:156:ARG:HG3	1:B:221:HIS:CD2	2.54	0.43
1:C:148:THR:HG23	1:C:246:THR:OG1	2.19	0.43
1:D:506:LEU:O	1:D:509:LEU:N	2.38	0.43
1:D:506:LEU:HA	1:D:509:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:THR:O	1:E:221:HIS:ND1	2.52	0.43
1:D:219:THR:O	1:D:221:HIS:ND1	2.52	0.43
1:C:490:THR:HA	1:C:493:LYS:HE3	2.01	0.43
1:D:235:ASP:HA	1:D:236:PRO:HD2	1.84	0.43
1:B:419:THR:OG1	1:B:420:ASP:N	2.52	0.43
1:A:527:TYR:CE2	1:A:538:ILE:HG23	2.54	0.43
1:B:367:ASP:N	1:B:367:ASP:OD1	2.51	0.42
1:A:139:ASP:HB3	1:A:144:LEU:HB2	2.01	0.42
1:A:358:PHE:CE1	1:A:362:PHE:HE1	2.38	0.42
1:B:552:SER:HA	1:B:553:PRO:HD3	1.93	0.42
1:D:490:THR:HA	1:D:493:LYS:HE3	2.01	0.42
1:B:120:LEU:HD22	1:B:444:LEU:HD11	2.01	0.42
1:D:419:THR:OG1	1:D:420:ASP:N	2.52	0.42
1:D:164:GLY:HA2	1:D:230:PHE:CE2	2.54	0.42
1:C:568:LEU:HD22	1:C:573:ASP:HB3	2.00	0.42
1:B:130:GLU:OE1	1:C:500:HIS:NE2	2.52	0.42
1:C:527:TYR:CE2	1:C:538:ILE:HG23	2.54	0.42
1:C:531:MET:HE1	1:C:586:LYS:HD2	2.01	0.42
1:D:100:PHE:CG	1:D:101:LEU:N	2.88	0.42
1:A:552:SER:HA	1:A:553:PRO:HD3	1.92	0.42
1:B:235:ASP:OD2	1:B:237:ARG:NH2	2.52	0.42
1:E:135:LYS:HB3	1:E:333:TRP:CH2	2.55	0.42
1:B:362:PHE:O	1:B:362:PHE:HD2	2.02	0.42
1:B:131:GLU:CG	1:B:150:THR:HG21	2.50	0.42
1:E:490:THR:HG23	1:E:572:VAL:HG11	2.01	0.42
1:A:429:TYR:CD2	1:A:495:GLY:HA2	2.55	0.41
1:E:156:ARG:HB2	1:E:221:HIS:NE2	2.35	0.41
1:C:129:ASN:O	1:C:243:ARG:NH1	2.39	0.41
1:D:460:ILE:O	1:D:464:LEU:HG	2.21	0.41
1:C:552:SER:HA	1:C:553:PRO:HD3	1.89	0.41
1:C:374:HIS:HD2	1:C:385:SER:O	2.03	0.41
1:E:429:TYR:O	1:E:491:ASN:HB3	2.20	0.41
1:E:429:TYR:CD2	1:E:495:GLY:HA2	2.55	0.41
1:C:139:ASP:HB3	1:C:144:LEU:HB2	2.02	0.41
1:E:156:ARG:HB2	1:E:221:HIS:CE1	2.55	0.41
1:A:100:PHE:CG	1:A:101:LEU:N	2.88	0.41
1:B:94:TYR:HB2	1:B:97:LYS:HZ1	1.85	0.41
1:A:274:PHE:CE1	1:A:358:PHE:HB2	2.55	0.41
1:E:274:PHE:CE1	1:E:358:PHE:HB2	2.56	0.41
1:B:174:PHE:HE2	1:B:191:LEU:O	2.03	0.41
1:B:261:LEU:HD11	1:B:331:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ASN:OD1	1:E:131:GLU:HG2	2.20	0.41
1:A:531:MET:HE1	1:A:586:LYS:HD2	2.02	0.41
1:B:171:THR:HG22	1:B:171:THR:O	2.21	0.41
1:C:125:ALA:O	1:C:216:ASN:ND2	2.51	0.41
1:A:356:LYS:HG2	1:A:369:PRO:HD2	2.03	0.41
1:B:340:LYS:HA	1:B:341:PRO:HD3	1.95	0.41
1:B:112:LEU:O	1:B:115:ILE:HG22	2.21	0.41
1:B:490:THR:HG23	1:B:572:VAL:HG11	2.02	0.41
1:E:359:TYR:HB2	1:E:388:PHE:CE1	2.55	0.41
1:E:112:LEU:HD22	1:E:132:LEU:HB3	2.02	0.41
1:B:135:LYS:HD3	1:B:333:TRP:CE2	2.55	0.41
1:D:223:TRP:CH2	1:D:225:SER:HB3	2.55	0.41
1:C:419:THR:OG1	1:C:420:ASP:N	2.54	0.41
1:B:103:GLU:O	1:B:106:SER:HB3	2.21	0.41
1:D:362:PHE:HD2	1:D:362:PHE:O	2.03	0.40
1:B:130:GLU:OE1	1:C:500:HIS:CE1	2.74	0.40
1:E:359:TYR:HE1	1:E:434:LYS:HD2	1.86	0.40
1:E:527:TYR:CE2	1:E:538:ILE:HG23	2.57	0.40
1:A:568:LEU:HD22	1:A:573:ASP:HB3	2.02	0.40
1:E:139:ASP:HB3	1:E:144:LEU:HB2	2.03	0.40
1:A:148:THR:HA	1:A:245:THR:O	2.21	0.40
1:B:445:ASN:O	1:C:581:PRO:CB	2.67	0.40
1:B:429:TYR:CD1	1:B:430:LEU:HG	2.57	0.40
1:C:490:THR:HG23	1:C:572:VAL:HG11	2.02	0.40
1:D:139:ASP:HB3	1:D:144:LEU:HB2	2.03	0.40
1:A:524:LEU:O	1:A:528:VAL:HG23	2.21	0.40
1:B:156:ARG:HB2	1:B:221:HIS:CE1	2.56	0.40
1:E:506:LEU:HA	1:E:509:LEU:HD12	2.03	0.40
1:E:422:PHE:HB3	1:E:425:MET:HG2	2.04	0.40
1:A:223:TRP:CH2	1:A:225:SER:HB3	2.55	0.40
1:C:146:HIS:CE1	1:C:248:THR:HG23	2.57	0.40
1:A:419:THR:OG1	1:A:420:ASP:N	2.54	0.40

All (5) 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:B:349:GLU:O	1:E:560:LYS:NZ[4_555]	1.61	0.59
1:B:561:LYS:NZ	1:C:544:SER:OG[2_655]	2.04	0.16
1:A:445:ASN:OD1	1:B:284:SER:OG[4_545]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:C	1:E:560:LYS:NZ[4_555]	2.12	0.08
1:B:352:ASP:N	1:E:557:ARG:NH2[4_555]	2.13	0.07

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	408/506 (81%)	381 (93%)	23 (6%)	4 (1%)	19	63
1	B	463/506 (92%)	409 (88%)	47 (10%)	7 (2%)	13	54
1	C	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	34	75
1	D	408/506 (81%)	379 (93%)	24 (6%)	5 (1%)	16	59
1	E	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	34	75
All	All	2095/2530 (83%)	1927 (92%)	148 (7%)	20 (1%)	19	63

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PHE
1	B	168	LYS
1	B	365	GLU
1	A	200	TYR
1	A	365	GLU
1	B	186	GLN
1	C	365	GLU
1	D	198	GLY
1	E	365	GLU
1	A	581	PRO
1	C	581	PRO
1	D	199	PHE
1	D	365	GLU
1	B	581	PRO

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Mol	Chain	Res	Type
1	D	581	PRO
1	E	581	PRO
1	B	173	GLU
1	B	474	LYS
1	D	556	GLU
1	B	170	GLY

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	365/456 (80%)	361 (99%)	4 (1%)	80	92
1	B	400/456 (88%)	386 (96%)	14 (4%)	43	78
1	C	365/456 (80%)	360 (99%)	5 (1%)	74	90
1	D	365/456 (80%)	361 (99%)	4 (1%)	80	92
1	E	365/456 (80%)	361 (99%)	4 (1%)	80	92
All	All	1860/2280 (82%)	1829 (98%)	31 (2%)	68	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	362	PHE
1	A	376	THR
1	A	448	ARG
1	B	73	SER
1	B	74	GLU
1	B	76	PHE
1	B	88	LEU
1	B	90	ILE
1	B	117	LEU
1	B	178	MET
1	B	179	THR
1	B	191	LEU

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Mol	Chain	Res	Type
1	B	362	PHE
1	B	376	THR
1	B	412	TYR
1	B	420	ASP
1	B	448	ARG
1	C	117	LEU
1	C	362	PHE
1	C	376	THR
1	C	391	THR
1	C	448	ARG
1	D	117	LEU
1	D	376	THR
1	D	448	ARG
1	D	522	THR
1	E	117	LEU
1	E	376	THR
1	E	391	THR
1	E	448	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	C	578	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.













5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/506 (82%)	1.50	122 (29%)  	179, 194, 209, 226	0
1	B	469/506 (92%)	1.31	96 (20%)  	179, 195, 223, 253	0
1	C	416/506 (82%)	1.29	109 (26%)  	179, 194, 209, 226	0
1	D	416/506 (82%)	1.76	136 (32%)  	179, 194, 209, 226	0
1	E	416/506 (82%)	3.12	200 (48%)  	179, 194, 209, 226	0
All	All	2133/2530 (84%)	1.78	663 (31%)  	179, 194, 211, 253	0

All (663) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	285	LYS	55.2
1	E	286	THR	27.2
1	E	198	GLY	23.6
1	E	281	VAL	17.1
1	E	277	PHE	16.7
1	E	247	ILE	16.5
1	D	138	CYS	14.7
1	E	147	VAL	14.4
1	E	264	ILE	14.3
1	D	163	LEU	14.2
1	E	280	TYR	14.0
1	E	163	LEU	13.8
1	E	284	SER	13.1
1	E	205	VAL	12.9
1	E	226	ASP	12.3
1	D	258	TYR	12.1
1	D	259	LEU	11.5
1	E	228	ASN	11.0
1	E	234	ALA	10.8
1	E	227	SER	10.6

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Mol	Chain	Res	Type	RSRZ
1	B	73	SER	10.3
1	E	279	ILE	10.3
1	C	253	GLU	10.2
1	E	383	PHE	10.1
1	E	334	GLU	9.9
1	B	380	GLU	9.8
1	E	335	LEU	9.8
1	E	452	GLN	9.8
1	E	206	ALA	9.7
1	E	258	TYR	9.6
1	E	235	ASP	9.3
1	A	594	GLU	9.3
1	E	246	THR	9.2
1	E	442	LEU	9.1
1	D	152	VAL	9.1
1	E	199	PHE	9.1
1	E	266	ASN	9.1
1	E	212	THR	8.9
1	E	443	PRO	8.9
1	E	542	ALA	8.8
1	E	262	ASP	8.8
1	A	125	ALA	8.8
1	E	202	ALA	8.8
1	D	222	ILE	8.7
1	D	442	LEU	8.6
1	A	159	LEU	8.6
1	E	125	ALA	8.5
1	E	245	THR	8.4
1	C	281	VAL	8.2
1	E	233	ILE	8.2
1	B	329	THR	8.1
1	E	451	LEU	8.0
1	E	136	ILE	7.9
1	B	548	GLU	7.8
1	E	330	VAL	7.7
1	E	197	VAL	7.7
1	E	126	LEU	7.7
1	E	263	THR	7.6
1	B	563	TYR	7.6
1	D	330	VAL	7.5
1	C	230	PHE	7.5
1	E	208	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	225	SER	7.3
1	A	521	ILE	7.3
1	C	444	LEU	7.2
1	E	154	MET	7.2
1	E	248	THR	7.2
1	E	265	LYS	7.2
1	E	278	PRO	7.2
1	E	100	PHE	7.1
1	D	205	VAL	7.0
1	E	249	LEU	6.9
1	E	155	THR	6.9
1	D	208	LYS	6.8
1	E	152	VAL	6.8
1	A	126	LEU	6.7
1	D	225	SER	6.7
1	A	562	GLY	6.7
1	D	230	PHE	6.6
1	B	286	THR	6.6
1	A	163	LEU	6.6
1	D	131	GLU	6.6
1	E	329	THR	6.5
1	D	223	TRP	6.5
1	E	541	MET	6.4
1	B	519	SER	6.4
1	E	207	ASP	6.4
1	E	113	ASP	6.4
1	A	208	LYS	6.3
1	E	239	ASN	6.3
1	E	382	THR	6.3
1	C	227	SER	6.2
1	C	203	PHE	6.2
1	A	496	VAL	6.2
1	E	588	PHE	6.1
1	D	444	LEU	6.1
1	D	232	VAL	6.1
1	C	136	ILE	6.1
1	E	550	GLU	6.1
1	A	237	ARG	6.0
1	A	97	LYS	6.0
1	C	228	ASN	6.0
1	E	422	PHE	6.0
1	E	162	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	200	TYR	6.0
1	A	95	LYS	5.9
1	A	162	ASN	5.9
1	D	237	ARG	5.8
1	E	498	GLU	5.8
1	E	481	ASN	5.8
1	E	134	VAL	5.8
1	E	160	VAL	5.7
1	E	213	SER	5.7
1	E	236	PRO	5.7
1	D	211	VAL	5.7
1	C	146	HIS	5.7
1	E	149	ASP	5.6
1	E	268	VAL	5.6
1	E	276	ASN	5.6
1	D	159	LEU	5.6
1	E	558	LEU	5.6
1	A	541	MET	5.6
1	A	549	ALA	5.6
1	A	533	GLU	5.6
1	D	141	GLU	5.6
1	D	278	PRO	5.6
1	A	551	SER	5.5
1	D	331	TRP	5.5
1	E	110	ASP	5.5
1	C	144	LEU	5.3
1	B	178	MET	5.3
1	C	448	ARG	5.3
1	C	138	CYS	5.3
1	B	551	SER	5.3
1	D	227	SER	5.3
1	D	212	THR	5.3
1	E	549	ALA	5.3
1	A	277	PHE	5.2
1	E	209	VAL	5.2
1	D	285	LYS	5.2
1	D	260	GLU	5.2
1	D	202	ALA	5.2
1	D	115	ILE	5.1
1	D	162	ASN	5.1
1	E	283	SER	5.0
1	D	445	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	228	ASN	5.0
1	E	229	GLU	5.0
1	D	280	TYR	4.9
1	B	451	LEU	4.9
1	E	211	VAL	4.9
1	E	548	GLU	4.9
1	D	151	GLY	4.9
1	E	138	CYS	4.8
1	E	444	LEU	4.8
1	D	209	VAL	4.8
1	A	96	ASN	4.8
1	A	213	SER	4.8
1	C	222	ILE	4.7
1	D	255	ALA	4.7
1	E	563	TYR	4.7
1	C	409	ILE	4.7
1	D	215	HIS	4.7
1	D	207	ASP	4.7
1	D	98	GLU	4.7
1	E	203	PHE	4.7
1	C	221	HIS	4.7
1	E	567	TYR	4.7
1	D	125	ALA	4.7
1	E	553	PRO	4.6
1	D	124	ASN	4.6
1	E	250	VAL	4.6
1	A	343	TRP	4.6
1	C	137	LYS	4.6
1	E	566	ILE	4.6
1	B	571	PRO	4.6
1	D	203	PHE	4.5
1	E	456	LEU	4.5
1	C	145	LEU	4.5
1	E	568	LEU	4.5
1	C	219	THR	4.5
1	C	282	TRP	4.5
1	D	262	ASP	4.5
1	E	377	ALA	4.5
1	D	443	PRO	4.5
1	D	221	HIS	4.4
1	E	145	LEU	4.4
1	B	429	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	213	SER	4.4
1	E	231	SER	4.4
1	D	519	SER	4.4
1	C	390	PRO	4.4
1	A	445	ASN	4.4
1	E	157	GLU	4.4
1	A	563	TYR	4.3
1	A	279	ILE	4.3
1	C	213	SER	4.3
1	A	147	VAL	4.3
1	B	575	TYR	4.3
1	D	276	ASN	4.3
1	E	259	LEU	4.3
1	E	512	PHE	4.3
1	C	422	PHE	4.3
1	E	594	GLU	4.3
1	E	464	LEU	4.3
1	A	539	TYR	4.3
1	A	132	LEU	4.2
1	B	328	LYS	4.2
1	C	534	LYS	4.2
1	E	450	THR	4.2
1	B	535	GLN	4.2
1	A	553	PRO	4.2
1	E	224	GLU	4.2
1	C	333	TRP	4.2
1	A	432	PHE	4.1
1	D	219	THR	4.1
1	E	104	LEU	4.1
1	E	156	ARG	4.1
1	D	448	ARG	4.1
1	E	460	ILE	4.1
1	E	521	ILE	4.1
1	C	231	SER	4.1
1	E	426	MET	4.1
1	E	411	LEU	4.1
1	C	454	HIS	4.0
1	E	257	ASP	4.0
1	C	568	LEU	4.0
1	C	533	GLU	4.0
1	A	286	THR	4.0
1	A	228	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	117	LEU	4.0
1	C	220	GLN	3.9
1	D	126	LEU	3.9
1	A	214	LYS	3.9
1	D	414	ARG	3.9
1	C	331	TRP	3.9
1	E	274	PHE	3.9
1	E	343	TRP	3.9
1	B	503	ARG	3.9
1	E	559	LEU	3.9
1	D	226	ASP	3.9
1	B	228	ASN	3.9
1	B	456	LEU	3.8
1	A	226	ASP	3.8
1	D	341	PRO	3.8
1	B	588	PHE	3.8
1	D	117	LEU	3.8
1	B	227	SER	3.8
1	E	101	LEU	3.8
1	E	445	ASN	3.8
1	B	569	THR	3.8
1	A	567	TYR	3.7
1	D	233	ILE	3.7
1	B	568	LEU	3.7
1	B	74	GLU	3.7
1	E	336	MET	3.7
1	D	199	PHE	3.7
1	A	559	LEU	3.7
1	C	259	LEU	3.7
1	A	145	LEU	3.7
1	E	95	LYS	3.6
1	E	282	TRP	3.6
1	B	86	MET	3.6
1	D	140	LYS	3.6
1	B	559	LEU	3.6
1	B	532	LYS	3.6
1	D	240	THR	3.6
1	E	222	ILE	3.6
1	B	330	VAL	3.6
1	E	223	TRP	3.6
1	A	383	PHE	3.6
1	E	253	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	539	TYR	3.6
1	A	446	VAL	3.5
1	C	343	TRP	3.5
1	D	343	TRP	3.5
1	E	380	GLU	3.5
1	B	540	PHE	3.5
1	E	139	ASP	3.5
1	E	142	LYS	3.5
1	B	172	SER	3.5
1	D	554	PHE	3.5
1	C	284	SER	3.5
1	D	218	ASP	3.5
1	E	146	HIS	3.5
1	D	97	LYS	3.5
1	D	383	PHE	3.5
1	B	78	PHE	3.5
1	D	164	GLY	3.5
1	B	531	MET	3.5
1	E	120	LEU	3.4
1	A	442	LEU	3.4
1	D	229	GLU	3.4
1	D	541	MET	3.4
1	A	331	TRP	3.4
1	C	442	LEU	3.4
1	E	159	LEU	3.4
1	C	223	TRP	3.4
1	A	231	SER	3.4
1	B	232	VAL	3.4
1	A	529	GLU	3.4
1	D	214	LYS	3.4
1	E	538	ILE	3.4
1	E	555	VAL	3.4
1	A	245	THR	3.3
1	A	256	SER	3.3
1	B	444	LEU	3.3
1	E	221	HIS	3.3
1	E	545	SER	3.3
1	A	138	CYS	3.3
1	B	204	LEU	3.3
1	E	241	LEU	3.3
1	C	232	VAL	3.3
1	D	359	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	206	ALA	3.3
1	C	147	VAL	3.3
1	B	539	TYR	3.3
1	C	385	SER	3.3
1	D	340	LYS	3.3
1	A	556	GLU	3.3
1	A	156	ARG	3.2
1	C	439	SER	3.2
1	D	539	TYR	3.2
1	D	413	VAL	3.2
1	C	445	ASN	3.2
1	A	98	GLU	3.2
1	C	355	TYR	3.2
1	C	250	VAL	3.2
1	A	426	MET	3.2
1	D	264	ILE	3.2
1	E	375	PHE	3.2
1	B	518	PRO	3.2
1	A	243	ARG	3.2
1	D	129	ASN	3.2
1	C	279	ILE	3.2
1	A	395	ARG	3.2
1	A	378	GLU	3.2
1	B	594	GLU	3.2
1	D	334	GLU	3.2
1	E	592	ALA	3.2
1	C	513	GLN	3.2
1	E	391	THR	3.2
1	B	166	ILE	3.2
1	E	118	ILE	3.2
1	D	238	GLY	3.2
1	E	243	ARG	3.2
1	C	240	THR	3.1
1	A	581	PRO	3.1
1	D	355	TYR	3.1
1	C	524	LEU	3.1
1	E	543	GLY	3.1
1	A	513	GLN	3.1
1	D	130	GLU	3.1
1	C	135	LYS	3.1
1	C	272	SER	3.1
1	B	89	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	3.1
1	D	239	ASN	3.1
1	A	215	HIS	3.1
1	B	537	LYS	3.0
1	D	136	ILE	3.0
1	C	258	TYR	3.0
1	C	283	SER	3.0
1	C	414	ARG	3.0
1	A	568	LEU	3.0
1	E	230	PHE	3.0
1	C	563	TYR	3.0
1	E	537	LYS	3.0
1	C	97	LYS	3.0
1	B	344	GLN	3.0
1	E	148	THR	3.0
1	E	410	LYS	3.0
1	E	98	GLU	3.0
1	C	566	ILE	3.0
1	A	100	PHE	3.0
1	B	557	ARG	3.0
1	D	263	THR	3.0
1	E	522	THR	3.0
1	C	362	PHE	3.0
1	C	159	LEU	2.9
1	D	96	ASN	2.9
1	A	255	ALA	2.9
1	E	425	MET	2.9
1	C	286	THR	2.9
1	E	459	VAL	2.9
1	A	460	ILE	2.9
1	E	210	ILE	2.9
1	D	329	THR	2.9
1	D	457	LEU	2.9
1	A	149	ASP	2.9
1	A	565	VAL	2.9
1	C	539	TYR	2.9
1	E	536	ASP	2.9
1	D	216	ASN	2.9
1	A	258	TYR	2.9
1	A	524	LEU	2.9
1	B	370	MET	2.9
1	A	501	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	538	ILE	2.9
1	D	434	LYS	2.9
1	C	559	LEU	2.9
1	A	512	PHE	2.9
1	C	268	VAL	2.9
1	C	381	VAL	2.9
1	C	567	TYR	2.8
1	C	278	PRO	2.8
1	A	480	TYR	2.8
1	C	280	TYR	2.8
1	D	243	ARG	2.8
1	A	355	TYR	2.8
1	A	555	VAL	2.8
1	A	207	ASP	2.8
1	D	456	LEU	2.8
1	D	134	VAL	2.8
1	E	158	GLU	2.8
1	E	370	MET	2.8
1	A	105	ILE	2.8
1	A	503	ARG	2.8
1	C	233	ILE	2.8
1	C	126	LEU	2.8
1	A	437	VAL	2.8
1	B	572	VAL	2.8
1	B	475	ILE	2.7
1	B	536	ASP	2.7
1	A	393	ALA	2.7
1	E	256	SER	2.7
1	C	560	LYS	2.7
1	C	271	TYR	2.7
1	A	444	LEU	2.7
1	B	457	LEU	2.7
1	E	482	ASP	2.7
1	D	370	MET	2.7
1	D	217	ASN	2.7
1	E	127	ALA	2.7
1	A	527	TYR	2.7
1	D	565	VAL	2.7
1	A	278	PRO	2.7
1	D	256	SER	2.7
1	C	541	MET	2.7
1	A	408	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	113	ASP	2.7
1	E	121	THR	2.7
1	B	411	LEU	2.7
1	B	524	LEU	2.7
1	C	275	ILE	2.7
1	C	205	VAL	2.7
1	A	280	TYR	2.7
1	E	432	PHE	2.7
1	A	113	ASP	2.7
1	A	101	LEU	2.6
1	A	576	CYS	2.6
1	A	522	THR	2.6
1	D	281	VAL	2.6
1	E	220	GLN	2.6
1	C	229	GLU	2.6
1	E	384	LYS	2.6
1	D	449	GLU	2.6
1	D	520	ASP	2.6
1	E	122	ASP	2.6
1	E	457	LEU	2.6
1	B	343	TRP	2.6
1	D	139	ASP	2.6
1	C	197	VAL	2.6
1	D	365	GLU	2.6
1	B	168	LYS	2.6
1	C	408	TYR	2.6
1	A	368	ASP	2.6
1	B	544	SER	2.6
1	E	514	SER	2.6
1	A	387	LEU	2.5
1	E	128	GLY	2.5
1	D	95	LYS	2.5
1	C	133	THR	2.5
1	B	143	ASN	2.5
1	D	557	ARG	2.5
1	D	425	MET	2.5
1	D	363	SER	2.5
1	B	460	ILE	2.5
1	E	518	PRO	2.5
1	D	408	TYR	2.5
1	D	542	ALA	2.5
1	E	441	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	521	ILE	2.5
1	A	591	VAL	2.5
1	C	115	ILE	2.5
1	C	261	LEU	2.5
1	E	261	LEU	2.5
1	E	546	ARG	2.5
1	D	265	LYS	2.5
1	B	497	ILE	2.5
1	C	330	VAL	2.5
1	A	264	ILE	2.5
1	D	388	PHE	2.5
1	B	85	MET	2.5
1	E	492	ILE	2.5
1	A	112	LEU	2.5
1	E	114	LYS	2.5
1	A	202	ALA	2.4
1	A	238	GLY	2.4
1	C	113	ASP	2.4
1	C	573	ASP	2.4
1	D	272	SER	2.4
1	B	512	PHE	2.4
1	A	588	PHE	2.4
1	E	547	LYS	2.4
1	A	411	LEU	2.4
1	E	109	SER	2.4
1	E	331	TRP	2.4
1	E	368	ASP	2.4
1	A	575	TYR	2.4
1	D	249	LEU	2.4
1	C	245	THR	2.4
1	D	494	LEU	2.4
1	A	221	HIS	2.4
1	D	347	SER	2.4
1	B	372	TYR	2.4
1	D	372	TYR	2.4
1	B	383	PHE	2.4
1	A	532	LYS	2.4
1	A	250	VAL	2.4
1	B	534	LYS	2.4
1	A	427	PRO	2.4
1	D	574	GLU	2.4
1	E	554	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	450	THR	2.4
1	D	123	GLU	2.4
1	D	384	LYS	2.4
1	B	496	VAL	2.4
1	E	417	PHE	2.4
1	C	527	TYR	2.4
1	E	453	GLN	2.4
1	B	547	LYS	2.3
1	A	550	GLU	2.3
1	B	436	VAL	2.3
1	C	437	VAL	2.3
1	C	510	LEU	2.3
1	C	149	ASP	2.3
1	E	430	LEU	2.3
1	B	223	TRP	2.3
1	B	437	VAL	2.3
1	C	556	GLU	2.3
1	A	375	PHE	2.3
1	E	551	SER	2.3
1	E	516	HIS	2.3
1	E	513	GLN	2.3
1	C	98	GLU	2.3
1	C	503	ARG	2.3
1	D	452	GLN	2.3
1	E	218	ASP	2.3
1	E	255	ALA	2.3
1	D	366	SER	2.3
1	A	526	GLN	2.3
1	D	144	LEU	2.3
1	D	204	LEU	2.3
1	D	503	ARG	2.3
1	C	95	LYS	2.3
1	C	212	THR	2.3
1	E	395	ARG	2.3
1	B	542	ALA	2.3
1	E	130	GLU	2.3
1	E	362	PHE	2.3
1	A	577	ILE	2.3
1	A	477	ASP	2.3
1	B	336	MET	2.3
1	C	249	LEU	2.3
1	D	145	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	2.3
1	C	594	GLU	2.3
1	D	533	GLU	2.3
1	A	199	PHE	2.2
1	A	584	ASP	2.2
1	D	362	PHE	2.2
1	E	332	ASP	2.2
1	B	386	ILE	2.2
1	E	135	LYS	2.2
1	E	440	ASP	2.2
1	D	231	SER	2.2
1	C	96	ASN	2.2
1	E	416	VAL	2.2
1	E	437	VAL	2.2
1	A	212	THR	2.2
1	E	385	SER	2.2
1	B	208	LYS	2.2
1	A	456	LEU	2.2
1	A	152	VAL	2.2
1	A	209	VAL	2.2
1	C	436	VAL	2.2
1	E	415	ARG	2.2
1	D	283	SER	2.2
1	B	434	LYS	2.2
1	D	105	ILE	2.2
1	B	379	GLY	2.2
1	C	132	LEU	2.2
1	E	540	PHE	2.2
1	D	381	VAL	2.2
1	A	394	PRO	2.2
1	C	456	LEU	2.2
1	E	424	ASP	2.2
1	B	409	ILE	2.2
1	A	275	ILE	2.2
1	E	275	ILE	2.2
1	B	513	GLN	2.2
1	A	219	THR	2.2
1	B	369	PRO	2.2
1	D	246	THR	2.2
1	C	481	ASN	2.2
1	C	380	GLU	2.1
1	D	418	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	TYR	2.1
1	A	381	VAL	2.1
1	D	374	HIS	2.1
1	C	211	VAL	2.1
1	D	361	SER	2.1
1	C	251	LEU	2.1
1	D	235	ASP	2.1
1	C	104	LEU	2.1
1	C	120	LEU	2.1
1	E	132	LEU	2.1
1	D	127	ALA	2.1
1	A	272	SER	2.1
1	E	515	SER	2.1
1	C	156	ARG	2.1
1	E	487	GLU	2.1
1	B	105	ILE	2.1
1	A	500	HIS	2.1
1	B	408	TYR	2.1
1	B	96	ASN	2.1
1	A	225	SER	2.1
1	A	422	PHE	2.1
1	B	580	LEU	2.1
1	B	165	THR	2.1
1	C	386	ILE	2.1
1	D	200	TYR	2.1
1	B	169	SER	2.1
1	C	468	THR	2.1
1	B	282	TRP	2.1
1	E	562	GLY	2.1
1	D	441	ASP	2.1
1	E	337	ASN	2.1
1	B	443	PRO	2.1
1	C	507	ALA	2.1
1	B	264	ILE	2.1
1	A	337	ASN	2.1
1	A	360	LYS	2.1
1	D	342	ILE	2.0
1	B	333	TRP	2.0
1	C	367	ASP	2.0
1	C	361	SER	2.0
1	B	216	ASN	2.0
1	B	472	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	417	PHE	2.0
1	E	161	LYS	2.0
1	B	272	SER	2.0
1	B	124	ASN	2.0
1	B	565	VAL	2.0
1	E	414	ARG	2.0
1	B	334	GLU	2.0
1	D	594	GLU	2.0
1	B	567	TYR	2.0
1	E	433	VAL	2.0
1	A	504	THR	2.0
1	A	583	PHE	2.0
1	B	510	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.