



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:02 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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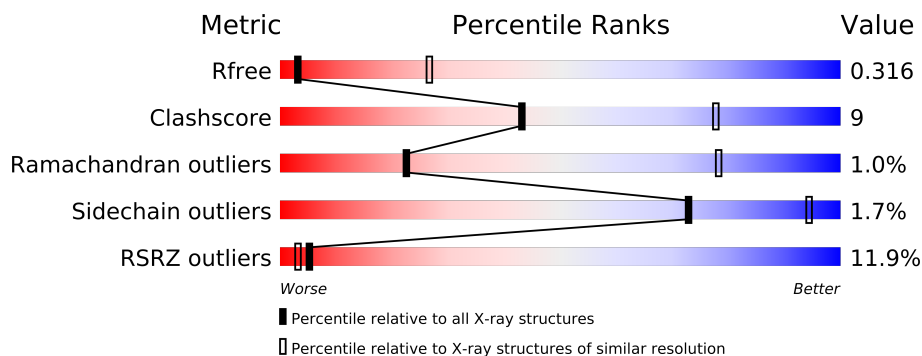
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	506	
1	B	506	
1	C	506	
1	D	506	
1	E	506	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17042 atoms, of which 0 are hydrogen and 0 are deuterium.

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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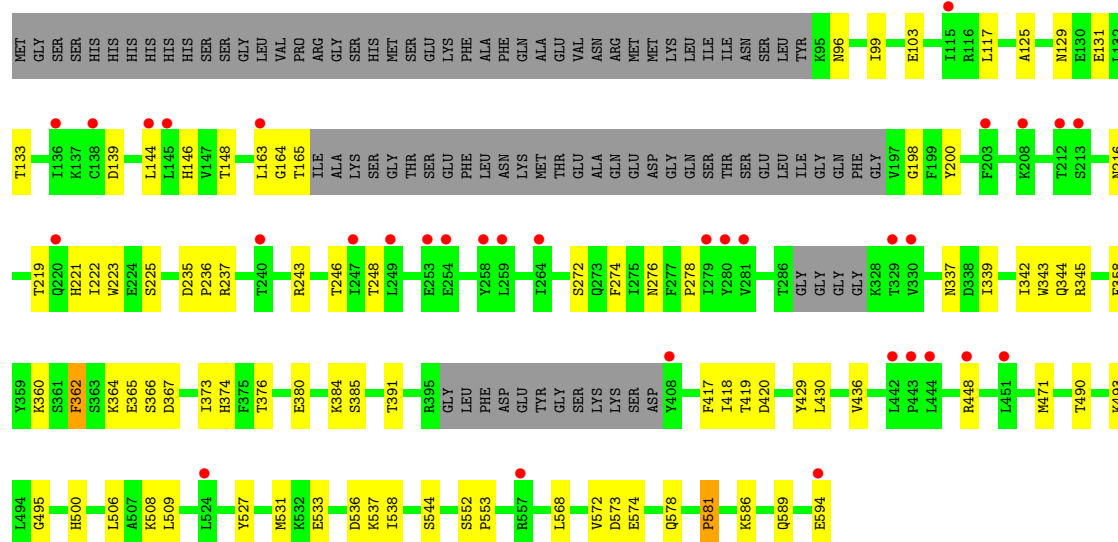
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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	SER	-	EXPRESSION TAG	UNP P41148
C	64	GLY	-	EXPRESSION TAG	UNP P41148
C	65	LEU	-	EXPRESSION TAG	UNP P41148
C	66	VAL	-	EXPRESSION TAG	UNP P41148
C	67	PRO	-	EXPRESSION TAG	UNP P41148
C	68	ARG	-	EXPRESSION 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



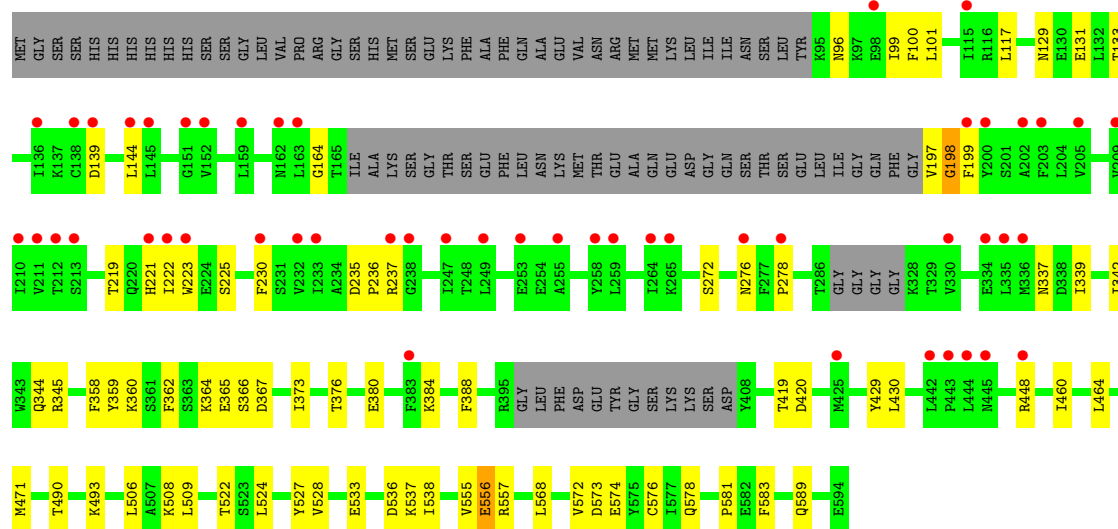
- Molecule 1: Endoplasmic

Chain C:



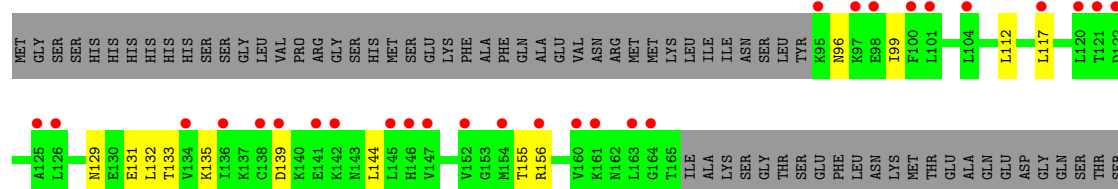
- Molecule 1: Endoplasmic

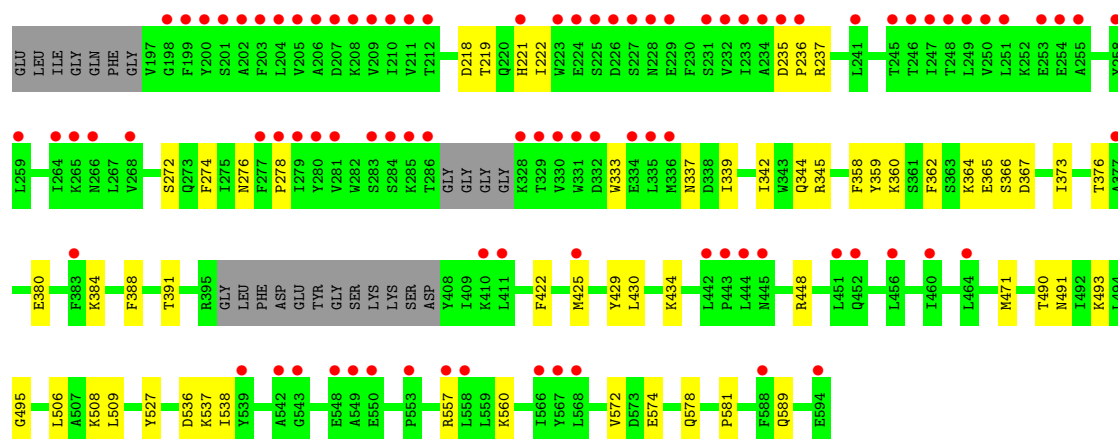
Chain D:



- Molecule 1: Endoplasmic

Chain E:







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.314 , 0.332 0.298 , 0.316	Depositor DCC
$R_{free}$ test set	2122 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	148.6	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 248.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.49	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (297) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:C:380:GLU:OE1	1:D:533:GLU:HB2	1.67	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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
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

### 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	408/506 (81%)	381 (93%)	23 (6%)	4 (1%)	22	78
1	B	463/506 (92%)	409 (88%)	47 (10%)	7 (2%)	15	68
1	C	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	38	87
1	D	408/506 (81%)	379 (93%)	24 (6%)	5 (1%)	19	74
1	E	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	38	87
All	All	2095/2530 (83%)	1927 (92%)	148 (7%)	20 (1%)	22	78

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
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%)	84	96
1	B	400/456 (88%)	386 (96%)	14 (4%)	48	87
1	C	365/456 (80%)	360 (99%)	5 (1%)	78	95
1	D	365/456 (80%)	361 (99%)	4 (1%)	84	96
1	E	365/456 (80%)	361 (99%)	4 (1%)	84	96
All	All	1860/2280 (82%)	1829 (98%)	31 (2%)	73	94

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
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 chains 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	416/506 (82%)	0.71	31 (7%) 14 6	179, 194, 209, 226	0
1	B	469/506 (92%)	0.58	20 (4%) 34 13	179, 195, 223, 253	0
1	C	416/506 (82%)	0.68	33 (7%) 13 6	179, 194, 209, 226	0
1	D	416/506 (82%)	0.85	51 (12%) 5 3	179, 194, 209, 226	0
1	E	416/506 (82%)	1.64	119 (28%) 1 1	179, 194, 209, 226	0
All	All	2133/2530 (84%)	0.88	254 (11%) 5 3	179, 194, 211, 253	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	285	LYS	39.0
1	E	286	THR	20.0
1	E	258	TYR	9.8
1	E	202	ALA	9.2
1	E	205	VAL	9.1
1	E	200	TYR	8.2
1	D	258	TYR	7.8
1	E	247	ILE	7.8
1	E	442	LEU	7.8
1	D	138	CYS	7.3
1	E	199	PHE	6.9
1	E	163	LEU	6.9
1	E	206	ALA	6.7
1	E	281	VAL	6.6
1	A	594	GLU	6.6
1	C	253	GLU	6.6
1	D	163	LEU	6.4
1	E	542	ALA	6.1
1	E	334	GLU	6.1
1	E	284	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	249	LEU	5.9
1	E	264	ILE	5.9
1	E	147	VAL	5.8
1	E	279	ILE	5.7
1	E	443	PRO	5.5
1	E	207	ASP	5.5
1	A	163	LEU	5.4
1	E	451	LEU	5.4
1	C	444	LEU	5.4
1	E	138	CYS	5.2
1	E	160	VAL	5.2
1	D	255	ALA	5.2
1	E	277	PHE	5.1
1	E	100	PHE	5.0
1	E	136	ILE	5.0
1	D	237	ARG	5.0
1	E	248	THR	5.0
1	D	259	LEU	4.9
1	B	329	THR	4.7
1	B	286	THR	4.7
1	E	330	VAL	4.7
1	A	159	LEU	4.7
1	E	253	GLU	4.6
1	D	144	LEU	4.6
1	E	208	LYS	4.6
1	A	563	TYR	4.5
1	E	134	VAL	4.5
1	E	444	LEU	4.4
1	E	198	GLY	4.4
1	B	513	GLN	4.3
1	D	442	LEU	4.3
1	E	98	GLU	4.3
1	E	335	LEU	4.2
1	D	162	ASN	4.2
1	A	138	CYS	4.1
1	E	280	TYR	4.1
1	E	212	THR	4.1
1	E	329	THR	4.1
1	E	95	LYS	4.0
1	E	141	GLU	4.0
1	A	445	ASN	4.0
1	C	138	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	203	PHE	3.8
1	A	156	ARG	3.8
1	C	258	TYR	3.8
1	B	73	SER	3.8
1	E	234	ALA	3.8
1	E	203	PHE	3.8
1	E	283	SER	3.7
1	E	278	PRO	3.7
1	E	122	ASP	3.7
1	E	233	ILE	3.7
1	D	222	ILE	3.7
1	E	204	LEU	3.7
1	A	97	LYS	3.5
1	E	568	LEU	3.5
1	C	212	THR	3.5
1	D	200	TYR	3.5
1	D	221	HIS	3.5
1	B	328	LYS	3.5
1	D	336	MET	3.4
1	D	444	LEU	3.4
1	E	268	VAL	3.4
1	E	588	PHE	3.4
1	E	452	GLN	3.4
1	D	205	VAL	3.4
1	E	104	LEU	3.3
1	C	144	LEU	3.3
1	E	456	LEU	3.3
1	C	281	VAL	3.3
1	E	201	SER	3.3
1	E	211	VAL	3.3
1	D	249	LEU	3.2
1	D	152	VAL	3.2
1	C	280	TYR	3.2
1	E	152	VAL	3.2
1	E	226	ASP	3.2
1	B	512	PHE	3.2
1	D	233	ILE	3.2
1	E	566	ILE	3.2
1	E	125	ALA	3.2
1	B	74	GLU	3.1
1	A	539	TYR	3.1
1	A	212	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	567	TYR	3.1
1	E	464	LEU	3.1
1	C	213	SER	3.1
1	E	266	ASN	3.0
1	C	557	ARG	3.0
1	E	145	LEU	3.0
1	E	445	ASN	3.0
1	E	558	LEU	3.0
1	A	258	TYR	3.0
1	A	95	LYS	3.0
1	D	265	LYS	3.0
1	B	178	MET	3.0
1	A	202	ALA	3.0
1	C	136	ILE	3.0
1	E	209	VAL	3.0
1	D	145	LEU	3.0
1	D	330	VAL	3.0
1	B	568	LEU	3.0
1	A	237	ARG	2.9
1	A	541	MET	2.9
1	E	245	THR	2.9
1	E	101	LEU	2.9
1	E	255	ALA	2.9
1	C	279	ILE	2.9
1	E	548	GLU	2.9
1	B	204	LEU	2.9
1	E	227	SER	2.9
1	A	255	ALA	2.8
1	E	460	ILE	2.8
1	E	126	LEU	2.8
1	D	445	ASN	2.8
1	B	380	GLU	2.8
1	D	202	ALA	2.8
1	E	246	THR	2.8
1	A	591	VAL	2.8
1	C	448	ARG	2.8
1	E	121	THR	2.8
1	A	529	GLU	2.8
1	E	120	LEU	2.7
1	D	278	PRO	2.7
1	E	550	GLU	2.7
1	E	383	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	210	ILE	2.7
1	C	329	THR	2.7
1	E	336	MET	2.7
1	B	451	LEU	2.7
1	C	247	ILE	2.7
1	D	334	GLU	2.7
1	E	377	ALA	2.7
1	C	451	LEU	2.7
1	D	223	TRP	2.7
1	A	557	ARG	2.6
1	D	151	GLY	2.6
1	D	238	GLY	2.6
1	D	199	PHE	2.6
1	E	97	LYS	2.6
1	C	208	LYS	2.6
1	D	209	VAL	2.6
1	E	411	LEU	2.6
1	E	146	HIS	2.6
1	E	265	LYS	2.6
1	D	335	LEU	2.5
1	B	548	GLU	2.5
1	C	330	VAL	2.5
1	B	557	ARG	2.5
1	E	156	ARG	2.5
1	D	264	ILE	2.5
1	E	225	SER	2.5
1	A	444	LEU	2.5
1	D	159	LEU	2.5
1	E	259	LEU	2.4
1	C	259	LEU	2.4
1	E	553	PRO	2.4
1	C	163	LEU	2.4
1	E	549	ALA	2.4
1	B	539	TYR	2.4
1	E	328	LYS	2.4
1	C	442	LEU	2.4
1	E	543	GLY	2.4
1	A	126	LEU	2.4
1	C	115	ILE	2.4
1	E	224	GLU	2.4
1	D	443	PRO	2.4
1	A	232	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	228	ASN	2.4
1	A	199	PHE	2.3
1	E	231	SER	2.3
1	C	249	LEU	2.3
1	C	240	THR	2.3
1	A	533	GLU	2.3
1	C	254	GLU	2.3
1	C	203	PHE	2.3
1	E	142	LYS	2.3
1	E	164	GLY	2.3
1	C	220	GLN	2.3
1	A	556	GLU	2.3
1	D	210	ILE	2.3
1	E	232	VAL	2.3
1	B	594	GLU	2.3
1	E	331	TRP	2.3
1	D	211	VAL	2.3
1	D	212	THR	2.3
1	E	235	ASP	2.3
1	E	229	GLU	2.2
1	B	185	GLY	2.2
1	C	524	LEU	2.2
1	E	250	VAL	2.2
1	D	247	ILE	2.2
1	E	154	MET	2.2
1	E	236	PRO	2.2
1	E	557	ARG	2.2
1	A	219	THR	2.2
1	E	539	TYR	2.2
1	B	542	ALA	2.2
1	A	521	ILE	2.2
1	C	443	PRO	2.2
1	A	567	TYR	2.2
1	D	383	PHE	2.2
1	D	448	ARG	2.2
1	D	98	GLU	2.2
1	E	223	TRP	2.2
1	E	254	GLU	2.2
1	E	332	ASP	2.2
1	D	232	VAL	2.1
1	A	221	HIS	2.1
1	A	231	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	276	ASN	2.1
1	E	567	TYR	2.1
1	C	594	GLU	2.1
1	D	136	ILE	2.1
1	D	115	ILE	2.1
1	E	410	LYS	2.1
1	D	230	PHE	2.1
1	E	425	MET	2.1
1	A	214	LYS	2.1
1	D	213	SER	2.1
1	E	161	LYS	2.1
1	D	425	MET	2.1
1	E	251	LEU	2.1
1	B	575	TYR	2.1
1	C	145	LEU	2.1
1	D	253	GLU	2.1
1	C	408	TYR	2.0
1	D	139	ASP	2.0
1	E	221	HIS	2.0
1	E	117	LEU	2.0
1	E	139	ASP	2.0
1	C	264	ILE	2.0
1	E	241	LEU	2.0
1	E	594	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.