



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 07:54 AM UTC

PDB ID : 3E6U / pdb_00003e6u
Title : Crystal structure of Human LanCL1
Authors : Zhang, W.; Zhu, G.; Li, X.; Rao, Z.; Zhang, C.
Deposited on : 2008-08-16
Resolution : 2.60 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

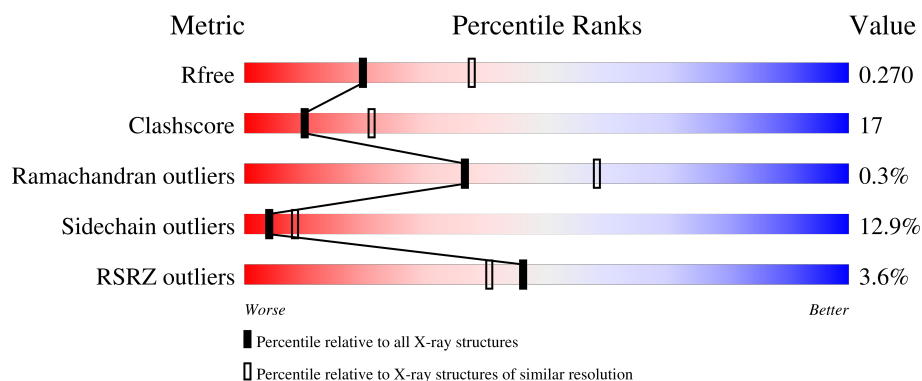
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

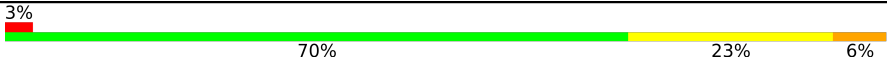
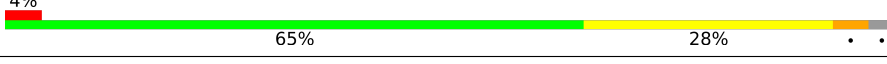
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	411	
1	B	411	
1	C	411	
1	D	411	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13228 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 LanC-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3283	2123	551	586	23			
1	C	409	Total	C	N	O	S	0	0	0
			3283	2123	551	586	23			
1	B	401	Total	C	N	O	S	0	0	0
			3213	2081	535	575	22			
1	D	399	Total	C	N	O	S	0	0	0
			3193	2067	533	571	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP O43813
A	-10	HIS	-	expression tag	UNP O43813
A	-9	HIS	-	expression tag	UNP O43813
A	-8	HIS	-	expression tag	UNP O43813
A	-7	HIS	-	expression tag	UNP O43813
A	-6	HIS	-	expression tag	UNP O43813
A	-5	SER	-	expression tag	UNP O43813
A	-4	MET	-	expression tag	UNP O43813
A	-3	ASP	-	expression tag	UNP O43813
A	-2	ILE	-	expression tag	UNP O43813
A	-1	GLU	-	expression tag	UNP O43813
A	0	PHE	-	expression tag	UNP O43813
C	-11	HIS	-	expression tag	UNP O43813
C	-10	HIS	-	expression tag	UNP O43813
C	-9	HIS	-	expression tag	UNP O43813
C	-8	HIS	-	expression tag	UNP O43813
C	-7	HIS	-	expression tag	UNP O43813
C	-6	HIS	-	expression tag	UNP O43813
C	-5	SER	-	expression tag	UNP O43813
C	-4	MET	-	expression tag	UNP O43813
C	-3	ASP	-	expression tag	UNP O43813

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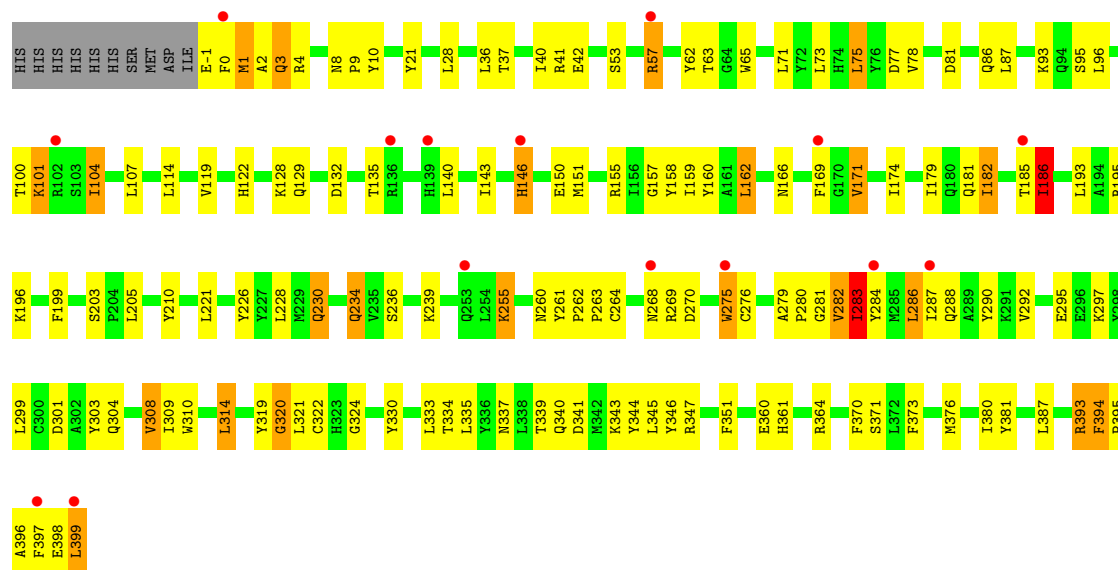
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ILE	-	expression tag	UNP O43813
C	-1	GLU	-	expression tag	UNP O43813
C	0	PHE	-	expression tag	UNP O43813
B	-11	HIS	-	expression tag	UNP O43813
B	-10	HIS	-	expression tag	UNP O43813
B	-9	HIS	-	expression tag	UNP O43813
B	-8	HIS	-	expression tag	UNP O43813
B	-7	HIS	-	expression tag	UNP O43813
B	-6	HIS	-	expression tag	UNP O43813
B	-5	SER	-	expression tag	UNP O43813
B	-4	MET	-	expression tag	UNP O43813
B	-3	ASP	-	expression tag	UNP O43813
B	-2	ILE	-	expression tag	UNP O43813
B	-1	GLU	-	expression tag	UNP O43813
B	0	PHE	-	expression tag	UNP O43813
D	-11	HIS	-	expression tag	UNP O43813
D	-10	HIS	-	expression tag	UNP O43813
D	-9	HIS	-	expression tag	UNP O43813
D	-8	HIS	-	expression tag	UNP O43813
D	-7	HIS	-	expression tag	UNP O43813
D	-6	HIS	-	expression tag	UNP O43813
D	-5	SER	-	expression tag	UNP O43813
D	-4	MET	-	expression tag	UNP O43813
D	-3	ASP	-	expression tag	UNP O43813
D	-2	ILE	-	expression tag	UNP O43813
D	-1	GLU	-	expression tag	UNP O43813
D	0	PHE	-	expression tag	UNP O43813

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

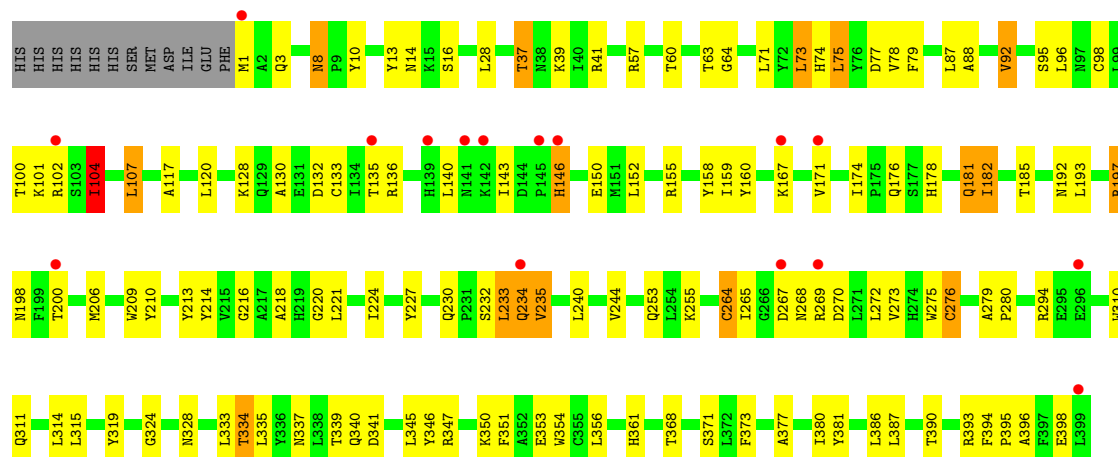
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	C	62	Total	O	0	0
			62	62		
3	B	67	Total	O	0	0
			67	67		
3	D	45	Total	O	0	0
			45	45		



• Molecule 1: LanC-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.28Å 194.28Å 211.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.58 – 2.60 32.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.58-2.60) 92.2 (32.58-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.275 0.243 , 0.270	Depositor DCC
R_{free} test set	5266 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13228	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.56	0/3379	0.96	7/4582 (0.2%)
1	B	0.60	3/3305 (0.1%)	0.95	5/4482 (0.1%)
1	C	0.56	0/3379	0.95	6/4582 (0.1%)
1	D	0.56	0/3284	0.96	11/4454 (0.2%)
All	All	0.57	3/13347 (0.0%)	0.96	29/18100 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ILE	CA-CB	6.59	1.61	1.54
1	B	282	VAL	CA-CB	5.85	1.61	1.54
1	B	186	ILE	CA-CB	5.30	1.61	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ARG	N-CA-C	10.20	122.35	111.03
1	C	398	GLU	N-CA-C	8.75	121.61	111.11
1	B	283	ILE	CB-CA-C	7.91	121.82	111.70
1	A	398	GLU	N-CA-C	7.04	118.74	111.14
1	B	234	GLN	N-CA-C	6.73	120.66	111.17
1	A	234	GLN	N-CA-C	6.45	120.30	111.39
1	C	394	PHE	CA-C-N	6.40	126.38	119.78
1	C	394	PHE	C-N-CA	6.40	126.38	119.78
1	C	151	MET	N-CA-C	6.28	118.69	111.02
1	B	287	ILE	N-CA-CB	6.24	117.43	110.51
1	D	268	ASN	N-CA-C	6.19	117.71	110.41
1	A	271	LEU	N-CA-C	6.16	122.52	114.75
1	D	234	GLN	N-CA-C	-6.04	101.69	110.64
1	B	282	VAL	N-CA-C	-5.91	104.36	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	THR	CA-C-N	5.88	125.59	119.82
1	D	368	THR	C-N-CA	5.88	125.59	119.82
1	D	197	ARG	CA-C-N	-5.81	115.00	122.79
1	D	197	ARG	C-N-CA	-5.81	115.00	122.79
1	D	152	LEU	N-CA-C	5.71	117.58	111.36
1	A	-8	HIS	CA-C-N	5.69	131.94	121.70
1	A	-8	HIS	C-N-CA	5.69	131.94	121.70
1	A	1	MET	N-CA-C	5.38	117.89	111.71
1	A	338	LEU	N-CA-C	-5.30	106.49	113.12
1	C	174	ILE	CA-C-N	5.26	126.41	119.84
1	C	174	ILE	C-N-CA	5.26	126.41	119.84
1	D	197	ARG	N-CA-C	-5.16	102.37	110.36
1	B	394	PHE	N-CA-C	-5.13	100.15	109.44
1	D	104	ILE	N-CA-C	5.09	117.01	112.17
1	D	275	TRP	N-CA-C	-5.01	105.71	111.07

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	3283	0	3197	108	0
1	B	3213	0	3140	127	0
1	C	3283	0	3197	130	0
1	D	3193	0	3125	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	78	0	0	27	0
3	B	67	0	0	20	0
3	C	62	0	0	16	0
3	D	45	0	0	10	0
All	All	13228	0	12659	447	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 17.

All (447) 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:D:176:GLN:CD	1:D:234:GLN:HE22	1.47	1.22
1:C:129:GLN:HG2	3:C:554:HOH:O	1.35	1.21
1:B:335:LEU:O	1:B:339:THR:HG22	1.44	1.17
1:D:176:GLN:NE2	1:D:234:GLN:HE22	1.42	1.15
1:B:160:TYR:CE1	1:B:396:ALA:HA	1.85	1.10
1:A:197:ARG:HB3	3:A:563:HOH:O	1.52	1.08
1:C:304:GLN:HG2	3:C:537:HOH:O	1.54	1.07
1:B:398:GLU:O	1:B:399:LEU:OXT	1.72	1.07
1:C:-9:HIS:HB3	3:C:542:HOH:O	1.54	1.06
1:B:151:MET:HE3	1:B:157:GLY:HA2	1.36	1.04
1:C:173:LYS:HE2	1:C:173:LYS:HA	1.40	1.04
1:C:128:LYS:HD2	1:C:128:LYS:O	1.58	1.03
1:C:172:GLU:O	1:C:172:GLU:HG3	1.60	1.02
1:B:160:TYR:HE1	1:B:396:ALA:HA	1.26	1.00
1:C:319:TYR:OH	1:C:361:HIS:HD2	1.43	1.00
1:B:0:PHE:HB2	1:B:3:GLN:OE1	1.61	0.98
1:D:176:GLN:CD	1:D:234:GLN:NE2	2.24	0.94
1:B:284:TYR:CD1	3:B:512:HOH:O	2.22	0.93
1:A:335:LEU:O	1:A:339:THR:HG22	1.70	0.91
1:C:314:LEU:HD13	1:C:351:PHE:CZ	2.04	0.91
1:A:-8:HIS:N	1:A:-7:HIS:HB2	1.85	0.91
1:C:182:ILE:O	1:C:186:ILE:HG22	1.71	0.91
1:C:335:LEU:O	1:C:339:THR:HG22	1.71	0.90
1:C:334:THR:HA	3:C:511:HOH:O	1.73	0.89
1:B:57:ARG:HD3	3:B:557:HOH:O	1.70	0.88
1:D:176:GLN:NE2	1:D:234:GLN:NE2	2.21	0.88
1:A:135:THR:HG23	3:A:520:HOH:O	1.73	0.87
1:B:304:GLN:HG2	3:B:514:HOH:O	1.73	0.87
1:A:214:TYR:HA	3:A:553:HOH:O	1.74	0.86
1:A:390:THR:HG22	3:A:513:HOH:O	1.75	0.86
1:A:-8:HIS:CA	1:A:-7:HIS:HB2	2.06	0.86
1:B:275:TRP:HH2	1:B:397:PHE:CD1	1.94	0.85
1:D:197:ARG:HB3	3:D:525:HOH:O	1.77	0.85
1:D:74:HIS:HD2	3:D:522:HOH:O	1.62	0.83
1:B:151:MET:CE	1:B:157:GLY:HA2	2.09	0.82
1:D:192:ASN:HB3	3:D:541:HOH:O	1.79	0.82
1:B:42:GLU:HG2	3:B:532:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:O	1:D:339:THR:HG22	1.78	0.81
1:C:391:LYS:HE3	3:C:532:HOH:O	1.80	0.81
1:C:-4:MET:HE3	1:C:-4:MET:HA	1.63	0.81
1:C:128:LYS:HD2	1:C:128:LYS:C	2.06	0.81
1:A:197:ARG:CB	3:A:563:HOH:O	2.20	0.80
1:B:275:TRP:HZ3	1:B:397:PHE:CD2	1.98	0.80
1:A:62:TYR:HD2	1:A:63:THR:HG23	1.46	0.79
1:C:128:LYS:O	1:C:128:LYS:CD	2.30	0.79
1:C:314:LEU:CD1	1:C:351:PHE:CZ	2.66	0.79
1:C:319:TYR:OH	1:C:361:HIS:CD2	2.32	0.78
1:A:4:ARG:HG2	3:A:540:HOH:O	1.84	0.77
1:A:41:ARG:CG	1:A:41:ARG:HH11	1.97	0.77
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.48	0.76
1:C:154:GLY:C	3:C:555:HOH:O	2.27	0.76
1:C:314:LEU:CD1	1:C:351:PHE:CE2	2.69	0.76
1:A:62:TYR:CD2	1:A:63:THR:HG23	2.20	0.75
1:C:255:LYS:HE3	3:C:537:HOH:O	1.87	0.75
1:D:319:TYR:OH	1:D:361:HIS:HD2	1.68	0.75
1:A:294:ARG:HH11	1:A:294:ARG:CG	2.00	0.74
1:A:197:ARG:CA	3:A:563:HOH:O	2.34	0.74
1:C:14:ASN:C	1:C:14:ASN:HD22	1.95	0.74
1:C:275:TRP:HZ3	1:C:397:PHE:CD2	2.06	0.74
1:A:63:THR:HA	1:A:371:SER:HB2	1.70	0.73
1:C:314:LEU:HD12	1:C:351:PHE:CE2	2.22	0.73
1:B:275:TRP:CH2	1:B:397:PHE:CD1	2.77	0.73
1:A:-8:HIS:H	1:A:-7:HIS:HB2	1.53	0.73
1:B:162:LEU:HD12	1:B:174:ILE:HD13	1.69	0.72
1:A:357:GLU:HB3	1:A:360:GLU:HG3	1.70	0.72
1:C:275:TRP:HZ3	1:C:397:PHE:CE2	2.08	0.72
1:B:0:PHE:HB3	3:B:556:HOH:O	1.90	0.72
1:C:101:LYS:HE2	3:C:515:HOH:O	1.89	0.72
1:B:284:TYR:CD1	1:B:397:PHE:HE2	2.08	0.72
1:B:398:GLU:O	1:B:399:LEU:C	2.32	0.72
1:A:214:TYR:CD1	3:A:553:HOH:O	2.43	0.71
1:A:275:TRP:CD1	1:A:276:CYS:N	2.58	0.71
1:C:314:LEU:HD13	1:C:351:PHE:CE1	2.25	0.71
1:D:233:LEU:O	1:D:234:GLN:C	2.32	0.71
1:A:198:ASN:N	3:A:563:HOH:O	2.22	0.70
1:B:104:ILE:HG12	1:B:158:TYR:HB2	1.73	0.70
1:A:319:TYR:OH	1:A:361:HIS:HD2	1.73	0.70
1:C:275:TRP:CZ3	1:C:397:PHE:CD2	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:CYS:HB2	3:C:559:HOH:O	1.90	0.70
1:A:317:LYS:HE3	1:C:-8:HIS:HE1	1.57	0.70
1:C:8:ASN:C	1:C:8:ASN:HD22	2.00	0.69
1:A:264:CYS:HB3	3:A:553:HOH:O	1.91	0.69
1:A:4:ARG:CG	3:A:540:HOH:O	2.39	0.69
1:D:178:HIS:O	1:D:182:ILE:HG22	1.92	0.69
1:A:132:ASP:C	1:A:132:ASP:OD1	2.36	0.69
1:B:360:GLU:HG2	3:B:560:HOH:O	1.93	0.69
1:B:8:ASN:C	1:B:8:ASN:HD22	1.99	0.69
1:A:1:MET:HB3	1:A:271:LEU:HA	1.75	0.68
1:A:230:GLN:HG2	1:A:399:LEU:HD13	1.76	0.68
1:A:317:LYS:HE3	1:C:-8:HIS:CE1	2.29	0.68
1:C:398:GLU:O	1:C:399:LEU:HB2	1.91	0.68
1:B:159:ILE:HA	1:B:162:LEU:HD23	1.74	0.68
1:C:172:GLU:O	1:C:172:GLU:CG	2.31	0.68
1:D:395:PRO:O	1:D:396:ALA:HB3	1.92	0.68
1:D:1:MET:N	3:D:533:HOH:O	2.26	0.68
1:A:210:TYR:CE1	1:C:-4:MET:HE1	2.29	0.68
1:C:66:ALA:O	1:C:70:VAL:HG23	1.93	0.67
1:C:14:ASN:ND2	1:C:17:LEU:H	1.93	0.66
1:B:151:MET:HE3	1:B:157:GLY:CA	2.21	0.66
1:A:178:HIS:O	1:A:182:ILE:HG22	1.96	0.65
1:A:288:GLN:O	1:A:292:VAL:HG23	1.96	0.65
1:B:275:TRP:CZ3	1:B:397:PHE:CG	2.85	0.65
1:C:128:LYS:C	1:C:128:LYS:CD	2.70	0.65
1:C:149:ASN:HD22	1:C:207:TYR:HD1	1.44	0.65
1:D:310:TRP:CE3	1:D:347:ARG:HG2	2.32	0.65
1:C:173:LYS:HE2	1:C:173:LYS:CA	2.18	0.64
1:C:339:THR:HG23	1:C:341:ASP:H	1.62	0.64
1:B:230:GLN:OE1	1:B:230:GLN:HA	1.97	0.64
1:D:8:ASN:ND2	1:D:10:TYR:H	1.95	0.64
1:A:181:GLN:O	1:A:185:THR:HG23	1.98	0.64
1:B:275:TRP:CH2	1:B:397:PHE:CG	2.85	0.64
1:D:160:TYR:CE1	1:D:396:ALA:HA	2.31	0.64
1:B:1:MET:HE3	1:B:270:ASP:OD2	1.97	0.64
1:B:334:THR:HA	3:B:510:HOH:O	1.98	0.64
1:B:275:TRP:CZ3	1:B:397:PHE:CD2	2.84	0.64
1:D:14:ASN:ND2	1:D:16:SER:HB3	2.13	0.64
1:B:0:PHE:O	1:B:1:MET:C	2.38	0.63
1:B:339:THR:O	1:B:340:GLN:HB2	1.98	0.63
1:B:393:ARG:HG3	1:B:398:GLU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:O	1:B:399:LEU:HG	1.97	0.63
1:D:8:ASN:HD22	1:D:10:TYR:H	1.44	0.63
1:A:357:GLU:O	1:A:360:GLU:HG2	1.98	0.63
1:D:339:THR:O	1:D:340:GLN:HB2	1.98	0.62
1:C:251:VAL:HA	1:C:254:LEU:HD12	1.80	0.62
1:A:290:TYR:CD1	1:A:299:LEU:HB2	2.36	0.61
1:B:160:TYR:CE1	1:B:396:ALA:CA	2.75	0.61
1:B:284:TYR:CD1	1:B:397:PHE:CE2	2.89	0.61
1:D:101:LYS:O	1:D:143:ILE:HD12	2.00	0.61
1:C:275:TRP:HH2	1:C:397:PHE:CD1	2.18	0.60
1:A:393:ARG:HD2	3:A:532:HOH:O	1.99	0.60
1:B:319:TYR:OH	1:B:361:HIS:HD2	1.83	0.60
1:D:181:GLN:O	1:D:185:THR:HG23	2.01	0.60
1:D:319:TYR:OH	1:D:361:HIS:CD2	2.54	0.60
1:A:41:ARG:HH11	1:A:41:ARG:HG3	1.67	0.60
1:B:395:PRO:O	1:B:396:ALA:HB3	2.01	0.60
1:B:1:MET:O	1:B:2:ALA:C	2.41	0.60
1:B:41:ARG:HD3	3:B:524:HOH:O	2.01	0.60
1:A:77:ASP:HB3	3:A:574:HOH:O	2.00	0.60
1:C:186:ILE:C	1:C:186:ILE:HD13	2.27	0.60
1:D:14:ASN:HD21	1:D:16:SER:HB3	1.67	0.60
1:B:279:ALA:O	1:B:283:ILE:HG22	2.02	0.59
1:B:166:ASN:O	1:B:169:PHE:O	2.21	0.59
1:B:86:GLN:HG3	3:B:571:HOH:O	2.02	0.59
1:C:230:GLN:HG2	1:C:399:LEU:HD13	1.82	0.59
1:C:364:ARG:HG2	3:C:539:HOH:O	2.02	0.59
1:D:92:VAL:HG11	1:D:117:ALA:HA	1.84	0.59
1:A:159:ILE:HG22	1:A:163:LEU:HD22	1.85	0.59
1:A:264:CYS:CB	3:A:553:HOH:O	2.51	0.59
1:B:339:THR:HG23	1:B:341:ASP:H	1.68	0.58
1:C:155:ARG:N	3:C:555:HOH:O	2.35	0.58
1:C:178:HIS:O	1:C:182:ILE:HG12	2.02	0.58
1:C:-4:MET:HA	1:C:-4:MET:CE	2.33	0.58
1:B:65:TRP:HB2	1:B:95:SER:HB3	1.86	0.58
1:D:310:TRP:CZ3	1:D:347:ARG:HG2	2.39	0.58
1:A:294:ARG:HG2	1:A:294:ARG:NH1	2.16	0.58
1:D:213:TYR:HB2	1:D:265:ILE:CG1	2.33	0.58
1:C:156:ILE:O	1:C:159:ILE:HB	2.04	0.58
1:B:155:ARG:HB3	1:B:182:ILE:HD11	1.84	0.58
1:A:218:ALA:HB2	1:A:276:CYS:HA	1.86	0.58
1:A:317:LYS:CE	1:C:-8:HIS:HE1	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:TYR:O	1:C:162:LEU:HD22	2.04	0.57
1:A:107:LEU:HD13	3:A:562:HOH:O	2.04	0.57
1:C:275:TRP:CZ3	1:C:397:PHE:CE2	2.92	0.57
1:D:235:VAL:HG12	1:D:235:VAL:O	2.03	0.57
1:C:275:TRP:CD1	1:C:276:CYS:N	2.73	0.57
1:D:8:ASN:HD22	1:D:8:ASN:C	2.13	0.57
1:A:145:PRO:HD2	3:A:576:HOH:O	2.04	0.57
1:C:197:ARG:HD3	1:B:210:TYR:CE1	2.40	0.57
1:B:8:ASN:ND2	1:B:10:TYR:H	2.02	0.56
1:A:301:ASP:O	1:A:304:GLN:HB3	2.05	0.56
1:A:35:ARG:NH2	1:A:356:LEU:HD12	2.20	0.56
1:B:0:PHE:O	1:B:2:ALA:N	2.39	0.56
1:A:275:TRP:CD1	1:A:322:CYS:HA	2.41	0.56
1:D:213:TYR:HB2	1:D:265:ILE:HG12	1.87	0.56
1:A:63:THR:HA	1:A:371:SER:CB	2.35	0.56
1:B:186:ILE:HD12	1:B:228:LEU:HD21	1.88	0.56
1:C:63:THR:HA	1:C:371:SER:HB2	1.86	0.56
1:B:179:ILE:O	1:B:182:ILE:HG22	2.06	0.56
1:C:226:TYR:OH	1:C:398:GLU:O	2.20	0.55
1:C:186:ILE:CD1	1:C:228:LEU:HD21	2.36	0.55
1:B:282:VAL:C	3:B:525:HOH:O	2.49	0.55
1:B:122:HIS:CG	1:B:169:PHE:CE1	2.94	0.55
1:B:284:TYR:CE1	3:B:512:HOH:O	2.55	0.55
1:A:195:ARG:HD3	3:A:523:HOH:O	2.06	0.55
1:C:275:TRP:CH2	1:C:397:PHE:CG	2.94	0.55
1:A:62:TYR:HD2	1:A:63:THR:CG2	2.20	0.54
1:B:286:LEU:HD22	1:B:301:ASP:CB	2.38	0.54
1:C:-4:MET:HE2	1:D:197:ARG:HD3	1.90	0.54
1:C:364:ARG:NH2	3:C:503:HOH:O	2.38	0.54
1:B:286:LEU:HD22	1:B:301:ASP:HB2	1.89	0.54
1:C:156:ILE:HA	1:C:159:ILE:HG13	1.90	0.54
1:A:66:ALA:O	1:A:70:VAL:HG23	2.08	0.54
1:A:275:TRP:CD1	1:A:276:CYS:H	2.23	0.54
1:D:74:HIS:CD2	3:D:522:HOH:O	2.47	0.53
1:C:275:TRP:HH2	1:C:397:PHE:CG	2.26	0.53
1:A:192:ASN:N	1:A:192:ASN:HD22	2.05	0.53
1:B:104:ILE:HG12	1:B:104:ILE:O	2.09	0.53
1:A:200:THR:HG22	3:A:507:HOH:O	2.09	0.53
1:A:319:TYR:OH	1:A:361:HIS:CD2	2.59	0.53
1:A:275:TRP:CG	1:A:276:CYS:N	2.76	0.53
1:D:214:TYR:O	1:D:220:GLY:HA3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLN:HA	1:C:132:ASP:HB2	1.90	0.53
1:A:178:HIS:O	1:A:182:ILE:CG2	2.57	0.52
1:B:295:GLU:OE2	1:B:297:LYS:HE2	2.09	0.52
1:B:262:PRO:HG2	3:B:550:HOH:O	2.08	0.52
1:C:296:GLU:HG3	3:C:559:HOH:O	2.09	0.52
1:B:399:LEU:OXT	1:B:399:LEU:HG	2.08	0.52
1:B:53:SER:HB3	3:B:553:HOH:O	2.08	0.52
1:B:186:ILE:CD1	1:B:228:LEU:HD21	2.40	0.52
1:B:288:GLN:NE2	1:B:292:VAL:HG23	2.24	0.52
1:A:4:ARG:CZ	3:A:540:HOH:O	2.57	0.52
1:B:0:PHE:H	1:B:3:GLN:NE2	2.07	0.52
1:B:8:ASN:HD22	1:B:9:PRO:N	2.07	0.52
1:A:4:ARG:CD	3:A:540:HOH:O	2.57	0.52
1:C:-4:MET:HE3	1:C:-4:MET:CA	2.35	0.52
1:A:52:LYS:HE2	3:A:536:HOH:O	2.08	0.52
1:D:155:ARG:HB3	1:D:182:ILE:HD11	1.92	0.52
1:D:107:LEU:HD12	3:D:510:HOH:O	2.10	0.52
1:D:240:LEU:HA	1:D:244:VAL:CG1	2.40	0.52
1:D:339:THR:HG23	1:D:341:ASP:H	1.75	0.52
1:A:339:THR:HG23	1:A:341:ASP:H	1.73	0.51
1:D:13:TYR:HB2	1:D:346:TYR:CD1	2.45	0.51
1:C:14:ASN:C	1:C:14:ASN:ND2	2.65	0.51
1:B:279:ALA:N	1:B:280:PRO:CD	2.72	0.51
1:D:100:THR:HG23	3:D:543:HOH:O	2.10	0.51
1:C:314:LEU:CD1	1:C:351:PHE:CE1	2.91	0.51
1:D:104:ILE:HG12	1:D:158:TYR:HB2	1.93	0.51
1:D:264:CYS:SG	1:D:267:ASP:OD2	2.54	0.51
1:A:366:PRO:HG2	1:A:369:PRO:HA	1.93	0.50
1:D:63:THR:HA	1:D:371:SER:HB2	1.94	0.50
1:B:319:TYR:OH	1:B:361:HIS:CD2	2.64	0.50
1:D:395:PRO:O	1:D:396:ALA:CB	2.58	0.50
1:C:8:ASN:HD22	1:C:9:PRO:N	2.09	0.50
1:C:313:GLY:O	1:C:328:ASN:ND2	2.28	0.50
1:D:140:LEU:O	1:D:143:ILE:HG12	2.12	0.50
1:C:320:GLY:N	1:C:324:GLY:HA3	2.26	0.50
1:B:304:GLN:O	1:B:308:VAL:HG23	2.10	0.50
1:B:314:LEU:CD1	1:B:351:PHE:CZ	2.94	0.50
1:C:225:TYR:CZ	1:C:247:SER:HB3	2.47	0.50
1:B:236:SER:OG	1:B:239:LYS:HD2	2.11	0.50
1:C:50:GLY:HA3	1:C:370:PHE:CE1	2.47	0.50
1:C:230:GLN:HB3	1:C:233:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:N	3:B:525:HOH:O	2.45	0.50
1:C:130:ALA:O	1:C:133:CYS:HB2	2.12	0.49
1:B:280:PRO:HG3	1:B:309:ILE:HG12	1.94	0.49
1:D:182:ILE:HD13	1:D:182:ILE:C	2.37	0.49
1:B:107:LEU:HD21	1:B:373:PHE:CE2	2.47	0.49
1:C:275:TRP:CD1	1:C:322:CYS:HA	2.47	0.49
1:B:230:GLN:HG3	1:B:399:LEU:HD11	1.94	0.49
1:D:218:ALA:HB2	1:D:276:CYS:HA	1.94	0.49
1:A:-8:HIS:N	1:A:-7:HIS:CB	2.66	0.49
1:A:41:ARG:CG	1:A:41:ARG:NH1	2.68	0.49
1:C:62:TYR:CD2	1:C:63:THR:HG23	2.46	0.49
1:C:236:SER:OG	1:C:239:LYS:HG3	2.13	0.49
1:C:173:LYS:CA	1:C:173:LYS:CE	2.86	0.49
1:A:41:ARG:HH11	1:A:41:ARG:HG2	1.74	0.49
1:B:37:THR:O	1:B:41:ARG:HG3	2.12	0.49
1:B:158:TYR:CE1	1:B:162:LEU:HD21	2.48	0.49
1:B:262:PRO:CG	3:B:550:HOH:O	2.61	0.49
1:D:220:GLY:O	1:D:224:ILE:HG13	2.13	0.49
1:A:35:ARG:HH22	1:A:356:LEU:HD12	1.77	0.49
1:D:78:VAL:HG23	1:D:79:PHE:CD1	2.47	0.49
1:B:62:TYR:HD2	1:B:63:THR:HG23	1.77	0.49
1:B:283:ILE:HA	1:B:286:LEU:HD12	1.95	0.49
1:A:275:TRP:HH2	1:A:397:PHE:CD1	2.30	0.48
1:C:243:LEU:O	1:C:246:PRO:HD2	2.13	0.48
1:A:62:TYR:CD2	1:A:63:THR:CG2	2.93	0.48
1:C:134:ILE:HD12	1:C:173:LYS:HG2	1.96	0.48
1:C:-4:MET:HE2	1:D:197:ARG:HA	1.95	0.48
1:C:343:LYS:O	1:C:346:TYR:HB3	2.13	0.48
1:A:41:ARG:NH1	3:A:526:HOH:O	2.47	0.48
1:A:213:TYR:CB	1:A:265:ILE:HD12	2.43	0.48
1:B:146:HIS:CD2	3:B:522:HOH:O	2.67	0.48
1:A:182:ILE:O	1:A:186:ILE:HG22	2.14	0.48
1:B:71:LEU:HG	1:B:75:LEU:HD22	1.95	0.47
1:C:186:ILE:HD12	1:C:228:LEU:HD21	1.94	0.47
1:A:121:TYR:CD1	1:A:129:GLN:HB3	2.50	0.47
1:C:159:ILE:HA	1:C:162:LEU:HD23	1.96	0.47
1:B:100:THR:C	1:B:101:LYS:HG2	2.39	0.47
1:C:67:GLY:O	1:C:70:VAL:HB	2.14	0.47
1:C:39:LYS:HD2	1:C:39:LYS:HA	1.68	0.47
1:B:203:SER:OG	1:B:205:LEU:O	2.29	0.47
1:B:226:TYR:CE2	1:B:284:TYR:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ASP:O	1:D:136:ARG:HB2	2.15	0.47
1:A:183:CYS:HA	1:A:186:ILE:HG23	1.96	0.47
1:A:197:ARG:HA	3:A:563:HOH:O	2.10	0.47
1:A:212:GLU:HB2	1:A:214:TYR:CE2	2.50	0.47
1:B:255:LYS:HB2	1:B:261:TYR:CE2	2.49	0.47
1:D:394:PHE:CD2	1:D:395:PRO:HD2	2.49	0.47
1:B:8:ASN:HD22	1:B:10:TYR:H	1.62	0.47
1:B:158:TYR:O	1:B:162:LEU:HD22	2.14	0.47
1:D:1:MET:HE2	1:D:273:VAL:CG2	2.44	0.47
1:B:62:TYR:CD2	1:B:63:THR:HG23	2.49	0.47
1:B:275:TRP:CD1	1:B:322:CYS:HA	2.50	0.47
1:D:240:LEU:HA	1:D:244:VAL:HG12	1.97	0.47
1:A:357:GLU:O	1:A:358:TYR:C	2.57	0.47
1:C:237:GLN:O	1:C:241:HIS:HD2	1.98	0.47
1:C:336:TYR:CD1	1:C:345:LEU:HB2	2.51	0.47
1:A:138:ILE:HD11	1:A:174:ILE:HG13	1.96	0.46
1:A:159:ILE:HG22	1:A:163:LEU:CD2	2.45	0.46
1:A:274:HIS:O	1:A:280:PRO:HD2	2.15	0.46
1:C:336:TYR:HA	1:C:339:THR:CG2	2.45	0.46
1:C:12:ASP:HB2	3:C:548:HOH:O	2.15	0.46
1:C:315:LEU:C	1:C:317:LYS:N	2.69	0.46
1:B:283:ILE:HG23	3:B:512:HOH:O	2.15	0.46
1:D:28:LEU:HD11	1:D:386:LEU:O	2.14	0.46
1:D:279:ALA:N	1:D:280:PRO:CD	2.78	0.46
1:A:186:ILE:O	1:A:186:ILE:HG13	2.12	0.46
1:B:321:LEU:O	1:B:394:PHE:HZ	1.98	0.46
1:D:334:THR:HG23	1:D:398:GLU:OE1	2.14	0.46
1:B:1:MET:HE2	1:B:260:ASN:HD22	1.80	0.46
1:D:71:LEU:HD22	1:D:377:ALA:HB1	1.96	0.46
1:A:314:LEU:HD13	1:A:351:PHE:CZ	2.51	0.46
1:C:262:PRO:HB2	1:C:267:ASP:HB2	1.97	0.46
1:C:244:VAL:O	1:C:245:LYS:C	2.58	0.46
1:C:335:LEU:C	1:C:339:THR:HG22	2.39	0.46
1:C:264:CYS:HB2	1:C:267:ASP:OD1	2.16	0.46
1:A:210:TYR:CZ	1:C:-4:MET:HE1	2.50	0.46
1:D:1:MET:HB2	1:D:270:ASP:O	2.16	0.46
1:A:297:LYS:HE2	3:A:567:HOH:O	2.16	0.46
1:B:310:TRP:CE3	1:B:347:ARG:HG2	2.51	0.46
1:D:233:LEU:O	1:D:235:VAL:HG23	2.16	0.45
1:C:315:LEU:C	1:C:317:LYS:H	2.24	0.45
1:C:350:LYS:HD3	1:C:350:LYS:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:O	1:B:40:ILE:HG13	2.16	0.45
1:D:234:GLN:CD	1:D:234:GLN:H	2.23	0.45
1:C:240:LEU:HA	1:C:244:VAL:HG13	1.98	0.45
1:B:122:HIS:CD2	1:B:169:PHE:CE1	3.04	0.45
1:C:39:LYS:O	1:C:40:ILE:C	2.59	0.45
1:C:209:TRP:O	1:C:210:TYR:C	2.57	0.45
1:B:186:ILE:HD13	1:B:186:ILE:C	2.42	0.45
1:B:288:GLN:HE21	1:B:292:VAL:HG23	1.82	0.45
1:B:322:CYS:HB2	1:B:373:PHE:HD1	1.82	0.45
1:D:213:TYR:HB2	1:D:265:ILE:HG13	1.98	0.45
1:C:156:ILE:N	3:C:555:HOH:O	2.50	0.45
1:C:314:LEU:CD1	1:C:351:PHE:CD2	2.99	0.45
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.85	0.45
1:B:260:ASN:CG	1:B:261:TYR:H	2.24	0.45
1:B:63:THR:HA	1:B:371:SER:HB2	1.99	0.44
1:B:330:TYR:HB2	1:B:394:PHE:HD1	1.81	0.44
1:A:357:GLU:O	1:A:360:GLU:CG	2.64	0.44
1:C:140:LEU:O	1:C:143:ILE:HG12	2.18	0.44
1:C:197:ARG:HD2	1:C:213:TYR:OH	2.18	0.44
1:C:283:ILE:HD13	1:C:287:ILE:HG12	1.99	0.44
1:B:-1:GLU:O	1:B:4:ARG:NH1	2.42	0.44
1:A:297:LYS:CE	3:A:567:HOH:O	2.65	0.44
1:B:303:TYR:HD2	1:B:344:TYR:HH	1.62	0.43
1:D:96:LEU:HD23	1:D:96:LEU:HA	1.56	0.43
1:A:381:TYR:C	1:A:381:TYR:CD2	2.96	0.43
1:B:320:GLY:O	1:B:324:GLY:HA3	2.18	0.43
1:D:351:PHE:O	1:D:354:TRP:HB3	2.17	0.43
1:A:-1:GLU:OE1	1:A:269:ARG:NH2	2.40	0.43
1:A:201:ALA:HB3	3:A:527:HOH:O	2.19	0.43
1:D:88:ALA:O	1:D:92:VAL:HG23	2.17	0.43
1:D:214:TYR:HA	1:D:264:CYS:HB3	1.99	0.43
1:D:240:LEU:HD12	1:D:244:VAL:HG11	2.00	0.43
1:A:81:ASP:OD2	1:A:81:ASP:C	2.62	0.43
1:A:120:LEU:O	1:A:120:LEU:HG	2.18	0.43
1:C:127:GLU:OE1	1:C:127:GLU:HA	2.18	0.43
1:C:235:VAL:O	1:C:236:SER:C	2.62	0.43
1:B:1:MET:C	1:B:3:GLN:N	2.77	0.43
1:B:1:MET:O	1:B:3:GLN:N	2.52	0.43
1:D:253:GLN:O	1:D:253:GLN:HG2	2.19	0.43
1:A:149:ASN:HD22	1:A:207:TYR:HD1	1.65	0.43
1:A:350:LYS:O	1:A:353:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ARG:O	1:C:159:ILE:HG12	2.19	0.43
1:B:122:HIS:CD2	1:B:169:PHE:HE1	2.37	0.43
1:D:14:ASN:HD22	1:D:16:SER:H	1.66	0.43
1:D:315:LEU:HD11	1:D:328:ASN:HD21	1.84	0.43
1:C:251:VAL:O	1:C:254:LEU:HB2	2.19	0.43
1:A:4:ARG:NH1	3:A:540:HOH:O	2.51	0.42
1:A:41:ARG:HG3	1:A:41:ARG:NH1	2.33	0.42
1:A:315:LEU:HD12	1:A:324:GLY:HA2	2.01	0.42
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.19	0.42
1:B:195:ARG:O	1:B:196:LYS:C	2.60	0.42
1:A:-8:HIS:CB	1:A:-7:HIS:HB2	2.49	0.42
1:A:314:LEU:CD1	1:A:351:PHE:CZ	3.02	0.42
1:D:206:MET:HE2	1:D:206:MET:HA	2.01	0.42
1:C:101:LYS:HB2	1:C:101:LYS:HE3	1.86	0.42
1:C:201:ALA:HB3	3:C:563:HOH:O	2.18	0.42
1:B:281:GLY:O	3:B:525:HOH:O	2.22	0.42
1:D:95:SER:O	1:D:98:CYS:HB2	2.20	0.42
1:D:60:THR:O	1:D:64:GLY:N	2.47	0.42
1:D:73:LEU:HD23	3:D:526:HOH:O	2.18	0.42
1:D:209:TRP:O	1:D:210:TYR:C	2.63	0.42
1:D:350:LYS:O	1:D:353:GLU:HB3	2.18	0.42
1:C:8:ASN:ND2	1:C:10:TYR:H	2.18	0.42
1:C:227:TYR:O	1:C:233:LEU:HD22	2.19	0.42
1:A:-7:HIS:HB3	1:A:-6:HIS:H	1.39	0.42
1:A:260:ASN:C	1:A:261:TYR:CD1	2.97	0.42
1:C:50:GLY:HA3	1:C:370:PHE:CZ	2.54	0.42
1:B:343:LYS:O	1:B:346:TYR:HB3	2.20	0.42
1:D:209:TRP:HE3	1:D:214:TYR:CE2	2.38	0.42
1:D:107:LEU:HD21	1:D:373:PHE:CZ	2.55	0.42
1:D:227:TYR:O	1:D:233:LEU:HD22	2.19	0.42
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.87	0.41
1:C:149:ASN:HA	1:C:155:ARG:H	1.86	0.41
1:B:330:TYR:CB	1:B:394:PHE:HD1	2.33	0.41
1:D:39:LYS:HG2	1:D:356:LEU:HD22	2.03	0.41
1:D:380:ILE:O	1:D:381:TYR:C	2.62	0.41
1:A:213:TYR:HB3	1:A:265:ILE:HD12	2.01	0.41
1:C:131:GLU:C	1:C:133:CYS:N	2.76	0.41
1:B:21:TYR:O	1:B:28:LEU:HA	2.21	0.41
1:C:138:ILE:C	1:C:140:LEU:H	2.28	0.41
1:D:130:ALA:O	1:D:133:CYS:HB2	2.20	0.41
1:D:146:HIS:CD2	3:D:512:HOH:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:O	1:A:131:GLU:HB2	2.21	0.41
1:B:275:TRP:HZ3	1:B:397:PHE:CE2	2.38	0.41
1:B:314:LEU:HD13	1:B:351:PHE:CZ	2.55	0.41
1:C:349:CYS:O	1:C:352:ALA:HB3	2.20	0.41
1:B:140:LEU:O	1:B:143:ILE:HG12	2.21	0.41
1:B:262:PRO:CD	3:B:550:HOH:O	2.68	0.41
1:B:381:TYR:CZ	1:B:395:PRO:HB3	2.56	0.41
1:B:395:PRO:O	1:B:396:ALA:CB	2.66	0.41
1:C:68:ILE:H	1:C:68:ILE:HG12	1.70	0.41
1:C:160:TYR:CD1	1:C:160:TYR:C	2.98	0.41
1:B:262:PRO:HA	1:B:263:PRO:HD3	1.86	0.41
1:B:290:TYR:CZ	1:B:299:LEU:HD22	2.56	0.41
1:D:75:LEU:HD12	1:D:75:LEU:HA	1.91	0.41
1:D:265:ILE:HG12	1:D:265:ILE:H	1.66	0.41
1:C:62:TYR:HD2	1:C:63:THR:HG23	1.86	0.41
1:C:138:ILE:HG23	1:C:178:HIS:NE2	2.35	0.41
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.88	0.41
1:A:105:THR:HG21	1:A:152:LEU:C	2.46	0.41
1:C:-4:MET:CE	1:D:197:ARG:HD3	2.51	0.41
1:C:51:LEU:C	1:C:53:SER:N	2.77	0.41
1:B:370:PHE:HA	1:B:376:MET:H	1.86	0.41
1:D:255:LYS:HB2	1:D:255:LYS:HE3	1.89	0.41
1:C:199:PHE:O	1:C:200:THR:C	2.64	0.41
1:B:81:ASP:OD2	1:B:81:ASP:C	2.64	0.41
1:D:37:THR:O	1:D:41:ARG:HG3	2.21	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.84	0.40
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.94	0.40
1:C:293:PHE:O	1:C:294:ARG:C	2.65	0.40
1:B:1:MET:HE1	1:B:260:ASN:HB2	2.02	0.40
1:B:93:LYS:HD3	3:B:517:HOH:O	2.21	0.40
1:D:337:ASN:HD21	1:D:390:THR:HA	1.86	0.40
1:C:251:VAL:O	1:C:252:CYS:C	2.63	0.40
1:B:380:ILE:O	1:B:381:TYR:C	2.65	0.40
1:D:198:ASN:N	3:D:525:HOH:O	2.34	0.40
1:A:22:PHE:CD1	1:A:345:LEU:HD13	2.57	0.40
1:A:122:HIS:HD2	1:A:127:GLU:OE1	2.04	0.40
1:B:169:PHE:C	1:B:171:VAL:N	2.78	0.40
1:B:288:GLN:HE21	1:B:292:VAL:CG2	2.35	0.40
1:D:315:LEU:HD12	1:D:324:GLY:HA2	2.02	0.40
1:D:159:ILE:HD11	1:D:182:ILE:HD12	2.04	0.40
1:D:233:LEU:O	1:D:235:VAL:N	2.54	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	407/411 (99%)	369 (91%)	37 (9%)	1 (0%)	43	66
1	B	399/411 (97%)	359 (90%)	38 (10%)	2 (0%)	24	46
1	C	407/411 (99%)	368 (90%)	38 (9%)	1 (0%)	43	66
1	D	397/411 (97%)	359 (90%)	37 (9%)	1 (0%)	36	58
All	All	1610/1644 (98%)	1455 (90%)	150 (9%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-7	HIS
1	B	1	MET
1	C	112	GLY
1	D	216	GLY
1	B	320	GLY

5.3.2 Protein sidechains [i](#)

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	341/343 (99%)	299 (88%)	42 (12%)	4	9
1	B	333/343 (97%)	288 (86%)	45 (14%)	4	7
1	C	341/343 (99%)	295 (86%)	46 (14%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	331/343 (96%)	291 (88%)	40 (12%)	5 10
All	All	1346/1372 (98%)	1173 (87%)	173 (13%)	4 8

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	HIS
1	A	41	ARG
1	A	42	GLU
1	A	52	LYS
1	A	71	LEU
1	A	75	LEU
1	A	78	VAL
1	A	87	LEU
1	A	101	LYS
1	A	114	LEU
1	A	119	VAL
1	A	120	LEU
1	A	132	ASP
1	A	135	THR
1	A	162	LEU
1	A	163	LEU
1	A	174	ILE
1	A	181	GLN
1	A	182	ILE
1	A	184	GLU
1	A	185	THR
1	A	186	ILE
1	A	192	ASN
1	A	193	LEU
1	A	202	LYS
1	A	221	LEU
1	A	232	SER
1	A	233	LEU
1	A	244	VAL
1	A	264	CYS
1	A	271	LEU
1	A	275	TRP
1	A	294	ARG
1	A	314	LEU
1	A	333	LEU
1	A	334	THR

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Mol	Chain	Res	Type
1	A	345	LEU
1	A	364	ARG
1	A	387	LEU
1	A	390	THR
1	A	393	ARG
1	A	399	LEU
1	C	-7	HIS
1	C	-2	ILE
1	C	-1	GLU
1	C	8	ASN
1	C	14	ASN
1	C	15	LYS
1	C	17	LEU
1	C	42	GLU
1	C	57	ARG
1	C	75	LEU
1	C	77	ASP
1	C	78	VAL
1	C	87	LEU
1	C	92	VAL
1	C	101	LYS
1	C	114	LEU
1	C	119	VAL
1	C	128	LYS
1	C	129	GLN
1	C	132	ASP
1	C	134	ILE
1	C	142	LYS
1	C	162	LEU
1	C	163	LEU
1	C	173	LYS
1	C	180	GLN
1	C	181	GLN
1	C	182	ILE
1	C	186	ILE
1	C	193	LEU
1	C	221	LEU
1	C	240	LEU
1	C	243	LEU
1	C	244	VAL
1	C	253	GLN
1	C	255	LYS

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Mol	Chain	Res	Type
1	C	275	TRP
1	C	283	ILE
1	C	287	ILE
1	C	333	LEU
1	C	338	LEU
1	C	345	LEU
1	C	364	ARG
1	C	387	LEU
1	C	390	THR
1	C	393	ARG
1	B	3	GLN
1	B	57	ARG
1	B	73	LEU
1	B	75	LEU
1	B	77	ASP
1	B	78	VAL
1	B	87	LEU
1	B	101	LYS
1	B	104	ILE
1	B	114	LEU
1	B	119	VAL
1	B	128	LYS
1	B	129	GLN
1	B	132	ASP
1	B	135	THR
1	B	146	HIS
1	B	150	GLU
1	B	162	LEU
1	B	171	VAL
1	B	181	GLN
1	B	182	ILE
1	B	185	THR
1	B	186	ILE
1	B	193	LEU
1	B	199	PHE
1	B	221	LEU
1	B	230	GLN
1	B	234	GLN
1	B	255	LYS
1	B	264	CYS
1	B	268	ASN
1	B	269	ARG

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Mol	Chain	Res	Type
1	B	275	TRP
1	B	276	CYS
1	B	283	ILE
1	B	286	LEU
1	B	308	VAL
1	B	314	LEU
1	B	333	LEU
1	B	337	ASN
1	B	345	LEU
1	B	364	ARG
1	B	387	LEU
1	B	393	ARG
1	B	399	LEU
1	D	3	GLN
1	D	8	ASN
1	D	37	THR
1	D	57	ARG
1	D	73	LEU
1	D	75	LEU
1	D	77	ASP
1	D	87	LEU
1	D	92	VAL
1	D	104	ILE
1	D	107	LEU
1	D	120	LEU
1	D	128	LYS
1	D	135	THR
1	D	146	HIS
1	D	150	GLU
1	D	167	LYS
1	D	171	VAL
1	D	174	ILE
1	D	181	GLN
1	D	182	ILE
1	D	193	LEU
1	D	200	THR
1	D	221	LEU
1	D	230	GLN
1	D	232	SER
1	D	233	LEU
1	D	235	VAL
1	D	264	CYS

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Mol	Chain	Res	Type
1	D	269	ARG
1	D	272	LEU
1	D	276	CYS
1	D	294	ARG
1	D	311	GLN
1	D	314	LEU
1	D	333	LEU
1	D	334	THR
1	D	345	LEU
1	D	387	LEU
1	D	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	89	HIS
1	A	97	ASN
1	A	122	HIS
1	A	129	GLN
1	A	192	ASN
1	A	268	ASN
1	A	274	HIS
1	A	277	HIS
1	A	337	ASN
1	A	361	HIS
1	C	-8	HIS
1	C	-6	HIS
1	C	8	ASN
1	C	14	ASN
1	C	34	GLN
1	C	38	ASN
1	C	86	GLN
1	C	97	ASN
1	C	192	ASN
1	C	237	GLN
1	C	241	HIS
1	C	253	GLN
1	C	274	HIS
1	C	311	GLN
1	C	337	ASN
1	C	340	GLN

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Mol	Chain	Res	Type
1	C	361	HIS
1	B	8	ASN
1	B	34	GLN
1	B	74	HIS
1	B	89	HIS
1	B	97	ASN
1	B	122	HIS
1	B	176	GLN
1	B	178	HIS
1	B	181	GLN
1	B	192	ASN
1	B	234	GLN
1	B	274	HIS
1	B	288	GLN
1	B	311	GLN
1	B	361	HIS
1	D	3	GLN
1	D	8	ASN
1	D	14	ASN
1	D	34	GLN
1	D	89	HIS
1	D	176	GLN
1	D	192	ASN
1	D	234	GLN
1	D	268	ASN
1	D	274	HIS
1	D	311	GLN
1	D	328	ASN
1	D	337	ASN
1	D	361	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	409/411 (99%)	0.34	14 (3%) 48 42	54, 70, 94, 98	0
1	B	401/411 (97%)	0.47	15 (3%) 45 39	18, 72, 96, 102	0
1	C	409/411 (99%)	0.38	14 (3%) 48 42	56, 72, 96, 100	0
1	D	399/411 (97%)	0.46	16 (4%) 42 37	37, 74, 99, 107	0
All	All	1618/1644 (98%)	0.41	59 (3%) 46 40	18, 72, 96, 107	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-9	HIS	4.3
1	D	135	THR	4.2
1	B	0	PHE	4.0
1	A	171	VAL	4.0
1	C	-8	HIS	4.0
1	B	399	LEU	3.3
1	C	-9	HIS	3.3
1	A	-8	HIS	3.2
1	D	146	HIS	3.2
1	A	139	HIS	3.0
1	B	146	HIS	3.0
1	B	139	HIS	3.0
1	D	102	ARG	2.9
1	D	171	VAL	2.9
1	A	-4	MET	2.9
1	B	169	PHE	2.9
1	B	284	TYR	2.8
1	D	142	LYS	2.8
1	B	275	TRP	2.8
1	A	128	LYS	2.7
1	D	167	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	2.7
1	A	102	ARG	2.7
1	C	102	ARG	2.6
1	A	196	LYS	2.6
1	B	253	GLN	2.6
1	C	196	LYS	2.5
1	B	136	ARG	2.5
1	C	275	TRP	2.5
1	D	267	ASP	2.5
1	A	185	THR	2.5
1	B	287	ILE	2.5
1	C	-7	HIS	2.5
1	C	-6	HIS	2.4
1	A	-7	HIS	2.4
1	C	184	GLU	2.4
1	C	193	LEU	2.3
1	D	139	HIS	2.3
1	D	399	LEU	2.3
1	B	185	THR	2.3
1	C	171	VAL	2.3
1	D	141	ASN	2.2
1	B	102	ARG	2.2
1	A	396	ALA	2.2
1	C	128	LYS	2.2
1	C	139	HIS	2.2
1	D	200	THR	2.2
1	D	296	GLU	2.2
1	B	268	ASN	2.2
1	D	1	MET	2.2
1	B	397	PHE	2.1
1	D	145	PRO	2.1
1	C	132	ASP	2.1
1	A	275	TRP	2.1
1	B	57	ARG	2.1
1	D	234	GLN	2.1
1	A	188	THR	2.0
1	C	97	ASN	2.0
1	D	269	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	504	1/1	0.98	0.04	67,67,67,67	0
2	ZN	C	502	1/1	0.99	0.05	66,66,66,66	0
2	ZN	B	503	1/1	0.99	0.04	65,65,65,65	0
2	ZN	A	501	1/1	0.99	0.04	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.