



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2017 – 09:21 PM EDT

PDB ID : 4IVJ  
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, triple mutant, I222 form  
Authors : Lai, Y.-T.; Sawaya, M.R.; Yeates, T.O.  
Deposited on : unknown  
Resolution : 7.35 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](mailto: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.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

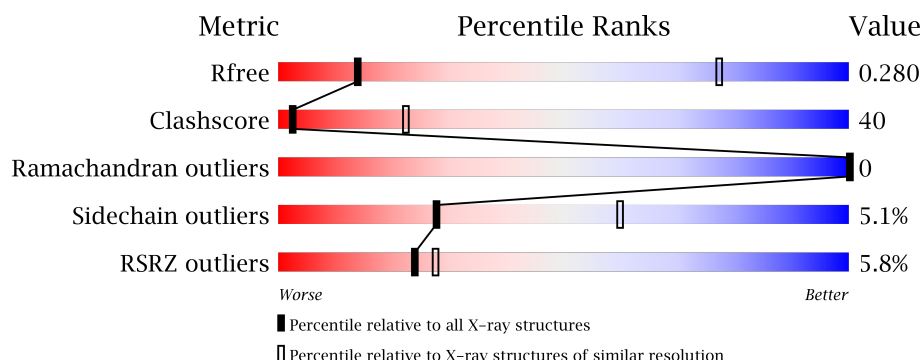
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 7.35 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))
$R_{free}$	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

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. 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	456	<div> <div>3%</div> <div>58%</div> <div>35%</div> <div>• •</div> </div>
1	B	456	<div> <div>9%</div> <div>55%</div> <div>37%</div> <div>5% •</div> </div>
1	C	456	<div> <div>4%</div> <div>54%</div> <div>39%</div> <div>• •</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10194 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	B	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	C	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
A	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
A	278	ALA	-	LINKER	UNP P03485
A	279	GLN	-	LINKER	UNP P03485
A	280	GLU	-	LINKER	UNP P03485
A	281	ALA	-	LINKER	UNP P03485
A	282	GLN	-	LINKER	UNP P03485
A	283	LYS	-	LINKER	UNP P03485
A	284	GLN	-	LINKER	UNP P03485
A	285	LYS	-	LINKER	UNP P03485
A	448	LEU	-	EXPRESSION TAG	UNP P03485
A	449	GLU	-	EXPRESSION TAG	UNP P03485
A	450	HIS	-	EXPRESSION TAG	UNP P03485
A	451	HIS	-	EXPRESSION TAG	UNP P03485
A	452	HIS	-	EXPRESSION TAG	UNP P03485
A	453	HIS	-	EXPRESSION TAG	UNP P03485
A	454	HIS	-	EXPRESSION TAG	UNP P03485
A	455	HIS	-	EXPRESSION TAG	UNP P03485
B	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
B	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
B	278	ALA	-	LINKER	UNP P03485
B	279	GLN	-	LINKER	UNP P03485
B	280	GLU	-	LINKER	UNP P03485

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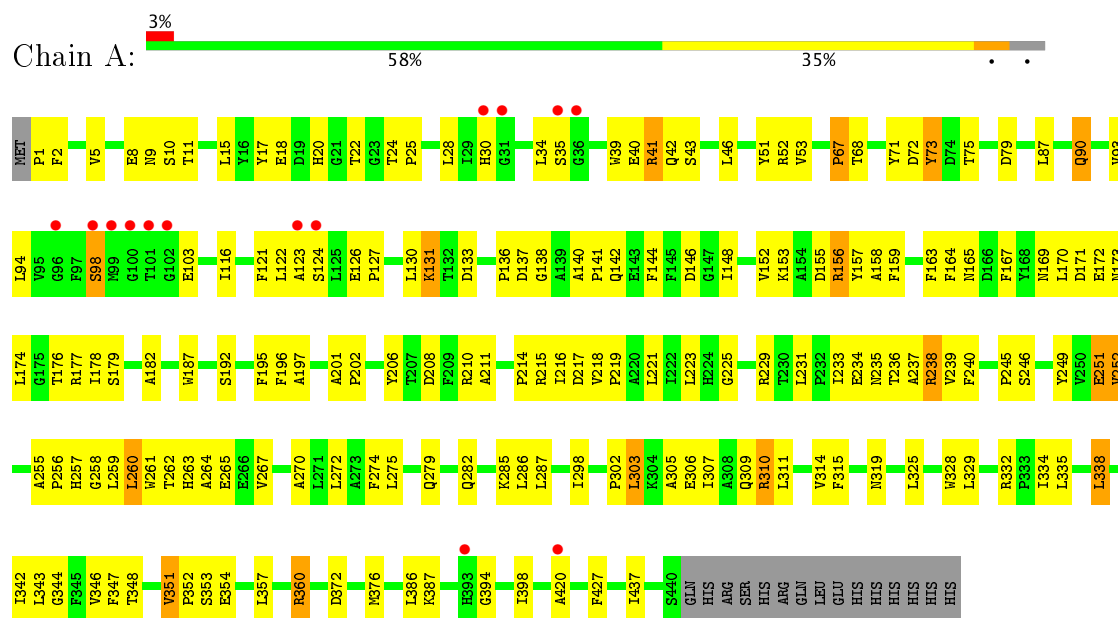
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Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	-	LINKER	UNP P03485
B	282	GLN	-	LINKER	UNP P03485
B	283	LYS	-	LINKER	UNP P03485
B	284	GLN	-	LINKER	UNP P03485
B	285	LYS	-	LINKER	UNP P03485
B	448	LEU	-	EXPRESSION TAG	UNP P03485
B	449	GLU	-	EXPRESSION TAG	UNP P03485
B	450	HIS	-	EXPRESSION TAG	UNP P03485
B	451	HIS	-	EXPRESSION TAG	UNP P03485
B	452	HIS	-	EXPRESSION TAG	UNP P03485
B	453	HIS	-	EXPRESSION TAG	UNP P03485
B	454	HIS	-	EXPRESSION TAG	UNP P03485
B	455	HIS	-	EXPRESSION TAG	UNP P03485
C	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
C	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
C	278	ALA	-	LINKER	UNP P03485
C	279	GLN	-	LINKER	UNP P03485
C	280	GLU	-	LINKER	UNP P03485
C	281	ALA	-	LINKER	UNP P03485
C	282	GLN	-	LINKER	UNP P03485
C	283	LYS	-	LINKER	UNP P03485
C	284	GLN	-	LINKER	UNP P03485
C	285	LYS	-	LINKER	UNP P03485
C	448	LEU	-	EXPRESSION TAG	UNP P03485
C	449	GLU	-	EXPRESSION TAG	UNP P03485
C	450	HIS	-	EXPRESSION TAG	UNP P03485
C	451	HIS	-	EXPRESSION TAG	UNP P03485
C	452	HIS	-	EXPRESSION TAG	UNP P03485
C	453	HIS	-	EXPRESSION TAG	UNP P03485
C	454	HIS	-	EXPRESSION TAG	UNP P03485
C	455	HIS	-	EXPRESSION TAG	UNP P03485

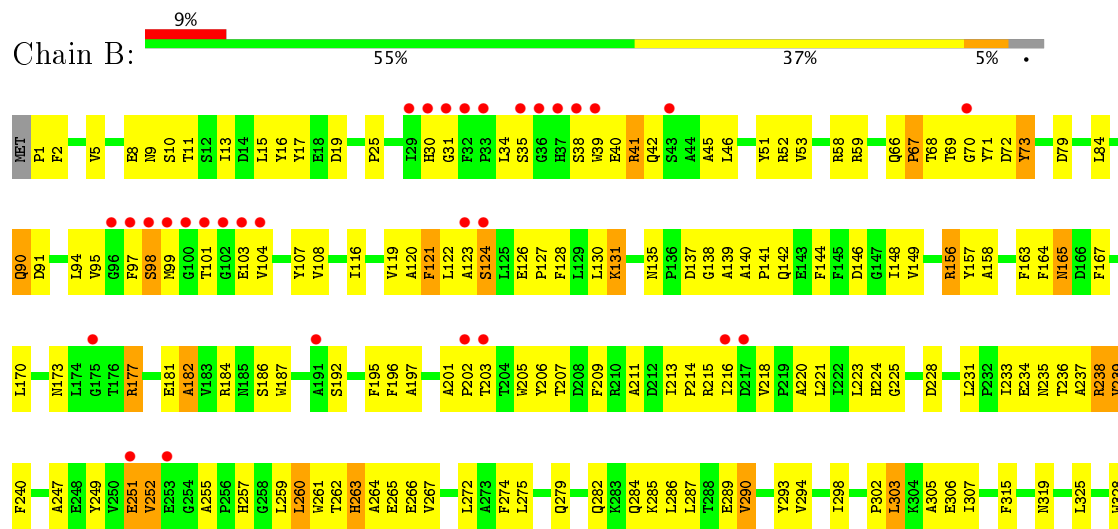
### 3 Residue-property plots

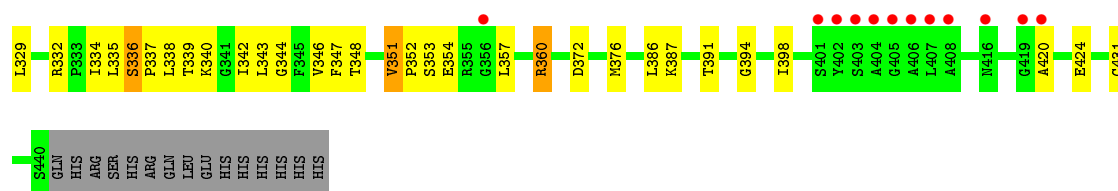
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

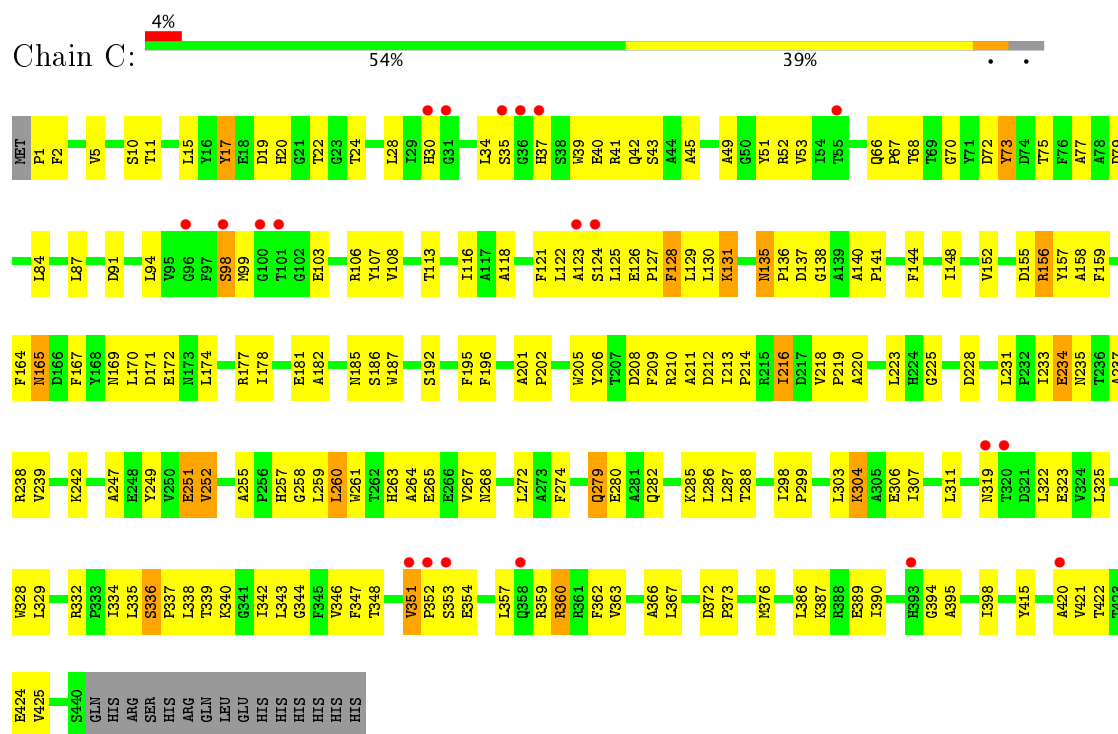


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1





- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.67Å 160.98Å 167.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.42 – 7.35 29.28 – 7.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.42-7.35) 97.2 (29.28-7.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 7.22Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, $R_{free}$	0.276 , 0.288 0.270 , 0.280	Depositor DCC
$R_{free}$ test set	121 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	400.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 204.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	10194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	318.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.79	2/3475 (0.1%)	1.23	22/4729 (0.5%)
1	B	0.75	2/3475 (0.1%)	1.17	20/4729 (0.4%)
1	C	0.77	3/3475 (0.1%)	1.16	21/4729 (0.4%)
All	All	0.77	7/10425 (0.1%)	1.19	63/14187 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	SER	CB-OG	5.35	1.49	1.42
1	C	136	PRO	N-CD	5.28	1.55	1.47
1	A	192	SER	CB-OG	5.16	1.49	1.42
1	C	192	SER	CB-OG	5.15	1.49	1.42
1	B	337	PRO	N-CD	5.07	1.54	1.47
1	C	337	PRO	N-CD	5.04	1.54	1.47
1	A	219	PRO	N-CD	5.02	1.54	1.47

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
1	C	53	VAL	CA-CB-CG2	5.98	119.87	110.90
1	C	98	SER	CB-CA-C	5.98	121.46	110.10
1	A	98	SER	CB-CA-C	5.97	121.45	110.10
1	A	53	VAL	CA-CB-CG2	5.96	119.84	110.90
1	A	121	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	B	239	VAL	CB-CA-C	5.92	122.64	111.40
1	C	121	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	218	VAL	C-N-CD	5.83	140.65	128.40
1	B	35	SER	N-CA-CB	-5.83	101.75	110.50
1	B	252	VAL	CA-C-N	-5.82	104.40	117.20
1	A	252	VAL	CA-C-N	-5.81	104.42	117.20
1	C	252	VAL	CA-C-N	-5.80	104.44	117.20
1	A	35	SER	N-CA-CB	-5.76	101.85	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	THR	CA-CB-CG2	5.76	120.47	112.40
1	C	336	SER	C-N-CD	5.76	140.50	128.40
1	B	336	SER	C-N-CD	5.74	140.46	128.40
1	A	22	THR	CA-CB-CG2	5.71	120.40	112.40
1	A	142	GLN	CG-CD-NE2	-5.70	103.02	116.70
1	B	182	ALA	N-CA-CB	5.70	118.07	110.10
1	B	142	GLN	CG-CD-NE2	-5.69	103.03	116.70
1	B	131	LYS	CB-CG-CD	-5.65	96.92	111.60
1	A	131	LYS	CB-CG-CD	-5.62	97.00	111.60
1	B	67	PRO	CA-C-O	5.59	133.62	120.20
1	C	131	LYS	CB-CG-CD	-5.59	97.06	111.60
1	A	103	GLU	N-CA-CB	5.58	120.64	110.60
1	C	124	SER	CB-CA-C	-5.56	99.54	110.10
1	A	124	SER	CB-CA-C	-5.55	99.55	110.10
1	C	135	ASN	C-N-CD	5.55	140.06	128.40
1	C	103	GLU	N-CA-CB	5.51	120.53	110.60
1	C	67	PRO	CA-C-O	5.50	133.41	120.20
1	A	67	PRO	CA-C-O	5.50	133.41	120.20
1	A	2	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	C	35	SER	N-CA-CB	-5.47	102.30	110.50
1	B	103	GLU	N-CA-CB	5.46	120.43	110.60
1	B	207	THR	N-CA-C	-5.45	96.29	111.00
1	B	2	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	75	THR	CA-CB-OG1	-5.34	97.78	109.00
1	C	2	PHE	CB-CG-CD2	-5.29	117.09	120.80
1	C	2	PHE	CB-CA-C	-5.28	99.85	110.40
1	A	2	PHE	CB-CA-C	-5.26	99.88	110.40
1	C	73	TYR	CA-CB-CG	-5.25	103.43	113.40
1	A	146	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	173	ASN	N-CA-C	5.22	125.11	111.00
1	B	73	TYR	CA-CB-CG	-5.22	103.48	113.40
1	B	2	PHE	CB-CA-C	-5.22	99.97	110.40
1	A	73	TYR	CA-CB-CG	-5.21	103.49	113.40
1	B	251	GLU	N-CA-CB	5.19	119.94	110.60
1	B	251	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	A	251	GLU	N-CA-CB	5.17	119.90	110.60
1	C	103	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	79	ASP	CA-CB-CG	5.14	124.71	113.40
1	B	146	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	251	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	C	79	ASP	CA-CB-CG	5.13	124.69	113.40
1	B	103	GLU	OE1-CD-OE2	-5.12	117.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	GLU	N-CA-CB	5.11	119.81	110.60
1	A	79	ASP	CA-CB-CG	5.05	124.50	113.40
1	C	113	THR	CA-CB-CG2	5.04	119.46	112.40
1	A	103	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	C	251	GLU	OE1-CD-OE2	5.03	129.33	123.30
1	B	16	TYR	CZ-CE2-CD2	-5.02	115.28	119.80
1	A	153	LYS	CD-CE-NZ	5.01	123.23	111.70

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	3398	0	3326	245	0
1	B	3398	0	3326	352	0
1	C	3398	0	3326	323	0
All	All	10194	0	9978	814	0

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 40.

All (814) 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:303:LEU:CD1	1:B:334:ILE:HB	1.46	1.46
1:B:10:SER:CB	1:C:87:LEU:HD22	1.53	1.39
1:B:303:LEU:HD12	1:B:334:ILE:CB	1.53	1.38
1:C:298:ILE:HD13	1:C:307:ILE:CD1	1.61	1.30
1:B:11:THR:HG22	1:C:17:TYR:CZ	1.65	1.29
1:C:298:ILE:CD1	1:C:307:ILE:HD13	1.66	1.25
1:B:158:ALA:HA	1:C:181:GLU:CD	1.67	1.14
1:B:10:SER:HB3	1:C:87:LEU:HD22	1.30	1.14
1:B:177:ARG:HB3	1:B:262:THR:CG2	1.78	1.13
1:A:233:ILE:HG13	1:A:237:ALA:HB3	1.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD11	1:A:261:TRP:O	1.47	1.11
1:C:359:ARG:HD2	1:C:415:TYR:CZ	1.85	1.10
1:C:360:ARG:HB2	1:C:363:VAL:HG23	1.35	1.08
1:B:108:VAL:HG11	1:B:216:ILE:HG12	1.14	1.07
1:C:24:THR:CG2	1:C:51:TYR:HD1	1.66	1.07
1:B:99:MET:SD	1:B:205:TRP:NE1	2.29	1.06
1:C:24:THR:HG22	1:C:51:TYR:HD1	1.20	1.06
1:B:10:SER:HB3	1:C:87:LEU:CD2	1.84	1.06
1:B:67:PRO:HA	1:C:20:HIS:HE1	1.20	1.06
1:B:177:ARG:HB3	1:B:262:THR:CB	1.87	1.05
1:B:9:ASN:HB2	1:C:19:ASP:CB	1.87	1.05
1:A:11:THR:HG22	1:B:17:TYR:CZ	1.91	1.05
1:B:9:ASN:CB	1:C:19:ASP:HB3	1.87	1.03
1:B:67:PRO:HA	1:C:20:HIS:CE1	1.94	1.03
1:A:287:LEU:HD13	1:A:315:PHE:HB3	1.42	1.02
1:A:40:GLU:OE1	1:C:156:ARG:HD3	1.57	1.02
1:B:10:SER:CB	1:C:87:LEU:CD2	2.37	1.01
1:C:24:THR:HG22	1:C:51:TYR:CD1	1.94	1.01
1:A:287:LEU:HD13	1:A:315:PHE:CB	1.90	1.00
1:B:177:ARG:HB3	1:B:262:THR:HG22	1.41	1.00
1:A:9:ASN:ND2	1:B:19:ASP:HB3	1.75	1.00
1:A:157:TYR:HB3	1:B:181:GLU:HB3	1.39	1.00
1:B:11:THR:HG22	1:C:17:TYR:CE2	1.95	0.99
1:C:144:PHE:CE2	1:C:148:ILE:HD11	1.97	0.99
1:C:303:LEU:HD22	1:C:334:ILE:HB	1.45	0.99
1:B:108:VAL:HG11	1:B:216:ILE:CG1	1.93	0.98
1:C:24:THR:CG2	1:C:51:TYR:CD1	2.46	0.97
1:B:10:SER:OG	1:C:87:LEU:HD22	1.63	0.97
1:A:157:TYR:HB3	1:B:181:GLU:CB	1.96	0.96
1:B:156:ARG:HD3	1:C:40:GLU:OE1	1.67	0.94
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.48	0.94
1:C:84:LEU:HD12	1:C:107:TYR:CZ	2.03	0.94
1:A:11:THR:CG2	1:B:17:TYR:CE2	2.51	0.94
1:B:139:ALA:CB	1:B:235:ASN:ND2	2.30	0.94
1:B:9:ASN:HB2	1:C:19:ASP:HB3	0.96	0.94
1:B:263:HIS:HB3	1:B:266:GLU:OE1	1.69	0.93
1:A:260:LEU:HD23	1:A:267:VAL:HG11	1.48	0.93
1:A:303:LEU:HD12	1:A:334:ILE:HB	1.50	0.93
1:C:360:ARG:HB2	1:C:363:VAL:CG2	1.98	0.93
1:B:108:VAL:CG1	1:B:216:ILE:HG12	1.98	0.93
1:A:260:LEU:O	1:A:264:ALA:HB2	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD12	1:B:107:TYR:CZ	2.03	0.93
1:B:303:LEU:HB2	1:B:334:ILE:CD1	1.98	0.93
1:B:30:HIS:HA	1:B:39:TRP:HE1	1.33	0.92
1:C:359:ARG:HD2	1:C:415:TYR:CE1	2.05	0.91
1:C:233:ILE:O	1:C:237:ALA:HB3	1.69	0.91
1:B:104:VAL:CG1	1:B:121:PHE:CE1	2.53	0.91
1:B:177:ARG:HB3	1:B:262:THR:HB	1.50	0.91
1:B:39:TRP:CZ2	1:B:97:PHE:HB3	2.05	0.91
1:A:127:PRO:CD	1:A:239:VAL:HG13	2.02	0.90
1:B:10:SER:HB2	1:C:19:ASP:OD2	1.70	0.90
1:C:303:LEU:CD2	1:C:334:ILE:HB	2.01	0.90
1:C:360:ARG:HG3	1:C:362:PHE:CZ	2.07	0.90
1:B:157:TYR:CD2	1:C:182:ALA:HA	2.06	0.90
1:B:11:THR:CG2	1:C:17:TYR:CE2	2.54	0.90
1:B:51:TYR:HE1	1:B:279:GLN:OE1	1.55	0.89
1:C:41:ARG:HD2	1:C:264:ALA:CB	2.02	0.89
1:A:178:ILE:HD11	1:A:261:TRP:C	1.94	0.88
1:A:127:PRO:HD2	1:A:239:VAL:CG1	2.03	0.88
1:B:195:PHE:CG	1:C:40:GLU:HB2	2.08	0.88
1:A:126:GLU:O	1:A:236:THR:HB	1.73	0.88
1:B:139:ALA:HB2	1:B:235:ASN:HD22	1.36	0.87
1:A:11:THR:HG22	1:B:17:TYR:OH	1.74	0.87
1:B:164:PHE:CE1	1:B:186:SER:HB3	2.09	0.87
1:B:233:ILE:HG13	1:B:237:ALA:HB3	1.55	0.87
1:A:233:ILE:HG13	1:A:237:ALA:CB	2.05	0.86
1:A:182:ALA:HB1	1:A:261:TRP:HZ2	1.39	0.86
1:C:129:LEU:CD1	1:C:205:TRP:HB3	2.06	0.86
1:C:303:LEU:HD21	1:C:335:LEU:HG	1.57	0.85
1:A:234:GLU:HA	1:A:238:ARG:HB2	1.58	0.85
1:B:139:ALA:HB2	1:B:235:ASN:ND2	1.89	0.85
1:A:127:PRO:HD2	1:A:239:VAL:HG13	1.58	0.85
1:A:164:PHE:HE2	1:A:187:TRP:HB2	1.40	0.85
1:C:108:VAL:HG11	1:C:216:ILE:HG12	1.59	0.85
1:B:287:LEU:O	1:B:290:VAL:HG12	1.76	0.85
1:C:360:ARG:CB	1:C:363:VAL:HG23	2.06	0.85
1:B:139:ALA:CB	1:B:235:ASN:HD22	1.87	0.84
1:C:129:LEU:HD12	1:C:205:TRP:HB3	1.55	0.84
1:B:39:TRP:HZ2	1:B:97:PHE:HB3	1.38	0.84
1:B:259:LEU:HD23	1:B:259:LEU:H	1.43	0.84
1:C:285:LYS:O	1:C:288:THR:HG22	1.77	0.84
1:C:165:ASN:OD1	1:C:170:LEU:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:HD23	1:C:398:ILE:HD11	1.59	0.83
1:B:303:LEU:HB2	1:B:334:ILE:HD12	1.59	0.83
1:B:158:ALA:HA	1:C:181:GLU:CG	2.08	0.83
1:A:386:LEU:HD23	1:A:398:ILE:HD11	1.59	0.83
1:B:303:LEU:HD12	1:B:334:ILE:CG1	2.09	0.82
1:B:386:LEU:HD23	1:B:398:ILE:HD11	1.59	0.82
1:A:262:THR:HG22	1:A:263:HIS:ND1	1.95	0.82
1:C:298:ILE:HD13	1:C:307:ILE:HD13	0.87	0.82
1:A:8:GLU:OE1	1:A:67:PRO:CB	2.27	0.81
1:C:127:PRO:HB2	1:C:210:ARG:HG2	1.60	0.81
1:C:303:LEU:HD21	1:C:335:LEU:CD2	2.10	0.81
1:B:303:LEU:HD12	1:B:334:ILE:HB	0.83	0.81
1:C:128:PHE:HE1	1:C:206:TYR:O	1.63	0.81
1:C:164:PHE:HE2	1:C:187:TRP:HA	1.43	0.81
1:B:164:PHE:CZ	1:B:186:SER:HB3	2.16	0.81
1:C:322:LEU:HD23	1:C:357:LEU:HD12	1.63	0.81
1:A:303:LEU:CD1	1:A:334:ILE:HB	2.11	0.80
1:A:164:PHE:HE2	1:A:187:TRP:CB	1.93	0.80
1:A:51:TYR:CZ	1:A:279:GLN:HG3	2.15	0.80
1:B:195:PHE:CD1	1:C:40:GLU:HB2	2.16	0.80
1:C:303:LEU:HD21	1:C:335:LEU:CG	2.11	0.80
1:A:262:THR:HG22	1:A:263:HIS:CE1	2.17	0.80
1:C:135:ASN:HD21	1:C:137:ASP:HB2	1.44	0.80
1:C:390:ILE:O	1:C:390:ILE:HG22	1.82	0.80
1:B:233:ILE:HD11	1:B:249:TYR:OH	1.83	0.79
1:A:173:ASN:ND2	1:A:177:ARG:HG3	1.96	0.79
1:B:11:THR:CG2	1:C:17:TYR:CZ	2.58	0.79
1:B:177:ARG:CB	1:B:262:THR:HG22	2.12	0.79
1:A:178:ILE:HD13	1:A:261:TRP:CD1	2.18	0.79
1:B:126:GLU:HB3	1:B:127:PRO:HA	1.64	0.79
1:B:164:PHE:HE2	1:B:187:TRP:HA	1.48	0.79
1:C:126:GLU:HB3	1:C:127:PRO:HA	1.64	0.78
1:B:157:TYR:C	1:C:181:GLU:HB3	2.03	0.78
1:A:286:LEU:HD11	1:A:427:PHE:CE2	2.19	0.78
1:B:177:ARG:HG3	1:B:263:HIS:CE1	2.18	0.78
1:A:360:ARG:HG2	1:A:360:ARG:HH11	1.50	0.77
1:A:11:THR:HG22	1:B:17:TYR:CE2	2.14	0.77
1:A:11:THR:CG2	1:B:17:TYR:CZ	2.68	0.76
1:B:360:ARG:HH11	1:B:360:ARG:HG2	1.50	0.76
1:A:287:LEU:CD1	1:A:315:PHE:HB3	2.15	0.76
1:C:360:ARG:CG	1:C:362:PHE:CE1	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:PHE:CE2	1:C:363:VAL:HG22	2.21	0.76
1:C:129:LEU:HB2	1:C:206:TYR:HA	1.68	0.76
1:A:17:TYR:CZ	1:C:11:THR:HG22	2.21	0.75
1:A:234:GLU:HA	1:A:238:ARG:HD2	1.69	0.75
1:A:303:LEU:HD12	1:A:334:ILE:CB	2.17	0.75
1:C:421:VAL:HB	1:C:425:VAL:HG11	1.69	0.75
1:B:234:GLU:HA	1:B:238:ARG:HB2	1.67	0.75
1:C:329:LEU:HD22	1:C:335:LEU:CD1	2.17	0.75
1:A:260:LEU:CD2	1:A:267:VAL:HG11	2.17	0.75
1:B:211:ALA:O	1:B:214:PRO:HD2	1.86	0.75
1:B:252:VAL:HG12	1:B:255:ALA:HB2	1.69	0.75
1:A:182:ALA:HB1	1:A:261:TRP:CZ2	2.21	0.75
1:A:259:LEU:HD23	1:A:259:LEU:H	1.50	0.75
1:A:211:ALA:O	1:A:214:PRO:HD2	1.86	0.75
1:C:252:VAL:HG12	1:C:255:ALA:HB2	1.69	0.74
1:C:359:ARG:CD	1:C:415:TYR:CZ	2.69	0.74
1:B:104:VAL:HG12	1:B:121:PHE:CE1	2.22	0.74
1:C:130:LEU:O	1:C:138:GLY:HA3	1.86	0.74
1:B:303:LEU:CG	1:B:334:ILE:HD12	2.18	0.74
1:A:51:TYR:OH	1:A:279:GLN:HG3	1.88	0.74
1:B:104:VAL:HG11	1:B:121:PHE:CE1	2.22	0.74
1:B:177:ARG:CB	1:B:262:THR:CG2	2.64	0.74
1:C:41:ARG:HD2	1:C:264:ALA:HB2	1.70	0.74
1:C:359:ARG:HD2	1:C:415:TYR:CE2	2.23	0.73
1:B:157:TYR:HB3	1:C:181:GLU:HB3	1.68	0.73
1:C:360:ARG:HG3	1:C:362:PHE:CE1	2.23	0.73
1:A:131:LYS:HD2	1:A:138:GLY:O	1.88	0.73
1:A:24:THR:HG21	1:A:279:GLN:OE1	1.89	0.73
1:A:252:VAL:HG12	1:A:255:ALA:HB2	1.69	0.73
1:B:41:ARG:HD2	1:B:264:ALA:HB2	1.71	0.73
1:B:282:GLN:O	1:B:286:LEU:HG	1.88	0.73
1:C:156:ARG:NE	1:C:157:TYR:CZ	2.56	0.73
1:B:344:GLY:O	1:B:348:THR:HG23	1.89	0.73
1:A:177:ARG:HD2	1:A:263:HIS:CE1	2.24	0.73
1:A:344:GLY:O	1:A:348:THR:HG23	1.89	0.73
1:C:211:ALA:O	1:C:214:PRO:HD2	1.88	0.72
1:C:344:GLY:O	1:C:348:THR:HG23	1.89	0.72
1:A:303:LEU:HB2	1:A:334:ILE:HD12	1.70	0.72
1:C:233:ILE:HG13	1:C:237:ALA:CB	2.19	0.72
1:C:164:PHE:CE1	1:C:186:SER:HB3	2.23	0.72
1:B:128:PHE:HE1	1:B:206:TYR:C	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:HD12	1:B:334:ILE:CD1	2.19	0.72
1:A:179:SER:OG	1:C:158:ALA:HB2	1.90	0.71
1:B:221:LEU:HB2	1:B:274:PHE:CE1	2.25	0.71
1:A:41:ARG:CD	1:A:264:ALA:CB	2.67	0.71
1:A:164:PHE:CZ	1:A:187:TRP:HA	2.24	0.71
1:C:233:ILE:O	1:C:237:ALA:CB	2.39	0.71
1:C:421:VAL:HB	1:C:425:VAL:CG1	2.20	0.71
1:A:71:TYR:OH	1:A:197:ALA:HB2	1.90	0.71
1:A:164:PHE:CE2	1:A:187:TRP:HB2	2.25	0.71
1:A:8:GLU:OE1	1:A:67:PRO:HB3	1.90	0.71
1:B:303:LEU:CB	1:B:334:ILE:HD12	2.20	0.71
1:A:41:ARG:HD2	1:A:264:ALA:CB	2.22	0.70
1:C:360:ARG:HB3	1:C:362:PHE:CE1	2.26	0.70
1:B:38:SER:HA	1:B:261:TRP:HZ2	1.55	0.70
1:B:39:TRP:CZ2	1:B:97:PHE:CB	2.73	0.70
1:B:177:ARG:CB	1:B:262:THR:HB	2.22	0.70
1:B:156:ARG:CD	1:C:40:GLU:OE1	2.38	0.70
1:C:285:LYS:HG3	1:C:286:LEU:N	2.07	0.70
1:B:51:TYR:CE1	1:B:279:GLN:OE1	2.44	0.70
1:B:158:ALA:N	1:C:181:GLU:HB2	2.07	0.69
1:B:68:THR:OG1	1:C:20:HIS:HB3	1.92	0.69
1:A:18:GLU:CG	1:A:20:HIS:CE1	2.75	0.69
1:C:165:ASN:ND2	1:C:170:LEU:HD12	2.06	0.69
1:A:71:TYR:CE1	1:A:197:ALA:HA	2.28	0.69
1:B:1:PRO:CB	1:B:17:TYR:CE1	2.75	0.69
1:B:307:ILE:HD11	1:B:335:LEU:HD21	1.75	0.69
1:B:303:LEU:HB2	1:B:334:ILE:HD13	1.72	0.69
1:B:158:ALA:N	1:C:181:GLU:CB	2.55	0.69
1:B:157:TYR:CB	1:C:181:GLU:HB3	2.23	0.69
1:C:329:LEU:CD2	1:C:335:LEU:HD11	2.23	0.69
1:A:234:GLU:HA	1:A:238:ARG:CD	2.23	0.69
1:B:236:THR:O	1:B:240:PHE:HB2	1.93	0.69
1:C:303:LEU:HD21	1:C:335:LEU:HD23	1.73	0.69
1:A:259:LEU:O	1:A:263:HIS:N	2.25	0.68
1:B:71:TYR:CE1	1:B:197:ALA:HA	2.28	0.68
1:A:18:GLU:CG	1:A:20:HIS:NE2	2.56	0.68
1:A:260:LEU:O	1:A:264:ALA:CB	2.42	0.68
1:C:164:PHE:CZ	1:C:186:SER:HB3	2.28	0.68
1:C:304:LYS:HA	1:C:307:ILE:HD12	1.75	0.68
1:A:259:LEU:O	1:A:263:HIS:CA	2.42	0.68
1:C:298:ILE:HG23	1:C:299:PRO:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HD2	1:A:264:ALA:HB2	1.74	0.68
1:A:287:LEU:HD13	1:A:315:PHE:CG	2.29	0.68
1:B:8:GLU:OE2	1:B:13:ILE:HD11	1.94	0.67
1:A:164:PHE:CE2	1:A:187:TRP:HA	2.28	0.67
1:A:221:LEU:HB2	1:A:274:PHE:CD1	2.29	0.67
1:B:135:ASN:HD21	1:B:137:ASP:CB	2.08	0.67
1:B:139:ALA:CA	1:B:235:ASN:ND2	2.58	0.67
1:C:164:PHE:CE2	1:C:187:TRP:HA	2.28	0.67
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.77	0.67
1:B:135:ASN:HD21	1:B:137:ASP:HB2	1.58	0.67
1:B:66:GLN:OE1	1:C:37:HIS:CE1	2.48	0.67
1:A:127:PRO:HD3	1:A:239:VAL:HG13	1.76	0.67
1:B:157:TYR:C	1:C:181:GLU:CB	2.63	0.67
1:B:259:LEU:CD2	1:B:259:LEU:H	2.08	0.67
1:B:287:LEU:HD13	1:B:315:PHE:CG	2.30	0.67
1:C:303:LEU:HD23	1:C:334:ILE:CG2	2.24	0.67
1:B:139:ALA:HA	1:B:235:ASN:ND2	2.09	0.67
1:A:158:ALA:HA	1:B:181:GLU:OE2	1.95	0.66
1:A:303:LEU:HD12	1:A:334:ILE:CG1	2.25	0.66
1:B:158:ALA:CA	1:C:181:GLU:CD	2.57	0.66
1:C:164:PHE:HE2	1:C:187:TRP:CA	2.08	0.66
1:A:127:PRO:HD2	1:A:239:VAL:HG11	1.76	0.66
1:C:362:PHE:O	1:C:366:ALA:N	2.23	0.66
1:C:360:ARG:N	1:C:415:TYR:OH	2.27	0.66
1:B:71:TYR:OH	1:B:197:ALA:HB2	1.95	0.66
1:B:157:TYR:HB3	1:C:181:GLU:C	2.16	0.66
1:B:164:PHE:CE2	1:B:187:TRP:HA	2.30	0.66
1:A:18:GLU:HG3	1:A:20:HIS:CE1	2.29	0.66
1:B:8:GLU:HG3	1:B:67:PRO:HB3	1.77	0.66
1:C:17:TYR:HE2	1:C:19:ASP:OD2	1.79	0.66
1:B:11:THR:HB	1:C:1:PRO:HB3	1.76	0.65
1:C:155:ASP:HB3	1:C:158:ALA:HB3	1.77	0.65
1:A:221:LEU:HB2	1:A:274:PHE:CG	2.31	0.65
1:A:30:HIS:CE1	1:A:34:LEU:O	2.50	0.65
1:B:104:VAL:CG1	1:B:121:PHE:CZ	2.79	0.65
1:B:360:ARG:NH1	1:B:360:ARG:HG2	2.12	0.65
1:B:10:SER:CB	1:C:19:ASP:OD2	2.43	0.65
1:B:195:PHE:HB2	1:C:40:GLU:OE1	1.95	0.65
1:A:163:PHE:O	1:A:167:PHE:HB2	1.97	0.65
1:B:249:TYR:HE1	1:B:251:GLU:HG3	1.62	0.65
1:C:84:LEU:HD12	1:C:107:TYR:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.76	0.65
1:C:390:ILE:CG2	1:C:390:ILE:O	2.45	0.65
1:A:40:GLU:OE1	1:C:156:ARG:CD	2.42	0.65
1:B:303:LEU:CD1	1:B:334:ILE:CB	2.35	0.65
1:B:336:SER:HB2	1:B:339:THR:CB	2.27	0.65
1:C:144:PHE:HE2	1:C:148:ILE:HD11	1.61	0.65
1:C:395:ALA:HB2	1:C:425:VAL:HG23	1.78	0.65
1:A:157:TYR:CB	1:B:181:GLU:CB	2.73	0.64
1:A:93:VAL:HG11	1:A:275:LEU:CD2	2.24	0.64
1:B:137:ASP:OD2	1:B:239:VAL:HG11	1.97	0.64
1:B:259:LEU:N	1:B:259:LEU:HD23	2.11	0.64
1:B:84:LEU:CD1	1:B:107:TYR:CZ	2.79	0.64
1:C:233:ILE:O	1:C:237:ALA:N	2.30	0.64
1:A:298:ILE:HD13	1:A:307:ILE:HD12	1.78	0.64
1:B:30:HIS:CE1	1:B:34:LEU:O	2.50	0.64
1:C:329:LEU:CD2	1:C:335:LEU:CD1	2.75	0.64
1:A:1:PRO:HB2	1:A:17:TYR:O	1.98	0.64
1:A:18:GLU:HG2	1:A:20:HIS:NE2	2.13	0.64
1:B:11:THR:HG23	1:C:19:ASP:CG	2.17	0.64
1:B:95:VAL:HG22	1:B:120:ALA:HB3	1.80	0.64
1:C:298:ILE:CG2	1:C:299:PRO:HD2	2.27	0.64
1:B:84:LEU:HD12	1:B:107:TYR:CE2	2.32	0.64
1:A:360:ARG:HG2	1:A:360:ARG:NH1	2.12	0.64
1:A:164:PHE:CE2	1:A:187:TRP:CA	2.80	0.64
1:B:1:PRO:HB2	1:B:17:TYR:CE1	2.33	0.64
1:C:259:LEU:O	1:C:263:HIS:N	2.29	0.64
1:B:319:ASN:HA	1:B:352:PRO:HG2	1.80	0.63
1:C:84:LEU:CD1	1:C:107:TYR:CZ	2.79	0.63
1:C:137:ASP:CG	1:C:239:VAL:CG2	2.66	0.63
1:C:319:ASN:HA	1:C:352:PRO:HG2	1.80	0.63
1:C:178:ILE:HD12	1:C:261:TRP:HD1	1.62	0.63
1:C:359:ARG:CD	1:C:415:TYR:CE1	2.81	0.63
1:A:319:ASN:HA	1:A:352:PRO:HG2	1.80	0.63
1:B:11:THR:HG23	1:C:19:ASP:OD2	1.99	0.63
1:A:262:THR:CG2	1:A:263:HIS:CE1	2.82	0.63
1:A:152:VAL:HG22	1:A:159:PHE:CE1	2.34	0.63
1:A:235:ASN:O	1:A:239:VAL:HG11	1.99	0.62
1:C:127:PRO:HG3	1:C:239:VAL:HG12	1.81	0.62
1:A:259:LEU:O	1:A:263:HIS:C	2.38	0.62
1:B:126:GLU:HG3	1:B:209:PHE:CB	2.30	0.62
1:B:73:TYR:OH	1:B:99:MET:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:HB	1:C:1:PRO:CB	2.29	0.62
1:B:335:LEU:HB3	1:B:340:LYS:CG	2.29	0.62
1:C:129:LEU:HD12	1:C:205:TRP:C	2.20	0.62
1:A:311:LEU:O	1:A:315:PHE:CG	2.52	0.62
1:B:234:GLU:H	1:B:234:GLU:CD	2.03	0.61
1:B:158:ALA:HA	1:C:181:GLU:OE2	1.99	0.61
1:C:30:HIS:CE1	1:C:34:LEU:O	2.53	0.61
1:A:18:GLU:HG3	1:A:20:HIS:NE2	2.15	0.61
1:A:87:LEU:HD22	1:C:10:SER:CB	2.29	0.61
1:B:119:VAL:HG23	1:B:121:PHE:HE2	1.65	0.61
1:A:9:ASN:HD21	1:B:52:ARG:HE	1.48	0.61
1:A:298:ILE:HD13	1:A:307:ILE:CD1	2.30	0.61
1:A:8:GLU:OE1	1:A:67:PRO:CA	2.49	0.61
1:B:303:LEU:HD11	1:B:334:ILE:HB	1.70	0.61
1:C:178:ILE:HD12	1:C:261:TRP:CD1	2.36	0.60
1:A:9:ASN:OD1	1:A:10:SER:N	2.35	0.60
1:B:286:LEU:HD13	1:B:424:GLU:CG	2.30	0.60
1:B:336:SER:HB2	1:B:339:THR:OG1	2.01	0.60
1:A:17:TYR:CE2	1:C:11:THR:HG22	2.35	0.60
1:A:152:VAL:HG22	1:A:159:PHE:CD1	2.37	0.60
1:B:135:ASN:ND2	1:B:137:ASP:HB2	2.16	0.60
1:B:157:TYR:HD2	1:C:182:ALA:HA	1.65	0.60
1:C:137:ASP:OD2	1:C:239:VAL:HG13	2.02	0.60
1:B:101:THR:OG1	1:B:124:SER:HA	2.02	0.60
1:B:164:PHE:HE2	1:B:187:TRP:CA	2.13	0.60
1:B:284:GLN:O	1:B:287:LEU:HB2	2.01	0.60
1:B:303:LEU:HD12	1:B:334:ILE:HD12	1.84	0.60
1:B:104:VAL:HG12	1:B:121:PHE:CZ	2.36	0.60
1:A:8:GLU:OE1	1:A:67:PRO:HA	2.00	0.60
1:B:11:THR:HG22	1:C:17:TYR:CE1	2.33	0.60
1:B:72:ASP:OD1	1:B:73:TYR:N	2.35	0.60
1:B:206:TYR:CD2	1:B:206:TYR:O	2.55	0.59
1:B:99:MET:SD	1:B:205:TRP:CD1	2.94	0.59
1:C:129:LEU:HD12	1:C:205:TRP:CB	2.29	0.59
1:A:259:LEU:HD23	1:A:259:LEU:N	2.17	0.59
1:C:208:ASP:OD1	1:C:210:ARG:HG3	2.03	0.59
1:B:285:LYS:O	1:B:289:GLU:HG3	2.02	0.59
1:C:303:LEU:CD2	1:C:335:LEU:HD23	2.33	0.59
1:B:42:GLN:NE2	1:B:260:LEU:HB3	2.17	0.59
1:C:360:ARG:HD2	1:C:362:PHE:HE1	1.68	0.59
1:A:41:ARG:HD3	1:A:264:ALA:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PHE:CE1	1:C:206:TYR:O	2.51	0.59
1:C:137:ASP:HB3	1:C:239:VAL:HG21	1.83	0.59
1:C:249:TYR:HE1	1:C:251:GLU:HG3	1.67	0.59
1:C:282:GLN:HA	1:C:285:LYS:HG2	1.84	0.59
1:C:108:VAL:HG11	1:C:216:ILE:CG1	2.31	0.59
1:C:233:ILE:CG1	1:C:237:ALA:HB3	2.33	0.59
1:C:51:TYR:HE1	1:C:279:GLN:OE1	1.86	0.59
1:B:104:VAL:HG11	1:B:121:PHE:CZ	2.37	0.58
1:B:336:SER:HB2	1:B:339:THR:HB	1.85	0.58
1:B:131:LYS:HD2	1:B:138:GLY:O	2.03	0.58
1:B:108:VAL:CG1	1:B:216:ILE:CG1	2.70	0.58
1:B:41:ARG:HD3	1:B:264:ALA:CB	2.33	0.58
1:A:71:TYR:CZ	1:A:197:ALA:HA	2.39	0.58
1:B:201:ALA:HB3	1:B:202:PRO:HD3	1.85	0.58
1:B:386:LEU:CD2	1:B:398:ILE:HD11	2.32	0.58
1:C:360:ARG:CB	1:C:362:PHE:CE1	2.86	0.58
1:B:68:THR:HA	1:B:196:PHE:CD1	2.38	0.58
1:C:303:LEU:HD11	1:C:332:ARG:HG3	1.85	0.58
1:A:259:LEU:CD2	1:A:259:LEU:H	2.14	0.58
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.69	0.58
1:C:216:ILE:HG22	1:C:218:VAL:H	1.69	0.58
1:C:360:ARG:CD	1:C:362:PHE:CE1	2.87	0.57
1:A:235:ASN:O	1:A:239:VAL:CG1	2.52	0.57
1:B:67:PRO:CA	1:C:20:HIS:CE1	2.79	0.57
1:C:231:LEU:HD12	1:C:257:HIS:HE1	1.69	0.57
1:C:362:PHE:CE2	1:C:363:VAL:CG2	2.86	0.57
1:C:422:THR:O	1:C:425:VAL:HG12	2.03	0.57
1:A:303:LEU:HD12	1:A:334:ILE:HD12	1.85	0.57
1:A:72:ASP:OD1	1:A:73:TYR:N	2.37	0.57
1:B:41:ARG:CD	1:B:264:ALA:CB	2.82	0.57
1:C:137:ASP:OD2	1:C:239:VAL:CG1	2.52	0.57
1:C:360:ARG:CD	1:C:362:PHE:HE1	2.17	0.57
1:A:122:LEU:CD2	1:A:223:LEU:HB3	2.35	0.57
1:B:69:THR:HG22	1:B:70:GLY:N	2.19	0.57
1:B:307:ILE:CD1	1:B:335:LEU:HD21	2.35	0.57
1:A:287:LEU:HD13	1:A:315:PHE:CA	2.34	0.57
1:A:164:PHE:HE2	1:A:187:TRP:CA	2.16	0.57
1:A:262:THR:CG2	1:A:263:HIS:ND1	2.67	0.57
1:A:9:ASN:ND2	1:B:19:ASP:CB	2.61	0.57
1:B:249:TYR:CE1	1:B:251:GLU:HG3	2.40	0.57
1:C:164:PHE:CE2	1:C:187:TRP:CA	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD11	1:A:427:PHE:HE2	1.69	0.57
1:A:386:LEU:CD2	1:A:398:ILE:HD11	2.32	0.57
1:B:126:GLU:HG3	1:B:209:PHE:HB2	1.85	0.57
1:B:195:PHE:CG	1:C:40:GLU:CB	2.85	0.57
1:C:228:ASP:OD2	1:C:257:HIS:HA	2.05	0.56
1:A:259:LEU:O	1:A:263:HIS:HB2	2.05	0.56
1:B:119:VAL:HG23	1:B:121:PHE:CE2	2.40	0.56
1:B:68:THR:HG23	1:C:20:HIS:CD2	2.40	0.56
1:B:335:LEU:HD13	1:B:343:LEU:HD12	1.87	0.56
1:A:157:TYR:CB	1:B:181:GLU:HB2	2.36	0.56
1:C:137:ASP:CG	1:C:239:VAL:HG21	2.24	0.56
1:C:260:LEU:HA	1:C:267:VAL:HG21	1.87	0.56
1:A:178:ILE:HG22	1:A:179:SER:O	2.06	0.56
1:C:303:LEU:HD23	1:C:334:ILE:HG22	1.86	0.56
1:C:359:ARG:HA	1:C:415:TYR:OH	2.05	0.56
1:A:286:LEU:HD11	1:A:427:PHE:CD2	2.40	0.56
1:B:8:GLU:HG2	1:B:13:ILE:HD11	1.86	0.56
1:C:122:LEU:CD2	1:C:223:LEU:HB3	2.34	0.56
1:C:259:LEU:HD23	1:C:259:LEU:N	2.21	0.56
1:A:256:PRO:CD	1:A:263:HIS:CE1	2.88	0.56
1:A:137:ASP:O	1:A:235:ASN:ND2	2.39	0.56
1:A:179:SER:CB	1:C:158:ALA:HB2	2.36	0.56
1:C:259:LEU:CD2	1:C:259:LEU:H	2.19	0.56
1:C:386:LEU:CD2	1:C:398:ILE:HD11	2.32	0.56
1:B:231:LEU:HD12	1:B:257:HIS:HE1	1.69	0.56
1:A:163:PHE:CE2	1:A:167:PHE:HD2	2.24	0.56
1:C:131:LYS:HD2	1:C:138:GLY:O	2.06	0.55
1:A:157:TYR:CB	1:B:181:GLU:HB3	2.26	0.55
1:B:228:ASP:OD2	1:B:257:HIS:HA	2.06	0.55
1:B:303:LEU:CB	1:B:334:ILE:CD1	2.77	0.55
1:B:329:LEU:HD22	1:B:335:LEU:CD1	2.36	0.55
1:B:335:LEU:HB3	1:B:340:LYS:HG2	1.88	0.55
1:B:149:VAL:HG21	1:B:203:THR:HG22	1.89	0.55
1:B:289:GLU:O	1:B:293:TYR:HD2	1.89	0.55
1:C:155:ASP:O	1:C:159:PHE:HB3	2.06	0.55
1:B:164:PHE:CZ	1:B:186:SER:CB	2.88	0.55
1:B:95:VAL:HA	1:B:120:ALA:O	2.07	0.55
1:B:260:LEU:HD23	1:B:267:VAL:HG11	1.88	0.55
1:B:177:ARG:CG	1:B:262:THR:HB	2.36	0.55
1:B:287:LEU:HD13	1:B:315:PHE:CD1	2.41	0.55
1:C:137:ASP:CG	1:C:239:VAL:HG22	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:HB3	1:C:362:PHE:CD1	2.42	0.55
1:A:163:PHE:O	1:A:167:PHE:CB	2.55	0.55
1:A:260:LEU:HD23	1:A:267:VAL:CG1	2.30	0.55
1:B:94:LEU:HG	1:B:116:ILE:HD12	1.89	0.55
1:B:135:ASN:OD1	1:B:137:ASP:HB2	2.06	0.55
1:C:360:ARG:CG	1:C:362:PHE:CZ	2.85	0.55
1:C:164:PHE:CZ	1:C:186:SER:C	2.80	0.55
1:B:336:SER:O	1:B:340:LYS:HG3	2.07	0.54
1:A:256:PRO:HD3	1:A:263:HIS:CE1	2.42	0.54
1:B:157:TYR:CB	1:C:181:GLU:C	2.75	0.54
1:C:359:ARG:HB3	1:C:415:TYR:CE2	2.43	0.54
1:C:42:GLN:NE2	1:C:260:LEU:HB3	2.22	0.54
1:A:223:LEU:CD1	1:A:270:ALA:CB	2.85	0.54
1:B:164:PHE:CE2	1:B:187:TRP:CA	2.89	0.54
1:B:303:LEU:CD1	1:B:334:ILE:HD12	2.38	0.54
1:B:335:LEU:HB3	1:B:340:LYS:HG3	1.88	0.54
1:C:99:MET:HA	1:C:125:LEU:HD11	1.89	0.54
1:A:163:PHE:CE2	1:A:167:PHE:CD2	2.96	0.54
1:A:41:ARG:HB3	1:A:264:ALA:HB1	1.89	0.54
1:B:286:LEU:CD1	1:B:424:GLU:HG2	2.37	0.54
1:C:233:ILE:HG13	1:C:237:ALA:HB3	1.90	0.54
1:C:354:GLU:O	1:C:357:LEU:HG	2.08	0.54
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.90	0.54
1:A:18:GLU:OE2	1:A:20:HIS:CE1	2.61	0.54
1:C:72:ASP:OD1	1:C:73:TYR:N	2.40	0.54
1:A:94:LEU:HG	1:A:116:ILE:HD12	1.89	0.54
1:A:131:LYS:HE2	1:A:136:PRO:O	2.08	0.54
1:A:11:THR:HG21	1:B:17:TYR:CE2	2.41	0.54
1:C:137:ASP:CB	1:C:239:VAL:HG21	2.38	0.54
1:C:94:LEU:HG	1:C:116:ILE:HD12	1.89	0.53
1:C:122:LEU:HD23	1:C:223:LEU:HB3	1.90	0.53
1:A:158:ALA:HA	1:B:181:GLU:CD	2.29	0.53
1:B:263:HIS:HB3	1:B:266:GLU:CD	2.29	0.53
1:B:69:THR:CG2	1:B:70:GLY:N	2.71	0.53
1:B:42:GLN:HE22	1:B:260:LEU:HB3	1.72	0.53
1:C:249:TYR:CE1	1:C:251:GLU:HG3	2.42	0.53
1:C:303:LEU:CD1	1:C:332:ARG:HG3	2.39	0.53
1:B:66:GLN:OE1	1:C:37:HIS:NE2	2.41	0.53
1:C:213:ILE:N	1:C:214:PRO:CD	2.72	0.53
1:C:303:LEU:HB2	1:C:334:ILE:HD12	1.89	0.53
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:CZ	1:C:185:ASN:CG	2.82	0.53
1:B:342:ILE:O	1:B:346:VAL:HG23	2.08	0.53
1:C:323:GLU:HB2	1:C:357:LEU:HD21	1.91	0.53
1:C:342:ILE:O	1:C:346:VAL:HG23	2.09	0.53
1:A:18:GLU:OE2	1:A:20:HIS:HE1	1.92	0.53
1:A:259:LEU:HD12	1:A:267:VAL:HG22	1.90	0.53
1:A:310:ARG:O	1:A:314:VAL:HG13	2.09	0.53
1:B:9:ASN:ND2	1:C:52:ARG:HG3	2.24	0.53
1:A:249:TYR:CE1	1:A:251:GLU:HG3	2.44	0.53
1:A:342:ILE:O	1:A:346:VAL:HG23	2.08	0.53
1:C:167:PHE:CE1	1:C:258:GLY:CA	2.91	0.53
1:A:25:PRO:HA	1:A:52:ARG:HB3	1.92	0.52
1:B:10:SER:N	1:C:19:ASP:OD2	2.42	0.52
1:B:9:ASN:HD21	1:C:52:ARG:HG3	1.74	0.52
1:C:24:THR:CG2	1:C:51:TYR:CE1	2.92	0.52
1:C:306:GLU:HB3	1:C:328:TRP:CH2	2.44	0.52
1:A:164:PHE:HZ	1:A:187:TRP:HA	1.74	0.52
1:A:233:ILE:HD11	1:A:249:TYR:OH	2.09	0.52
1:A:215:ARG:O	1:A:216:ILE:C	2.45	0.52
1:B:157:TYR:CD1	1:C:185:ASN:HB2	2.45	0.52
1:B:177:ARG:O	1:B:262:THR:HA	2.09	0.52
1:B:157:TYR:CE1	1:C:185:ASN:HB2	2.44	0.52
1:A:122:LEU:HD23	1:A:223:LEU:HB3	1.91	0.52
1:B:236:THR:O	1:B:240:PHE:CB	2.58	0.52
1:B:360:ARG:HH11	1:B:360:ARG:CG	2.22	0.52
1:C:336:SER:HB2	1:C:339:THR:OG1	2.10	0.52
1:A:182:ALA:HA	1:C:157:TYR:CB	2.40	0.52
1:B:71:TYR:CZ	1:B:197:ALA:HA	2.45	0.52
1:C:259:LEU:H	1:C:259:LEU:HD23	1.73	0.52
1:A:157:TYR:O	1:B:181:GLU:HG2	2.09	0.52
1:B:303:LEU:HD12	1:B:334:ILE:CG2	2.34	0.52
1:A:182:ALA:HA	1:C:157:TYR:CG	2.45	0.52
1:A:360:ARG:HH11	1:A:360:ARG:CG	2.22	0.52
1:B:141:PRO:O	1:B:144:PHE:HB3	2.10	0.52
1:B:67:PRO:CA	1:C:20:HIS:HE1	2.07	0.52
1:B:126:GLU:CD	1:B:126:GLU:H	2.13	0.51
1:B:135:ASN:ND2	1:B:138:GLY:H	2.07	0.51
1:A:24:THR:CG2	1:A:279:GLN:OE1	2.58	0.51
1:B:104:VAL:HG12	1:B:121:PHE:HE1	1.75	0.51
1:B:156:ARG:NE	1:B:157:TYR:CZ	2.79	0.51
1:C:335:LEU:HB3	1:C:340:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TRP:CH2	1:B:97:PHE:HB2	2.45	0.51
1:C:155:ASP:O	1:C:159:PHE:CB	2.59	0.51
1:A:234:GLU:H	1:A:234:GLU:CD	2.14	0.51
1:B:68:THR:HG22	1:B:196:PHE:CG	2.46	0.51
1:B:10:SER:CA	1:C:19:ASP:OD2	2.58	0.51
1:A:141:PRO:O	1:A:144:PHE:HB3	2.10	0.51
1:B:108:VAL:HG11	1:B:216:ILE:HG23	1.93	0.51
1:B:38:SER:HA	1:B:261:TRP:CZ2	2.43	0.51
1:C:165:ASN:O	1:C:169:ASN:N	2.44	0.51
1:A:178:ILE:HD13	1:A:261:TRP:NE1	2.25	0.51
1:A:286:LEU:HD22	1:A:286:LEU:O	2.10	0.51
1:B:157:TYR:HB3	1:C:181:GLU:CB	2.40	0.51
1:A:169:ASN:HA	1:A:229:ARG:NH1	2.25	0.51
1:B:123:ALA:HA	1:B:224:HIS:CE1	2.46	0.50
1:B:1:PRO:HB2	1:B:17:TYR:CD1	2.46	0.50
1:A:155:ASP:O	1:A:159:PHE:HB2	2.11	0.50
1:C:118:ALA:HB1	1:C:274:PHE:CZ	2.47	0.50
1:C:24:THR:HG21	1:C:51:TYR:CE1	2.46	0.50
1:B:104:VAL:CG1	1:B:121:PHE:HE1	2.16	0.50
1:B:126:GLU:HA	1:B:127:PRO:C	2.32	0.50
1:B:11:THR:HB	1:C:1:PRO:CG	2.41	0.50
1:C:216:ILE:CG2	1:C:218:VAL:HG22	2.41	0.50
1:A:303:LEU:CB	1:A:334:ILE:HD12	2.38	0.50
1:B:164:PHE:CZ	1:B:186:SER:C	2.85	0.50
1:B:290:VAL:O	1:B:294:VAL:HG23	2.12	0.50
1:B:158:ALA:CA	1:C:181:GLU:CG	2.85	0.50
1:C:17:TYR:CE2	1:C:19:ASP:OD2	2.61	0.50
1:A:260:LEU:O	1:A:264:ALA:CA	2.60	0.50
1:A:9:ASN:CG	1:A:10:SER:H	2.15	0.50
1:B:1:PRO:HB3	1:B:17:TYR:CE1	2.45	0.50
1:C:335:LEU:HB2	1:C:340:LYS:HE2	1.94	0.50
1:C:322:LEU:CD2	1:C:357:LEU:HD12	2.39	0.50
1:A:233:ILE:O	1:A:237:ALA:HB3	2.11	0.50
1:B:233:ILE:HD11	1:B:249:TYR:HH	1.73	0.50
1:B:221:LEU:HB2	1:B:274:PHE:CZ	2.46	0.49
1:B:46:LEU:HD22	1:B:51:TYR:HD2	1.77	0.49
1:A:41:ARG:CD	1:A:264:ALA:HB3	2.42	0.49
1:B:220:ALA:HB3	1:B:247:ALA:HB2	1.94	0.49
1:C:303:LEU:HD23	1:C:334:ILE:HB	1.88	0.49
1:A:303:LEU:HA	1:A:306:GLU:OE1	2.13	0.49
1:A:68:THR:HA	1:A:196:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD12	1:B:107:TYR:OH	2.12	0.49
1:C:286:LEU:HD21	1:C:424:GLU:HG3	1.94	0.49
1:A:303:LEU:HD12	1:A:334:ILE:CD1	2.42	0.49
1:B:157:TYR:O	1:C:181:GLU:HG2	2.13	0.49
1:A:178:ILE:CD1	1:A:261:TRP:CD1	2.93	0.49
1:A:182:ALA:CB	1:A:261:TRP:HZ2	2.20	0.49
1:B:30:HIS:CA	1:B:39:TRP:HE1	2.16	0.49
1:B:209:PHE:O	1:B:213:ILE:HG13	2.13	0.49
1:C:164:PHE:HZ	1:C:186:SER:C	2.15	0.49
1:A:127:PRO:HD3	1:A:240:PHE:HB2	1.95	0.49
1:B:221:LEU:HB2	1:B:274:PHE:CD1	2.47	0.49
1:C:135:ASN:ND2	1:C:137:ASP:HB2	2.21	0.49
1:C:303:LEU:CD2	1:C:334:ILE:CB	2.83	0.49
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.48	0.48
1:A:335:LEU:HD13	1:A:343:LEU:HD12	1.95	0.48
1:A:195:PHE:HB3	1:B:40:GLU:OE1	2.13	0.48
1:C:259:LEU:O	1:C:263:HIS:HB2	2.13	0.48
1:C:84:LEU:HD12	1:C:107:TYR:OH	2.12	0.48
1:A:126:GLU:O	1:A:236:THR:CB	2.55	0.48
1:A:71:TYR:CE2	1:A:196:PHE:HD1	2.32	0.48
1:C:335:LEU:O	1:C:340:LYS:HE3	2.13	0.48
1:C:70:GLY:O	1:C:75:THR:HG21	2.13	0.48
1:B:233:ILE:HG23	1:B:238:ARG:HD2	1.94	0.48
1:B:31:GLY:HA3	1:B:98:SER:HB3	1.95	0.48
1:A:177:ARG:HD2	1:A:262:THR:HG22	1.94	0.48
1:B:164:PHE:CE1	1:B:186:SER:CB	2.91	0.48
1:A:354:GLU:O	1:A:357:LEU:HG	2.13	0.48
1:A:41:ARG:HD3	1:A:264:ALA:HB3	1.96	0.48
1:A:9:ASN:ND2	1:B:52:ARG:HE	2.10	0.48
1:A:195:PHE:CB	1:B:40:GLU:OE1	2.62	0.48
1:B:144:PHE:CZ	1:B:148:ILE:HD11	2.48	0.48
1:C:249:TYR:HE1	1:C:251:GLU:CG	2.26	0.48
1:A:156:ARG:NE	1:A:157:TYR:CZ	2.81	0.48
1:A:208:ASP:OD1	1:A:210:ARG:HG3	2.12	0.48
1:B:354:GLU:O	1:B:357:LEU:HG	2.13	0.48
1:B:157:TYR:CB	1:C:181:GLU:CB	2.91	0.48
1:B:123:ALA:HA	1:B:224:HIS:ND1	2.29	0.48
1:B:303:LEU:HA	1:B:306:GLU:OE1	2.13	0.48
1:C:164:PHE:CZ	1:C:186:SER:CB	2.96	0.48
1:C:127:PRO:HG3	1:C:239:VAL:CG1	2.42	0.48
1:A:256:PRO:HD2	1:A:263:HIS:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ALA:N	1:B:202:PRO:CD	2.77	0.48
1:A:24:THR:OG1	1:A:279:GLN:OE1	2.28	0.47
1:A:171:ASP:OD1	1:A:172:GLU:N	2.46	0.47
1:B:122:LEU:CD2	1:B:223:LEU:HB3	2.44	0.47
1:C:234:GLU:HG2	1:C:235:ASN:N	2.30	0.47
1:C:303:LEU:HD23	1:C:334:ILE:CB	2.43	0.47
1:B:31:GLY:CA	1:B:98:SER:HB3	2.44	0.47
1:C:167:PHE:CE1	1:C:258:GLY:HA2	2.50	0.47
1:B:11:THR:HG23	1:C:17:TYR:CE2	2.44	0.47
1:A:287:LEU:HB3	1:A:315:PHE:CD2	2.49	0.47
1:B:31:GLY:HA3	1:B:98:SER:CB	2.45	0.47
1:B:234:GLU:HA	1:B:238:ARG:CB	2.42	0.47
1:B:10:SER:HB3	1:C:87:LEU:HD21	1.89	0.47
1:B:157:TYR:CE1	1:C:185:ASN:CB	2.98	0.47
1:B:157:TYR:HB3	1:C:181:GLU:O	2.14	0.47
1:A:223:LEU:HD12	1:A:270:ALA:HB1	1.97	0.47
1:A:171:ASP:OD1	1:A:172:GLU:HG3	2.14	0.47
1:B:25:PRO:HA	1:B:52:ARG:HB3	1.97	0.47
1:B:41:ARG:CD	1:B:264:ALA:HB2	2.37	0.47
1:C:171:ASP:OD1	1:C:172:GLU:HG3	2.14	0.47
1:C:77:ALA:HB2	1:C:106:ARG:HG3	1.96	0.47
1:B:260:LEU:CD2	1:B:267:VAL:HG11	2.45	0.46
1:C:165:ASN:CG	1:C:170:LEU:HB2	2.35	0.46
1:B:157:TYR:CE1	1:C:185:ASN:CG	2.89	0.46
1:A:223:LEU:HD11	1:A:270:ALA:CB	2.45	0.46
1:C:220:ALA:HB3	1:C:247:ALA:HB2	1.98	0.46
1:A:249:TYR:CE1	1:A:251:GLU:CG	2.98	0.46
1:A:249:TYR:HE1	1:A:251:GLU:HG3	1.79	0.46
1:A:259:LEU:O	1:A:263:HIS:CB	2.63	0.46
1:B:119:VAL:CG2	1:B:121:PHE:CE2	2.99	0.46
1:C:167:PHE:CE1	1:C:258:GLY:HA3	2.51	0.46
1:A:39:TRP:CE3	1:A:42:GLN:HG2	2.51	0.46
1:A:43:SER:HB2	1:C:195:PHE:CZ	2.51	0.46
1:B:260:LEU:HA	1:B:267:VAL:HG21	1.98	0.46
1:C:126:GLU:CB	1:C:127:PRO:HA	2.37	0.46
1:B:156:ARG:HG3	1:B:157:TYR:CE2	2.51	0.46
1:C:45:ALA:HB2	1:C:268:ASN:ND2	2.31	0.46
1:C:298:ILE:HD13	1:C:307:ILE:HD12	1.81	0.46
1:C:68:THR:HA	1:C:196:PHE:CD1	2.51	0.46
1:A:329:LEU:HD11	1:A:347:PHE:HD2	1.81	0.46
1:B:121:PHE:CD2	1:B:121:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:CD1	1:B:334:ILE:CG2	2.94	0.46
1:C:148:ILE:O	1:C:152:VAL:HG23	2.16	0.46
1:C:233:ILE:HG12	1:C:237:ALA:HB3	1.97	0.46
1:A:245:PRO:HG2	1:A:246:SER:H	1.81	0.46
1:C:329:LEU:HD22	1:C:335:LEU:HD11	1.92	0.46
1:A:173:ASN:HD22	1:A:177:ARG:HG3	1.74	0.46
1:A:275:LEU:O	1:A:279:GLN:HG2	2.16	0.46
1:B:303:LEU:HG	1:B:334:ILE:HD12	1.94	0.46
1:B:319:ASN:CA	1:B:352:PRO:HG2	2.46	0.46
1:C:68:THR:HG22	1:C:196:PHE:CG	2.51	0.46
1:A:234:GLU:CA	1:A:238:ARG:HB2	2.40	0.45
1:B:101:THR:HB	1:B:124:SER:HB3	1.98	0.45
1:B:249:TYR:CE1	1:B:251:GLU:CG	2.99	0.45
1:C:329:LEU:HD23	1:C:335:LEU:HD11	1.98	0.45
1:C:70:GLY:O	1:C:75:THR:HB	2.15	0.45
1:A:265:GLU:HA	1:A:265:GLU:OE1	2.17	0.45
1:A:30:HIS:ND1	1:A:34:LEU:O	2.49	0.45
1:C:394:GLY:O	1:C:398:ILE:HG23	2.16	0.45
1:B:108:VAL:HG11	1:B:216:ILE:CG2	2.45	0.45
1:B:329:LEU:HD11	1:B:347:PHE:HD2	1.81	0.45
1:C:238:ARG:NH1	1:C:242:LYS:NZ	2.65	0.45
1:C:249:TYR:CE1	1:C:251:GLU:CG	3.00	0.45
1:B:394:GLY:O	1:B:398:ILE:HG23	2.17	0.45
1:C:329:LEU:HD11	1:C:347:PHE:HD2	1.81	0.45
1:A:394:GLY:O	1:A:398:ILE:HG23	2.16	0.45
1:A:223:LEU:CD1	1:A:270:ALA:HB1	2.47	0.45
1:A:258:GLY:O	1:A:262:THR:HB	2.17	0.45
1:C:259:LEU:CD2	1:C:259:LEU:N	2.79	0.45
1:C:372:ASP:HA	1:C:373:PRO:HD3	1.86	0.45
1:B:71:TYR:CE2	1:B:196:PHE:HD1	2.35	0.45
1:A:319:ASN:CA	1:A:352:PRO:HG2	2.46	0.45
1:B:135:ASN:ND2	1:B:137:ASP:N	2.64	0.45
1:B:10:SER:O	1:C:17:TYR:OH	2.35	0.45
1:B:249:TYR:HE1	1:B:251:GLU:CG	2.28	0.44
1:B:286:LEU:CD1	1:B:424:GLU:CG	2.93	0.44
1:C:360:ARG:HB2	1:C:363:VAL:HG21	1.91	0.44
1:B:156:ARG:H	1:B:156:ARG:HG2	1.55	0.44
1:B:290:VAL:HG23	1:B:431:CYS:SG	2.57	0.44
1:C:118:ALA:HB1	1:C:274:PHE:HZ	1.82	0.44
1:C:98:SER:HA	1:C:123:ALA:O	2.18	0.44
1:A:20:HIS:CE1	1:C:66:GLN:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PHE:CE2	1:C:148:ILE:CD1	2.86	0.44
1:C:363:VAL:HG12	1:C:367:LEU:HD12	2.00	0.44
1:C:421:VAL:HB	1:C:425:VAL:HG13	1.98	0.44
1:A:182:ALA:HA	1:C:157:TYR:CD2	2.53	0.44
1:C:233:ILE:HG13	1:C:237:ALA:HB2	1.99	0.44
1:C:237:ALA:HB1	1:C:249:TYR:OH	2.18	0.44
1:C:156:ARG:NE	1:C:157:TYR:OH	2.36	0.44
1:C:49:ALA:CB	1:C:272:LEU:HD22	2.48	0.44
1:A:195:PHE:CD2	1:B:40:GLU:HB2	2.52	0.44
1:C:339:THR:HG22	1:C:343:LEU:CD1	2.46	0.44
1:B:104:VAL:HB	1:B:121:PHE:CE1	2.53	0.44
1:B:286:LEU:HD13	1:B:424:GLU:HG3	2.00	0.44
1:B:30:HIS:ND1	1:B:34:LEU:O	2.49	0.44
1:B:58:ARG:O	1:B:59:ARG:C	2.56	0.44
1:C:177:ARG:CD	1:C:263:HIS:CE1	3.01	0.44
1:C:319:ASN:CA	1:C:352:PRO:HG2	2.46	0.44
1:B:164:PHE:HZ	1:B:186:SER:C	2.21	0.44
1:A:249:TYR:HE1	1:A:251:GLU:CG	2.31	0.43
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.59	0.43
1:A:98:SER:HA	1:A:123:ALA:O	2.18	0.43
1:C:155:ASP:CB	1:C:158:ALA:HB3	2.46	0.43
1:A:176:THR:HG22	1:A:177:ARG:N	2.33	0.43
1:B:135:ASN:CG	1:B:137:ASP:HB2	2.38	0.43
1:C:303:LEU:O	1:C:307:ILE:HG13	2.18	0.43
1:B:130:LEU:HA	1:B:130:LEU:HD12	1.81	0.43
1:B:177:ARG:C	1:B:262:THR:HG22	2.38	0.43
1:C:49:ALA:CB	1:C:272:LEU:CD2	2.96	0.43
1:A:239:VAL:HG13	1:A:240:PHE:N	2.33	0.43
1:C:225:GLY:HA2	1:C:255:ALA:HB3	2.00	0.43
1:A:225:GLY:HA2	1:A:255:ALA:HB3	2.00	0.43
1:B:135:ASN:HD21	1:B:137:ASP:CA	2.31	0.43
1:C:17:TYR:HE2	1:C:19:ASP:CG	2.21	0.43
1:C:265:GLU:OE1	1:C:265:GLU:HA	2.18	0.43
1:B:329:LEU:CD2	1:B:335:LEU:HD11	2.48	0.43
1:A:68:THR:HG22	1:A:196:PHE:CG	2.53	0.43
1:C:228:ASP:CG	1:C:257:HIS:HA	2.39	0.43
1:A:68:THR:HG22	1:A:196:PHE:CB	2.49	0.43
1:B:177:ARG:HA	1:B:177:ARG:HD3	1.57	0.43
1:B:139:ALA:HB1	1:B:235:ASN:ND2	2.30	0.43
1:A:178:ILE:CG2	1:A:179:SER:N	2.81	0.43
1:A:178:ILE:HG22	1:A:179:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PRO:CG	1:C:239:VAL:HG12	2.48	0.43
1:C:322:LEU:HB3	1:C:357:LEU:CD1	2.49	0.43
1:A:140:ALA:HB1	1:A:141:PRO:HD2	2.01	0.42
1:C:170:LEU:HD22	1:C:174:LEU:HD13	2.01	0.42
1:A:170:LEU:HD22	1:A:174:LEU:HD13	2.01	0.42
1:B:328:TRP:O	1:B:332:ARG:HG2	2.20	0.42
1:B:71:TYR:CE1	1:B:197:ALA:CB	3.01	0.42
1:C:41:ARG:CD	1:C:264:ALA:CB	2.88	0.42
1:C:335:LEU:HD13	1:C:343:LEU:HD12	2.01	0.42
1:B:126:GLU:HG3	1:B:209:PHE:CG	2.54	0.42
1:C:171:ASP:OD1	1:C:172:GLU:N	2.47	0.42
1:C:238:ARG:NH1	1:C:242:LYS:HZ1	2.17	0.42
1:B:329:LEU:CD2	1:B:335:LEU:CD1	2.98	0.42
1:C:140:ALA:HB1	1:C:141:PRO:HD2	2.01	0.42
1:C:322:LEU:HB3	1:C:357:LEU:HD12	2.01	0.42
1:A:39:TRP:HE3	1:A:42:GLN:HG2	1.83	0.42
1:B:163:PHE:O	1:B:167:PHE:HB2	2.20	0.42
1:B:122:LEU:HD22	1:B:223:LEU:HD22	2.01	0.42
1:C:329:LEU:HD11	1:C:347:PHE:CD2	2.54	0.42
1:B:225:GLY:HA2	1:B:255:ALA:HB3	2.00	0.42
1:B:287:LEU:HD22	1:B:315:PHE:CE1	2.55	0.42
1:B:329:LEU:HD11	1:B:347:PHE:CD2	2.54	0.42
1:A:223:LEU:CD1	1:A:270:ALA:HB3	2.50	0.42
1:A:71:TYR:CE1	1:A:197:ALA:CB	3.03	0.42
1:B:289:GLU:O	1:B:293:TYR:CD2	2.72	0.42
1:C:201:ALA:N	1:C:202:PRO:CD	2.82	0.42
1:B:122:LEU:HA	1:B:223:LEU:O	2.20	0.42
1:C:328:TRP:O	1:C:332:ARG:HG2	2.19	0.42
1:B:104:VAL:CB	1:B:121:PHE:CE1	3.02	0.41
1:B:220:ALA:HB3	1:B:247:ALA:CB	2.51	0.41
1:B:302:PRO:O	1:B:305:ALA:HB3	2.19	0.41
1:B:372:ASP:O	1:B:376:MET:HG3	2.20	0.41
1:C:129:LEU:HA	1:C:129:LEU:HD23	1.80	0.41
1:C:307:ILE:HG22	1:C:311:LEU:CD1	2.50	0.41
1:B:195:PHE:CD2	1:C:40:GLU:CB	3.03	0.41
1:A:157:TYR:CD2	1:B:182:ALA:HA	2.55	0.41
1:A:201:ALA:N	1:A:202:PRO:CD	2.83	0.41
1:A:302:PRO:O	1:A:305:ALA:HB3	2.19	0.41
1:A:329:LEU:HD11	1:A:347:PHE:CD2	2.54	0.41
1:B:231:LEU:HD12	1:B:257:HIS:CE1	2.54	0.41
1:B:71:TYR:CE1	1:B:197:ALA:CA	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:HB3	1:C:52:ARG:HH21	1.85	0.41
1:C:387:LYS:NZ	1:C:420:ALA:O	2.53	0.41
1:C:70:GLY:O	1:C:75:THR:CG2	2.68	0.41
1:A:20:HIS:CG	1:C:68:THR:HG23	2.55	0.41
1:B:8:GLU:HG2	1:B:13:ILE:CG1	2.50	0.41
1:B:228:ASP:CG	1:B:257:HIS:HA	2.40	0.41
1:C:260:LEU:O	1:C:264:ALA:CA	2.69	0.41
1:A:347:PHE:O	1:A:351:VAL:HB	2.20	0.41
1:A:338:LEU:HD13	1:A:437:ILE:HD13	2.01	0.41
1:B:177:ARG:HG3	1:B:262:THR:HB	2.02	0.41
1:B:39:TRP:CZ2	1:B:97:PHE:HB2	2.55	0.41
1:C:128:PHE:CE2	1:C:130:LEU:HB3	2.55	0.41
1:A:236:THR:HA	1:A:239:VAL:HG12	2.01	0.41
1:B:140:ALA:HB1	1:B:141:PRO:HD2	2.01	0.41
1:A:156:ARG:HG2	1:A:156:ARG:H	1.57	0.41
1:B:234:GLU:O	1:B:239:VAL:HG23	2.20	0.41
1:B:347:PHE:O	1:B:351:VAL:HB	2.21	0.41
1:B:40:GLU:OE2	1:B:261:TRP:HH2	2.04	0.41
1:A:178:ILE:HD13	1:A:261:TRP:CG	2.56	0.41
1:A:187:TRP:CE2	1:B:184:ARG:NH2	2.85	0.41
1:B:195:PHE:CZ	1:C:43:SER:HB2	2.56	0.41
1:B:387:LYS:NZ	1:B:420:ALA:O	2.53	0.41
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.56	0.41
1:B:216:ILE:HG22	1:B:218:VAL:HG22	2.01	0.41
1:B:263:HIS:O	1:B:266:GLU:N	2.54	0.41
1:B:45:ALA:HB1	1:B:272:LEU:HD11	2.01	0.41
1:B:335:LEU:HB2	1:B:340:LYS:HE2	2.02	0.41
1:B:5:VAL:HG11	1:B:15:LEU:CD1	2.51	0.41
1:C:5:VAL:HG11	1:C:15:LEU:CD1	2.51	0.41
1:C:233:ILE:O	1:C:237:ALA:CA	2.68	0.41
1:C:347:PHE:O	1:C:351:VAL:HB	2.20	0.41
1:C:323:GLU:N	1:C:357:LEU:HD11	2.36	0.41
1:A:5:VAL:HG11	1:A:15:LEU:CD1	2.51	0.41
1:A:252:VAL:CG1	1:A:255:ALA:HB2	2.46	0.41
1:C:372:ASP:O	1:C:376:MET:HG3	2.20	0.41
1:A:328:TRP:O	1:A:332:ARG:HG2	2.20	0.41
1:A:387:LYS:NZ	1:A:420:ALA:O	2.53	0.41
1:B:165:ASN:OD1	1:B:170:LEU:HB2	2.20	0.41
1:B:335:LEU:CB	1:B:340:LYS:HG2	2.50	0.41
1:C:225:GLY:CA	1:C:255:ALA:HB3	2.51	0.41
1:C:30:HIS:ND1	1:C:34:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:O	1:A:376:MET:HG3	2.20	0.41
1:B:260:LEU:HG	1:B:260:LEU:H	1.52	0.41
1:B:265:GLU:HA	1:B:265:GLU:OE1	2.20	0.41
1:B:46:LEU:HD21	1:B:275:LEU:CD1	2.51	0.41
1:B:298:ILE:HD13	1:B:307:ILE:HD13	2.03	0.41
1:B:263:HIS:ND1	1:B:263:HIS:N	2.68	0.40
1:B:19:ASP:HA	1:B:53:VAL:O	2.21	0.40
1:C:106:ARG:NH2	1:C:209:PHE:CE1	2.89	0.40
1:A:225:GLY:CA	1:A:255:ALA:HB3	2.51	0.40
1:A:305:ALA:O	1:A:309:GLN:HG2	2.22	0.40
1:B:319:ASN:HA	1:B:352:PRO:CG	2.49	0.40
1:C:129:LEU:HD12	1:C:205:TRP:O	2.21	0.40
1:C:209:PHE:O	1:C:212:ASP:HB2	2.22	0.40
1:C:28:LEU:HB3	1:C:39:TRP:CE2	2.56	0.40
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.82	0.40
1:A:236:THR:CA	1:A:239:VAL:HG12	2.52	0.40
1:B:225:GLY:CA	1:B:255:ALA:HB3	2.51	0.40
1:B:90:GLN:HB2	1:B:391:THR:HG21	2.03	0.40
1:C:299:PRO:HG2	1:C:334:ILE:CG2	2.51	0.40
1:A:46:LEU:HD23	1:A:272:LEU:HD21	2.04	0.40
1:B:158:ALA:HA	1:C:181:GLU:HG2	1.97	0.40
1:B:195:PHE:HZ	1:C:43:SER:HB2	1.86	0.40
1:C:218:VAL:O	1:C:219:PRO:C	2.60	0.40
1:C:70:GLY:O	1:C:75:THR:CB	2.70	0.40
1:B:263:HIS:O	1:B:264:ALA:C	2.59	0.40

There are no symmetry-related clashes.

## 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	438/456 (96%)	427 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/456 (96%)	428 (98%)	10 (2%)	0	100	100
1	C	438/456 (96%)	427 (98%)	11 (2%)	0	100	100
All	All	1314/1368 (96%)	1282 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	354/370 (96%)	337 (95%)	17 (5%)	30	61
1	B	354/370 (96%)	334 (94%)	20 (6%)	25	57
1	C	354/370 (96%)	337 (95%)	17 (5%)	30	61
All	All	1062/1110 (96%)	1008 (95%)	54 (5%)	28	60

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	90	GLN
1	A	133	ASP
1	A	156	ARG
1	A	165	ASN
1	A	217	ASP
1	A	238	ARG
1	A	260	LEU
1	A	282	GLN
1	A	285	LYS
1	A	303	LEU
1	A	310	ARG
1	A	325	LEU
1	A	338	LEU
1	A	351	VAL
1	A	353	SER

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Mol	Chain	Res	Type
1	A	360	ARG
1	B	41	ARG
1	B	90	GLN
1	B	91	ASP
1	B	98	SER
1	B	121	PHE
1	B	124	SER
1	B	156	ARG
1	B	165	ASN
1	B	177	ARG
1	B	215	ARG
1	B	238	ARG
1	B	260	LEU
1	B	263	HIS
1	B	290	VAL
1	B	303	LEU
1	B	325	LEU
1	B	338	LEU
1	B	351	VAL
1	B	353	SER
1	B	360	ARG
1	C	91	ASP
1	C	128	PHE
1	C	156	ARG
1	C	165	ASN
1	C	216	ILE
1	C	234	GLU
1	C	260	LEU
1	C	279	GLN
1	C	280	GLU
1	C	287	LEU
1	C	304	LYS
1	C	325	LEU
1	C	338	LEU
1	C	351	VAL
1	C	353	SER
1	C	360	ARG
1	C	389	GLU

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



Mol	Chain	Res	Type
1	A	90	GLN
1	A	135	ASN
1	A	173	ASN
1	A	188	ASN
1	B	9	ASN
1	B	42	GLN
1	B	90	GLN
1	B	135	ASN
1	B	173	ASN
1	B	188	ASN
1	B	235	ASN
1	B	279	GLN
1	C	42	GLN
1	C	135	ASN
1	C	173	ASN
1	C	188	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	440/456 (96%)	0.11	14 (3%) 48 46	184, 286, 365, 403	0
1	B	440/456 (96%)	0.68	43 (9%) 8 15	268, 397, 443, 467	0
1	C	440/456 (96%)	0.16	20 (4%) 34 35	165, 260, 336, 373	0
All	All	1320/1368 (96%)	0.32	77 (5%) 24 27	165, 306, 426, 467	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	GLY	9.9
1	B	96	GLY	9.3
1	B	101	THR	8.6
1	B	30	HIS	8.1
1	A	30	HIS	7.8
1	C	36	GLY	7.3
1	B	31	GLY	7.3
1	B	123	ALA	6.9
1	A	36	GLY	6.0
1	C	30	HIS	6.0
1	B	124	SER	6.0
1	C	31	GLY	5.9
1	A	101	THR	5.8
1	A	100	GLY	5.7
1	B	36	GLY	5.7
1	A	96	GLY	5.4
1	B	98	SER	5.4
1	B	102	GLY	5.2
1	B	403	SER	5.1
1	B	356	GLY	5.1
1	A	98	SER	4.9
1	B	99	MET	4.7
1	A	31	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	96	GLY	4.4
1	B	406	ALA	4.3
1	B	420	ALA	4.3
1	B	404	ALA	4.2
1	A	123	ALA	4.1
1	C	98	SER	3.9
1	B	405	GLY	3.8
1	B	38	SER	3.7
1	B	419	GLY	3.6
1	A	35	SER	3.6
1	B	103	GLU	3.5
1	B	29	ILE	3.5
1	C	320	THR	3.3
1	B	408	ALA	3.2
1	C	393	HIS	3.2
1	C	37	HIS	3.2
1	C	35	SER	3.2
1	C	55	THR	3.1
1	B	35	SER	3.1
1	A	124	SER	3.0
1	B	33	PRO	3.0
1	B	203	THR	2.9
1	B	407	LEU	2.9
1	B	416	ASN	2.8
1	C	319	ASN	2.7
1	A	99	MET	2.7
1	C	101	THR	2.7
1	B	401	SER	2.6
1	B	104	VAL	2.5
1	A	393	HIS	2.5
1	B	191	ALA	2.5
1	A	102	GLY	2.4
1	C	124	SER	2.4
1	B	253	GLU	2.4
1	B	39	TRP	2.4
1	B	217	ASP	2.4
1	C	420	ALA	2.3
1	C	358	GLN	2.3
1	C	352	PRO	2.3
1	B	202	PRO	2.3
1	B	216	ILE	2.3
1	C	123	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	251	GLU	2.3
1	C	351	VAL	2.3
1	C	100	GLY	2.2
1	B	43	SER	2.2
1	C	353	SER	2.2
1	A	420	ALA	2.2
1	B	175	GLY	2.2
1	B	37	HIS	2.2
1	B	70	GLY	2.1
1	B	402	TYR	2.1
1	B	97	PHE	2.1
1	B	32	PHE	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.