



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 1E1E / pdb_00001e1e
Title : Crystal structure of a Monocot (Maize ZMGlu1) beta-glucosidase
Authors : Czjzek, M.; Cicek, M.; Bevan, D.R.; Henrissat, B.; Esen, A.
Deposited on : 2000-05-03
Resolution : 2.50 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

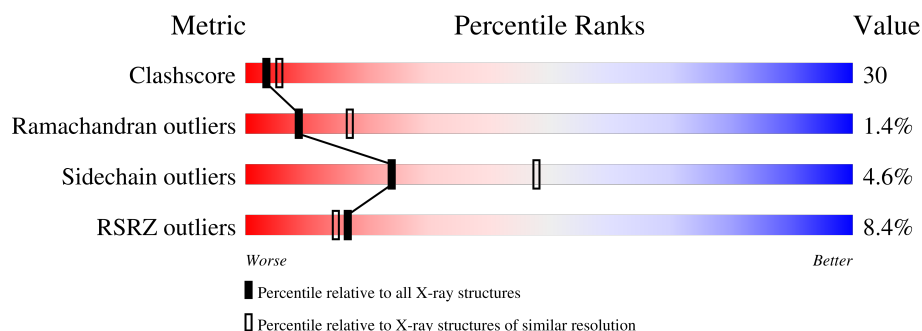
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	512	4% 54% 36% 5% . .
1	B	512	12% 46% 46% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8302 atoms, of which 0 are hydrogens and 0 are deuteriums.

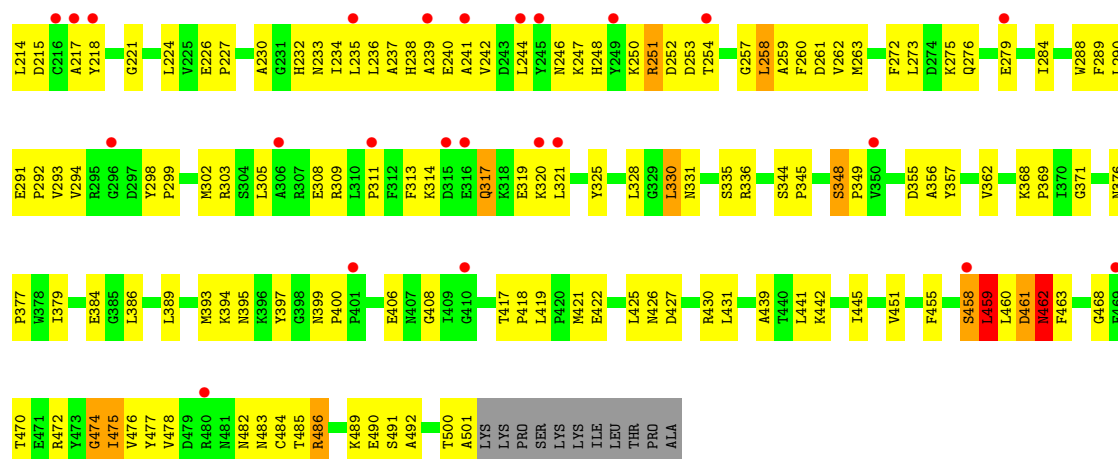
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3967	2544	656	749	18			
1	B	495	Total	C	N	O	S	0	0	0
			4004	2565	664	757	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	215	Total	O	0	0
			215	215		
2	B	116	Total	O	0	0
			116	116		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.88Å 118.34Å 77.10Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	27.00 – 2.50 27.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (27.00-2.50) 98.2 (27.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.322 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8302	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

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	0.52	0/4088	1.03	27/5550 (0.5%)
1	B	0.54	0/4125	0.99	20/5600 (0.4%)
All	All	0.53	0/8213	1.01	47/11150 (0.4%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ILE	N-CA-C	-11.25	102.10	112.90
1	A	362	VAL	N-CA-C	-10.35	103.52	111.90
1	B	475	ILE	N-CA-C	-9.17	101.94	113.22
1	B	459	LEU	N-CA-C	-8.57	102.09	112.54
1	B	395	ASN	N-CA-C	8.28	122.95	113.01
1	A	459	LEU	N-CA-C	-7.89	102.91	112.54
1	A	112	GLY	N-CA-C	-7.85	104.93	114.66
1	B	362	VAL	N-CA-C	-7.75	105.21	112.96
1	B	40	GLU	N-CA-C	7.54	120.16	111.11
1	A	40	GLU	N-CA-C	7.53	119.18	110.97
1	B	317	GLN	N-CA-C	-7.02	104.59	113.43
1	A	138	VAL	N-CA-C	6.96	118.61	108.58
1	A	115	ASN	CA-C-N	6.89	126.49	119.19
1	A	115	ASN	C-N-CA	6.89	126.49	119.19
1	A	462	ASN	N-CA-C	6.82	117.49	107.88
1	A	348	SER	CA-C-N	6.79	127.16	119.83
1	A	348	SER	C-N-CA	6.79	127.16	119.83
1	A	379	ILE	N-CA-C	6.43	116.99	107.15
1	A	395	ASN	N-CA-C	6.32	120.99	113.28
1	B	275	LYS	N-CA-C	-6.27	104.52	111.36
1	B	204	VAL	N-CA-C	-6.27	105.51	113.22
1	A	474	GLY	N-CA-C	6.24	120.53	112.54
1	B	461	ASP	N-CA-C	-6.24	101.05	110.28
1	B	462	ASN	N-CA-C	6.19	116.61	107.88
1	A	429	LYS	N-CA-C	-6.04	104.81	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	GLY	N-CA-C	5.95	121.02	112.82
1	B	39	ILE	N-CA-C	5.92	116.70	111.90
1	B	74	ALA	N-CA-C	-5.89	105.40	112.59
1	A	272	PHE	N-CA-C	-5.88	105.96	113.01
1	A	23	TRP	N-CA-C	-5.83	106.33	113.50
1	A	326	ASN	N-CA-C	-5.78	106.57	113.97
1	A	261	ASP	N-CA-C	-5.62	102.16	110.48
1	A	202	THR	N-CA-C	-5.57	105.11	111.07
1	A	275	LYS	N-CA-C	-5.56	105.30	111.36
1	A	398	GLY	N-CA-C	5.46	122.89	115.30
1	A	74	ALA	N-CA-C	-5.45	105.33	112.41
1	B	397	TYR	N-CA-C	5.39	119.37	112.26
1	A	461	ASP	N-CA-C	-5.33	102.39	110.28
1	A	393	MET	N-CA-C	-5.30	105.39	111.07
1	B	348	SER	CA-C-N	5.28	125.20	119.76
1	B	348	SER	C-N-CA	5.28	125.20	119.76
1	A	306	ALA	N-CA-C	-5.21	106.16	112.88
1	B	379	ILE	N-CA-C	5.12	115.73	107.73
1	B	393	MET	N-CA-C	-5.12	105.69	111.28
1	B	138	VAL	N-CA-C	5.10	116.62	108.87
1	A	135	GLU	N-CA-C	5.09	116.06	109.65
1	B	272	PHE	N-CA-C	-5.01	106.68	112.89

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	3967	0	3759	184	0
1	B	4004	0	3793	287	0
2	A	215	0	0	33	0
2	B	116	0	0	34	0
All	All	8302	0	7552	466	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 30.

All (466) 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:A:376:ASN:HB2	1:A:377:PRO:HD2	1.46	0.98
1:B:77:TYR:HA	1:B:121:TYR:CZ	2.00	0.96
1:B:146:PRO:HG2	1:B:149:LEU:HG	1.48	0.94
1:A:461:ASP:HA	2:A:2198:HOH:O	1.67	0.94
1:B:49:GLY:O	1:B:102:PRO:HB2	1.65	0.94
1:B:236:LEU:HD12	2:B:2058:HOH:O	1.69	0.93
1:B:376:ASN:HB2	1:B:377:PRO:HD2	1.55	0.88
1:B:101:TRP:HA	1:B:171:PHE:CZ	2.10	0.86
1:A:436:ARG:CZ	2:A:2187:HOH:O	2.24	0.86
1:B:147:GLN:HE21	1:B:147:GLN:HA	1.40	0.85
1:A:482:ASN:HD22	1:A:483:ASN:H	1.20	0.85
1:B:51:SER:O	2:B:2024:HOH:O	1.95	0.84
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.59	0.84
1:A:482:ASN:ND2	1:A:483:ASN:H	1.76	0.84
1:B:34:THR:HG21	2:B:2032:HOH:O	1.79	0.83
1:B:77:TYR:HA	1:B:121:TYR:OH	1.79	0.82
1:A:95:TYR:HD2	1:A:129:LEU:HD11	1.45	0.82
1:B:482:ASN:ND2	1:B:483:ASN:H	1.78	0.82
1:A:12:MET:C	1:A:13:LEU:HD23	2.05	0.81
1:B:149:LEU:HB3	1:B:153:TYR:HE1	1.45	0.81
1:B:119:ILE:HD13	1:B:119:ILE:H	1.45	0.81
1:B:110:LYS:HG2	1:B:170:TYR:CZ	2.15	0.81
1:B:460:LEU:HD22	2:B:2108:HOH:O	1.80	0.81
1:A:194:THR:CB	2:A:2110:HOH:O	2.29	0.81
1:A:384:GLU:HB3	2:A:2167:HOH:O	1.80	0.80
1:B:48:LYS:HD2	1:B:103:ARG:HG3	1.62	0.80
1:B:87:LEU:HD21	1:B:459:LEU:HG	1.64	0.80
1:A:87:LEU:HD21	1:A:459:LEU:HG	1.64	0.79
1:B:49:GLY:C	1:B:102:PRO:HB2	2.08	0.78
1:A:194:THR:HB	2:A:2110:HOH:O	1.82	0.78
1:A:251:ARG:HB2	1:A:254:THR:HG23	1.65	0.78
1:B:9:GLY:O	2:B:2003:HOH:O	2.02	0.77
1:B:171:PHE:HE2	2:B:2046:HOH:O	1.69	0.75
1:B:119:ILE:HD13	1:B:119:ILE:N	2.02	0.74
1:B:408:GLY:HA3	2:B:2107:HOH:O	1.88	0.74
1:B:177:ASP:HA	2:B:2050:HOH:O	1.87	0.74
1:B:19:PRO:HG3	1:B:439:ALA:HB2	1.68	0.74
1:B:54:ASP:HB2	2:B:2024:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ASN:HD22	1:B:483:ASN:H	1.34	0.74
1:B:171:PHE:CE2	2:B:2046:HOH:O	2.42	0.73
1:A:298:TYR:O	2:A:2139:HOH:O	2.06	0.73
1:A:162:LYS:HD3	2:A:2095:HOH:O	1.88	0.73
1:B:232:HIS:CE1	1:B:311:PRO:HB2	2.23	0.72
1:A:15:PRO:HG2	2:A:2001:HOH:O	1.89	0.72
1:B:101:TRP:CG	1:B:146:PRO:HD3	2.25	0.72
1:A:120:LYS:HE3	2:A:2067:HOH:O	1.88	0.72
1:B:173:LYS:HA	1:B:176:PHE:CD2	2.24	0.72
1:B:460:LEU:HB3	2:B:2108:HOH:O	1.88	0.72
1:A:427:ASP:OD2	1:A:430:ARG:HD2	1.90	0.72
1:A:52:ASN:N	1:A:52:ASN:HD22	1.86	0.72
1:A:82:THR:O	1:A:86:LEU:HD22	1.89	0.71
1:B:84:VAL:HG13	1:B:129:LEU:HD23	1.71	0.71
1:A:157:LEU:HD11	1:A:200:TYR:CE1	2.26	0.71
1:B:140:ILE:HG23	2:B:2042:HOH:O	1.90	0.71
1:A:370:ILE:O	2:A:2162:HOH:O	2.09	0.71
1:B:52:ASN:N	1:B:52:ASN:HD22	1.88	0.71
1:B:104:ILE:O	1:B:105:LEU:HD23	1.91	0.71
1:A:239:ALA:HB2	1:A:321:LEU:HD23	1.72	0.70
1:B:232:HIS:CE1	1:B:313:PHE:CE2	2.79	0.70
1:A:462:ASN:C	1:A:462:ASN:HD22	2.00	0.70
1:B:101:TRP:HE1	1:B:108:GLY:CA	2.03	0.70
1:B:123:ARG:HH21	1:B:123:ARG:HG3	1.57	0.70
1:A:82:THR:HG22	1:A:85:ARG:NH2	2.06	0.69
1:B:240:GLU:OE2	1:B:240:GLU:HA	1.92	0.69
1:B:279:GLU:OE1	1:B:279:GLU:HA	1.92	0.69
1:B:55:HIS:N	2:B:2024:HOH:O	1.89	0.69
1:B:180:GLY:HA2	1:B:186:TRP:HZ2	1.56	0.69
1:B:244:LEU:HD12	1:B:248:HIS:HD2	1.57	0.69
1:A:107:LYS:HB2	1:A:112:GLY:HA3	1.75	0.69
1:B:149:LEU:HB3	1:B:153:TYR:CE1	2.26	0.68
1:A:130:LEU:HD11	1:A:182:LYS:HB3	1.74	0.68
1:B:147:GLN:HA	1:B:147:GLN:NE2	2.07	0.68
1:A:153:TYR:CE2	1:A:163:SER:HB3	2.28	0.68
1:A:279:GLU:HA	1:A:279:GLU:OE1	1.93	0.68
1:B:123:ARG:HH12	1:B:182:LYS:HZ2	1.42	0.68
1:B:52:ASN:HD22	1:B:52:ASN:H	1.42	0.67
1:B:21:ARG:HB3	2:B:2011:HOH:O	1.94	0.67
1:B:114:ILE:CG2	1:B:119:ILE:HD11	2.24	0.67
1:B:88:LYS:HD3	1:B:132:ASN:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:MET:HE2	1:A:425:LEU:HD11	1.77	0.67
1:B:101:TRP:HE1	1:B:108:GLY:HA2	1.60	0.67
1:B:442:LYS:O	1:B:442:LYS:HD3	1.95	0.66
1:A:79:MET:HE1	1:A:484:CYS:HB2	1.78	0.66
1:B:107:LYS:HB2	1:B:112:GLY:HA3	1.77	0.66
1:B:150:GLU:OE2	1:B:155:GLY:HA3	1.95	0.66
1:A:156:PHE:O	1:A:230:ALA:HA	1.95	0.66
1:B:173:LYS:CB	1:B:244:LEU:HD21	2.24	0.66
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.60	0.66
1:A:14:SER:O	1:A:18:ILE:HG12	1.95	0.65
1:A:217:ALA:C	1:A:219:PRO:HD3	2.21	0.65
1:B:80:TYR:O	1:B:84:VAL:HG23	1.96	0.65
1:A:75:ASN:HD21	1:A:78:HIS:HD2	1.44	0.65
1:B:289:PHE:C	1:B:292:PRO:HD2	2.21	0.65
1:B:460:LEU:CB	2:B:2108:HOH:O	2.44	0.65
1:B:163:SER:O	1:B:167:ASP:OD2	2.15	0.64
1:A:303:ARG:HH22	1:A:312:PHE:HA	1.61	0.64
1:B:191:GLU:HG2	1:B:261:ASP:HB3	1.79	0.64
1:A:191:GLU:HG2	1:A:261:ASP:HB3	1.79	0.64
1:A:191:GLU:CG	1:A:261:ASP:HB3	2.28	0.64
1:B:101:TRP:HA	1:B:171:PHE:CE1	2.32	0.64
1:B:461:ASP:OD2	1:B:472:ARG:HB3	1.98	0.64
1:B:179:PHE:C	1:B:181:ASP:H	2.06	0.63
1:A:464:GLU:OE1	2:A:2201:HOH:O	2.15	0.63
1:B:460:LEU:CD2	2:B:2108:HOH:O	2.40	0.63
1:B:258:LEU:H	1:B:258:LEU:HD23	1.61	0.63
1:A:31:GLY:O	1:A:455:PHE:HA	1.99	0.62
1:A:193:GLN:HA	1:A:289:PHE:HE2	1.64	0.62
1:A:101:TRP:HB3	1:A:102:PRO:HD3	1.81	0.62
1:A:135:GLU:HG3	2:A:2025:HOH:O	2.00	0.61
1:A:312:PHE:CE2	1:B:345:PRO:HD3	2.34	0.61
1:A:13:LEU:O	1:A:14:SER:HB2	1.99	0.60
1:A:75:ASN:HB3	1:A:79:MET:CE	2.30	0.60
1:A:52:ASN:HD22	1:A:52:ASN:H	1.48	0.60
1:A:415:LYS:O	1:A:418:PRO:HD3	2.01	0.60
1:A:231:GLY:HA2	1:A:234:ILE:HD12	1.81	0.60
1:A:312:PHE:CE2	1:B:344:SER:HA	2.36	0.60
1:A:36:ALA:O	1:A:40:GLU:HB2	2.02	0.60
1:A:111:GLU:HG3	2:A:2064:HOH:O	2.00	0.60
1:B:211:SER:HA	1:B:221:GLY:O	2.02	0.60
1:B:52:ASN:N	1:B:145:VAL:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:C	1:B:23:TRP:H	2.10	0.59
1:B:250:LYS:HD3	1:B:251:ARG:H	1.66	0.59
1:A:373:PRO:HG3	1:A:380:TYR:CE2	2.36	0.59
1:B:22:ASP:N	2:B:2011:HOH:O	2.34	0.59
1:A:111:GLU:CG	2:A:2064:HOH:O	2.50	0.59
1:B:52:ASN:H	1:B:52:ASN:ND2	2.01	0.59
1:B:162:LYS:HA	1:B:165:VAL:HB	1.85	0.59
1:B:462:ASN:HD22	1:B:462:ASN:C	2.09	0.59
1:A:295:ARG:HD2	1:B:273:LEU:HD11	1.84	0.59
1:A:482:ASN:ND2	1:A:483:ASN:N	2.48	0.59
1:B:65:LEU:HD23	1:B:470:THR:HG21	1.84	0.59
1:B:184:LYS:C	1:B:185:ASN:HD22	2.11	0.59
1:B:478:VAL:CG2	2:B:2108:HOH:O	2.50	0.59
1:B:48:LYS:CD	1:B:103:ARG:HG3	2.30	0.58
1:B:174:VAL:O	1:B:177:ASP:HB2	2.03	0.58
1:B:123:ARG:HH12	1:B:182:LYS:NZ	1.99	0.58
1:B:124:ASN:HA	2:B:2038:HOH:O	2.03	0.58
1:B:123:ARG:HG3	1:B:123:ARG:NH2	2.18	0.58
1:B:20:GLN:O	1:B:23:TRP:HB2	2.03	0.57
1:B:459:LEU:HD13	1:B:460:LEU:HG	1.85	0.57
1:A:191:GLU:OE2	1:A:261:ASP:HB3	2.05	0.57
1:B:251:ARG:NH1	2:B:2062:HOH:O	2.37	0.57
1:A:75:ASN:HB3	1:A:79:MET:HE3	1.85	0.57
1:B:145:VAL:HG13	1:B:146:PRO:HD2	1.86	0.57
1:A:472:ARG:HG2	2:A:2203:HOH:O	2.05	0.57
1:B:141:PHE:HD2	1:B:189:PHE:HD2	1.53	0.57
1:A:60:HIS:NE2	1:A:218:TYR:HE1	2.02	0.56
1:B:458:SER:O	1:B:474:GLY:HA2	2.04	0.56
1:B:173:LYS:HB2	1:B:244:LEU:HD21	1.86	0.56
1:B:251:ARG:HB3	2:B:2064:HOH:O	2.04	0.56
1:B:119:ILE:H	1:B:119:ILE:CD1	2.03	0.56
1:A:168:TYR:CD2	1:A:237:ALA:HB1	2.40	0.56
1:A:482:ASN:ND2	1:A:485:THR:OG1	2.38	0.56
1:B:101:TRP:HE1	1:B:108:GLY:HA3	1.70	0.56
1:B:250:LYS:O	1:B:251:ARG:HG2	2.05	0.56
1:A:449:SER:OG	1:A:451:VAL:HG22	2.05	0.56
1:A:459:LEU:HD13	1:A:460:LEU:HG	1.87	0.56
1:B:258:LEU:HD23	1:B:258:LEU:N	2.20	0.56
1:A:461:ASP:OD2	1:A:472:ARG:HB3	2.06	0.56
1:B:110:LYS:HG2	1:B:170:TYR:CE1	2.40	0.56
1:A:194:THR:O	1:A:195:PHE:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.26	0.56
1:B:51:SER:HB3	2:B:2023:HOH:O	2.05	0.55
1:B:25:PRO:HB2	1:B:27:ASP:OD1	2.07	0.55
1:B:49:GLY:O	1:B:102:PRO:CB	2.47	0.55
1:B:105:LEU:C	1:B:107:LYS:H	2.14	0.55
1:A:52:ASN:H	1:A:52:ASN:ND2	2.05	0.55
1:A:52:ASN:N	1:A:52:ASN:ND2	2.55	0.55
1:B:247:LYS:HA	2:B:2060:HOH:O	2.07	0.55
1:B:179:PHE:O	1:B:181:ASP:N	2.40	0.55
1:B:224:LEU:O	1:B:309:ARG:HD2	2.06	0.55
1:B:239:ALA:HB1	1:B:320:LYS:HB3	1.87	0.55
1:A:83:ASP:O	1:A:87:LEU:HG	2.06	0.54
1:A:142:HIS:NE2	1:A:190:ASN:ND2	2.55	0.54
1:B:173:LYS:HE2	1:B:174:VAL:CG2	2.37	0.54
1:B:421:MET:HE3	1:B:425:LEU:HD11	1.89	0.54
1:B:160:SER:O	1:B:161:HIS:HB2	2.07	0.54
1:A:344:SER:HB2	1:A:345:PRO:HD2	1.89	0.54
1:A:419:LEU:HD23	1:A:420:PRO:HD2	1.89	0.54
1:B:209:ARG:HG2	1:B:209:ARG:NH1	2.23	0.54
1:B:290:LEU:O	1:B:294:VAL:HG23	2.08	0.54
1:A:60:HIS:HE2	1:A:218:TYR:HE1	1.54	0.54
1:A:130:LEU:CD1	1:A:182:LYS:HB3	2.38	0.54
1:A:86:LEU:HD21	1:A:486:ARG:HD3	1.88	0.54
1:A:421:MET:O	1:A:425:LEU:HG	2.08	0.54
1:B:19:PRO:CG	1:B:439:ALA:HB2	2.36	0.54
1:B:226:GLU:HB2	1:B:227:PRO:HD3	1.91	0.54
1:B:427:ASP:HB2	1:B:430:ARG:HB3	1.89	0.54
1:A:373:PRO:HG3	1:A:380:TYR:HE2	1.73	0.53
1:B:49:GLY:N	1:B:102:PRO:O	2.40	0.53
1:B:46:ASP:O	1:B:115:ASN:OD1	2.26	0.53
1:B:77:TYR:CA	1:B:121:TYR:OH	2.54	0.53
1:B:184:LYS:C	1:B:185:ASN:ND2	2.66	0.53
1:A:289:PHE:C	1:A:292:PRO:HD2	2.33	0.53
1:A:312:PHE:CD2	1:B:345:PRO:HD3	2.44	0.53
1:A:191:GLU:OE1	2:A:2107:HOH:O	2.19	0.53
1:B:284:ILE:HD12	1:B:302:MET:HE3	1.90	0.53
1:B:232:HIS:ND1	1:B:311:PRO:HB2	2.23	0.52
1:B:426:ASN:HA	1:B:490:GLU:HG2	1.92	0.52
1:B:459:LEU:HD13	1:B:460:LEU:CD2	2.39	0.52
1:A:387:LYS:HD2	1:A:447:LEU:HD12	1.91	0.52
1:A:14:SER:HB3	1:A:17:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:HG22	1:A:470:THR:HB	1.91	0.52
1:B:75:ASN:HD21	1:B:78:HIS:CD2	2.28	0.52
1:B:122:TYR:O	1:B:126:ILE:HG13	2.10	0.52
1:B:196:THR:HG22	1:B:230:ALA:HB3	1.90	0.52
1:B:97:PHE:CZ	1:B:138:VAL:HG22	2.44	0.52
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.91	0.52
1:A:135:GLU:CG	2:A:2025:HOH:O	2.56	0.52
1:B:172:ALA:O	1:B:175:CYS:HB2	2.10	0.52
1:B:168:TYR:C	1:B:170:TYR:N	2.68	0.52
1:A:356:ALA:O	1:A:357:TYR:C	2.53	0.51
1:A:147:GLN:NE2	1:A:150:GLU:HB3	2.24	0.51
1:A:200:TYR:HB3	1:A:226:GLU:HB3	1.93	0.51
1:A:326:ASN:HA	2:A:2151:HOH:O	2.09	0.51
1:B:141:PHE:HD2	1:B:189:PHE:CD2	2.28	0.51
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.74	0.51
1:B:478:VAL:HG23	2:B:2108:HOH:O	2.11	0.51
1:A:477:TYR:O	1:A:486:ARG:HA	2.11	0.51
1:B:60:HIS:HA	1:B:62:GLU:OE1	2.11	0.51
1:B:427:ASP:OD1	1:B:427:ASP:N	2.42	0.51
1:A:218:TYR:O	1:A:220:THR:N	2.36	0.51
1:A:342:ASP:HB3	2:A:2155:HOH:O	2.10	0.51
1:B:24:PHE:CD1	1:B:24:PHE:N	2.78	0.51
1:B:173:LYS:HA	1:B:176:PHE:HD2	1.72	0.51
1:B:101:TRP:HB3	1:B:102:PRO:HD3	1.93	0.51
1:B:119:ILE:O	1:B:123:ARG:HB2	2.10	0.51
1:B:173:LYS:HE2	1:B:174:VAL:HG23	1.93	0.51
1:A:235:LEU:HD21	1:A:289:PHE:HD1	1.76	0.51
1:B:263:MET:HE1	2:B:2065:HOH:O	2.10	0.51
1:B:252:ASP:N	2:B:2064:HOH:O	2.38	0.51
1:B:303:ARG:HG2	1:B:303:ARG:NH1	2.24	0.51
1:B:317:GLN:C	1:B:319:GLU:H	2.19	0.51
1:B:431:LEU:HD13	1:B:491:SER:HA	1.92	0.51
1:A:371:GLY:HA2	2:A:2079:HOH:O	2.09	0.50
1:B:173:LYS:HG3	1:B:174:VAL:N	2.26	0.50
1:A:51:SER:HB3	1:A:102:PRO:HG2	1.93	0.50
1:A:61:PRO:O	1:A:67:GLY:HA2	2.11	0.50
1:A:251:ARG:HB2	1:A:254:THR:CG2	2.39	0.50
1:B:146:PRO:O	1:B:148:ALA:N	2.45	0.50
1:B:442:LYS:HD3	1:B:442:LYS:C	2.36	0.50
1:A:164:ILE:HG23	1:A:165:VAL:N	2.26	0.50
1:B:31:GLY:HA2	1:B:92:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:SER:HB2	2:B:2018:HOH:O	2.11	0.50
1:B:146:PRO:C	1:B:148:ALA:N	2.66	0.50
1:B:235:LEU:O	1:B:321:LEU:HD21	2.12	0.50
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.77	0.50
1:A:364:GLY:HA3	2:A:2160:HOH:O	2.12	0.50
1:B:251:ARG:HG3	1:B:251:ARG:HH11	1.75	0.50
1:A:89:GLU:HB3	2:A:2211:HOH:O	2.11	0.50
1:B:246:ASN:HA	1:B:250:LYS:HG2	1.94	0.50
1:B:251:ARG:HB2	1:B:254:THR:HG23	1.93	0.50
1:A:288:TRP:CD1	1:A:302:MET:HE1	2.47	0.49
1:B:35:SER:HB3	1:B:38:GLN:OE1	2.11	0.49
1:B:48:LYS:CG	1:B:103:ARG:HG3	2.42	0.49
1:B:291:GLU:OE2	1:B:299:PRO:HA	2.12	0.49
1:B:293:VAL:O	1:B:325:TYR:HE2	1.95	0.49
1:B:241:ALA:O	1:B:244:LEU:HB3	2.13	0.49
1:B:305:LEU:HD13	1:B:355:ASP:O	2.12	0.49
1:A:152:LYS:HD2	1:A:153:TYR:CD2	2.47	0.49
1:B:20:GLN:HB2	1:B:23:TRP:CD1	2.48	0.49
1:B:107:LYS:CB	1:B:112:GLY:HA3	2.43	0.49
1:B:118:GLY:C	1:B:120:LYS:H	2.20	0.49
1:A:57:CYS:HB3	1:A:69:ASN:HB3	1.94	0.48
1:A:60:HIS:HB3	1:A:62:GLU:OE2	2.13	0.48
1:B:195:PHE:O	1:B:199:SER:HB2	2.13	0.48
1:B:232:HIS:CE1	1:B:313:PHE:HE2	2.31	0.48
1:A:331:ASN:CG	1:A:406:GLU:HB2	2.39	0.48
1:B:54:ASP:CB	2:B:2024:HOH:O	2.56	0.48
1:B:173:LYS:HB3	1:B:244:LEU:HD21	1.95	0.48
1:B:187:LEU:HA	1:B:257:GLY:O	2.13	0.48
1:A:480:ARG:NH1	2:A:2207:HOH:O	2.47	0.48
1:B:149:LEU:N	1:B:149:LEU:HD23	2.27	0.48
1:B:191:GLU:CG	1:B:261:ASP:HB3	2.43	0.48
1:B:482:ASN:ND2	1:B:485:THR:OG1	2.46	0.48
1:A:20:GLN:O	1:A:23:TRP:HB2	2.13	0.48
1:B:54:ASP:N	2:B:2024:HOH:O	2.45	0.48
1:B:477:TYR:O	1:B:486:ARG:HA	2.12	0.48
1:A:60:HIS:C	1:A:62:GLU:H	2.21	0.48
1:B:83:ASP:OD1	1:B:460:LEU:HD11	2.13	0.48
1:B:107:LYS:O	1:B:149:LEU:HD21	2.14	0.48
1:B:482:ASN:ND2	1:B:483:ASN:N	2.55	0.48
1:A:369:PRO:C	1:A:371:GLY:H	2.21	0.48
1:A:417:THR:HG22	1:A:417:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TRP:CD2	1:B:146:PRO:HD3	2.47	0.48
1:B:215:ASP:CG	1:B:215:ASP:O	2.56	0.48
1:B:331:ASN:CG	1:B:406:GLU:HB2	2.39	0.48
1:B:101:TRP:HB3	1:B:102:PRO:CD	2.43	0.48
1:B:190:ASN:HA	1:B:259:ALA:HB3	1.94	0.48
1:A:411:ASP:HA	2:A:2178:HOH:O	2.13	0.48
1:B:66:ASP:OD1	1:B:468:GLY:HA3	2.14	0.48
1:B:173:LYS:HG3	1:B:174:VAL:H	1.78	0.48
1:A:60:HIS:NE2	1:A:218:TYR:CE1	2.81	0.47
1:B:142:HIS:NE2	1:B:190:ASN:ND2	2.62	0.47
1:A:82:THR:HG22	1:A:85:ARG:HH22	1.77	0.47
1:A:193:GLN:HA	1:A:289:PHE:CE2	2.48	0.47
1:B:77:TYR:O	1:B:121:TYR:CE1	2.68	0.47
1:A:38:GLN:O	1:A:462:ASN:HB2	2.14	0.47
1:B:74:ALA:O	1:B:75:ASN:C	2.57	0.47
1:B:368:LYS:HB3	1:B:369:PRO:HD2	1.97	0.47
1:B:258:LEU:N	1:B:258:LEU:CD2	2.78	0.47
1:B:399:ASN:N	1:B:400:PRO:CD	2.78	0.47
1:A:52:ASN:HD22	1:A:53:TRP:H	1.63	0.47
1:A:96:ARG:NH1	1:A:405:THR:HB	2.30	0.47
1:B:105:LEU:HD11	1:B:171:PHE:HA	1.96	0.47
1:B:114:ILE:HG22	1:B:119:ILE:HD11	1.97	0.47
1:B:153:TYR:CD2	1:B:163:SER:HB3	2.49	0.47
1:B:230:ALA:O	1:B:234:ILE:HG13	2.14	0.47
1:A:312:PHE:HE2	1:B:344:SER:HA	1.79	0.47
1:A:339:LYS:HE3	2:A:2153:HOH:O	2.15	0.47
1:B:105:LEU:HD12	1:B:108:GLY:HA2	1.97	0.46
1:A:266:VAL:HG13	1:A:267:PRO:HD2	1.97	0.46
1:B:200:TYR:C	1:B:227:PRO:HG3	2.41	0.46
1:B:217:ALA:C	1:B:218:TYR:HD1	2.23	0.46
1:A:80:TYR:O	1:A:84:VAL:HG23	2.15	0.46
1:B:54:ASP:CA	2:B:2024:HOH:O	2.64	0.46
1:A:191:GLU:HB3	2:A:2110:HOH:O	2.15	0.46
1:B:49:GLY:HA3	1:B:106:PRO:HA	1.98	0.46
1:B:149:LEU:CB	1:B:153:TYR:HE1	2.23	0.46
1:B:34:THR:CG2	2:B:2032:HOH:O	2.52	0.46
1:B:38:GLN:O	1:B:462:ASN:HB2	2.16	0.46
1:A:154:GLY:O	1:A:155:GLY:C	2.59	0.46
1:B:52:ASN:N	1:B:52:ASN:ND2	2.56	0.46
1:B:52:ASN:HD22	1:B:53:TRP:H	1.64	0.46
1:A:142:HIS:O	1:A:143:TRP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:VAL:HG13	1:B:237:ALA:HA	1.98	0.45
1:B:194:THR:HG1	1:B:261:ASP:CG	2.23	0.45
1:A:95:TYR:CD2	1:A:129:LEU:HD11	2.37	0.45
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.79	0.45
1:A:105:LEU:O	1:A:108:GLY:N	2.45	0.45
1:B:115:ASN:O	1:B:119:ILE:HD11	2.16	0.45
1:B:298:TYR:HB3	1:B:299:PRO:HD2	1.99	0.45
1:B:417:THR:N	1:B:418:PRO:HD3	2.32	0.45
1:B:500:THR:O	1:B:501:ALA:C	2.58	0.45
1:B:106:PRO:O	1:B:107:LYS:HD3	2.16	0.45
1:B:170:TYR:HD1	1:B:173:LYS:HZ3	1.63	0.45
1:B:194:THR:O	1:B:198:PHE:HB2	2.17	0.45
1:A:66:ASP:OD1	1:A:468:GLY:HA3	2.15	0.45
1:A:144:ASP:OD2	1:A:144:ASP:N	2.48	0.45
1:A:96:ARG:HH12	1:A:406:GLU:HG3	1.81	0.45
1:A:436:ARG:NE	2:A:2187:HOH:O	2.44	0.45
1:A:98:SER:HB3	2:A:2081:HOH:O	2.17	0.45
1:B:335:SER:O	1:B:336:ARG:HG2	2.17	0.45
1:B:251:ARG:HB2	1:B:254:THR:CG2	2.47	0.45
1:B:356:ALA:O	1:B:357:TYR:C	2.60	0.45
1:A:18:ILE:HD12	1:A:435:GLN:NE2	2.32	0.45
1:A:475:ILE:O	1:A:492:ALA:HB2	2.17	0.45
1:B:459:LEU:CD1	1:B:460:LEU:HG	2.46	0.44
1:A:268:TYR:CD2	1:A:339:LYS:HD2	2.52	0.44
1:B:172:ALA:O	1:B:175:CYS:N	2.46	0.44
1:A:255:ARG:HD3	2:A:2129:HOH:O	2.16	0.44
1:B:156:PHE:O	1:B:233:ASN:ND2	2.41	0.44
1:B:168:TYR:O	1:B:170:TYR:N	2.50	0.44
1:B:161:HIS:O	1:B:165:VAL:HG21	2.17	0.44
1:B:288:TRP:CG	1:B:302:MET:HE1	2.52	0.44
1:A:333:TYR:HH	1:A:457:TRP:CG	2.36	0.44
1:B:105:LEU:HD23	1:B:114:ILE:HG12	2.00	0.44
1:B:115:ASN:O	1:B:119:ILE:CD1	2.66	0.44
1:B:123:ARG:NH2	1:B:127:ASN:HD21	2.15	0.44
1:A:239:ALA:HB2	1:A:321:LEU:CD2	2.45	0.44
1:A:303:ARG:NH2	1:A:312:PHE:HA	2.28	0.44
1:A:459:LEU:O	1:A:459:LEU:HD22	2.18	0.44
1:B:317:GLN:C	1:B:319:GLU:N	2.76	0.44
1:A:194:THR:O	1:A:197:SER:N	2.51	0.44
1:A:299:PRO:HD2	1:A:302:MET:SD	2.58	0.44
1:A:369:PRO:C	1:A:371:GLY:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLU:OE2	2:B:2094:HOH:O	2.21	0.44
1:A:200:TYR:O	1:A:223:SER:HA	2.18	0.44
1:A:198:PHE:C	1:A:205:PHE:HB2	2.43	0.43
1:A:472:ARG:HA	2:A:2203:HOH:O	2.18	0.43
1:B:114:ILE:CG2	1:B:119:ILE:CD1	2.94	0.43
1:B:147:GLN:NE2	1:B:147:GLN:CA	2.74	0.43
1:A:60:HIS:C	1:A:62:GLU:N	2.77	0.43
1:A:19:PRO:HA	1:A:23:TRP:CZ3	2.53	0.43
1:B:200:TYR:HA	1:B:209:ARG:O	2.19	0.43
1:B:394:LYS:HA	1:B:399:ASN:HA	2.01	0.43
1:A:19:PRO:HG3	1:A:439:ALA:HB2	2.00	0.43
1:A:65:LEU:HD23	1:A:470:THR:HG21	1.99	0.43
1:A:101:TRP:N	1:A:102:PRO:CD	2.81	0.43
1:A:309:ARG:CB	1:A:309:ARG:HH11	2.32	0.43
1:B:308:GLU:HG2	1:B:309:ARG:N	2.32	0.43
1:A:161:HIS:O	1:A:162:LYS:HB2	2.18	0.43
1:B:31:GLY:O	1:B:455:PHE:HA	2.19	0.43
1:B:118:GLY:C	1:B:120:LYS:N	2.77	0.43
1:B:158:ASP:HB3	1:B:164:ILE:HG22	2.01	0.43
1:B:169:THR:O	1:B:173:LYS:HB3	2.17	0.43
1:B:289:PHE:O	1:B:292:PRO:HD2	2.18	0.43
1:B:335:SER:C	1:B:336:ARG:HG2	2.44	0.43
1:B:459:LEU:HD22	1:B:459:LEU:O	2.19	0.43
1:A:232:HIS:CE1	1:A:313:PHE:CE2	3.06	0.43
1:B:205:PHE:O	1:B:206:ALA:C	2.61	0.43
1:B:276:GLN:NE2	2:B:2071:HOH:O	2.45	0.43
1:B:348:SER:HA	1:B:349:PRO:HD3	1.84	0.43
1:A:63:ARG:HH21	1:A:217:ALA:HA	1.83	0.43
1:B:21:ARG:C	1:B:23:TRP:N	2.77	0.43
1:B:123:ARG:HH22	1:B:127:ASN:HD21	1.66	0.43
1:B:149:LEU:HD22	1:B:153:TYR:OH	2.19	0.43
1:B:335:SER:O	1:B:336:ARG:NH1	2.52	0.43
1:A:20:GLN:HB2	1:A:23:TRP:CD1	2.54	0.42
1:A:122:TYR:O	1:A:126:ILE:HD12	2.19	0.42
1:B:55:HIS:ND1	1:B:147:GLN:OE1	2.52	0.42
1:B:325:TYR:CD1	1:B:325:TYR:C	2.96	0.42
1:B:330:LEU:HG	1:B:389:LEU:HD21	1.99	0.42
1:B:146:PRO:O	1:B:147:GLN:C	2.61	0.42
1:B:260:PHE:CZ	1:B:290:LEU:HA	2.55	0.42
1:B:164:ILE:HA	1:B:167:ASP:OD2	2.19	0.42
1:A:305:LEU:HD13	1:A:355:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:CB	1:A:377:PRO:HD2	2.28	0.42
1:B:38:GLN:HG2	1:B:463:PHE:O	2.20	0.42
1:B:142:HIS:CE1	1:B:190:ASN:ND2	2.87	0.42
1:A:32:ALA:CB	1:A:459:LEU:HB2	2.50	0.42
1:B:251:ARG:NH2	1:B:253:ASP:OD1	2.52	0.42
1:A:155:GLY:N	2:A:2086:HOH:O	2.52	0.42
1:B:19:PRO:HA	1:B:23:TRP:CZ3	2.55	0.42
1:B:51:SER:HB3	1:B:102:PRO:HG3	2.02	0.42
1:B:52:ASN:ND2	1:B:145:VAL:H	2.17	0.42
1:A:298:TYR:CD2	1:A:310:LEU:HD21	2.54	0.42
1:B:61:PRO:O	1:B:67:GLY:HA2	2.19	0.42
1:B:376:ASN:CB	1:B:377:PRO:HD2	2.36	0.42
1:A:101:TRP:CD1	1:A:146:PRO:HG2	2.55	0.42
1:A:21:ARG:C	1:A:23:TRP:H	2.27	0.42
1:B:173:LYS:CG	1:B:174:VAL:N	2.82	0.42
1:B:212:PRO:C	1:B:214:LEU:H	2.28	0.42
1:A:335:SER:C	1:A:336:ARG:HG2	2.45	0.41
1:B:14:SER:HB2	1:B:17:GLU:HG3	2.02	0.41
1:B:238:HIS:O	1:B:242:VAL:HG23	2.20	0.41
1:B:458:SER:C	1:B:460:LEU:N	2.74	0.41
1:A:63:ARG:NH1	2:A:2038:HOH:O	2.53	0.41
1:A:96:ARG:NH1	1:A:406:GLU:HG3	2.35	0.41
1:B:76:SER:C	1:B:121:TYR:OH	2.63	0.41
1:B:263:MET:CE	2:B:2065:HOH:O	2.66	0.41
1:B:314:LYS:HG3	1:B:317:GLN:OE1	2.20	0.41
1:B:486:ARG:H	1:B:486:ARG:HG2	1.55	0.41
1:B:60:HIS:NE2	1:B:218:TYR:HE1	2.18	0.41
1:B:76:SER:O	1:B:121:TYR:OH	2.34	0.41
1:B:103:ARG:O	1:B:104:ILE:HD13	2.20	0.41
1:B:146:PRO:C	1:B:148:ALA:H	2.26	0.41
1:A:187:LEU:HA	1:A:257:GLY:O	2.21	0.41
1:A:335:SER:O	1:A:336:ARG:NH1	2.53	0.41
1:B:80:TYR:HD1	1:B:80:TYR:H	1.67	0.41
1:A:193:GLN:HB3	1:A:261:ASP:OD2	2.21	0.41
1:B:105:LEU:C	1:B:107:LYS:N	2.76	0.41
1:B:369:PRO:C	1:B:371:GLY:N	2.76	0.41
1:A:217:ALA:O	1:A:219:PRO:HD3	2.20	0.41
1:A:296:GLY:O	1:A:318:LYS:HG2	2.21	0.41
1:A:334:THR:OG1	1:A:335:SER:N	2.54	0.41
1:A:335:SER:O	1:A:336:ARG:HG2	2.21	0.41
1:A:458:SER:O	1:A:474:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:HD2	1:B:123:ARG:HA	1.91	0.41
1:B:483:ASN:O	1:B:484:CYS:HB2	2.21	0.41
1:A:129:LEU:HD23	1:A:134:ILE:HD12	2.03	0.41
1:A:224:LEU:HD13	1:A:350:VAL:O	2.21	0.41
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.82	0.41
1:A:238:HIS:CE1	1:A:242:VAL:HG21	2.55	0.40
1:B:165:VAL:O	1:B:165:VAL:HG12	2.21	0.40
1:B:459:LEU:O	1:B:476:VAL:HB	2.22	0.40
1:B:475:ILE:O	1:B:492:ALA:HB2	2.22	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.95	0.40
1:B:153:TYR:CD1	1:B:153:TYR:N	2.69	0.40
1:B:246:ASN:HA	1:B:250:LYS:CG	2.51	0.40
1:B:474:GLY:O	1:B:489:LYS:HD2	2.22	0.40
1:A:32:ALA:HB1	1:A:459:LEU:HB2	2.03	0.40
1:A:81:LYS:HB2	2:A:2049:HOH:O	2.22	0.40
1:A:152:LYS:HD2	1:A:153:TYR:HD2	1.87	0.40
1:B:193:GLN:HA	1:B:289:PHE:HE2	1.85	0.40
1:B:441:LEU:O	1:B:445:ILE:HG13	2.22	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	488/512 (95%)	430 (88%)	50 (10%)	8 (2%)	7	14
1	B	493/512 (96%)	425 (86%)	62 (13%)	6 (1%)	10	20
All	All	981/1024 (96%)	855 (87%)	112 (11%)	14 (1%)	9	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	A	162	LYS
1	A	307	ARG
1	B	180	GLY
1	A	15	PRO
1	B	75	ASN
1	B	147	GLN
1	A	13	LEU
1	A	161	HIS
1	A	219	PRO
1	A	65	LEU
1	B	68	SER
1	B	104	ILE
1	B	106	PRO

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	423/441 (96%)	407 (96%)	16 (4%)	29	56
1	B	427/441 (97%)	404 (95%)	23 (5%)	20	41
All	All	850/882 (96%)	811 (95%)	39 (5%)	24	48

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	52	ASN
1	A	86	LEU
1	A	98	SER
1	A	152	LYS
1	A	159	LYS
1	A	204	VAL
1	A	224	LEU
1	A	328	LEU
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	386	LEU
1	A	419	LEU
1	A	451	VAL
1	A	458	SER
1	A	459	LEU
1	A	462	ASN
1	B	52	ASN
1	B	86	LEU
1	B	105	LEU
1	B	109	THR
1	B	119	ILE
1	B	153	TYR
1	B	156	PHE
1	B	167	ASP
1	B	173	LYS
1	B	181	ASP
1	B	251	ARG
1	B	258	LEU
1	B	262	VAL
1	B	328	LEU
1	B	330	LEU
1	B	386	LEU
1	B	419	LEU
1	B	422	GLU
1	B	451	VAL
1	B	458	SER
1	B	459	LEU
1	B	462	ASN
1	B	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	75	ASN
1	A	115	ASN
1	A	178	ASN
1	A	193	GLN
1	A	246	ASN
1	A	360	GLN
1	A	407	ASN
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	435	GLN
1	A	462	ASN
1	A	481	ASN
1	A	482	ASN
1	A	499	ASN
1	B	52	ASN
1	B	75	ASN
1	B	78	HIS
1	B	115	ASN
1	B	127	ASN
1	B	190	ASN
1	B	232	HIS
1	B	248	HIS
1	B	276	GLN
1	B	399	ASN
1	B	481	ASN
1	B	482	ASN
1	B	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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	490/512 (95%)	0.53	22 (4%) 38 33	7, 45, 75, 94	1 (0%)
1	B	495/512 (96%)	0.87	61 (12%) 8 7	8, 52, 85, 99	1 (0%)
All	All	985/1024 (96%)	0.70	83 (8%) 17 15	7, 48, 82, 99	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	SER	6.2
1	B	458	SER	5.0
1	B	153	TYR	4.1
1	B	148	ALA	3.9
1	B	171	PHE	3.8
1	B	245	TYR	3.8
1	B	164	ILE	3.7
1	B	46	ASP	3.7
1	B	49	GLY	3.5
1	B	108	GLY	3.4
1	B	112	GLY	3.4
1	B	113	GLY	3.2
1	B	216	CYS	3.1
1	A	425	LEU	3.1
1	A	370	ILE	3.0
1	A	202	THR	3.0
1	B	254	THR	3.0
1	B	241	ALA	3.0
1	B	235	LEU	3.0
1	A	12	MET	3.0
1	A	37	TYR	2.9
1	B	101	TRP	2.7
1	A	347	TYR	2.7
1	B	175	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASP	2.7
1	B	47	GLY	2.7
1	A	466	PHE	2.7
1	B	217	ALA	2.7
1	B	209	ARG	2.6
1	B	316	GLU	2.6
1	B	122	TYR	2.6
1	B	102	PRO	2.6
1	B	162	LYS	2.5
1	B	109	THR	2.5
1	B	169	THR	2.5
1	B	249	TYR	2.5
1	B	48	LYS	2.5
1	B	179	PHE	2.4
1	B	469	PHE	2.4
1	A	82	THR	2.4
1	A	269	GLY	2.4
1	A	316	GLU	2.4
1	B	56	PHE	2.4
1	B	59	ASN	2.4
1	A	424	ALA	2.4
1	B	401	PRO	2.3
1	B	55	HIS	2.3
1	B	239	ALA	2.3
1	B	167	ASP	2.3
1	B	35	SER	2.3
1	B	218	TYR	2.3
1	B	155	GLY	2.3
1	A	14	SER	2.2
1	B	177	ASP	2.2
1	B	178	ASN	2.2
1	A	213	GLY	2.2
1	B	176	PHE	2.2
1	B	320	LYS	2.2
1	B	201	GLY	2.2
1	B	199	SER	2.2
1	B	279	GLU	2.2
1	B	311	PRO	2.2
1	A	482	ASN	2.1
1	A	410	GLY	2.1
1	B	182	LYS	2.1
1	B	244	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	TYR	2.1
1	A	342	ASP	2.1
1	A	359	SER	2.1
1	B	158	ASP	2.1
1	A	312	PHE	2.1
1	B	161	HIS	2.1
1	B	130	LEU	2.1
1	A	307	ARG	2.1
1	A	349	PRO	2.1
1	B	97	PHE	2.1
1	B	306	ALA	2.1
1	B	480	ARG	2.1
1	B	321	LEU	2.0
1	B	410	GLY	2.0
1	B	350	VAL	2.0
1	B	296	GLY	2.0
1	B	315	ASP	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.