



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 02:17 PM JST

PDB ID : 6KHT  
Title : Chimeric beta-glucosidase Cel1b-H13  
Authors : Niu, K.L.  
Deposited on : 2019-07-16  
Resolution : 3.31 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

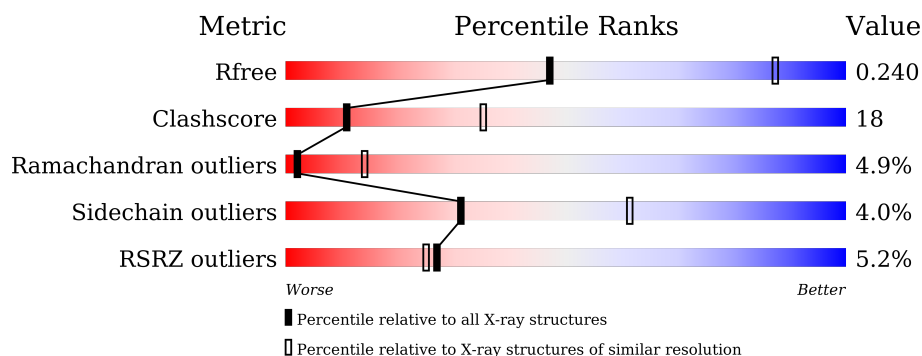
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	513	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>.. 7%</div> </div> </div>
1	B	513	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>.. 7%</div> </div> </div>
1	C	513	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>.. 7%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11529 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 Glycoside hydrolase family 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3843	2451	661	718	13			
1	B	477	Total	C	N	O	S	0	0	0
			3843	2451	661	718	13			
1	C	477	Total	C	N	O	S	0	0	0
			3843	2451	661	718	13			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP G0RIF5
A	-12	HIS	-	expression tag	UNP G0RIF5
A	-11	HIS	-	expression tag	UNP G0RIF5
A	-10	HIS	-	expression tag	UNP G0RIF5
A	-9	HIS	-	expression tag	UNP G0RIF5
A	-8	HIS	-	expression tag	UNP G0RIF5
A	-7	SER	-	expression tag	UNP G0RIF5
A	-6	SER	-	expression tag	UNP G0RIF5
A	-5	GLY	-	expression tag	UNP G0RIF5
A	-4	LEU	-	expression tag	UNP G0RIF5
A	-3	VAL	-	expression tag	UNP G0RIF5
A	-2	PRO	-	expression tag	UNP G0RIF5
A	-1	ARG	-	expression tag	UNP G0RIF5
A	0	GLY	-	expression tag	UNP G0RIF5
A	1	SER	-	expression tag	UNP G0RIF5
A	200	ASP	ASN	conflict	UNP G0RIF5
A	319	TYR	PHE	conflict	UNP G0RIF5
A	479	ILE	-	expression tag	UNP G0RIF5
A	480	PRO	-	expression tag	UNP G0RIF5
A	481	GLU	-	expression tag	UNP G0RIF5
A	482	GLU	-	expression tag	UNP G0RIF5
A	483	LEU	-	expression tag	UNP G0RIF5
A	484	ALA	-	expression tag	UNP G0RIF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	485	HIS	-	expression tag	UNP G0RIF5
A	486	LEU	-	expression tag	UNP G0RIF5
A	487	ALA	-	expression tag	UNP G0RIF5
A	488	ASP	-	expression tag	UNP G0RIF5
A	489	LEU	-	expression tag	UNP G0RIF5
A	490	LYS	-	expression tag	UNP G0RIF5
A	491	PHE	-	expression tag	UNP G0RIF5
A	492	LEU	-	expression tag	UNP G0RIF5
A	493	GLU	-	expression tag	UNP G0RIF5
A	494	HIS	-	expression tag	UNP G0RIF5
A	495	HIS	-	expression tag	UNP G0RIF5
A	496	HIS	-	expression tag	UNP G0RIF5
A	497	HIS	-	expression tag	UNP G0RIF5
A	498	HIS	-	expression tag	UNP G0RIF5
A	499	HIS	-	expression tag	UNP G0RIF5
B	-13	HIS	-	expression tag	UNP G0RIF5
B	-12	HIS	-	expression tag	UNP G0RIF5
B	-11	HIS	-	expression tag	UNP G0RIF5
B	-10	HIS	-	expression tag	UNP G0RIF5
B	-9	HIS	-	expression tag	UNP G0RIF5
B	-8	HIS	-	expression tag	UNP G0RIF5
B	-7	SER	-	expression tag	UNP G0RIF5
B	-6	SER	-	expression tag	UNP G0RIF5
B	-5	GLY	-	expression tag	UNP G0RIF5
B	-4	LEU	-	expression tag	UNP G0RIF5
B	-3	VAL	-	expression tag	UNP G0RIF5
B	-2	PRO	-	expression tag	UNP G0RIF5
B	-1	ARG	-	expression tag	UNP G0RIF5
B	0	GLY	-	expression tag	UNP G0RIF5
B	1	SER	-	expression tag	UNP G0RIF5
B	200	ASP	ASN	conflict	UNP G0RIF5
B	319	TYR	PHE	conflict	UNP G0RIF5
B	479	ILE	-	expression tag	UNP G0RIF5
B	480	PRO	-	expression tag	UNP G0RIF5
B	481	GLU	-	expression tag	UNP G0RIF5
B	482	GLU	-	expression tag	UNP G0RIF5
B	483	LEU	-	expression tag	UNP G0RIF5
B	484	ALA	-	expression tag	UNP G0RIF5
B	485	HIS	-	expression tag	UNP G0RIF5
B	486	LEU	-	expression tag	UNP G0RIF5
B	487	ALA	-	expression tag	UNP G0RIF5
B	488	ASP	-	expression tag	UNP G0RIF5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	489	LEU	-	expression tag	UNP G0RIF5
B	490	LYS	-	expression tag	UNP G0RIF5
B	491	PHE	-	expression tag	UNP G0RIF5
B	492	LEU	-	expression tag	UNP G0RIF5
B	493	GLU	-	expression tag	UNP G0RIF5
B	494	HIS	-	expression tag	UNP G0RIF5
B	495	HIS	-	expression tag	UNP G0RIF5
B	496	HIS	-	expression tag	UNP G0RIF5
B	497	HIS	-	expression tag	UNP G0RIF5
B	498	HIS	-	expression tag	UNP G0RIF5
B	499	HIS	-	expression tag	UNP G0RIF5
C	-13	HIS	-	expression tag	UNP G0RIF5
C	-12	HIS	-	expression tag	UNP G0RIF5
C	-11	HIS	-	expression tag	UNP G0RIF5
C	-10	HIS	-	expression tag	UNP G0RIF5
C	-9	HIS	-	expression tag	UNP G0RIF5
C	-8	HIS	-	expression tag	UNP G0RIF5
C	-7	SER	-	expression tag	UNP G0RIF5
C	-6	SER	-	expression tag	UNP G0RIF5
C	-5	GLY	-	expression tag	UNP G0RIF5
C	-4	LEU	-	expression tag	UNP G0RIF5
C	-3	VAL	-	expression tag	UNP G0RIF5
C	-2	PRO	-	expression tag	UNP G0RIF5
C	-1	ARG	-	expression tag	UNP G0RIF5
C	0	GLY	-	expression tag	UNP G0RIF5
C	1	SER	-	expression tag	UNP G0RIF5
C	200	ASP	ASN	conflict	UNP G0RIF5
C	319	TYR	PHE	conflict	UNP G0RIF5
C	479	ILE	-	expression tag	UNP G0RIF5
C	480	PRO	-	expression tag	UNP G0RIF5
C	481	GLU	-	expression tag	UNP G0RIF5
C	482	GLU	-	expression tag	UNP G0RIF5
C	483	LEU	-	expression tag	UNP G0RIF5
C	484	ALA	-	expression tag	UNP G0RIF5
C	485	HIS	-	expression tag	UNP G0RIF5
C	486	LEU	-	expression tag	UNP G0RIF5
C	487	ALA	-	expression tag	UNP G0RIF5
C	488	ASP	-	expression tag	UNP G0RIF5
C	489	LEU	-	expression tag	UNP G0RIF5
C	490	LYS	-	expression tag	UNP G0RIF5
C	491	PHE	-	expression tag	UNP G0RIF5
C	492	LEU	-	expression tag	UNP G0RIF5

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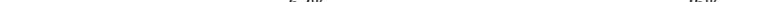
Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP G0RIF5
C	494	HIS	-	expression tag	UNP G0RIF5
C	495	HIS	-	expression tag	UNP G0RIF5
C	496	HIS	-	expression tag	UNP G0RIF5
C	497	HIS	-	expression tag	UNP G0RIF5
C	498	HIS	-	expression tag	UNP G0RIF5
C	499	HIS	-	expression tag	UNP G0RIF5

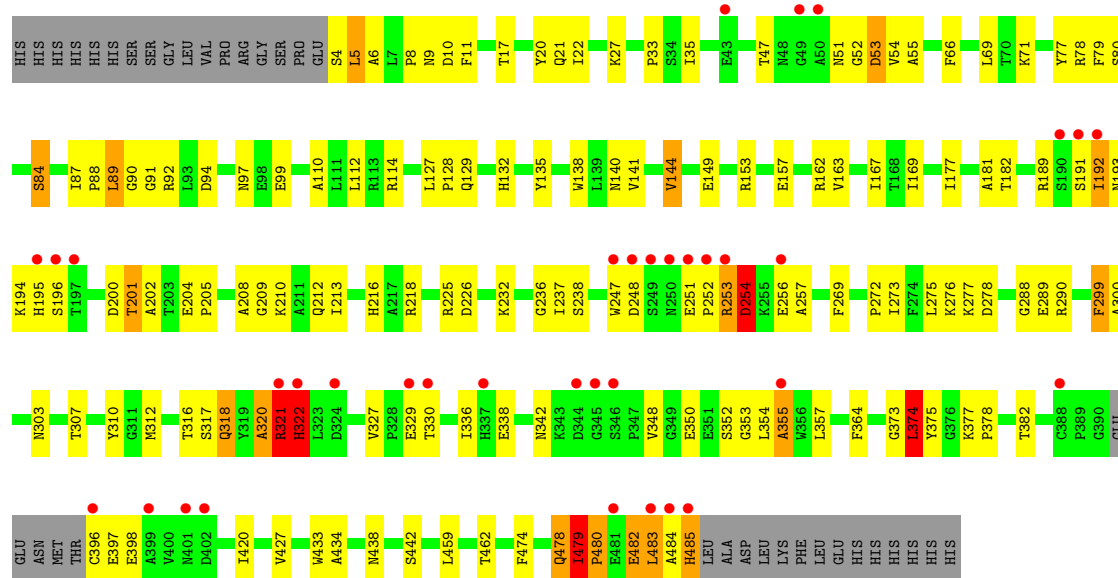


- Molecule 1: Glycoside hydrolase family 1





Chain C:  7% 63% 26% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.58Å 182.39Å 210.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.23 – 3.31 38.23 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.23-3.31) 99.5 (38.23-3.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496, PHENIX	Depositor
R, $R_{free}$	0.174 , 0.237 0.181 , 0.240	Depositor DCC
$R_{free}$ test set	1590 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.55	0/3960	0.75	5/5380 (0.1%)
1	B	0.53	0/3960	0.76	8/5380 (0.1%)
1	C	0.52	0/3960	0.75	4/5380 (0.1%)
All	All	0.53	0/11880	0.75	17/16140 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	4
All	All	0	9

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	CA-CB-CG	12.25	143.47	115.30
1	C	322	HIS	N-CA-C	7.91	132.37	111.00
1	B	485	HIS	N-CA-C	7.69	131.78	111.00
1	C	374	LEU	CA-CB-CG	7.67	132.95	115.30
1	B	484	ALA	CB-CA-C	7.56	121.44	110.10
1	B	321	ARG	CG-CD-NE	-6.27	98.64	111.80
1	B	374	LEU	CA-CB-CG	6.14	129.41	115.30
1	B	253	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	374	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	479	ILE	C-N-CD	-5.45	108.61	120.60
1	A	89	LEU	N-CA-CB	5.43	121.26	110.40
1	A	374	LEU	N-CA-C	-5.37	96.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	HIS	N-CA-CB	-5.32	101.02	110.60
1	C	321	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	C	479	ILE	C-N-CD	-5.18	109.20	120.60
1	B	374	LEU	N-CA-C	-5.09	97.26	111.00
1	B	322	HIS	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	GLY	Peptide
1	A	374	LEU	Peptide
1	A	5	LEU	Peptide
1	A	88	PRO	Peptide
1	B	373	GLY	Peptide
1	C	254	ASP	Peptide
1	C	320	ALA	Peptide
1	C	321	ARG	Peptide
1	C	373	GLY	Peptide

## 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	3843	0	3635	136	0
1	B	3843	0	3635	134	0
1	C	3843	0	3635	141	0
All	All	11529	0	10905	409	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 18.

All (409) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ILE:CG2	1:C:480:PRO:HA	1.46	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ILE:CG2	1:A:480:PRO:HA	1.57	1.33
1:C:478:GLN:O	1:C:479:ILE:HD13	1.17	1.30
1:C:479:ILE:CB	1:C:480:PRO:HA	1.57	1.30
1:C:478:GLN:O	1:C:479:ILE:CD1	1.80	1.30
1:A:479:ILE:CB	1:A:480:PRO:HA	1.62	1.28
1:B:479:ILE:HG22	1:B:480:PRO:CA	1.64	1.26
1:A:479:ILE:HG22	1:A:480:PRO:CA	1.74	1.17
1:B:479:ILE:CG2	1:B:480:PRO:HA	1.75	1.16
1:B:479:ILE:CB	1:B:480:PRO:HA	1.72	1.16
1:C:479:ILE:HG22	1:C:480:PRO:CA	1.79	1.13
1:C:479:ILE:CB	1:C:480:PRO:CA	2.30	1.10
1:C:479:ILE:CG2	1:C:480:PRO:CA	2.29	1.10
1:C:479:ILE:HG22	1:C:480:PRO:HA	1.33	1.10
1:A:479:ILE:HB	1:A:480:PRO:HA	1.28	1.08
1:A:479:ILE:CG2	1:A:480:PRO:CA	2.29	1.08
1:B:479:ILE:HB	1:B:480:PRO:HA	1.33	1.07
1:B:195:HIS:HB3	1:B:196:SER:HA	1.32	1.07
1:C:479:ILE:HB	1:C:480:PRO:CA	1.85	1.07
1:C:479:ILE:HB	1:C:480:PRO:HA	1.30	1.07
1:B:479:ILE:CG2	1:B:480:PRO:CA	2.29	1.06
1:B:485:HIS:N	1:B:485:HIS:ND1	2.00	1.05
1:A:479:ILE:CB	1:A:480:PRO:CA	2.38	1.02
1:C:485:HIS:H	1:C:485:HIS:CD2	1.70	1.00
1:A:195:HIS:HB3	1:A:196:SER:HA	1.41	0.99
1:A:478:GLN:O	1:A:479:ILE:HG12	1.66	0.95
1:C:257:ALA:HB1	1:C:336:ILE:HD11	1.46	0.94
1:A:33:PRO:HD2	1:A:89:LEU:HD11	1.50	0.93
1:B:479:ILE:HG22	1:B:480:PRO:N	1.72	0.92
1:A:479:ILE:HB	1:A:480:PRO:CA	1.96	0.92
1:A:288:GLY:HA3	1:A:290:ARG:H	1.34	0.90
1:A:482:GLU:C	1:A:484:ALA:H	1.68	0.89
1:B:479:ILE:CB	1:B:480:PRO:CA	2.48	0.88
1:A:194:LYS:HA	1:A:195:HIS:HB2	1.54	0.86
1:C:474:PHE:O	1:C:478:GLN:HG3	1.75	0.86
1:A:196:SER:OG	1:A:197:THR:N	2.04	0.85
1:C:485:HIS:H	1:C:485:HIS:HD2	1.19	0.85
1:B:89:LEU:HD12	1:B:130:ALA:H	1.42	0.85
1:B:197:THR:HG22	1:B:198:GLU:HG3	1.61	0.82
1:C:318:GLN:NE2	1:C:338:GLU:OE1	2.12	0.82
1:A:396:CYS:SG	1:A:397:GLU:N	2.53	0.82
1:C:153:ARG:NH2	1:C:226:ASP:OD2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLY:HA3	1:C:289:GLU:HB2	1.60	0.81
1:B:253:ARG:HD2	1:B:321:ARG:NH2	1.96	0.81
1:B:251:GLU:OE2	1:B:253:ARG:HG3	1.82	0.80
1:C:195:HIS:HB3	1:C:196:SER:HA	1.62	0.79
1:A:257:ALA:HB1	1:A:336:ILE:HD11	1.62	0.79
1:A:478:GLN:O	1:A:479:ILE:CG1	2.30	0.79
1:B:323:LEU:HD12	1:B:327:VAL:HG12	1.62	0.79
1:A:479:ILE:HG22	1:A:480:PRO:N	1.94	0.79
1:B:481:GLU:O	1:B:481:GLU:CG	2.30	0.78
1:A:482:GLU:C	1:A:484:ALA:N	2.37	0.78
1:A:241:GLY:HA2	1:A:265:HIS:CE1	2.17	0.78
1:B:194:LYS:HA	1:B:195:HIS:HB2	1.65	0.77
1:C:482:GLU:C	1:C:484:ALA:N	2.36	0.76
1:C:479:ILE:HB	1:C:480:PRO:CB	2.16	0.76
1:C:135:TYR:HB2	1:C:140:ASN:HD22	1.50	0.75
1:B:253:ARG:HD2	1:B:321:ARG:HH22	1.51	0.75
1:B:127:LEU:HD12	1:B:128:PRO:HD2	1.69	0.75
1:C:254:ASP:N	1:C:254:ASP:OD1	2.20	0.74
1:B:195:HIS:CB	1:B:196:SER:HA	2.13	0.74
1:B:191:SER:H	1:B:201:THR:HG23	1.52	0.74
1:A:275:LEU:HB3	1:A:277:LYS:HG3	1.70	0.73
1:B:479:ILE:HG22	1:B:480:PRO:C	2.08	0.73
1:C:485:HIS:N	1:C:485:HIS:CD2	2.48	0.73
1:A:474:PHE:O	1:A:478:GLN:HG3	1.88	0.73
1:B:396:CYS:SG	1:B:397:GLU:N	2.62	0.73
1:A:218:ARG:HE	1:A:301:ILE:HD13	1.54	0.72
1:A:195:HIS:CB	1:A:196:SER:HA	2.18	0.72
1:C:247:TRP:N	1:C:321:ARG:HD3	2.04	0.72
1:A:35:ILE:HD13	1:A:127:LEU:HB3	1.71	0.71
1:C:396:CYS:SG	1:C:397:GLU:N	2.64	0.71
1:C:251:GLU:HB3	1:C:321:ARG:HH12	1.55	0.71
1:C:482:GLU:C	1:C:484:ALA:H	1.94	0.70
1:B:257:ALA:HB1	1:B:336:ILE:HD11	1.73	0.70
1:C:478:GLN:C	1:C:479:ILE:HD13	2.07	0.70
1:B:288:GLY:HA3	1:B:289:GLU:HB3	1.74	0.69
1:C:474:PHE:O	1:C:478:GLN:CG	2.40	0.69
1:B:254:ASP:OD1	1:B:321:ARG:NE	2.26	0.69
1:B:153:ARG:NH2	1:B:226:ASP:OD2	2.25	0.69
1:B:278:ASP:HB2	1:B:294:LEU:HD12	1.74	0.69
1:A:191:SER:H	1:A:201:THR:HG23	1.56	0.69
1:C:254:ASP:HB2	1:C:321:ARG:HD2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:GLN:O	1:C:479:ILE:CG1	2.40	0.68
1:B:481:GLU:HG3	1:B:481:GLU:O	1.94	0.68
1:A:181:ALA:HB2	1:A:205:PRO:HG3	1.75	0.68
1:A:484:ALA:O	1:A:485:HIS:C	2.30	0.68
1:A:20:TYR:CZ	1:A:52:GLY:HA3	2.29	0.68
1:B:89:LEU:CD1	1:B:130:ALA:H	2.07	0.67
1:A:478:GLN:C	1:A:479:ILE:HG12	2.14	0.67
1:B:260:ARG:NH2	1:B:335:ALA:O	2.27	0.67
1:B:191:SER:H	1:B:201:THR:CG2	2.08	0.67
1:C:127:LEU:HD12	1:C:128:PRO:HD2	1.77	0.66
1:A:90:GLY:HA3	1:A:94:ASP:OD2	1.95	0.66
1:B:479:ILE:HB	1:B:480:PRO:CA	2.16	0.66
1:C:20:TYR:CZ	1:C:52:GLY:HA3	2.29	0.66
1:B:474:PHE:O	1:B:478:GLN:HG3	1.95	0.66
1:A:112:LEU:HD11	1:A:162:ARG:HB3	1.77	0.65
1:A:478:GLN:O	1:A:479:ILE:CD1	2.45	0.65
1:B:253:ARG:HB2	1:B:321:ARG:NH2	2.11	0.65
1:A:482:GLU:O	1:A:484:ALA:N	2.30	0.65
1:C:353:GLY:HA2	1:C:354:LEU:C	2.18	0.65
1:C:479:ILE:HG22	1:C:480:PRO:N	2.12	0.64
1:C:482:GLU:O	1:C:484:ALA:N	2.30	0.64
1:C:247:TRP:O	1:C:342:ASN:HB2	1.98	0.64
1:A:353:GLY:HA2	1:A:354:LEU:C	2.18	0.64
1:A:317:SER:HB3	1:A:363:MET:HE2	1.80	0.64
1:A:401:ASN:HA	1:A:465:LYS:HD2	1.78	0.64
1:B:19:ALA:H	1:B:80:SER:HB3	1.62	0.64
1:C:288:GLY:CA	1:C:289:GLU:HB2	2.27	0.64
1:B:316:THR:OG1	1:B:317:SER:N	2.29	0.63
1:A:191:SER:H	1:A:201:THR:CG2	2.13	0.62
1:A:365:ARG:HB2	1:A:415:SER:HB2	1.81	0.62
1:B:31:ARG:HB2	1:B:85:ARG:HG3	1.81	0.62
1:B:396:CYS:HB3	1:B:398:GLU:HG3	1.80	0.62
1:B:288:GLY:HA3	1:B:290:ARG:H	1.65	0.62
1:A:479:ILE:HG22	1:A:480:PRO:C	2.20	0.62
1:A:92:ARG:HD3	1:A:147:ASP:OD1	2.00	0.61
1:B:275:LEU:HB3	1:B:277:LYS:HG3	1.83	0.61
1:C:189:ARG:NH1	1:C:204:GLU:OE2	2.34	0.61
1:C:397:GLU:OE2	1:C:462:THR:OG1	2.17	0.61
1:C:479:ILE:HB	1:C:480:PRO:HB3	1.80	0.61
1:A:275:LEU:HD23	1:A:375:TYR:HD1	1.66	0.61
1:C:478:GLN:C	1:C:479:ILE:CG1	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HD3	1:B:147:ASP:OD1	2.00	0.61
1:C:191:SER:H	1:C:201:THR:CG2	2.14	0.61
1:A:321:ARG:HD3	1:A:339:HIS:CE1	2.36	0.61
1:C:484:ALA:O	1:C:485:HIS:C	2.40	0.60
1:C:194:LYS:HG2	1:C:194:LYS:O	2.01	0.60
1:B:373:GLY:H	1:B:376:GLY:HA3	1.65	0.60
1:C:35:ILE:HD13	1:C:127:LEU:HB3	1.83	0.60
1:A:321:ARG:HD3	1:A:339:HIS:HE1	1.67	0.60
1:C:90:GLY:HA3	1:C:94:ASP:OD2	2.01	0.60
1:B:189:ARG:NH2	1:B:198:GLU:OE1	2.34	0.59
1:B:353:GLY:HA2	1:B:354:LEU:C	2.22	0.59
1:C:135:TYR:HE1	1:C:144:VAL:HG23	1.67	0.59
1:B:153:ARG:HG3	1:B:222:VAL:HG11	1.83	0.59
1:C:208:ALA:O	1:C:212:GLN:HG3	2.02	0.59
1:C:247:TRP:HB3	1:C:321:ARG:HE	1.67	0.59
1:A:312:MET:HE2	1:A:364:PHE:HE1	1.68	0.58
1:B:181:ALA:HB2	1:B:205:PRO:HG3	1.85	0.58
1:C:478:GLN:C	1:C:479:ILE:HG12	2.23	0.58
1:C:288:GLY:HA3	1:C:289:GLU:CB	2.30	0.58
1:B:479:ILE:CG2	1:B:480:PRO:N	2.49	0.58
1:A:88:PRO:HD2	1:A:95:PRO:O	2.04	0.58
1:C:191:SER:H	1:C:201:THR:HG23	1.69	0.58
1:A:21:GLN:NE2	1:A:441:TRP:NE1	2.51	0.57
1:B:481:GLU:HG2	1:B:481:GLU:O	2.04	0.57
1:A:182:THR:O	1:A:193:ASN:ND2	2.37	0.57
1:A:401:ASN:HB2	1:A:465:LYS:HZ2	1.70	0.57
1:C:88:PRO:O	1:C:89:LEU:HB2	2.05	0.57
1:C:352:SER:OG	1:C:357:LEU:O	2.23	0.57
1:B:87:ILE:O	1:B:89:LEU:N	2.38	0.56
1:B:275:LEU:HD23	1:B:375:TYR:HD1	1.70	0.56
1:B:20:TYR:CZ	1:B:52:GLY:HA3	2.41	0.56
1:C:478:GLN:C	1:C:479:ILE:CD1	2.69	0.56
1:B:244:TYR:CD1	1:B:320:ALA:HB2	2.40	0.56
1:B:321:ARG:NH1	1:B:322:HIS:CD2	2.74	0.56
1:C:479:ILE:HG21	1:C:480:PRO:HA	1.71	0.56
1:A:288:GLY:CA	1:A:290:ARG:H	2.13	0.56
1:B:88:PRO:O	1:B:89:LEU:HB2	2.05	0.56
1:A:297:ALA:O	1:A:300:ALA:HB3	2.05	0.55
1:A:310:TYR:CE1	1:A:312:MET:HB2	2.41	0.55
1:A:57:ASP:HB3	1:A:61:ARG:HD2	1.88	0.55
1:B:247:TRP:HD1	1:B:342:ASN:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLY:HA2	1:B:355:ALA:N	2.21	0.55
1:A:402:ASP:OD2	1:A:466:SER:OG	2.19	0.55
1:C:33:PRO:O	1:C:89:LEU:HD11	2.07	0.55
1:A:89:LEU:HD23	1:A:130:ALA:H	1.71	0.54
1:B:98:GLU:O	1:B:102:GLU:HG3	2.07	0.54
1:C:247:TRP:HB3	1:C:321:ARG:NE	2.22	0.54
1:C:320:ALA:O	1:C:321:ARG:HG3	2.08	0.54
1:B:352:SER:OG	1:B:357:LEU:O	2.24	0.54
1:A:310:TYR:HE1	1:A:312:MET:HB2	1.72	0.54
1:C:290:ARG:NH1	1:C:329:GLU:O	2.41	0.54
1:C:149:GLU:OE1	1:C:218:ARG:HD2	2.07	0.54
1:A:241:GLY:HA2	1:A:265:HIS:ND1	2.23	0.54
1:A:288:GLY:HA3	1:A:290:ARG:N	2.13	0.53
1:B:218:ARG:O	1:B:222:VAL:HG23	2.09	0.53
1:B:343:LYS:C	1:B:345:GLY:H	2.11	0.53
1:B:240:ASN:HB3	1:B:313:ASN:HB2	1.90	0.53
1:C:253:ARG:O	1:C:322:HIS:HE1	1.91	0.53
1:C:135:TYR:CE1	1:C:144:VAL:HG23	2.44	0.53
1:A:209:GLY:O	1:A:213:ILE:HG13	2.09	0.53
1:C:236:GLY:HA2	1:C:307:THR:HG23	1.89	0.53
1:C:479:ILE:HG22	1:C:480:PRO:C	2.29	0.53
1:B:141:VAL:HG22	1:B:211:ALA:HB2	1.91	0.53
1:A:437:ASP:OD2	1:A:448:ARG:NH1	2.39	0.52
1:A:86:ILE:HG23	1:A:101:ILE:HG12	1.90	0.52
1:A:478:GLN:O	1:A:479:ILE:HD13	2.10	0.52
1:B:192:ILE:HG12	1:B:201:THR:HG21	1.92	0.52
1:B:245:GLU:HB2	1:B:246:PRO:HD2	1.91	0.52
1:C:254:ASP:HB3	1:C:257:ALA:HB3	1.91	0.52
1:A:479:ILE:CG2	1:A:480:PRO:N	2.65	0.52
1:C:135:TYR:O	1:C:140:ASN:HB2	2.10	0.52
1:B:181:ALA:HB2	1:B:205:PRO:CG	2.39	0.51
1:A:135:TYR:HB2	1:A:140:ASN:HD22	1.74	0.51
1:B:192:ILE:HD11	1:B:330:THR:HG21	1.92	0.51
1:C:248:ASP:HB3	1:C:321:ARG:NH2	2.25	0.51
1:C:78:ARG:HE	1:C:167:ILE:HD12	1.76	0.51
1:C:482:GLU:O	1:C:483:LEU:C	2.48	0.51
1:A:92:ARG:HD2	1:A:146:LEU:HB3	1.92	0.51
1:A:479:ILE:HG21	1:A:480:PRO:HA	1.78	0.51
1:A:353:GLY:HA2	1:A:355:ALA:N	2.26	0.51
1:A:78:ARG:NH1	1:A:383:GLU:HG3	2.26	0.50
1:A:21:GLN:HB3	1:A:438:ASN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:CE1	1:A:237:ILE:HB	2.46	0.50
1:A:65:ASP:OD1	1:A:461:ARG:NE	2.43	0.50
1:C:251:GLU:CD	1:C:253:ARG:HE	2.15	0.50
1:B:482:GLU:C	1:B:484:ALA:N	2.63	0.50
1:C:216:HIS:CE1	1:C:237:ILE:HB	2.46	0.50
1:C:278:ASP:HB3	1:C:299:PHE:HZ	1.76	0.50
1:B:90:GLY:HA2	1:B:131:LEU:HG	1.92	0.50
1:C:20:TYR:CE2	1:C:52:GLY:HA3	2.46	0.50
1:C:181:ALA:HB2	1:C:205:PRO:HG3	1.93	0.50
1:A:319:TYR:CE2	1:A:348:VAL:HG22	2.46	0.50
1:B:257:ALA:HB1	1:B:336:ILE:CD1	2.39	0.50
1:C:195:HIS:HB3	1:C:196:SER:CA	2.37	0.50
1:C:484:ALA:O	1:C:485:HIS:O	2.30	0.50
1:A:484:ALA:O	1:A:485:HIS:O	2.30	0.50
1:B:473:MET:O	1:B:477:ARG:HG3	2.11	0.50
1:C:247:TRP:H	1:C:321:ARG:HD3	1.77	0.50
1:A:141:VAL:HG22	1:A:211:ALA:HB2	1.93	0.49
1:B:247:TRP:CD1	1:B:342:ASN:HA	2.47	0.49
1:A:127:LEU:HD12	1:A:128:PRO:HD2	1.93	0.49
1:A:440:GLU:O	1:A:443:ASP:HB2	2.12	0.49
1:B:479:ILE:HD11	1:C:27:LYS:HE3	1.94	0.49
1:C:251:GLU:CG	1:C:253:ARG:HG3	2.41	0.49
1:C:288:GLY:HA3	1:C:290:ARG:H	1.77	0.49
1:A:87:ILE:O	1:A:89:LEU:N	2.45	0.49
1:C:51:ASN:ND2	1:C:53:ASP:OD2	2.46	0.49
1:B:89:LEU:HD13	1:B:128:PRO:HB3	1.93	0.49
1:C:254:ASP:HA	1:C:257:ALA:H	1.77	0.49
1:A:88:PRO:O	1:A:89:LEU:HD12	2.13	0.49
1:C:353:GLY:HA2	1:C:355:ALA:N	2.26	0.49
1:A:174:ILE:HG23	1:A:178:TYR:CD2	2.48	0.49
1:B:290:ARG:O	1:B:292:PRO:HD3	2.12	0.49
1:C:181:ALA:HB2	1:C:205:PRO:CG	2.43	0.49
1:C:275:LEU:HB3	1:C:277:LYS:HG3	1.95	0.48
1:A:458:THR:HB	1:A:460:LYS:HB2	1.95	0.48
1:C:182:THR:O	1:C:193:ASN:ND2	2.47	0.48
1:C:4:SER:O	1:C:5:LEU:HB2	2.12	0.48
1:C:91:GLY:N	1:C:94:ASP:OD2	2.47	0.48
1:A:32:GLY:HA3	1:A:89:LEU:CD1	2.44	0.48
1:B:322:HIS:C	1:B:322:HIS:CD2	2.86	0.48
1:C:66:PHE:O	1:C:69:LEU:HB2	2.14	0.48
1:B:321:ARG:NH1	1:B:322:HIS:CG	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:O	1:A:290:ARG:HD2	2.12	0.48
1:B:281:GLU:C	1:B:283:MET:H	2.15	0.48
1:B:482:GLU:C	1:B:484:ALA:H	2.16	0.48
1:C:396:CYS:HB3	1:C:398:GLU:OE2	2.13	0.48
1:A:78:ARG:HH12	1:A:383:GLU:HG3	1.79	0.47
1:C:169:ILE:HD13	1:C:212:GLN:HB3	1.96	0.47
1:A:238:SER:HA	1:A:311:GLY:O	2.13	0.47
1:C:479:ILE:HG13	1:C:483:LEU:HD13	1.95	0.47
1:A:377:LYS:HB3	1:A:378:PRO:HD2	1.97	0.47
1:C:254:ASP:HB2	1:C:321:ARG:CD	2.42	0.47
1:C:193:ASN:CG	1:C:194:LYS:H	2.17	0.47
1:C:141:VAL:HG21	1:C:210:LYS:HD3	1.96	0.47
1:C:310:TYR:CE1	1:C:312:MET:HB2	2.49	0.47
1:B:480:PRO:HD2	1:B:481:GLU:H	1.78	0.47
1:A:248:ASP:OD1	1:A:343:LYS:HD3	2.15	0.47
1:A:479:ILE:HB	1:A:480:PRO:CB	2.44	0.47
1:B:110:ALA:HB1	1:B:114:ARG:HH12	1.80	0.47
1:B:86:ILE:HG23	1:B:101:ILE:HG12	1.97	0.47
1:A:177:ILE:HD13	1:A:205:PRO:HB3	1.97	0.47
1:C:420:ILE:HD11	1:C:427:VAL:HB	1.96	0.46
1:B:239:LEU:HD12	1:B:310:TYR:CE2	2.50	0.46
1:B:288:GLY:CA	1:B:290:ARG:H	2.26	0.46
1:A:225:ARG:HD3	1:A:225:ARG:HA	1.76	0.46
1:A:14:GLY:HA3	1:A:76:ALA:O	2.16	0.46
1:B:433:TRP:HA	1:B:434:ALA:HA	1.72	0.46
1:A:245:GLU:HB2	1:A:246:PRO:HD2	1.97	0.46
1:B:465:LYS:HB3	1:B:465:LYS:HE3	1.76	0.46
1:C:316:THR:OG1	1:C:317:SER:N	2.49	0.46
1:B:66:PHE:O	1:B:69:LEU:HB2	2.16	0.46
1:C:248:ASP:H	1:C:321:ARG:CZ	2.29	0.46
1:C:153:ARG:O	1:C:157:GLU:HG3	2.16	0.46
1:C:88:PRO:HD3	1:C:97:ASN:H	1.79	0.46
1:B:253:ARG:HH11	1:B:321:ARG:CZ	2.29	0.46
1:B:373:GLY:O	1:B:374:LEU:HB3	2.16	0.46
1:B:405:ARG:HG2	1:B:409:PHE:CE2	2.51	0.46
1:A:171:GLU:HB3	1:A:174:ILE:HD12	1.98	0.46
1:A:191:SER:OG	1:A:200:ASP:HA	2.15	0.46
1:B:253:ARG:HB2	1:B:321:ARG:HH21	1.79	0.46
1:A:51:ASN:O	1:A:445:TYR:OH	2.24	0.45
1:B:101:ILE:HD13	1:B:158:ARG:HG3	1.98	0.45
1:A:257:ALA:HB1	1:A:336:ILE:CD1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD13	1:A:356:TRP:CE2	2.51	0.45
1:B:86:ILE:HD11	1:B:104:TYR:CD2	2.50	0.45
1:B:321:ARG:NH2	1:B:322:HIS:HB3	2.31	0.45
1:C:21:GLN:HE22	1:C:433:TRP:HZ2	1.65	0.45
1:A:193:ASN:HB3	1:A:195:HIS:HA	1.99	0.45
1:B:191:SER:HB2	1:B:201:THR:HG23	1.99	0.45
1:C:135:TYR:HB2	1:C:140:ASN:ND2	2.25	0.45
1:A:290:ARG:O	1:A:292:PRO:HD3	2.17	0.45
1:C:177:ILE:O	1:C:181:ALA:HB3	2.16	0.45
1:A:420:ILE:HD11	1:A:427:VAL:HB	1.99	0.45
1:A:437:ASP:H	1:A:454:THR:HG23	1.81	0.45
1:A:149:GLU:OE1	1:A:218:ARG:HD2	2.17	0.45
1:A:397:GLU:OE2	1:A:462:THR:OG1	2.25	0.45
1:A:33:PRO:CD	1:A:89:LEU:HD11	2.34	0.45
1:B:278:ASP:CB	1:B:294:LEU:HD12	2.45	0.45
1:B:65:ASP:OD1	1:B:461:ARG:NE	2.50	0.44
1:C:84:SER:O	1:C:88:PRO:HA	2.17	0.44
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.62	0.44
1:B:15:PHE:CE1	1:B:451:VAL:HG21	2.52	0.44
1:C:312:MET:HE2	1:C:364:PHE:HE1	1.82	0.44
1:C:433:TRP:CD2	1:C:434:ALA:HB2	2.53	0.44
1:C:478:GLN:O	1:C:479:ILE:HD11	1.98	0.44
1:B:322:HIS:HA	1:B:336:ILE:HD13	1.99	0.44
1:A:396:CYS:HB3	1:A:398:GLU:CD	2.38	0.44
1:B:251:GLU:HA	1:B:252:PRO:HD2	1.72	0.44
1:B:340:GLN:O	1:B:348:VAL:HG23	2.18	0.44
1:A:173:TRP:CE2	1:A:177:ILE:HG13	2.53	0.44
1:B:374:LEU:HA	1:B:375:TYR:HA	1.81	0.44
1:A:462:THR:HA	1:A:463:PRO:HD3	1.87	0.43
1:B:89:LEU:HD12	1:B:130:ALA:N	2.22	0.43
1:A:406:ILE:HG23	1:A:473:MET:CE	2.48	0.43
1:B:87:ILE:C	1:B:89:LEU:H	2.20	0.43
1:C:17:THR:HB	1:C:22:ILE:HD13	2.00	0.43
1:A:251:GLU:OE2	1:A:253:ARG:HB2	2.18	0.43
1:A:241:GLY:HA2	1:A:265:HIS:HE1	1.79	0.43
1:A:278:ASP:HB2	1:A:294:LEU:HD12	1.99	0.43
1:A:71:LYS:HB2	1:A:71:LYS:HE3	1.63	0.43
1:C:191:SER:OG	1:C:200:ASP:HA	2.17	0.43
1:C:202:ALA:O	1:C:290:ARG:HD2	2.18	0.43
1:A:173:TRP:CD1	1:A:265:HIS:HD2	2.36	0.43
1:A:299:PHE:HB3	1:A:303:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:O	1:B:345:GLY:N	2.52	0.43
1:C:374:LEU:HA	1:C:375:TYR:HA	1.55	0.43
1:A:374:LEU:HD23	1:A:374:LEU:O	2.18	0.43
1:B:322:HIS:O	1:B:323:LEU:HD23	2.18	0.43
1:C:129:GLN:HE21	1:C:132:HIS:HB3	1.83	0.43
1:C:310:TYR:HE1	1:C:312:MET:HB2	1.83	0.43
1:C:336:ILE:HA	1:C:336:ILE:HD13	1.73	0.43
1:A:189:ARG:NH2	1:A:198:GLU:HB3	2.33	0.43
1:A:218:ARG:HE	1:A:301:ILE:CD1	2.26	0.43
1:B:92:ARG:HD2	1:B:146:LEU:HB3	2.00	0.43
1:C:276:LYS:HE2	1:C:303:ASN:HA	2.01	0.43
1:B:238:SER:HA	1:B:311:GLY:O	2.18	0.43
1:B:321:ARG:HG2	1:B:322:HIS:H	1.82	0.43
1:B:269:PHE:O	1:B:273:ILE:HG13	2.19	0.43
1:B:21:GLN:NE2	1:B:433:TRP:HZ2	2.17	0.43
1:C:87:ILE:O	1:C:89:LEU:N	2.52	0.43
1:A:181:ALA:HB2	1:A:205:PRO:CG	2.48	0.43
1:B:437:ASP:HB2	1:B:454:THR:OG1	2.18	0.43
1:C:27:LYS:HB3	1:C:27:LYS:HE2	1.90	0.43
1:A:433:TRP:HA	1:A:434:ALA:HA	1.79	0.42
1:B:238:SER:HB2	1:B:382:THR:OG1	2.19	0.42
1:A:279:TYR:CE2	1:A:291:LEU:HG	2.53	0.42
1:A:173:TRP:CD2	1:A:265:HIS:CD2	3.07	0.42
1:B:377:LYS:HB3	1:B:378:PRO:HD2	2.01	0.42
1:A:415:SER:HA	1:A:418:LYS:HB2	2.00	0.42
1:B:433:TRP:CE2	1:B:434:ALA:HB2	2.55	0.42
1:B:480:PRO:CD	1:B:481:GLU:H	2.31	0.42
1:C:149:GLU:HB2	1:C:218:ARG:HB3	2.01	0.42
1:C:225:ARG:HD3	1:C:225:ARG:HA	1.70	0.42
1:B:51:ASN:ND2	1:B:53:ASP:OD2	2.53	0.42
1:A:251:GLU:HA	1:A:252:PRO:HD2	1.87	0.42
1:B:121:THR:HA	1:B:167:ILE:O	2.20	0.42
1:B:254:ASP:C	1:B:256:GLU:N	2.73	0.42
1:B:21:GLN:HE22	1:B:433:TRP:HZ2	1.68	0.42
1:B:32:GLY:HA3	1:B:89:LEU:HD23	2.02	0.42
1:A:278:ASP:HB3	1:A:299:PHE:HZ	1.85	0.42
1:B:321:ARG:CZ	1:B:322:HIS:CG	3.03	0.42
1:C:251:GLU:HA	1:C:252:PRO:HD2	1.90	0.42
1:A:406:ILE:HG23	1:A:473:MET:HE1	2.01	0.41
1:C:433:TRP:HA	1:C:434:ALA:HA	1.81	0.41
1:A:336:ILE:HD13	1:A:336:ILE:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:PHE:O	1:B:478:GLN:CG	2.68	0.41
1:C:47:THR:HG22	1:C:442:SER:HA	2.02	0.41
1:A:352:SER:HB2	1:A:387:PRO:O	2.19	0.41
1:B:327:VAL:HG11	1:B:335:ALA:HB2	2.02	0.41
1:C:238:SER:HB2	1:C:382:THR:OG1	2.20	0.41
1:B:336:ILE:HD13	1:B:336:ILE:HA	1.84	0.41
1:C:127:LEU:HD22	1:C:138:TRP:CD1	2.55	0.41
1:C:77:TYR:CE2	1:C:79:PHE:HB3	2.54	0.41
1:A:400:VAL:O	1:A:465:LYS:N	2.50	0.41
1:C:269:PHE:O	1:C:272:PRO:HD2	2.20	0.41
1:A:290:ARG:NH1	1:A:329:GLU:O	2.36	0.41
1:B:343:LYS:HB2	1:B:343:LYS:HE3	1.82	0.41
1:B:436:LEU:HD13	1:B:454:THR:HG21	2.02	0.41
1:A:33:PRO:HG3	1:C:485:HIS:HB2	2.03	0.41
1:A:89:LEU:CD2	1:A:130:ALA:H	2.34	0.41
1:A:218:ARG:NE	1:A:301:ILE:HD13	2.30	0.41
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.84	0.41
1:B:21:GLN:OE1	1:B:441:TRP:NE1	2.54	0.41
1:A:192:ILE:HD11	1:A:330:THR:HG21	2.02	0.41
1:A:51:ASN:ND2	1:A:53:ASP:OD2	2.54	0.41
1:B:87:ILE:HG12	1:B:150:ARG:NH1	2.36	0.41
1:C:192:ILE:HD11	1:C:330:THR:HG21	2.02	0.41
1:C:53:ASP:O	1:C:55:ALA:N	2.53	0.41
1:A:235:ILE:N	1:A:308:ASP:OD2	2.47	0.41
1:A:53:ASP:O	1:A:55:ALA:N	2.53	0.41
1:B:354:LEU:HD23	1:B:356:TRP:CE2	2.56	0.41
1:C:377:LYS:HB3	1:C:378:PRO:HD2	2.03	0.41
1:C:479:ILE:HG13	1:C:483:LEU:CD1	2.51	0.41
1:B:171:GLU:HG3	1:B:313:ASN:HD22	1.86	0.41
1:B:338:GLU:HG2	1:B:338:GLU:H	1.54	0.41
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.88	0.41
1:B:42:LEU:HA	1:B:42:LEU:HD23	1.86	0.40
1:C:209:GLY:O	1:C:213:ILE:HG13	2.21	0.40
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.94	0.40
1:A:98:GLU:OE2	1:A:158:ARG:NH2	2.46	0.40
1:C:110:ALA:HB1	1:C:114:ARG:HH12	1.85	0.40
1:C:269:PHE:O	1:C:273:ILE:HG13	2.22	0.40
1:C:433:TRP:CE2	1:C:434:ALA:HB2	2.56	0.40
1:C:71:LYS:HB2	1:C:71:LYS:HE3	1.95	0.40

There are no symmetry-related clashes.

## 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	473/513 (92%)	407 (86%)	40 (8%)	26 (6%)	2	11
1	B	473/513 (92%)	399 (84%)	53 (11%)	21 (4%)	2	16
1	C	473/513 (92%)	402 (85%)	49 (10%)	22 (5%)	2	14
All	All	1419/1539 (92%)	1208 (85%)	142 (10%)	69 (5%)	2	14

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA
1	A	8	PRO
1	A	11	PHE
1	A	89	LEU
1	A	327	VAL
1	A	350	GLU
1	A	479	ILE
1	A	483	LEU
1	B	8	PRO
1	B	10	ASP
1	B	89	LEU
1	B	322	HIS
1	B	327	VAL
1	B	355	ALA
1	B	479	ILE
1	B	480	PRO
1	C	5	LEU
1	C	8	PRO
1	C	89	LEU
1	C	321	ARG
1	C	322	HIS
1	C	355	ALA
1	C	479	ILE
1	C	480	PRO

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Mol	Chain	Res	Type
1	A	9	ASN
1	A	288	GLY
1	A	300	ALA
1	A	355	ALA
1	B	11	PHE
1	B	288	GLY
1	B	300	ALA
1	B	344	ASP
1	B	350	GLU
1	B	353	GLY
1	C	6	ALA
1	C	9	ASN
1	C	10	ASP
1	C	11	PHE
1	C	92	ARG
1	C	232	LYS
1	C	374	LEU
1	C	483	LEU
1	A	5	LEU
1	A	195	HIS
1	A	326	PRO
1	A	373	GLY
1	A	480	PRO
1	B	163	VAL
1	C	54	VAL
1	C	299	PHE
1	A	54	VAL
1	A	92	ARG
1	A	163	VAL
1	B	6	ALA
1	B	9	ASN
1	B	232	LYS
1	C	163	VAL
1	C	350	GLU
1	A	322	HIS
1	A	387	PRO
1	B	92	ARG
1	B	195	HIS
1	C	300	ALA
1	A	345	GLY
1	B	387	PRO
1	C	327	VAL

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Mol	Chain	Res	Type
1	A	88	PRO
1	A	353	GLY
1	A	446	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	396/429 (92%)	385 (97%)	11 (3%)	43	70
1	B	396/429 (92%)	377 (95%)	19 (5%)	25	56
1	C	396/429 (92%)	378 (96%)	18 (4%)	27	58
All	All	1188/1287 (92%)	1140 (96%)	48 (4%)	31	61

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	191	SER
1	A	194	LYS
1	A	196	SER
1	A	253	ARG
1	A	259	GLU
1	A	386	CYS
1	A	398	GLU
1	A	438	ASN
1	A	459	LEU
1	A	478	GLN
1	B	5	LEU
1	B	26	VAL
1	B	53	ASP
1	B	89	LEU
1	B	144	VAL
1	B	253	ARG
1	B	254	ASP
1	B	259	GLU

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Mol	Chain	Res	Type
1	B	321	ARG
1	B	322	HIS
1	B	344	ASP
1	B	360	CYS
1	B	438	ASN
1	B	458	THR
1	B	459	LEU
1	B	478	GLN
1	B	481	GLU
1	B	483	LEU
1	B	485	HIS
1	C	53	ASP
1	C	80	SER
1	C	84	SER
1	C	99	GLU
1	C	144	VAL
1	C	162	ARG
1	C	192	ILE
1	C	201	THR
1	C	253	ARG
1	C	254	ASP
1	C	256	GLU
1	C	318	GLN
1	C	348	VAL
1	C	438	ASN
1	C	459	LEU
1	C	478	GLN
1	C	482	GLU
1	C	485	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	212	GLN
1	A	265	HIS
1	A	303	ASN
1	B	313	ASN
1	B	322	HIS
1	C	140	ASN
1	C	195	HIS
1	C	485	HIS

### 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 monosaccharides 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	477/513 (92%)	-0.19	15 (3%)	49 48	11, 27, 68, 90	0
1	B	477/513 (92%)	-0.10	23 (4%)	30 28	11, 32, 75, 99	0
1	C	477/513 (92%)	0.02	36 (7%)	14 13	13, 32, 76, 97	0
All	All	1431/1539 (92%)	-0.09	74 (5%)	27 25	11, 30, 73, 99	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	THR	6.2
1	C	250	ASN	5.0
1	A	485	HIS	5.0
1	C	483	LEU	4.7
1	A	250	ASN	4.7
1	B	250	ASN	4.6
1	C	485	HIS	4.6
1	C	195	HIS	4.2
1	B	344	ASP	4.2
1	B	346	SER	4.0
1	C	344	ASP	4.0
1	A	43	GLU	3.9
1	B	396	CYS	3.8
1	A	197	THR	3.8
1	C	248	ASP	3.6
1	B	197	THR	3.6
1	C	346	SER	3.5
1	B	345	GLY	3.4
1	A	326	PRO	3.4
1	C	196	SER	3.3
1	A	195	HIS	3.2
1	B	253	ARG	3.1
1	C	191	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	483	LEU	3.1
1	C	252	PRO	3.0
1	C	324	ASP	3.0
1	C	330	THR	3.0
1	C	337	HIS	2.9
1	B	251	GLU	2.9
1	B	252	PRO	2.9
1	B	249	SER	2.8
1	C	481	GLU	2.8
1	C	321	ARG	2.8
1	C	484	ALA	2.8
1	A	324	ASP	2.8
1	B	191	SER	2.8
1	B	199	GLY	2.7
1	B	255	LYS	2.7
1	B	324	ASP	2.7
1	B	195	HIS	2.7
1	B	347	PRO	2.7
1	B	342	ASN	2.7
1	B	483	LEU	2.6
1	B	330	THR	2.6
1	C	396	CYS	2.6
1	A	481	GLU	2.5
1	A	249	SER	2.5
1	C	256	GLU	2.5
1	C	355	ALA	2.5
1	C	329	GLU	2.5
1	C	322	HIS	2.5
1	A	396	CYS	2.5
1	B	43	GLU	2.5
1	C	43	GLU	2.4
1	B	343	LYS	2.4
1	C	401	ASN	2.4
1	C	251	GLU	2.4
1	C	345	GLY	2.4
1	C	247	TRP	2.3
1	C	388	CYS	2.3
1	A	198	GLU	2.3
1	B	401	ASN	2.3
1	C	402	ASP	2.3
1	C	192	ILE	2.3
1	B	485	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	190	SER	2.2
1	A	248	ASP	2.2
1	C	49	GLY	2.2
1	C	253	ARG	2.2
1	C	249	SER	2.2
1	C	399	ALA	2.2
1	A	196	SER	2.1
1	A	330	THR	2.1
1	C	50	ALA	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 monosaccharides 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.