



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:14 PM UTC

PDB ID : 6KHT / pdb_00006kht
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

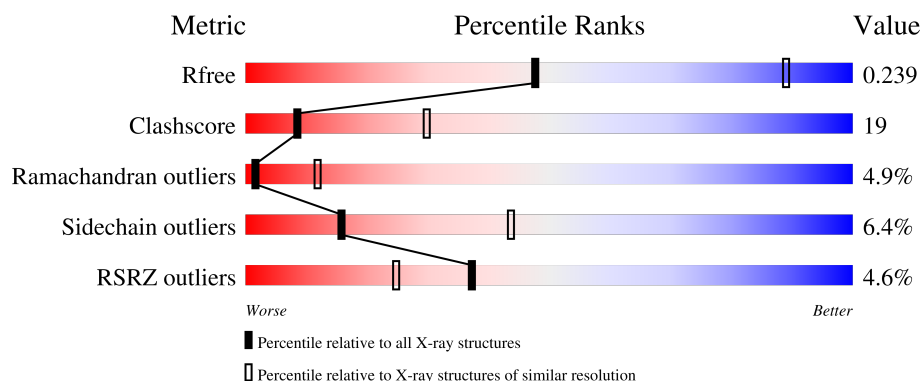
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

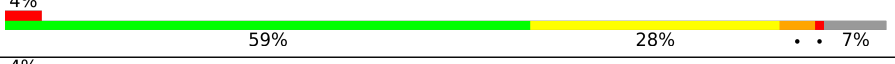
The reported resolution of this entry is 3.31 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	

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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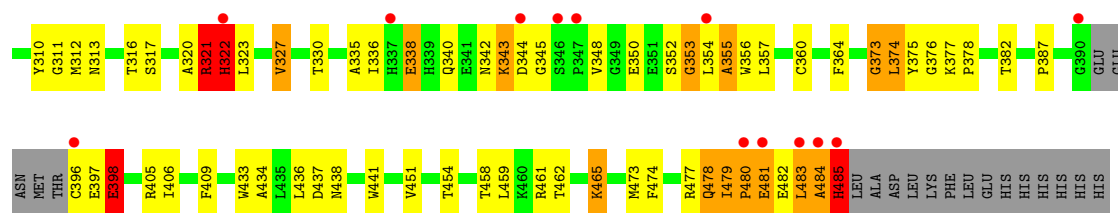
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Chain	Residue	Modelled	Actual	Comment	Reference
B	489	LEU	-	expression tag	UNP G0RIF5
B	490	LYS	-	expression tag	UNP G0RIF5
B	491	PHE	-	expression tag	UNP G0RIF5
B	492	LEU	-	expression tag	UNP G0RIF5
B	493	GLU	-	expression tag	UNP G0RIF5
B	494	HIS	-	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

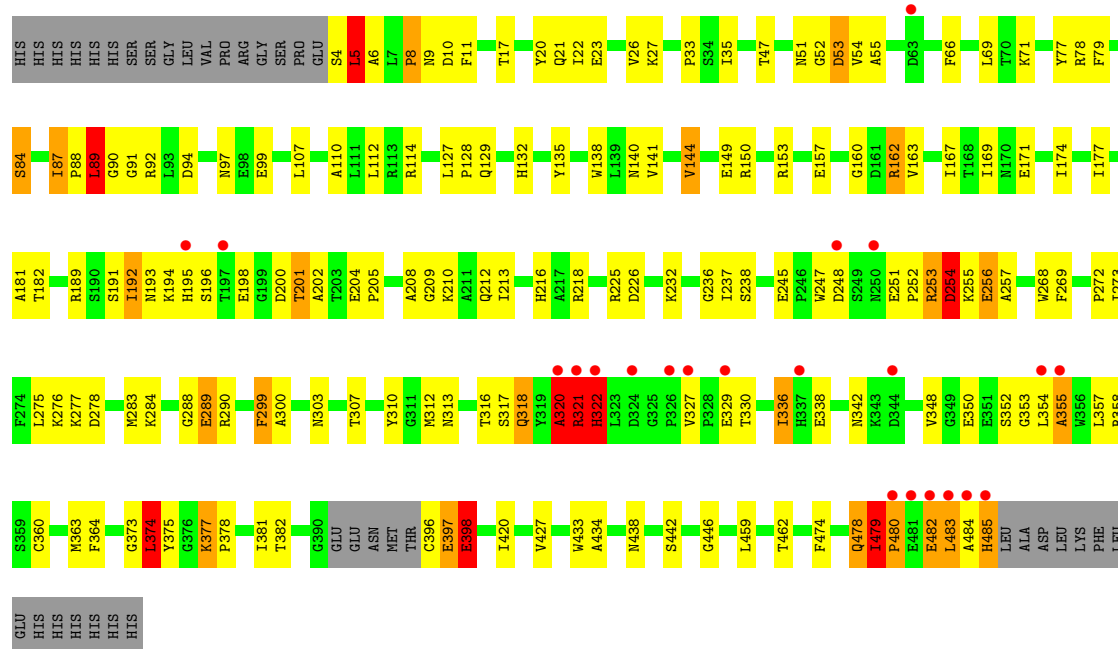
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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP G0RIF5
C	494	HIS	-	expression tag	UNP G0RIF5
C	495	HIS	-	expression tag	UNP G0RIF5
C	496	HIS	-	expression tag	UNP G0RIF5
C	497	HIS	-	expression tag	UNP G0RIF5
C	498	HIS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



• Molecule 1: Glycoside hydrolase family 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.4 (38.23-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496, PHENIX	Depositor
R, R_{free}	0.174 , 0.237 0.182 , 0.239	Depositor DCC
R_{free} test set	1590 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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	0.91	EDS
Total number of atoms	11529	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/3960	1.07	20/5380 (0.4%)
1	B	0.66	1/3960 (0.0%)	1.09	21/5380 (0.4%)
1	C	0.65	0/3960	1.06	16/5380 (0.3%)
All	All	0.66	1/11880 (0.0%)	1.07	57/16140 (0.4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	HIS	CG-ND1	-5.29	1.32	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	HIS	N-CA-C	10.12	132.37	110.80
1	A	446	GLY	CA-C-N	9.72	130.33	119.83
1	A	446	GLY	C-N-CA	9.72	130.33	119.83
1	B	483	LEU	N-CA-C	-8.90	102.59	113.19
1	B	484	ALA	N-CA-C	8.61	120.75	111.36
1	B	32	GLY	CA-C-N	8.33	128.84	119.93
1	B	32	GLY	C-N-CA	8.33	128.84	119.93
1	A	481	GLU	N-CA-C	-8.03	103.49	112.57
1	C	255	LYS	N-CA-C	-7.82	103.62	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	CA-CB-CG	7.76	143.47	116.30
1	C	398	GLU	N-CA-C	-7.71	102.97	113.30
1	B	321	ARG	N-CA-C	7.70	120.93	108.76
1	B	485	HIS	N-CA-C	7.42	131.78	111.00
1	B	251	GLU	CA-C-N	6.91	128.48	119.84
1	B	251	GLU	C-N-CA	6.91	128.48	119.84
1	A	374	LEU	N-CA-C	-6.71	96.50	110.80
1	A	398	GLU	N-CA-C	-6.58	105.22	113.18
1	B	322	HIS	N-CA-C	6.44	124.52	110.80
1	A	89	LEU	N-CA-CB	6.37	121.26	110.49
1	B	374	LEU	N-CA-C	-6.36	97.26	110.80
1	A	89	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	B	484	ALA	CB-CA-C	6.23	121.44	110.85
1	A	32	GLY	CA-C-N	6.17	126.08	119.85
1	A	32	GLY	C-N-CA	6.17	126.08	119.85
1	B	398	GLU	N-CA-C	-6.17	105.58	113.23
1	B	321	ARG	CG-CD-NE	-6.07	98.64	112.00
1	A	117	THR	CA-C-N	-5.99	113.62	119.90
1	A	117	THR	C-N-CA	-5.99	113.62	119.90
1	B	7	LEU	CA-C-N	5.76	127.05	119.84
1	B	7	LEU	C-N-CA	5.76	127.05	119.84
1	C	162	ARG	N-CA-C	-5.65	101.10	109.86
1	A	288	GLY	CA-C-N	5.59	131.76	121.70
1	A	288	GLY	C-N-CA	5.59	131.76	121.70
1	B	485	HIS	N-CA-CB	-5.58	101.02	110.50
1	C	320	ALA	CA-C-O	-5.56	116.17	122.01
1	A	351	GLU	N-CA-C	5.49	118.53	109.85
1	A	479	ILE	C-N-CD	-5.45	108.61	120.60
1	C	87	ILE	CA-C-N	5.44	126.65	119.84
1	C	87	ILE	C-N-CA	5.44	126.65	119.84
1	C	198	GLU	N-CA-C	5.38	116.82	109.18
1	A	291	LEU	CA-C-N	5.34	126.51	119.84
1	A	291	LEU	C-N-CA	5.34	126.51	119.84
1	A	87	ILE	CA-C-N	5.32	126.49	119.84
1	A	87	ILE	C-N-CA	5.32	126.49	119.84
1	B	288	GLY	CA-C-N	5.25	131.15	121.70
1	B	288	GLY	C-N-CA	5.25	131.15	121.70
1	C	360	CYS	CA-C-N	5.24	124.75	119.19
1	C	360	CYS	C-N-CA	5.24	124.75	119.19
1	C	23	GLU	N-CA-C	5.23	116.67	111.07
1	C	479	ILE	C-N-CD	-5.18	109.20	120.60
1	B	120	VAL	N-CA-C	5.14	116.09	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	LEU	N-CA-C	-5.11	99.91	110.80
1	B	271	ASN	CA-C-N	-5.05	113.72	118.97
1	B	271	ASN	C-N-CA	-5.05	113.72	118.97
1	C	160	GLY	N-CA-C	5.05	120.22	114.67
1	C	446	GLY	CA-C-N	5.04	126.42	120.23
1	C	446	GLY	C-N-CA	5.04	126.42	120.23

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	140	0
1	B	3843	0	3635	142	0
1	C	3843	0	3635	147	0
All	All	11529	0	10905	427	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 19.

All (427) 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
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:CG2	1:C:480:PRO:CA	2.29	1.10
1:C:479:ILE:CB	1:C:480:PRO:CA	2.30	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:482:GLU:C	1:A:484:ALA:H	1.68	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: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:482:GLU:C	1:A:484:ALA:N	2.37	0.81
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:A:396:CYS:SG	1:A:397:GLU:N	2.53	0.80
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:C:478:GLN:C	1:C:479:ILE:HD13	2.07	0.78
1:B:479:ILE:HG22	1:B:480:PRO:C	2.08	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:C:482:GLU:C	1:C:484:ALA:H	1.94	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:A:21:GLN:HE21	1:A:441:TRP:NE1	1.84	0.74
1:C:254:ASP:OD1	1:C:254:ASP:N	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:C:485:HIS:CD2	1:C:485:HIS:N	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:484:ALA:O	1:A:485:HIS:C	2.30	0.72
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:478:GLN:C	1:A:479:ILE:HG12	2.14	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:B:257:ALA:HB1	1:B:336:ILE:HD11	1.73	0.70
1:B:288:GLY:HA3	1:B:289:GLU:HB3	1.74	0.69
1:C:353:GLY:HA2	1:C:354:LEU:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:353:GLY:HA2	1:A:354:LEU:C	2.18	0.69
1:C:254:ASP:HB2	1:C:321:ARG:HD2	1.73	0.68
1:C:478:GLN:O	1:C:479:ILE:CG1	2.40	0.68
1:B:481:GLU:O	1:B:481:GLU:HG3	1.94	0.68
1:A:181:ALA:HB2	1:A:205:PRO:HG3	1.75	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: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:A:479:ILE:HG22	1:A:480:PRO:C	2.20	0.66
1:C:127:LEU:HD12	1:C:128:PRO:HD2	1.77	0.66
1:C:478:GLN:C	1:C:479:ILE:CG1	2.68	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:C:484:ALA:O	1:C:485:HIS:C	2.40	0.65
1:A:482:GLU:O	1:A:484:ALA:N	2.30	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: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:C:478:GLN:C	1:C:479:ILE:HG12	2.23	0.63
1:B:353:GLY:HA2	1:B:354:LEU:C	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:478:GLN:C	1:C:479:ILE:CD1	2.69	0.60
1:C:194:LYS:O	1:C:194:LYS:HG2	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: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:B:181:ALA:HB2	1:B:205:PRO:HG3	1.85	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:C:479:ILE:HG22	1:C:480:PRO:C	2.29	0.57
1:B:481:GLU:O	1:B:481:GLU:HG2	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	1.69	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:343:LYS:C	1:B:345:GLY:H	2.11	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: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:C:482:GLU:O	1:C:483:LEU:C	2.48	0.56
1:A:288:GLY:CA	1:A:290:ARG:H	2.13	0.56
1:A:57:ASP:HB3	1:A:61:ARG:HD2	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PRO:O	1:B:89:LEU:HB2	2.05	0.55
1:B:247:TRP:HD1	1:B:342:ASN:HA	1.71	0.55
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:B:482:GLU:C	1:B:484:ALA:N	2.63	0.55
1:C:33:PRO:O	1:C:89:LEU:HD11	2.07	0.55
1:C:251:GLU:CD	1:C:253:ARG:HE	2.15	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:A:245:GLU:HG2	1:A:363:MET:HE3	1.87	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: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:B:141:VAL:HG22	1:B:211:ALA:HB2	1.91	0.53
1:B:322:HIS:CD2	1:B:322:HIS:C	2.86	0.53
1:A:86:ILE:HG23	1:A:101:ILE:HG12	1.90	0.52
1:A:437:ASP:OD2	1:A:448:ARG:NH1	2.39	0.52
1:B:482:GLU:C	1:B:484:ALA:H	2.16	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:C:193:ASN:CG	1:C:194:LYS:H	2.17	0.52
1:B:245:GLU:HB2	1:B:246:PRO:HD2	1.91	0.52
1:B:281:GLU:C	1:B:283:MET:H	2.15	0.52
1:A:312:MET:HE2	1:A:364:PHE:HE1	1.75	0.52
1:C:254:ASP:HB3	1:C:257:ALA:HB3	1.91	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:B:268:TRP:CG	1:B:283:MET:HE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HE	1:C:167:ILE:HD12	1.76	0.51
1:C:248:ASP:HB3	1:C:321:ARG:NH2	2.25	0.51
1:A:92:ARG:HD2	1:A:146:LEU:HB3	1.92	0.51
1:C:268:TRP:CG	1:C:283:MET:HE1	2.46	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
1:A:65:ASP:OD1	1:A:461:ARG:NE	2.43	0.50
1:A:216:HIS:CE1	1:A:237:ILE:HB	2.46	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:A:406:ILE:HG23	1:A:473:MET:HE1	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:THR:O	1:C:193:ASN:ND2	2.47	0.48
1:B:87:ILE:C	1:B:89:LEU:H	2.20	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:396:CYS:HB3	1:A:398:GLU:CD	2.38	0.48
1:A:32:GLY:HA3	1:A:89:LEU:CD1	2.44	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
1:A:202:ALA:O	1:A:290:ARG:HD2	2.12	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:A:247:TRP:CD1	1:A:339:HIS:HD1	2.32	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:14:GLY:HA3	1:A:76:ALA:O	2.16	0.46
1:A:225:ARG:HA	1:A:225:ARG:HD3	1.76	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:HE3	1:B:465:LYS:HB3	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:88:PRO:HD3	1:C:97:ASN:H	1.79	0.46
1:C:153:ARG:O	1:C:157:GLU:HG3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:343:LYS:C	1:B:345:GLY:N	2.75	0.45
1:C:245:GLU:HG2	1:C:363:MET:HE3	1.99	0.45
1:A:149:GLU:OE1	1:A:218:ARG:HD2	2.17	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:15:PHE:CE1	1:B:451:VAL:HG21	2.52	0.44
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.62	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:A:196:SER:O	1:A:197:THR:C	2.61	0.44
1:B:322:HIS:HA	1:B:336:ILE:HD13	1.99	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:254:ASP:C	1:B:256:GLU:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HB2	1:A:71:LYS:HE3	1.63	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:B:312:MET:HE2	1:B:364:PHE:HE1	1.82	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
1:A:317:SER:HB3	1:A:363:MET:HE2	2.00	0.43
1:B:171:GLU:CD	1:B:313:ASN:HD22	2.26	0.43
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:O	1:A:374:LEU:HD23	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:251:GLU:CD	1:C:253:ARG:HG3	2.44	0.43
1:C:310:TYR:HE1	1:C:312:MET:HB2	1.83	0.43
1:C:336:ILE:HD13	1:C:336:ILE:HA	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:24:GLY:O	1:B:25:ALA:C	2.62	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:21:GLN:NE2	1:B:433:TRP:HZ2	2.17	0.43
1:B:269:PHE:O	1:B:273:ILE:HG13	2.19	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:HE2	1:C:27:LYS:HB3	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:281:GLU:C	1:B:283:MET:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ARG:HA	1:C:225:ARG:HD3	1.70	0.42
1:B:51:ASN:ND2	1:B:53:ASP:OD2	2.53	0.42
1:C:254:ASP:C	1:C:256:GLU:H	2.27	0.42
1:A:251:GLU:HA	1:A:252:PRO:HD2	1.87	0.42
1:A:275:LEU:C	1:A:277:LYS:H	2.28	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:B:121:THR:HA	1:B:167:ILE:O	2.20	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:268:TRP:CG	1:A:283:MET:HE1	2.55	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
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:77:TYR:CE2	1:C:79:PHE:HB3	2.54	0.41
1:C:127:LEU:HD22	1:C:138:TRP:CD1	2.55	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:33:PRO:HG3	1:C:485:HIS:HB2	2.03	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:C:171:GLU:CD	1:C:313:ASN:HD22	2.28	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:21:GLN:OE1	1:B:441:TRP:NE1	2.54	0.41
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.84	0.41
1:A:51:ASN:ND2	1:A:53:ASP:OD2	2.54	0.41
1:A:192:ILE:HD11	1:A:330:THR:HG21	2.02	0.41
1:B:87:ILE:HG12	1:B:150:ARG:NH1	2.36	0.41
1:C:53:ASP:O	1:C:55:ALA:N	2.53	0.41
1:C:192:ILE:HD11	1:C:330:THR:HG21	2.02	0.41
1:A:53:ASP:O	1:A:55:ALA:N	2.53	0.41
1:A:235:ILE:N	1:A:308:ASP:OD2	2.47	0.41
1:B:171:GLU:HG3	1:B:313:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:GLU:H	1:B:338:GLU:HG2	1.54	0.41
1:B:406:ILE:HG23	1:B:473:MET:HE1	2.03	0.41
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.88	0.41
1:C:254:ASP:C	1:C:256:GLU:N	2.78	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.86	0.40
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.94	0.40
1:C:209:GLY:O	1:C:213:ILE:HG13	2.21	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:B:254:ASP:C	1:B:256:GLU:H	2.29	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 ⓘ

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	473/513 (92%)	407 (86%)	40 (8%)	26 (6%)	1	10
1	B	473/513 (92%)	399 (84%)	53 (11%)	21 (4%)	2	13
1	C	473/513 (92%)	402 (85%)	49 (10%)	22 (5%)	2	12
All	All	1419/1539 (92%)	1208 (85%)	142 (10%)	69 (5%)	1	12

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	381 (96%)	15 (4%)	29	57
1	B	396/429 (92%)	367 (93%)	29 (7%)	13	39
1	C	396/429 (92%)	364 (92%)	32 (8%)	11	36
All	All	1188/1287 (92%)	1112 (94%)	76 (6%)	16	44

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	80	SER
1	A	191	SER
1	A	194	LYS
1	A	196	SER
1	A	266	ILE
1	A	306	GLU
1	A	336	ILE
1	A	348	VAL
1	A	386	CYS
1	A	398	GLU
1	A	442	SER
1	A	458	THR
1	A	459	LEU
1	A	482	GLU
1	B	5	LEU
1	B	26	VAL
1	B	86	ILE
1	B	89	LEU
1	B	144	VAL
1	B	174	ILE
1	B	197	THR
1	B	250	ASN
1	B	253	ARG
1	B	254	ASP
1	B	255	LYS
1	B	259	GLU
1	B	281	GLU
1	B	284	LYS
1	B	321	ARG
1	B	322	HIS
1	B	338	GLU
1	B	343	LYS
1	B	360	CYS
1	B	398	GLU
1	B	438	ASN
1	B	458	THR
1	B	459	LEU
1	B	462	THR
1	B	465	LYS
1	B	478	GLN
1	B	481	GLU

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Mol	Chain	Res	Type
1	B	483	LEU
1	B	485	HIS
1	C	5	LEU
1	C	8	PRO
1	C	26	VAL
1	C	53	ASP
1	C	84	SER
1	C	89	LEU
1	C	99	GLU
1	C	107	LEU
1	C	144	VAL
1	C	150	ARG
1	C	162	ARG
1	C	174	ILE
1	C	192	ILE
1	C	201	THR
1	C	253	ARG
1	C	254	ASP
1	C	256	GLU
1	C	284	LYS
1	C	289	GLU
1	C	318	GLN
1	C	336	ILE
1	C	348	VAL
1	C	358	ARG
1	C	377	LYS
1	C	381	ILE
1	C	397	GLU
1	C	398	GLU
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	195	HIS
1	A	234	GLN
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	265	HIS
1	A	303	ASN
1	A	384	ASN
1	B	51	ASN
1	B	132	HIS
1	B	164	GLN
1	B	265	HIS
1	B	313	ASN
1	B	322	HIS
1	B	384	ASN
1	B	401	ASN
1	B	438	ASN
1	C	21	GLN
1	C	132	HIS
1	C	140	ASN
1	C	165	ASN
1	C	195	HIS
1	C	250	ASN
1	C	422	GLN
1	C	485	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	477/513 (92%)	-0.01	21 (4%)	39 25	11, 27, 68, 90	0
1	B	477/513 (92%)	-0.00	23 (4%)	35 24	11, 32, 75, 99	0
1	C	477/513 (92%)	0.05	22 (4%)	37 25	13, 32, 76, 97	0
All	All	1431/1539 (92%)	0.01	66 (4%)	37 25	11, 30, 73, 99	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	483	LEU	6.5
1	A	485	HIS	6.5
1	C	485	HIS	5.3
1	A	481	GLU	4.9
1	C	481	GLU	4.7
1	C	484	ALA	4.2
1	A	483	LEU	3.8
1	B	483	LEU	3.7
1	A	197	THR	3.6
1	C	195	HIS	3.5
1	C	320	ALA	3.5
1	B	337	HIS	3.4
1	B	199	GLY	3.3
1	C	355	ALA	3.3
1	C	322	HIS	3.0
1	A	355	ALA	3.0
1	C	480	PRO	2.9
1	B	396	CYS	2.9
1	A	326	PRO	2.9
1	B	197	THR	2.9
1	B	249	SER	2.8
1	C	321	ARG	2.8
1	B	485	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	480	PRO	2.7
1	B	480	PRO	2.7
1	C	326	PRO	2.7
1	B	484	ALA	2.7
1	C	482	GLU	2.7
1	B	481	GLU	2.6
1	B	322	HIS	2.6
1	C	197	THR	2.6
1	C	329	GLU	2.5
1	A	354	LEU	2.5
1	A	349	GLY	2.5
1	B	346	SER	2.4
1	B	191	SER	2.4
1	A	324	ASP	2.3
1	C	63	ASP	2.3
1	C	327	VAL	2.3
1	A	250	ASN	2.3
1	A	67	ASP	2.3
1	B	344	ASP	2.3
1	A	48	ASN	2.3
1	B	347	PRO	2.2
1	A	43	GLU	2.2
1	A	254	ASP	2.2
1	C	344	ASP	2.2
1	B	251	GLU	2.2
1	B	252	PRO	2.2
1	C	354	LEU	2.2
1	A	53	ASP	2.2
1	A	133	ASP	2.2
1	A	195	HIS	2.2
1	A	484	ALA	2.2
1	B	354	LEU	2.1
1	B	247	TRP	2.1
1	B	195	HIS	2.1
1	B	390	GLY	2.1
1	B	245	GLU	2.1
1	C	250	ASN	2.1
1	A	194	LYS	2.1
1	C	337	HIS	2.1
1	C	248	ASP	2.1
1	C	324	ASP	2.1
1	A	252	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	194	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.