



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:43 am GMT

PDB ID : 5D06
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme
Authors : Zhai, L.; Xiang, S.
Deposited on : 2015-08-02
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

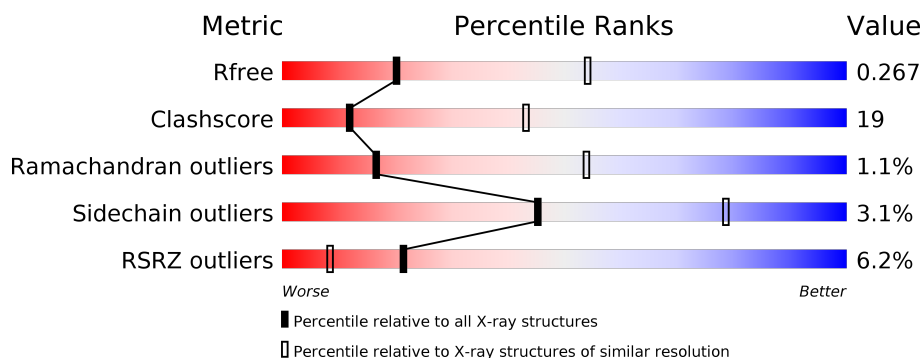
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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

Mol	Chain	Length	Quality of chain
1	A	1528	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	1528	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>..</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24403 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.

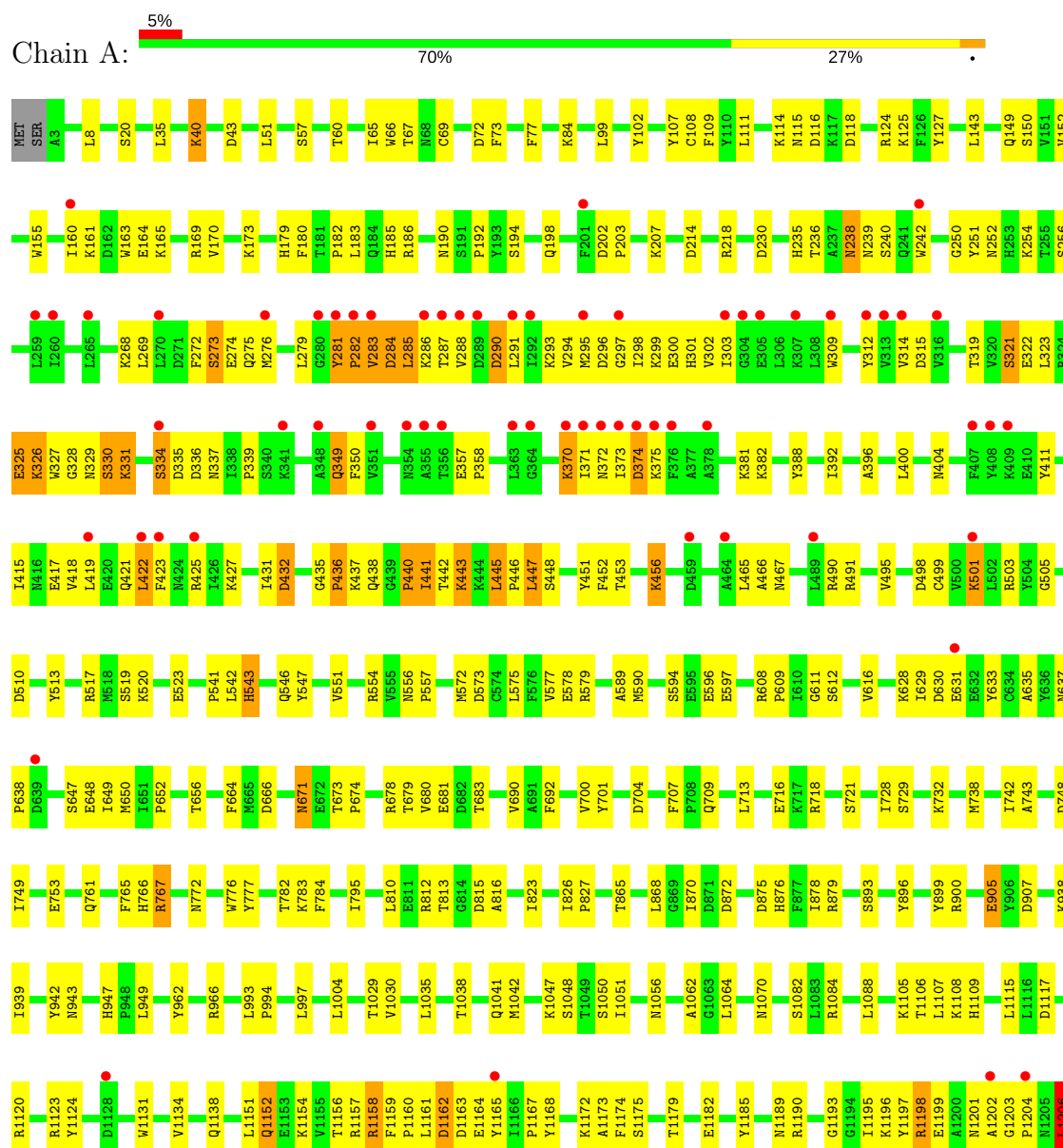
- Molecule 1 is a protein called Uncharacterized protein.

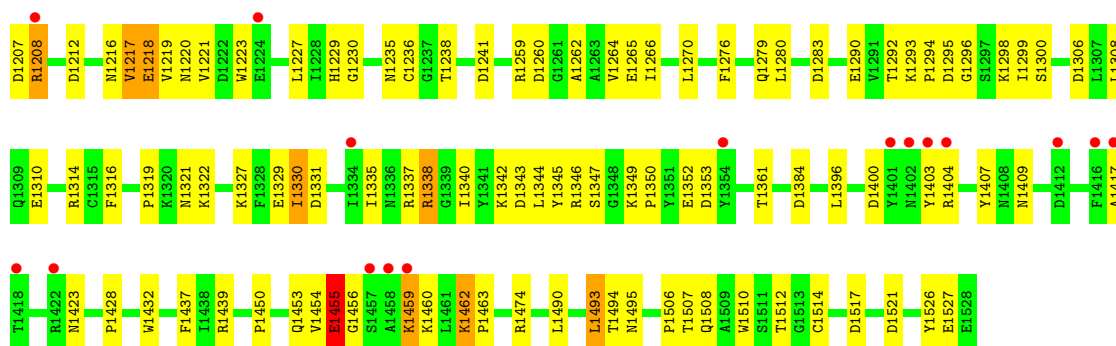
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2065	2331	52			
1	B	1506	Total	C	N	O	S	0	0	0
			12125	7736	2038	2299	52			

3 Residue-property plots

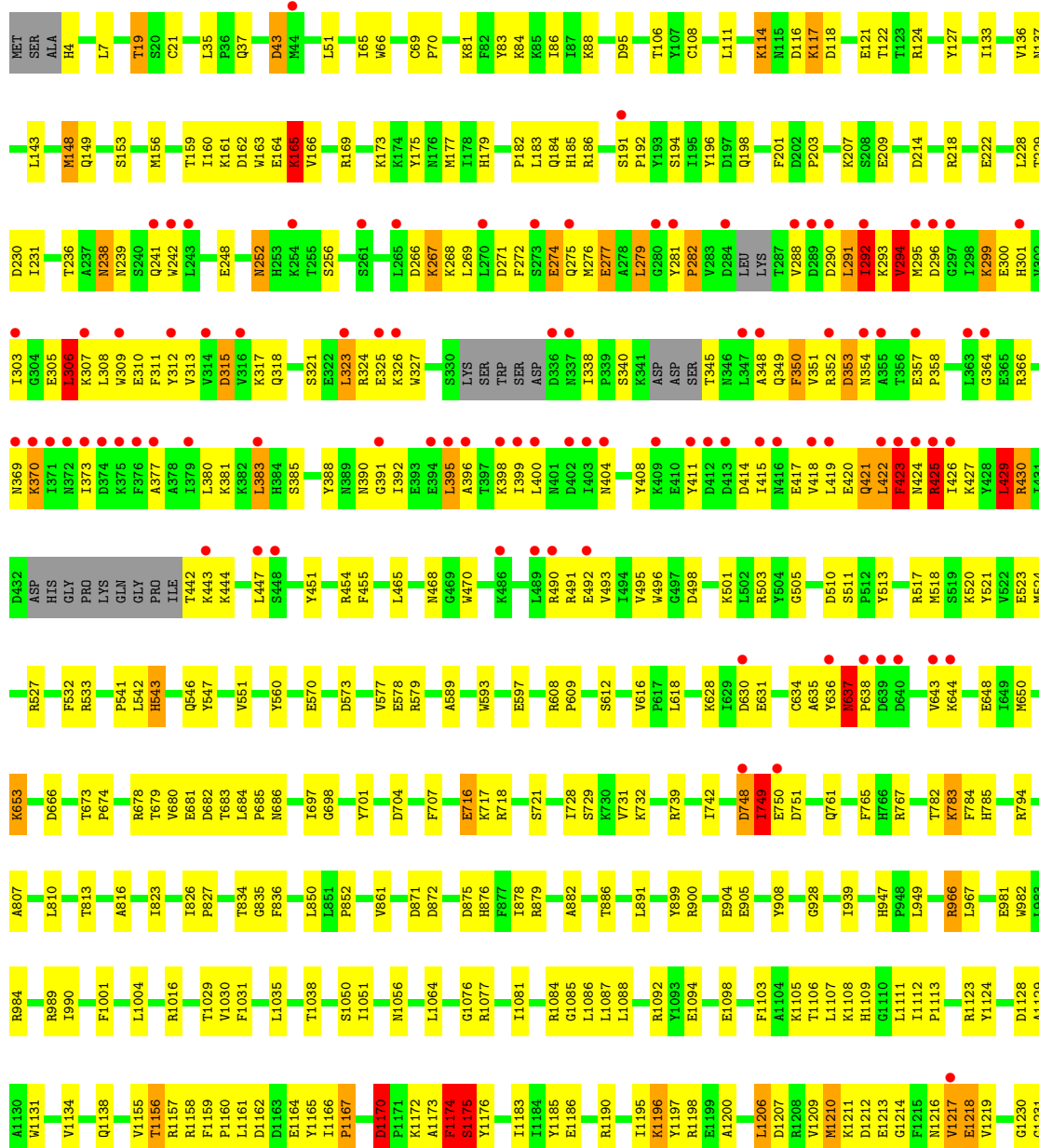
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncharacterized protein





• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.27Å 198.95Å 261.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.75 – 3.10 48.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.75-3.10) 97.3 (48.22-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.268 0.235 , 0.267	Depositor DCC
R_{free} test set	2608 reflections (3.56%)	DCC
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24403	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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	0.41	1/12589 (0.0%)	0.77	21/17071 (0.1%)
1	B	0.91	13/12427 (0.1%)	0.90	48/16845 (0.3%)
All	All	0.71	14/25016 (0.1%)	0.84	69/33916 (0.2%)

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	7
1	B	0	8
All	All	0	15

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1174	PHE	CG-CD1	67.60	2.40	1.38
1	B	1174	PHE	CD2-CE2	27.54	1.94	1.39
1	B	1174	PHE	CG-CD2	22.46	1.72	1.38
1	B	1174	PHE	CB-CG	20.87	1.86	1.51
1	B	1174	PHE	CD1-CE1	20.43	1.80	1.39
1	B	1174	PHE	CE1-CZ	20.41	1.76	1.37
1	B	1174	PHE	CE2-CZ	13.35	1.62	1.37
1	B	1510	TRP	CB-CG	11.64	1.71	1.50
1	B	1174	PHE	CA-CB	7.72	1.71	1.53
1	A	1208	ARG	CG-CD	6.96	1.69	1.51
1	B	1511	SER	N-CA	-5.65	1.35	1.46
1	B	1510	TRP	CA-CB	5.57	1.66	1.53
1	B	1217	VAL	CB-CG2	-5.47	1.41	1.52
1	B	1432	TRP	CB-CG	-5.37	1.40	1.50

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1174	PHE	CB-CG-CD1	25.99	138.99	120.80
1	B	1174	PHE	CB-CG-CD2	-16.14	109.50	120.80
1	A	285	LEU	CB-CG-CD2	-10.37	93.38	111.00
1	B	425	ARG	CB-CG-CD	10.31	138.41	111.60
1	B	291	LEU	CA-CB-CG	8.81	135.56	115.30
1	A	445	LEU	CA-CB-CG	8.77	135.46	115.30
1	B	429	LEU	CA-CB-CG	8.46	134.77	115.30
1	B	383	LEU	CA-CB-CG	-7.88	97.16	115.30
1	B	1490	LEU	CB-CG-CD2	-7.66	97.98	111.00
1	B	1510	TRP	CA-C-N	-7.61	100.46	117.20
1	B	1156	THR	CA-CB-CG2	-7.42	102.02	112.40
1	B	1510	TRP	CA-CB-CG	7.21	127.40	113.70
1	B	1512	THR	CA-CB-CG2	7.15	122.41	112.40
1	B	370	LYS	CD-CE-NZ	-6.95	95.72	111.70
1	B	1206	LEU	CA-CB-CG	6.95	131.28	115.30
1	B	1493	LEU	CA-CB-CG	6.84	131.04	115.30
1	B	1511	SER	N-CA-CB	-6.83	100.26	110.50
1	B	1512	THR	N-CA-CB	6.82	123.27	110.30
1	A	422	LEU	CB-CG-CD2	-6.82	99.41	111.00
1	B	1396	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	432	ASP	CB-CG-OD1	-6.75	112.23	118.30
1	B	395	LEU	CA-CB-CG	6.67	130.63	115.30
1	A	422	LEU	CA-CB-CG	6.55	130.38	115.30
1	B	165	LYS	CG-CD-CE	-6.52	92.35	111.90
1	B	966	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	1512	THR	CB-CA-C	-6.47	94.12	111.60
1	B	1509	ALA	CA-C-N	-6.39	103.15	117.20
1	A	1208	ARG	CB-CG-CD	6.27	127.91	111.60
1	A	1203	GLY	N-CA-C	-6.25	97.46	113.10
1	B	279	LEU	CA-CB-CG	6.22	129.61	115.30
1	B	291	LEU	CB-CG-CD1	-5.89	100.98	111.00
1	A	290	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	1174	PHE	N-CA-C	-5.81	95.32	111.00
1	B	1174	PHE	CZ-CE2-CD2	5.74	126.99	120.10
1	B	1490	LEU	CA-CB-CG	5.73	128.48	115.30
1	B	1174	PHE	CD1-CE1-CZ	-5.66	113.31	120.10
1	B	1174	PHE	CD1-CG-CD2	-5.62	110.99	118.30
1	B	292	ILE	CA-CB-CG1	-5.60	100.35	111.00
1	B	423	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	A	1493	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	B	1175	SER	N-CA-C	5.54	125.97	111.00
1	A	290	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	1208	ARG	NE-CZ-NH1	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	VAL	N-CA-C	-5.49	96.19	111.00
1	A	419	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	1426	GLN	CA-CB-CG	5.43	125.35	113.40
1	B	306	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	1174	PHE	CE1-CZ-CE2	5.42	129.75	120.00
1	A	281	TYR	C-N-CA	-5.41	99.30	122.00
1	B	294	VAL	CB-CA-C	-5.39	101.16	111.40
1	B	748	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	349	GLN	CA-CB-CG	5.36	125.19	113.40
1	B	1170	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	277	GLU	CA-CB-CG	-5.30	101.75	113.40
1	B	315	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	1493	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	1210	MET	CA-CB-CG	5.25	122.22	113.30
1	B	423	PHE	CB-CG-CD2	5.19	124.43	120.80
1	B	1509	ALA	N-CA-C	-5.19	97.00	111.00
1	A	1152	GLN	CA-CB-CG	-5.15	102.07	113.40
1	A	1208	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	353	ASP	N-CA-C	5.13	124.86	111.00
1	A	1206	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	309	TRP	CA-CB-CG	-5.12	103.98	113.70
1	B	1414	ASP	N-CA-C	5.09	124.74	111.00
1	B	429	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	447	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	1513	GLY	N-CA-C	-5.04	100.50	113.10
1	A	876	HIS	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1158	ARG	Peptide
1	A	1217	VAL	Peptide
1	A	1218	GLU	Peptide
1	A	330	SER	Peptide
1	A	331	LYS	Peptide
1	A	436	PRO	Peptide
1	A	650	MET	Peptide
1	B	1174	PHE	Peptide
1	B	1218	GLU	Peptide
1	B	1509	ALA	Peptide
1	B	277	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	306	LEU	Peptide
1	B	421	GLN	Peptide
1	B	442	THR	Peptide
1	B	783	LYS	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	12278	0	11960	403	0
1	B	12125	0	11812	522	4
All	All	24403	0	23772	925	4

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:PHE:CE1	1:B:1174:PHE:CZ	1.76	1.68
1:B:1174:PHE:CD1	1:B:1174:PHE:CE1	1.80	1.64
1:B:1174:PHE:CG	1:B:1174:PHE:CB	1.86	1.56
1:B:1174:PHE:CD2	1:B:1174:PHE:CE2	1.94	1.55
1:B:1508:GLN:HB3	1:B:1510:TRP:HB3	1.21	1.16
1:B:1510:TRP:CE3	1:B:1511:SER:HB2	1.88	1.08
1:B:1174:PHE:CD1	1:B:1174:PHE:CG	2.40	1.08
1:B:425:ARG:HG2	1:B:426:ILE:N	1.69	1.07
1:B:678:ARG:HB2	1:B:783:LYS:HD3	1.30	1.07
1:B:1196:LYS:HG3	1:B:1218:GLU:HG3	1.33	1.02
1:A:282:PRO:HG2	1:A:294:VAL:HG22	1.40	1.02
1:B:165:LYS:HG3	1:B:166:VAL:H	0.89	1.02
1:B:165:LYS:HG3	1:B:166:VAL:N	1.72	1.01
1:A:1196:LYS:HA	1:A:1218:GLU:CG	1.90	1.01
1:B:1160:PRO:HG3	1:B:1164:GLU:H	1.28	0.99
1:B:682:ASP:HB2	1:B:783:LYS:HB3	1.43	0.98
1:A:1196:LYS:CA	1:A:1218:GLU:HG3	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.46	0.97
1:B:425:ARG:HG2	1:B:426:ILE:H	1.19	0.95
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.46	0.95
1:B:165:LYS:CG	1:B:166:VAL:H	1.80	0.95
1:B:1510:TRP:HE3	1:B:1511:SER:HB2	1.27	0.94
1:B:198:GLN:OE1	1:B:517:ARG:NH1	2.01	0.92
1:B:156:MET:O	1:B:165:LYS:NZ	2.03	0.92
1:B:422:LEU:HB3	1:B:425:ARG:HD3	1.53	0.90
1:B:468:ASN:HB3	1:B:501:LYS:HB2	1.54	0.90
1:B:679:THR:O	1:B:783:LYS:NZ	2.04	0.90
1:B:1035:LEU:HD22	1:B:1512:THR:HG22	1.55	0.89
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.38	0.89
1:B:1490:LEU:HB2	1:B:1510:TRP:CZ2	2.07	0.88
1:B:1320:LYS:O	1:B:1338:ARG:NH1	2.06	0.87
1:A:1196:LYS:HA	1:A:1218:GLU:HG3	0.96	0.87
1:A:400:LEU:O	1:A:404:ASN:ND2	2.08	0.86
1:B:425:ARG:HD2	1:B:426:ILE:HD12	1.57	0.86
1:A:349:GLN:O	1:A:349:GLN:HG2	1.76	0.85
1:A:432:ASP:OD1	1:A:435:GLY:N	2.07	0.85
1:B:1401:TYR:O	1:B:1404:ARG:NH2	2.09	0.85
1:A:283:VAL:HG11	1:A:441:ILE:HG12	1.57	0.84
1:B:742:ILE:HG21	1:B:767:ARG:HH21	1.41	0.84
1:B:1508:GLN:CB	1:B:1510:TRP:HB3	2.04	0.84
1:B:323:LEU:HD21	1:B:377:ALA:HB2	1.60	0.83
1:B:307:LYS:O	1:B:309:TRP:N	2.11	0.83
1:A:1198:ARG:NH2	1:A:1212:ASP:O	2.11	0.83
1:B:426:ILE:HA	1:B:429:LEU:HB2	1.60	0.83
1:B:608:ARG:HE	1:B:750:GLU:HB3	1.44	0.82
1:A:452:PHE:HA	1:A:466:ALA:HA	1.59	0.82
1:B:1432:TRP:HB3	1:B:1511:SER:OG	1.80	0.82
1:B:678:ARG:CB	1:B:783:LYS:HD3	2.10	0.82
1:B:313:VAL:HG13	1:B:404:ASN:HD22	1.44	0.82
1:A:721:SER:OG	1:A:823:ILE:O	1.97	0.82
1:A:328:GLY:H	1:A:331:LYS:HZ3	1.28	0.81
1:B:682:ASP:OD2	1:B:686:ASN:HB2	1.79	0.81
1:B:721:SER:OG	1:B:823:ILE:O	1.97	0.81
1:A:1204:PRO:HB2	1:A:1208:ARG:HH11	1.45	0.81
1:A:1204:PRO:HB2	1:A:1208:ARG:NH1	1.96	0.81
1:A:295:MET:SD	1:A:423:PHE:HB3	2.20	0.81
1:B:682:ASP:HB2	1:B:783:LYS:CB	2.10	0.80
1:B:1158:ARG:HA	1:B:1173:ALA:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ASP:OD1	1:B:354:ASN:N	2.15	0.80
1:A:1217:VAL:O	1:A:1218:GLU:HG2	1.81	0.79
1:B:1172:LYS:HA	1:B:1175:SER:HB3	1.64	0.79
1:A:186:ARG:NH2	1:A:202:ASP:OD2	2.16	0.78
1:B:1103:PHE:HB3	1:B:1112:ILE:HD11	1.66	0.78
1:A:251:TYR:HB2	1:A:501:LYS:HE2	1.66	0.78
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.65	0.78
1:A:1342:LYS:HE2	1:A:1353:ASP:HB3	1.65	0.77
1:A:325:GLU:OE1	1:A:325:GLU:N	2.17	0.77
1:A:1220:ASN:OD1	1:A:1221:VAL:N	2.13	0.77
1:A:72:ASP:OD1	1:A:73:PHE:N	2.15	0.77
1:B:1217:VAL:HG13	1:B:1231:GLY:HA2	1.65	0.77
1:B:1508:GLN:HB3	1:B:1510:TRP:CB	2.10	0.77
1:B:520:LYS:HA	1:B:523:GLU:HB2	1.67	0.77
1:A:326:LYS:CE	1:A:374:ASP:HB3	2.14	0.77
1:A:1322:LYS:HD2	1:A:1322:LYS:H	1.49	0.77
1:A:1158:ARG:O	1:A:1159:PHE:HD2	1.68	0.76
1:B:353:ASP:CG	1:B:354:ASN:HD22	1.89	0.75
1:A:442:THR:HG22	1:A:443:LYS:H	1.51	0.75
1:B:315:ASP:H	1:B:370:LYS:NZ	1.84	0.75
1:B:1510:TRP:CZ2	1:B:1512:THR:HG23	2.22	0.74
1:A:291:LEU:HA	1:A:294:VAL:HG23	1.69	0.74
1:A:748:ASP:OD1	1:A:749:ILE:N	2.20	0.74
1:B:1396:LEU:HD23	1:B:1426:GLN:HB2	1.70	0.74
1:B:156:MET:HB3	1:B:165:LYS:HZ1	1.53	0.73
1:A:114:LYS:NZ	1:A:118:ASP:OD1	2.21	0.73
1:B:117:LYS:N	1:B:117:LYS:HD3	2.02	0.73
1:B:1196:LYS:CG	1:B:1218:GLU:HG3	2.14	0.73
1:B:1160:PRO:HG3	1:B:1164:GLU:N	2.03	0.73
1:A:1062:ALA:HB1	1:A:1510:TRP:HZ3	1.54	0.73
1:A:238:ASN:OD1	1:A:239:ASN:ND2	2.21	0.73
1:B:634:CYS:HB3	1:B:636:TYR:HE1	1.52	0.73
1:B:1400:ASP:OD2	1:B:1402:ASN:N	2.17	0.73
1:B:162:ASP:O	1:B:165:LYS:NZ	2.21	0.73
1:B:143:LEU:HD23	1:B:560:TYR:HE2	1.53	0.72
1:B:443:LYS:O	1:B:444:LYS:HG2	1.89	0.72
1:B:1108:LYS:HE2	1:B:1109:HIS:CE1	2.23	0.72
1:A:1108:LYS:HG2	1:A:1109:HIS:CD2	2.24	0.72
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.22	0.72
1:B:1165:TYR:O	1:B:1167:PRO:HD3	1.89	0.72
1:B:185:HIS:HB2	1:B:203:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ALA:HB3	1:A:501:LYS:HE3	1.72	0.72
1:B:1156:THR:O	1:B:1156:THR:HG22	1.83	0.72
1:B:1197:TYR:H	1:B:1218:GLU:CD	1.92	0.72
1:B:422:LEU:O	1:B:424:ASN:N	2.23	0.72
1:A:1316:PHE:O	1:A:1342:LYS:HB2	1.89	0.72
1:B:680:VAL:HG11	1:B:826:ILE:HD13	1.72	0.71
1:B:306:LEU:HD23	1:B:309:TRP:HE1	1.56	0.71
1:A:1117:ASP:O	1:A:1120:ARG:HG2	1.91	0.71
1:A:738:MET:HB3	1:A:776:TRP:CH2	2.26	0.71
1:A:1306:ASP:O	1:A:1310:GLU:HG3	1.91	0.70
1:B:1108:LYS:HD2	1:B:1159:PHE:CE2	2.27	0.70
1:B:636:TYR:CE1	1:B:643:VAL:HG13	2.27	0.70
1:A:335:ASP:OD1	1:A:336:ASP:N	2.24	0.70
1:A:680:VAL:HG11	1:A:826:ILE:HD13	1.74	0.70
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.27	0.70
1:B:1407:TYR:CE1	1:B:1424:TYR:HD1	2.10	0.69
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.24	0.69
1:B:608:ARG:NE	1:B:750:GLU:HB3	2.07	0.69
1:B:143:LEU:HD23	1:B:560:TYR:CE2	2.28	0.69
1:A:251:TYR:O	1:A:501:LYS:NZ	2.26	0.69
1:A:251:TYR:HB2	1:A:501:LYS:CE	2.21	0.69
1:A:328:GLY:N	1:A:331:LYS:HZ3	1.91	0.69
1:B:292:ILE:HA	1:B:294:VAL:HG22	1.75	0.69
1:A:40:LYS:N	1:A:43:ASP:OD2	2.25	0.69
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.25	0.69
1:B:636:TYR:O	1:B:637:ASN:HB3	1.92	0.69
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.57	0.69
1:B:306:LEU:HD23	1:B:309:TRP:NE1	2.08	0.69
1:B:716:GLU:OE2	1:B:718:ARG:NH1	2.25	0.69
1:A:629:ILE:HD13	1:A:631:GLU:HB2	1.73	0.68
1:B:420:GLU:HA	1:B:423:PHE:CB	2.23	0.68
1:A:647:SER:OG	1:A:648:GLU:N	2.27	0.68
1:B:513:TYR:CZ	1:B:517:ARG:HD3	2.29	0.68
1:A:326:LYS:HE2	1:A:329:ASN:HB2	1.75	0.67
1:B:1432:TRP:N	1:B:1511:SER:HB3	2.10	0.67
1:A:1163:ASP:OD1	1:A:1190:ARG:NH2	2.28	0.67
1:B:1508:GLN:O	1:B:1510:TRP:HD1	1.76	0.67
1:B:238:ASN:OD1	1:B:239:ASN:ND2	2.25	0.67
1:A:1407:TYR:OH	1:A:1409:ASN:ND2	2.27	0.67
1:B:784:PHE:O	1:B:785:HIS:ND1	2.27	0.67
1:B:1213:GLU:HG3	1:B:1234:PHE:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HB3	1:B:165:LYS:NZ	2.09	0.66
1:B:290:ASP:OD1	1:B:293:LYS:HB2	1.96	0.66
1:B:520:LYS:O	1:B:520:LYS:HD2	1.96	0.66
1:B:1232:SER:N	1:B:1235:ASN:HD22	1.92	0.66
1:A:287:THR:HG22	1:A:288:VAL:H	1.60	0.65
1:B:292:ILE:HD13	1:B:427:LYS:HE2	1.76	0.65
1:A:1327:LYS:HG2	1:A:1327:LYS:O	1.97	0.65
1:B:299:LYS:HG2	1:B:300:GLU:N	2.10	0.65
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.26	0.65
1:B:1391:VAL:O	1:B:1431:VAL:HG13	1.97	0.65
1:A:240:SER:HB3	1:A:242:TRP:NE1	2.11	0.65
1:A:422:LEU:HA	1:A:425:ARG:HG3	1.79	0.65
1:A:150:SER:OG	1:A:700:VAL:HA	1.96	0.65
1:A:326:LYS:NZ	1:A:326:LYS:O	2.21	0.65
1:A:161:LYS:O	1:A:161:LYS:HD2	1.96	0.64
1:A:327:TRP:CE2	1:A:381:LYS:HE2	2.32	0.64
1:A:422:LEU:HG	1:A:425:ARG:HH21	1.62	0.64
1:B:268:LYS:O	1:B:268:LYS:HG3	1.95	0.64
1:B:1232:SER:OG	1:B:1235:ASN:ND2	2.31	0.64
1:A:520:LYS:HA	1:A:523:GLU:HG2	1.78	0.64
1:B:323:LEU:HD22	1:B:327:TRP:HE3	1.62	0.64
1:A:748:ASP:OD1	1:A:749:ILE:HG22	1.97	0.64
1:A:1108:LYS:HE3	1:A:1159:PHE:CD1	2.33	0.64
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.80	0.64
1:A:671:ASN:N	1:A:671:ASN:OD1	2.31	0.64
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.33	0.63
1:B:267:LYS:HE3	1:B:454:ARG:NH1	2.14	0.63
1:B:682:ASP:HB2	1:B:783:LYS:CD	2.28	0.63
1:B:1481:TRP:HB3	1:B:1490:LEU:HD21	1.80	0.63
1:A:284:ASP:OD1	1:A:440:PRO:HA	1.99	0.63
1:B:1157:ARG:HH12	1:B:1186:GLU:CD	2.02	0.63
1:B:312:TYR:OH	1:B:414:ASP:OD2	2.15	0.63
1:B:451:TYR:CZ	1:B:491:ARG:HD2	2.34	0.63
1:B:1164:GLU:HG3	1:B:1165:TYR:O	1.99	0.62
1:B:267:LYS:HE3	1:B:454:ARG:HH11	1.64	0.62
1:B:628:LYS:HE2	1:B:630:ASP:O	2.00	0.62
1:B:682:ASP:HB2	1:B:783:LYS:HE3	1.81	0.62
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.17	0.62
1:B:269:LEU:HA	1:B:272:PHE:HB3	1.82	0.62
1:B:317:LYS:O	1:B:321:SER:OG	2.15	0.62
1:A:273:SER:OG	1:A:273:SER:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:O	1:B:348:ALA:HB3	2.00	0.62
1:B:116:ASP:HB2	1:B:117:LYS:NZ	2.15	0.62
1:B:608:ARG:HE	1:B:750:GLU:CB	2.12	0.62
1:B:749:ILE:HG23	1:B:750:GLU:H	1.65	0.62
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.32	0.62
1:B:1159:PHE:HB3	1:B:1160:PRO:CD	2.30	0.62
1:B:1402:ASN:HB3	1:B:1426:GLN:HE21	1.63	0.62
1:B:1490:LEU:HB2	1:B:1510:TRP:CH2	2.34	0.62
1:A:466:ALA:H	1:A:501:LYS:HZ2	1.47	0.62
1:B:1481:TRP:HB3	1:B:1490:LEU:CD2	2.30	0.62
1:A:327:TRP:CZ2	1:A:381:LYS:HE2	2.34	0.61
1:A:427:LYS:O	1:A:431:ILE:N	2.33	0.61
1:B:114:LYS:HE2	1:B:118:ASP:HA	1.82	0.61
1:B:423:PHE:HA	1:B:425:ARG:NH2	2.15	0.61
1:A:1160:PRO:HG2	1:A:1164:GLU:HB3	1.82	0.61
1:A:314:VAL:N	1:A:404:ASN:OD1	2.30	0.61
1:B:1293:LYS:HB3	1:B:1294:PRO:HD2	1.81	0.61
1:B:682:ASP:CB	1:B:783:LYS:HB3	2.26	0.61
1:A:513:TYR:CZ	1:A:517:ARG:HG3	2.35	0.61
1:B:156:MET:C	1:B:165:LYS:HZ2	2.01	0.61
1:B:417:GLU:OE1	1:B:417:GLU:N	2.33	0.61
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.32	0.61
1:B:323:LEU:HD22	1:B:327:TRP:CE3	2.34	0.61
1:B:505:GLY:HA3	1:B:510:ASP:HB3	1.83	0.61
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.81	0.61
1:B:1381:GLU:O	1:B:1385:GLN:HG3	2.00	0.61
1:A:326:LYS:HE3	1:A:374:ASP:HB3	1.82	0.61
1:B:185:HIS:CD2	1:B:196:TYR:CD1	2.89	0.61
1:B:875:ASP:OD2	1:B:879:ARG:NH1	2.34	0.61
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.82	0.61
1:B:182:PRO:HG2	1:B:192:PRO:O	2.01	0.60
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.02	0.60
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.66	0.60
1:B:1510:TRP:CE2	1:B:1512:THR:HG23	2.36	0.60
1:A:1432:TRP:CB	1:A:1510:TRP:HD1	2.14	0.60
1:A:608:ARG:HD2	1:A:749:ILE:HG12	1.83	0.60
1:A:1490:LEU:HD12	1:A:1512:THR:HG22	1.83	0.60
1:B:1337:ARG:HD3	1:B:1382:LEU:HD22	1.83	0.60
1:B:748:ASP:CG	1:B:749:ILE:H	2.00	0.60
1:B:1398:PRO:HA	1:B:1403:TYR:CD2	2.37	0.60
1:A:425:ARG:NH2	1:A:491:ARG:HB3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1105:LYS:HE2	1:B:1156:THR:O	2.01	0.60
1:B:422:LEU:CB	1:B:425:ARG:HD3	2.29	0.60
1:A:236:THR:HG21	1:A:242:TRP:CZ2	2.37	0.59
1:A:321:SER:OG	1:A:322:GLU:N	2.33	0.59
1:A:520:LYS:HA	1:A:523:GLU:CG	2.32	0.59
1:B:900:ARG:NH1	1:B:904:GLU:O	2.34	0.59
1:A:421:GLN:O	1:A:425:ARG:HG2	2.02	0.59
1:B:1138:GLN:HE22	1:B:1275:ARG:HH21	1.49	0.59
1:A:198:GLN:NE2	1:A:236:THR:OG1	2.35	0.59
1:B:1508:GLN:O	1:B:1510:TRP:CD1	2.55	0.59
1:B:1035:LEU:CD2	1:B:1512:THR:HG22	2.31	0.59
1:A:441:ILE:O	1:A:442:THR:OG1	2.18	0.59
1:A:1108:LYS:HE3	1:A:1159:PHE:HD1	1.66	0.59
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.34	0.59
1:A:1350:PRO:O	1:A:1353:ASP:HB2	2.02	0.59
1:A:328:GLY:H	1:A:331:LYS:NZ	1.99	0.59
1:A:1204:PRO:CB	1:A:1208:ARG:HG2	2.33	0.58
1:A:1229:HIS:HE1	1:A:1346:ARG:HG2	1.68	0.58
1:A:281:TYR:CE2	1:A:293:LYS:HD3	2.37	0.58
1:B:1166:ILE:HD12	1:B:1166:ILE:N	2.18	0.58
1:B:1217:VAL:HG22	1:B:1235:ASN:CG	2.23	0.58
1:B:420:GLU:HA	1:B:423:PHE:HB2	1.84	0.58
1:A:185:HIS:HB2	1:A:203:PRO:HD3	1.85	0.58
1:B:1213:GLU:HG3	1:B:1234:PHE:CB	2.33	0.58
1:B:1314:ARG:NH1	1:B:1329:GLU:OE2	2.35	0.58
1:B:1402:ASN:HB3	1:B:1426:GLN:NE2	2.18	0.58
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.38	0.58
1:B:420:GLU:HA	1:B:423:PHE:HB3	1.85	0.58
1:B:682:ASP:HB2	1:B:783:LYS:CE	2.33	0.58
1:B:421:GLN:HE22	1:B:492:GLU:CG	2.16	0.58
1:B:673:THR:HG21	1:B:707:PHE:O	2.02	0.58
1:B:425:ARG:CG	1:B:426:ILE:N	2.57	0.58
1:A:765:PHE:HE2	1:A:767:ARG:HB2	1.68	0.58
1:B:1407:TYR:OH	1:B:1409:ASN:OD1	2.21	0.58
1:A:1042:MET:HE1	1:A:1507:THR:HG22	1.86	0.58
1:A:1217:VAL:HG12	1:A:1235:ASN:OD1	2.04	0.58
1:A:326:LYS:NZ	1:A:374:ASP:HB3	2.18	0.58
1:B:398:LYS:HG3	1:B:399:ILE:N	2.18	0.58
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	2.04	0.57
1:A:1292:THR:HG22	1:A:1298:LYS:NZ	2.18	0.57
1:A:1299:ILE:HG22	1:A:1300:SER:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:CG1	1:A:441:ILE:HG12	2.32	0.57
1:B:1403:TYR:O	1:B:1404:ARG:HD3	2.03	0.57
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.05	0.57
1:B:682:ASP:CB	1:B:783:LYS:HD2	2.35	0.57
1:A:290:ASP:OD1	1:A:290:ASP:N	2.37	0.57
1:B:1272:SER:HB2	1:B:1275:ARG:NH2	2.20	0.57
1:B:315:ASP:HB2	1:B:370:LYS:HZ1	1.68	0.57
1:A:1204:PRO:HB3	1:A:1208:ARG:HG2	1.85	0.57
1:B:309:TRP:CD1	1:B:411:TYR:CE1	2.93	0.57
1:B:312:TYR:HE2	1:B:411:TYR:HD1	1.52	0.57
1:A:312:TYR:HE2	1:A:411:TYR:HD1	1.52	0.57
1:A:1417:ALA:O	1:A:1423:ASN:ND2	2.37	0.57
1:B:636:TYR:C	1:B:638:PRO:HD3	2.25	0.57
1:A:325:GLU:CD	1:A:326:LYS:HB3	2.25	0.56
1:B:1510:TRP:CG	1:B:1511:SER:N	2.68	0.56
1:A:1190:ARG:HG3	1:A:1195:ILE:HG22	1.87	0.56
1:B:369:ASN:C	1:B:370:LYS:HG2	2.25	0.56
1:A:1105:LYS:NZ	1:A:1158:ARG:HE	2.03	0.56
1:A:1106:THR:O	1:A:1124:TYR:OH	2.05	0.56
1:A:1038:THR:HG21	1:A:1512:THR:OG1	2.06	0.56
1:A:276:MET:HA	1:A:279:LEU:HG	1.88	0.56
1:A:423:PHE:O	1:A:427:LYS:HG3	2.06	0.56
1:A:630:ASP:OD1	1:A:635:ALA:HB3	2.06	0.56
1:B:682:ASP:OD1	1:B:685:PRO:HG2	2.05	0.56
1:A:1195:ILE:HD11	1:A:1219:VAL:HB	1.87	0.56
1:A:331:LYS:HG3	1:A:381:LYS:HZ1	1.70	0.56
1:B:148:MET:HE1	1:B:228:LEU:HD11	1.88	0.56
1:B:313:VAL:HG21	1:B:408:TYR:CE1	2.40	0.56
1:B:1195:ILE:O	1:B:1218:GLU:HB3	2.05	0.56
1:B:292:ILE:HD13	1:B:427:LYS:CE	2.35	0.56
1:A:1117:ASP:HB3	1:A:1120:ARG:O	2.06	0.56
1:A:466:ALA:H	1:A:501:LYS:NZ	2.03	0.56
1:B:1361:THR:HG21	1:B:1437:PHE:CA	2.29	0.56
1:B:505:GLY:HA3	1:B:510:ASP:CB	2.36	0.56
1:A:893:SER:HA	1:A:896:TYR:CD2	2.40	0.56
1:B:121:GLU:HG2	1:B:122:THR:H	1.71	0.55
1:B:315:ASP:H	1:B:370:LYS:HZ3	1.55	0.55
1:B:315:ASP:CB	1:B:370:LYS:NZ	2.68	0.55
1:A:1197:TYR:CD2	1:A:1218:GLU:OE2	2.59	0.55
1:B:1510:TRP:CE3	1:B:1511:SER:CB	2.77	0.55
1:A:312:TYR:CE2	1:A:411:TYR:HD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1396:LEU:HD11	1:B:1400:ASP:HB3	1.88	0.55
1:B:1482:ILE:HB	1:B:1490:LEU:CD1	2.36	0.55
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.07	0.55
1:B:1217:VAL:HG22	1:B:1235:ASN:ND2	2.22	0.55
1:B:1330:ILE:HD11	1:B:1335:ILE:HD12	1.89	0.55
1:A:1195:ILE:HD12	1:A:1218:GLU:CD	2.27	0.55
1:B:1245:GLU:O	1:B:1245:GLU:HG2	2.07	0.55
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.88	0.55
1:B:1050:SER:HB2	1:B:1056:ASN:HA	1.87	0.55
1:B:1350:PRO:O	1:B:1353:ASP:HB2	2.07	0.55
1:A:326:LYS:NZ	1:A:331:LYS:NZ	2.55	0.55
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.88	0.55
1:A:505:GLY:HA3	1:A:510:ASP:HB3	1.87	0.55
1:A:519:SER:O	1:A:523:GLU:HG2	2.06	0.55
1:B:717:LYS:HD2	1:B:717:LYS:O	2.06	0.55
1:A:1158:ARG:HA	1:A:1173:ALA:O	2.07	0.54
1:A:1361:THR:HG21	1:A:1437:PHE:CA	2.28	0.54
1:A:1450:PRO:HA	1:A:1453:GLN:OE1	2.07	0.54
1:B:1211:LYS:HB2	1:B:1213:GLU:CD	2.28	0.54
1:B:1418:THR:HA	1:B:1423:ASN:HB2	1.87	0.54
1:B:1465:SER:O	1:B:1469:ARG:HG2	2.07	0.54
1:A:1493:LEU:HD23	1:A:1494:THR:N	2.22	0.54
1:A:273:SER:HA	1:A:276:MET:HB3	1.90	0.54
1:A:251:TYR:HD1	1:A:501:LYS:HD3	1.73	0.54
1:A:1342:LYS:HD3	1:A:1344:LEU:O	2.07	0.54
1:A:330:SER:C	1:A:331:LYS:HD3	2.28	0.54
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.90	0.54
1:B:1157:ARG:NH1	1:B:1186:GLU:OE2	2.37	0.54
1:B:184:GLN:HA	1:B:201:PHE:HA	1.90	0.54
1:B:291:LEU:O	1:B:294:VAL:HG13	2.08	0.54
1:B:218:ARG:O	1:B:222:GLU:HG2	2.08	0.54
1:B:327:TRP:HZ3	1:B:392:ILE:HG21	1.72	0.54
1:B:391:GLY:O	1:B:395:LEU:HB2	2.08	0.54
1:B:395:LEU:HG	1:B:398:LYS:HZ2	1.73	0.54
1:B:116:ASP:HB2	1:B:117:LYS:HZ2	1.73	0.53
1:B:1510:TRP:CD2	1:B:1512:THR:N	2.76	0.53
1:B:718:ARG:HH21	1:B:823:ILE:HG13	1.73	0.53
1:B:276:MET:O	1:B:279:LEU:HB3	2.08	0.53
1:B:1031:PHE:CG	1:B:1479:ARG:HG3	2.43	0.53
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.43	0.53
1:B:1404:ARG:HB2	1:B:1423:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:O	1:B:256:SER:OG	2.23	0.53
1:B:276:MET:O	1:B:279:LEU:N	2.37	0.53
1:A:1432:TRP:HB3	1:A:1510:TRP:HD1	1.73	0.53
1:B:1170:ASP:HB2	1:B:1172:LYS:H	1.74	0.53
1:B:19:THR:HG22	1:B:21:CYS:O	2.07	0.53
1:A:1050:SER:OG	1:A:1051:ILE:N	2.39	0.53
1:B:248:GLU:HA	1:B:252:ASN:HD21	1.74	0.53
1:B:761:GLN:O	1:B:782:THR:HG22	2.09	0.53
1:A:1292:THR:HG22	1:A:1298:LYS:HZ2	1.73	0.53
1:A:315:ASP:O	1:A:319:THR:OG1	2.24	0.53
1:B:1160:PRO:O	1:B:1176:TYR:OH	2.05	0.53
1:B:1166:ILE:HD11	1:B:1200:ALA:HB1	1.90	0.53
1:B:1186:GLU:O	1:B:1190:ARG:HB2	2.09	0.53
1:B:1213:GLU:HG2	1:B:1214:GLY:N	2.23	0.53
1:B:470:TRP:HZ3	1:B:496:TRP:HE1	1.56	0.53
1:B:7:LEU:HD22	1:B:653:LYS:HB2	1.91	0.53
1:A:1279:GLN:NE2	1:A:1283:ASP:OD2	2.42	0.53
1:B:1474:ARG:HG2	1:B:1474:ARG:HH11	1.73	0.53
1:B:318:GLN:HA	1:B:321:SER:HG	1.74	0.53
1:B:1077:ARG:O	1:B:1081:ILE:HD12	2.09	0.53
1:B:1209:VAL:HG11	1:B:1245:GLU:HG3	1.91	0.53
1:B:1337:ARG:HD2	1:B:1340:ILE:HD11	1.90	0.53
1:B:185:HIS:HD2	1:B:196:TYR:CD1	2.26	0.53
1:B:395:LEU:O	1:B:398:LYS:HG2	2.09	0.53
1:A:630:ASP:HB3	1:A:633:TYR:HA	1.90	0.53
1:B:313:VAL:HG13	1:B:404:ASN:ND2	2.18	0.53
1:B:589:ALA:HB3	1:B:666:ASP:HA	1.91	0.53
1:A:1220:ASN:CG	1:A:1221:VAL:H	2.07	0.52
1:B:420:GLU:O	1:B:423:PHE:HB3	2.10	0.52
1:B:593:TRP:CD1	1:B:597:GLU:HG3	2.44	0.52
1:A:1432:TRP:HB3	1:A:1510:TRP:CD1	2.45	0.52
1:A:589:ALA:HB3	1:A:666:ASP:HA	1.91	0.52
1:B:1160:PRO:HG3	1:B:1164:GLU:HB3	1.89	0.52
1:A:1172:LYS:HA	1:A:1175:SER:HB2	1.92	0.52
1:B:1453:GLN:HB3	1:B:1461:LEU:HD23	1.91	0.52
1:B:422:LEU:O	1:B:425:ARG:HB3	2.09	0.52
1:B:939:ILE:HD11	1:B:947:HIS:CD2	2.44	0.52
1:B:981:GLU:OE1	1:B:984:ARG:NH2	2.39	0.52
1:A:1204:PRO:O	1:A:1208:ARG:HG3	2.10	0.52
1:A:1217:VAL:O	1:A:1218:GLU:CG	2.55	0.52
1:A:678:ARG:HB3	1:A:784:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:O	1:B:327:TRP:N	2.42	0.52
1:A:182:PRO:HG2	1:A:192:PRO:O	2.09	0.52
1:A:281:TYR:HE2	1:A:293:LYS:HD3	1.74	0.52
1:B:1352:GLU:HA	1:B:1355:GLN:HG3	1.90	0.52
1:A:326:LYS:HZ1	1:A:331:LYS:HZ2	1.56	0.52
1:A:673:THR:HG21	1:A:707:PHE:O	2.10	0.52
1:B:1106:THR:O	1:B:1124:TYR:OH	2.16	0.52
1:A:1494:THR:HG22	1:A:1495:ASN:O	2.10	0.52
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.90	0.52
1:A:337:ASN:HB3	1:A:350:PHE:CZ	2.44	0.52
1:A:870:ILE:HG12	1:A:993:LEU:HD22	1.91	0.52
1:B:1160:PRO:CG	1:B:1164:GLU:HB3	2.39	0.52
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.91	0.52
1:B:816:ALA:HB2	1:B:826:ILE:HG13	1.91	0.52
1:A:1156:THR:HG21	1:A:1174:PHE:CD1	2.45	0.52
1:A:1260:ASP:OD1	1:A:1347:SER:HB2	2.09	0.52
1:A:1270:LEU:HD23	1:A:1308:LEU:HD11	1.92	0.52
1:A:331:LYS:HB3	1:A:381:LYS:HZ2	1.74	0.52
1:A:505:GLY:HA3	1:A:510:ASP:CB	2.40	0.52
1:B:309:TRP:HD1	1:B:411:TYR:HH	1.58	0.52
1:A:1107:LEU:O	1:A:1157:ARG:NH2	2.43	0.51
1:A:296:ASP:HB3	1:A:299:LYS:HE3	1.92	0.51
1:A:870:ILE:HD11	1:A:997:LEU:CD1	2.40	0.51
1:B:1432:TRP:N	1:B:1511:SER:CB	2.73	0.51
1:B:315:ASP:H	1:B:370:LYS:HZ1	1.57	0.51
1:A:1109:HIS:CG	1:A:1197:TYR:CE2	2.98	0.51
1:A:288:VAL:N	1:A:290:ASP:OD1	2.43	0.51
1:A:452:PHE:CE1	1:A:466:ALA:HB2	2.45	0.51
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.39	0.51
1:A:629:ILE:HG22	1:A:649:ILE:HA	1.91	0.51
1:B:813:THR:O	1:B:827:PRO:HG2	2.10	0.51
1:B:1160:PRO:HG2	1:B:1162:ASP:C	2.29	0.51
1:A:1346:ARG:O	1:A:1346:ARG:HG3	2.09	0.51
1:B:1329:GLU:N	1:B:1329:GLU:OE1	2.43	0.51
1:A:813:THR:O	1:A:827:PRO:HG2	2.11	0.51
1:B:1210:MET:HE1	1:B:1234:PHE:O	2.11	0.51
1:A:1474:ARG:HG2	1:A:1474:ARG:HH11	1.76	0.51
1:B:1198:ARG:HG2	1:B:1216:ASN:HB3	1.93	0.51
1:B:323:LEU:HG	1:B:373:ILE:HG23	1.92	0.51
1:B:419:LEU:O	1:B:423:PHE:N	2.38	0.51
1:B:682:ASP:HA	1:B:685:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:HG21	1:B:242:TRP:CZ2	2.46	0.51
1:A:72:ASP:HA	1:A:102:TYR:CE2	2.46	0.51
1:A:1160:PRO:CG	1:A:1164:GLU:HB3	2.41	0.51
1:A:1474:ARG:NH1	1:A:1474:ARG:HG2	2.26	0.51
1:A:240:SER:HB3	1:A:242:TRP:CD1	2.46	0.51
1:A:337:ASN:O	1:A:339:PRO:HD3	2.11	0.51
1:B:252:ASN:OD1	1:B:465:LEU:HD22	2.11	0.51
1:B:765:PHE:HE2	1:B:767:ARG:HB2	1.76	0.51
1:A:322:GLU:O	1:A:373:ILE:HG21	2.11	0.50
1:B:1463:PRO:HD3	1:B:1526:TYR:CE1	2.46	0.50
1:A:1432:TRP:CG	1:A:1510:TRP:CD1	2.98	0.50
1:A:312:TYR:HE2	1:A:411:TYR:CD1	2.30	0.50
1:B:165:LYS:HD2	1:B:166:VAL:HG23	1.93	0.50
1:B:268:LYS:O	1:B:269:LEU:HD23	2.10	0.50
1:B:513:TYR:OH	1:B:517:ARG:HD3	2.10	0.50
1:B:836:PHE:CD1	1:B:852:PRO:HD3	2.46	0.50
1:B:1185:TYR:CG	1:B:1288:TYR:HD2	2.30	0.50
1:A:1029:THR:HG22	1:A:1030:VAL:H	1.77	0.50
1:A:114:LYS:NZ	1:A:118:ASP:HA	2.27	0.50
1:A:1403:TYR:O	1:A:1404:ARG:HD3	2.11	0.50
1:A:160:ILE:O	1:A:163:TRP:HB2	2.11	0.50
1:B:1404:ARG:O	1:B:1423:ASN:ND2	2.42	0.50
1:B:1432:TRP:CA	1:B:1511:SER:HB3	2.42	0.50
1:B:191:SER:HB3	1:B:498:ASP:OD2	2.12	0.50
1:A:296:ASP:CB	1:A:299:LYS:HE3	2.42	0.50
1:A:629:ILE:CD1	1:A:631:GLU:HB2	2.39	0.50
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.11	0.50
1:B:307:LYS:C	1:B:309:TRP:H	2.15	0.50
1:B:513:TYR:CE2	1:B:517:ARG:HD3	2.47	0.50
1:B:541:PRO:HB2	1:B:543:HIS:CE1	2.46	0.50
1:B:681:GLU:HA	1:B:810:LEU:HD23	1.93	0.50
1:A:411:TYR:CZ	1:A:415:ILE:HG13	2.47	0.50
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.47	0.50
1:B:318:GLN:HA	1:B:321:SER:OG	2.12	0.50
1:B:423:PHE:HA	1:B:425:ARG:CZ	2.42	0.50
1:A:325:GLU:HG2	1:A:326:LYS:HB3	1.94	0.50
1:A:812:ARG:NH2	1:A:815:ASP:OD1	2.45	0.50
1:B:1219:VAL:HG22	1:B:1230:GLY:HA3	1.94	0.50
1:B:1431:VAL:CG1	1:B:1510:TRP:HZ3	2.25	0.50
1:A:939:ILE:HD11	1:A:947:HIS:CD2	2.46	0.49
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:ARG:HA	1:A:1216:ASN:HA	1.93	0.49
1:A:1259:ARG:NH1	1:A:1343:ASP:OD2	2.44	0.49
1:A:453:THR:N	1:A:465:LEU:O	2.30	0.49
1:B:1402:ASN:HD22	1:B:1402:ASN:N	2.11	0.49
1:B:1403:TYR:C	1:B:1404:ARG:HD3	2.33	0.49
1:B:1431:VAL:HG11	1:B:1510:TRP:HZ3	1.78	0.49
1:A:114:LYS:HZ1	1:A:118:ASP:CG	2.14	0.49
1:A:273:SER:HA	1:A:276:MET:CB	2.42	0.49
1:A:447:LEU:HD12	1:A:448:SER:HB3	1.95	0.49
1:A:692:PHE:C	1:A:767:ARG:HH21	2.15	0.49
1:B:1396:LEU:C	1:B:1396:LEU:HD12	2.32	0.49
1:B:303:ILE:O	1:B:306:LEU:HD22	2.12	0.49
1:A:1105:LYS:NZ	1:A:1158:ARG:HH21	2.11	0.49
1:A:1330:ILE:HD12	1:A:1331:ASP:N	2.28	0.49
1:A:283:VAL:HG11	1:A:441:ILE:CG1	2.35	0.49
1:A:418:VAL:HG22	1:A:490:ARG:HA	1.94	0.49
1:B:742:ILE:HG21	1:B:767:ARG:NH2	2.20	0.49
1:B:882:ALA:HB2	1:B:982:TRP:CZ2	2.47	0.49
1:A:1462:LYS:HG3	1:A:1463:PRO:N	2.28	0.49
1:A:285:LEU:HD21	1:A:290:ASP:OD2	2.13	0.49
1:B:1213:GLU:CG	1:B:1214:GLY:N	2.76	0.49
1:B:679:THR:OG1	1:B:783:LYS:HE2	2.12	0.49
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.94	0.49
1:B:353:ASP:CG	1:B:354:ASN:N	2.65	0.49
1:B:1185:TYR:HE1	1:B:1290:GLU:O	1.95	0.49
1:B:162:ASP:O	1:B:165:LYS:HG2	2.12	0.49
1:A:1105:LYS:HE2	1:A:1156:THR:O	2.12	0.49
1:A:816:ALA:HB2	1:A:826:ILE:HG13	1.95	0.49
1:A:1229:HIS:CE1	1:A:1346:ARG:HG2	2.48	0.49
1:B:274:GLU:HG2	1:B:275:GLN:HG3	1.95	0.49
1:B:1432:TRP:CA	1:B:1511:SER:CB	2.91	0.48
1:B:315:ASP:CB	1:B:370:LYS:HZ1	2.26	0.48
1:A:1161:LEU:O	1:A:1161:LEU:HD23	2.13	0.48
1:A:1223:TRP:HD1	1:A:1293:LYS:HZ3	1.51	0.48
1:A:1330:ILE:HD11	1:A:1335:ILE:HD12	1.94	0.48
1:B:1396:LEU:CD2	1:B:1426:GLN:HB2	2.40	0.48
1:B:1407:TYR:CZ	1:B:1424:TYR:HD1	2.30	0.48
1:B:1459:LYS:HA	1:B:1459:LYS:HD2	1.36	0.48
1:A:1223:TRP:CD1	1:A:1293:LYS:NZ	2.76	0.48
1:B:357:GLU:HB3	1:B:358:PRO:HD2	1.95	0.48
1:B:127:TYR:HB2	1:B:578:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TRP:HE3	1:B:311:PHE:HB2	1.77	0.48
1:B:312:TYR:CE2	1:B:411:TYR:HD1	2.29	0.48
1:B:421:GLN:HE22	1:B:492:GLU:HG2	1.78	0.48
1:A:1115:LEU:HB3	1:A:1123:ARG:HB3	1.95	0.48
1:B:1287:LYS:HE3	1:B:1288:TYR:CE1	2.49	0.48
1:B:1291:VAL:HB	1:B:1299:ILE:HG13	1.96	0.48
1:B:338:ILE:HG23	1:B:383:LEU:HD22	1.96	0.48
1:B:231:ILE:HD12	1:B:532:PHE:CG	2.48	0.48
1:B:682:ASP:H	1:B:783:LYS:HE3	1.77	0.48
1:A:1238:THR:HG21	1:A:1259:ARG:HE	1.78	0.48
1:A:357:GLU:HB3	1:A:358:PRO:HD2	1.95	0.48
1:B:1259:ARG:HB3	1:B:1344:LEU:HD21	1.96	0.48
1:B:422:LEU:HA	1:B:425:ARG:HB3	1.96	0.48
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.95	0.48
1:A:299:LYS:HD2	1:A:300:GLU:HB3	1.95	0.48
1:B:748:ASP:CG	1:B:749:ILE:HG22	2.33	0.48
1:A:1107:LEU:C	1:A:1157:ARG:HH22	2.17	0.48
1:A:1342:LYS:NZ	1:A:1345:TYR:HA	2.29	0.48
1:A:252:ASN:OD1	1:A:254:LYS:HB2	2.14	0.48
1:A:683:THR:HG22	1:A:728:ILE:HG13	1.96	0.48
1:B:1400:ASP:OD2	1:B:1401:TYR:N	2.47	0.48
1:B:159:THR:O	1:B:163:TRP:CD1	2.67	0.48
1:A:761:GLN:O	1:A:782:THR:OG1	2.30	0.48
1:B:1230:GLY:O	1:B:1260:ASP:HA	2.13	0.48
1:B:274:GLU:OE1	1:B:274:GLU:N	2.47	0.48
1:B:396:ALA:O	1:B:400:LEU:HG	2.13	0.48
1:B:871:ASP:OD1	1:B:872:ASP:N	2.47	0.48
1:A:907:ASP:OD1	1:A:1047:LYS:HB2	2.14	0.47
1:A:1082:SER:OG	1:A:1510:TRP:HB3	2.13	0.47
1:A:251:TYR:CD1	1:A:503:ARG:HB2	2.49	0.47
1:A:326:LYS:O	1:A:331:LYS:NZ	2.44	0.47
1:A:326:LYS:CE	1:A:329:ASN:HB2	2.42	0.47
1:B:1272:SER:HB2	1:B:1275:ARG:HH22	1.79	0.47
1:B:1449:ASN:O	1:B:1453:GLN:NE2	2.46	0.47
1:A:1154:LYS:HB2	1:A:1154:LYS:HE2	1.65	0.47
1:A:326:LYS:NZ	1:A:331:LYS:HZ2	2.13	0.47
1:B:1342:LYS:HB2	1:B:1353:ASP:O	2.14	0.47
1:B:1431:VAL:C	1:B:1511:SER:HB3	2.35	0.47
1:B:161:LYS:HD3	1:B:161:LYS:N	2.28	0.47
1:B:749:ILE:HG23	1:B:750:GLU:HG2	1.96	0.47
1:B:900:ARG:HH22	1:B:908:TYR:HE1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:LYS:HG3	1:A:1294:PRO:N	2.29	0.47
1:A:256:SER:OG	1:A:256:SER:O	2.24	0.47
1:B:315:ASP:OD2	1:B:318:GLN:HB3	2.15	0.47
1:B:35:LEU:CD1	1:B:133:ILE:HD13	2.45	0.47
1:B:470:TRP:HZ3	1:B:496:TRP:NE1	2.13	0.47
1:A:1064:LEU:O	1:A:1506:PRO:HD2	2.14	0.47
1:B:1197:TYR:O	1:B:1218:GLU:OE2	2.33	0.47
1:A:1138:GLN:HG3	1:A:1276:PHE:CD1	2.50	0.47
1:A:1349:LYS:HG3	1:A:1352:GLU:HG3	1.97	0.47
1:A:269:LEU:HA	1:A:272:PHE:HB3	1.97	0.47
1:A:440:PRO:HB2	1:A:441:ILE:H	1.44	0.47
1:A:947:HIS:CD2	1:A:949:LEU:H	2.33	0.47
1:B:236:THR:HG21	1:B:242:TRP:CH2	2.50	0.47
1:A:1048:SER:HB2	1:A:1070:ASN:ND2	2.29	0.47
1:A:165:LYS:HD2	1:A:165:LYS:HA	1.57	0.47
1:A:334:SER:HA	1:A:382:LYS:NZ	2.29	0.47
1:A:235:HIS:CG	1:A:499:CYS:HB3	2.50	0.47
1:B:1159:PHE:HB3	1:B:1160:PRO:HD2	1.94	0.47
1:B:381:LYS:HA	1:B:385:SER:O	2.15	0.47
1:A:1084:ARG:HG3	1:A:1088:LEU:HD12	1.97	0.47
1:A:1259:ARG:HH21	1:A:1265:GLU:CD	2.18	0.47
1:A:284:ASP:HB3	1:A:438:GLN:HE21	1.78	0.47
1:B:1107:LEU:HD22	1:B:1183:ILE:HG23	1.97	0.47
1:B:682:ASP:HB2	1:B:783:LYS:HD2	1.95	0.47
1:B:679:THR:N	1:B:783:LYS:HE2	2.29	0.47
1:A:66:TRP:CH2	1:A:84:LYS:HG3	2.50	0.47
1:A:716:GLU:CD	1:A:718:ARG:HH21	2.18	0.47
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.96	0.47
1:A:966:ARG:NH1	1:A:966:ARG:HB3	2.30	0.47
1:B:377:ALA:O	1:B:381:LYS:HG2	2.15	0.47
1:A:1109:HIS:CE1	1:A:1163:ASP:HB3	2.50	0.47
1:A:312:TYR:CD2	1:A:411:TYR:HB2	2.50	0.47
1:B:148:MET:HA	1:B:177:MET:O	2.15	0.47
1:B:311:PHE:HE2	1:B:364:GLY:O	1.98	0.47
1:B:315:ASP:HB2	1:B:370:LYS:NZ	2.30	0.47
1:B:324:ARG:HB2	1:B:388:TYR:CZ	2.50	0.47
1:B:518:MET:HA	1:B:521:TYR:HB3	1.97	0.47
1:B:648:GLU:OE2	1:B:876:HIS:HD2	1.97	0.47
1:A:1062:ALA:HB1	1:A:1510:TRP:CZ3	2.42	0.47
1:A:251:TYR:CD1	1:A:501:LYS:HD3	2.50	0.47
1:B:1108:LYS:HD2	1:B:1159:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TRP:HA	1:B:165:LYS:NZ	2.30	0.47
1:B:443:LYS:HA	1:B:443:LYS:HD2	1.74	0.47
1:B:634:CYS:HB3	1:B:636:TYR:CE1	2.40	0.47
1:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.18	0.46
1:A:250:GLY:HA3	1:A:465:LEU:HD13	1.98	0.46
1:A:323:LEU:C	1:A:325:GLU:OE1	2.53	0.46
1:B:1112:ILE:HG13	1:B:1113:PRO:HD2	1.97	0.46
1:B:1198:ARG:NH1	1:B:1212:ASP:O	2.49	0.46
1:B:395:LEU:HG	1:B:398:LYS:NZ	2.31	0.46
1:B:451:TYR:CD1	1:B:495:VAL:HG21	2.50	0.46
1:B:966:ARG:HG3	1:B:967:LEU:N	2.31	0.46
1:A:1157:ARG:HH11	1:A:1157:ARG:HG3	1.80	0.46
1:A:1204:PRO:O	1:A:1208:ARG:CG	2.63	0.46
1:A:268:LYS:O	1:A:269:LEU:HD23	2.15	0.46
1:B:160:ILE:C	1:B:163:TRP:H	2.19	0.46
1:A:1342:LYS:CE	1:A:1353:ASP:HB3	2.40	0.46
1:A:170:VAL:HA	1:A:173:LYS:HE2	1.98	0.46
1:A:329:ASN:H	1:A:331:LYS:NZ	2.13	0.46
1:B:353:ASP:OD2	1:B:354:ASN:ND2	2.46	0.46
1:B:707:PHE:CD1	1:B:823:ILE:HD11	2.51	0.46
1:B:66:TRP:CZ3	1:B:84:LYS:HB2	2.51	0.46
1:A:1179:THR:OG1	1:A:1182:GLU:HG2	2.16	0.46
1:A:251:TYR:H	1:A:501:LYS:HD3	1.81	0.46
1:B:1109:HIS:O	1:B:1111:LEU:HD13	2.15	0.46
1:B:1196:LYS:HA	1:B:1218:GLU:CD	2.36	0.46
1:A:1035:LEU:O	1:A:1038:THR:HB	2.16	0.46
1:A:541:PRO:HB2	1:A:543:HIS:CE1	2.50	0.46
1:A:893:SER:HA	1:A:896:TYR:HD2	1.81	0.46
1:B:173:LYS:HE2	1:B:175:TYR:HE2	1.81	0.46
1:B:267:LYS:HE2	1:B:267:LYS:HB3	1.66	0.46
1:B:491:ARG:HA	1:B:491:ARG:HD3	1.79	0.46
1:B:573:ASP:O	1:B:577:VAL:HG23	2.16	0.46
1:A:161:LYS:HA	1:A:164:GLU:HB2	1.98	0.46
1:A:287:THR:HG22	1:A:288:VAL:N	2.27	0.46
1:A:331:LYS:HA	1:A:331:LYS:HD2	1.60	0.46
1:A:542:LEU:O	1:A:546:GLN:HG3	2.16	0.46
1:A:594:SER:OG	1:A:596:GLU:HG2	2.16	0.46
1:B:136:VAL:HG13	1:B:137:ASN:H	1.81	0.46
1:B:296:ASP:HB3	1:B:299:LYS:HD3	1.96	0.46
1:B:327:TRP:CZ3	1:B:392:ILE:HG21	2.51	0.46
1:A:279:LEU:HD12	1:A:279:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1064:LEU:O	1:B:1506:PRO:HD2	2.15	0.46
1:A:275:GLN:N	1:A:275:GLN:OE1	2.49	0.46
1:A:417:GLU:O	1:A:421:GLN:HB2	2.15	0.46
1:A:738:MET:HB3	1:A:776:TRP:CZ2	2.50	0.46
1:B:1174:PHE:CD1	1:B:1174:PHE:CZ	2.97	0.46
1:B:1349:LYS:HG3	1:B:1352:GLU:HG3	1.98	0.46
1:B:309:TRP:CD1	1:B:411:TYR:HE1	2.34	0.46
1:B:312:TYR:CD2	1:B:411:TYR:HB2	2.51	0.46
1:B:503:ARG:NH2	1:B:511:SER:OG	2.49	0.46
1:B:748:ASP:OD1	1:B:749:ILE:N	2.40	0.46
1:A:1123:ARG:NH2	1:A:1207:ASP:HB2	2.19	0.46
1:B:891:LEU:HA	1:B:891:LEU:HD23	1.81	0.46
1:A:1158:ARG:O	1:A:1159:PHE:CD2	2.59	0.45
1:A:127:TYR:HB2	1:A:578:GLU:HG2	1.98	0.45
1:B:1185:TYR:CE1	1:B:1290:GLU:O	2.69	0.45
1:B:1206:LEU:HD12	1:B:1207:ASP:N	2.31	0.45
1:B:149:GLN:HG2	1:B:175:TYR:CE1	2.51	0.45
1:A:1508:GLN:NE2	1:A:1510:TRP:CH2	2.85	0.45
1:A:329:ASN:H	1:A:331:LYS:HZ3	1.63	0.45
1:A:742:ILE:HG22	1:A:743:ALA:N	2.30	0.45
1:B:1270:LEU:HD23	1:B:1308:LEU:HD11	1.98	0.45
1:B:429:LEU:O	1:B:430:ARG:HB2	2.15	0.45
1:A:325:GLU:OE2	1:A:326:LYS:HB3	2.16	0.45
1:B:1432:TRP:HA	1:B:1511:SER:HB3	1.98	0.45
1:B:307:LYS:O	1:B:310:GLU:OE1	2.35	0.45
1:A:435:GLY:HA2	1:A:436:PRO:HD2	1.77	0.45
1:B:1196:LYS:HE2	1:B:1218:GLU:HB2	1.98	0.45
1:B:424:ASN:OD1	1:B:424:ASN:O	2.34	0.45
1:A:679:THR:HG21	1:A:783:LYS:HE3	1.98	0.45
1:A:896:TYR:HD1	1:A:900:ARG:HD3	1.80	0.45
1:B:1407:TYR:CZ	1:B:1424:TYR:CD1	3.04	0.45
1:B:1510:TRP:NE1	1:B:1512:THR:HG23	2.31	0.45
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.52	0.45
1:A:713:LEU:HD12	1:A:713:LEU:H	1.81	0.45
1:B:1108:LYS:HD2	1:B:1159:PHE:CD2	2.51	0.45
1:B:1128:ASP:OD1	1:B:1129:ALA:N	2.49	0.45
1:B:1211:LYS:HB2	1:B:1213:GLU:OE2	2.16	0.45
1:B:1235:ASN:O	1:B:1258:PRO:HB3	2.16	0.45
1:B:268:LYS:HZ1	1:B:301:HIS:CE1	2.35	0.45
1:B:274:GLU:H	1:B:274:GLU:CD	2.19	0.45
1:B:312:TYR:HE2	1:B:411:TYR:CD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASP:HB3	1:B:454:ARG:HH22	1.82	0.45
1:B:947:HIS:CD2	1:B:949:LEU:H	2.34	0.45
1:B:928:GLY:CA	1:B:966:ARG:HH12	2.30	0.45
1:A:681:GLU:HA	1:A:810:LEU:HD23	1.97	0.45
1:B:1421:GLY:O	1:B:1424:TYR:HB2	2.17	0.45
1:B:1467:LEU:O	1:B:1470:LYS:HB2	2.17	0.45
1:A:761:GLN:HE21	1:A:761:GLN:HB3	1.44	0.45
1:B:183:LEU:N	1:B:184:GLN:OE1	2.50	0.45
1:A:1105:LYS:HZ3	1:A:1158:ARG:HE	1.65	0.45
1:A:287:THR:HB	1:A:290:ASP:CG	2.36	0.45
1:B:1161:LEU:O	1:B:1161:LEU:HD23	2.17	0.45
1:B:267:LYS:O	1:B:271:ASP:HB2	2.17	0.45
1:A:325:GLU:CG	1:A:326:LYS:HB3	2.47	0.45
1:A:649:ILE:HG13	1:A:649:ILE:H	1.56	0.45
1:B:179:HIS:NE2	1:B:533:ARG:HD2	2.32	0.45
1:A:1193:GLY:O	1:A:1294:PRO:HD3	2.17	0.44
1:A:302:VAL:HG23	1:A:303:ILE:H	1.82	0.44
1:A:664:PHE:CE2	1:A:690:VAL:HG22	2.52	0.44
1:B:1397:ASP:OD2	1:B:1399:SER:N	2.48	0.44
1:B:43:ASP:OD1	1:B:43:ASP:N	2.49	0.44
1:A:1454:VAL:HG12	1:A:1455:GLU:N	2.32	0.44
1:A:938:LYS:HE2	1:A:942:TYR:HE2	1.83	0.44
1:B:1087:LEU:HA	1:B:1092:ARG:HB2	1.99	0.44
1:A:1050:SER:HB2	1:A:1056:ASN:HA	1.98	0.44
1:A:575:LEU:HD11	1:A:579:ARG:NH2	2.33	0.44
1:A:649:ILE:HD12	1:A:649:ILE:O	2.16	0.44
1:B:1029:THR:HG22	1:B:1030:VAL:N	2.33	0.44
1:B:186:ARG:HD2	1:B:192:PRO:HA	1.99	0.44
1:B:350:PHE:CD1	1:B:353:ASP:OD2	2.70	0.44
1:B:451:TYR:CE1	1:B:491:ARG:HD2	2.53	0.44
1:B:421:GLN:HE22	1:B:492:GLU:CA	2.30	0.44
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.48	0.44
1:A:1223:TRP:HD1	1:A:1293:LYS:NZ	2.15	0.44
1:A:69:CYS:SG	1:A:107:TYR:HB3	2.58	0.44
1:B:1324:ASP:OD2	1:B:1324:ASP:N	2.50	0.44
1:B:184:GLN:O	1:B:186:ARG:HG2	2.17	0.44
1:B:81:LYS:HG2	1:B:83:TYR:CZ	2.53	0.44
1:A:1029:THR:HG22	1:A:1030:VAL:N	2.33	0.44
1:A:388:TYR:HA	1:A:392:ILE:HG13	1.99	0.44
1:B:1094:GLU:O	1:B:1098:GLU:HG2	2.16	0.44
1:B:117:LYS:N	1:B:117:LYS:CD	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1185:TYR:CG	1:B:1288:TYR:CD2	3.05	0.44
1:B:274:GLU:CD	1:B:275:GLN:H	2.20	0.44
1:A:57:SER:O	1:A:60:THR:OG1	2.33	0.44
1:B:761:GLN:HB3	1:B:761:GLN:HE21	1.50	0.44
1:A:1108:LYS:NZ	1:A:1164:GLU:O	2.47	0.44
1:A:396:ALA:O	1:A:400:LEU:HG	2.17	0.44
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.99	0.44
1:A:186:ARG:HD2	1:A:190:ASN:OD1	2.18	0.44
1:B:1085:GLY:HA3	1:B:1513:GLY:CA	2.48	0.44
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.52	0.44
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.52	0.44
1:A:1514:CYS:O	1:A:1517:ASP:HB2	2.18	0.44
1:A:35:LEU:H	1:A:35:LEU:HD12	1.83	0.44
1:A:609:PRO:O	1:A:612:SER:HB2	2.18	0.44
1:A:875:ASP:OD2	1:A:879:ARG:NH1	2.51	0.44
1:B:1320:LYS:HE3	1:B:1320:LYS:HB3	1.84	0.44
1:B:520:LYS:NZ	1:B:527:ARG:NH2	2.66	0.44
1:B:782:THR:OG1	1:B:783:LYS:N	2.49	0.44
1:B:834:THR:HG22	1:B:835:GLY:H	1.83	0.44
1:A:291:LEU:HA	1:A:294:VAL:CG2	2.45	0.43
1:B:307:LYS:HG2	1:B:310:GLU:OE2	2.18	0.43
1:B:351:VAL:HG21	1:B:399:ILE:HD13	1.99	0.43
1:B:415:ILE:HG22	1:B:418:VAL:HG21	2.01	0.43
1:B:631:GLU:HB2	1:B:650:MET:SD	2.58	0.43
1:B:674:PRO:HB3	1:B:783:LYS:NZ	2.33	0.43
1:B:899:TYR:O	1:B:900:ARG:HB2	2.19	0.43
1:A:637:ASN:HA	1:A:638:PRO:HD3	1.85	0.43
1:B:404:ASN:N	1:B:404:ASN:OD1	2.52	0.43
1:B:542:LEU:O	1:B:546:GLN:HG3	2.18	0.43
1:B:717:LYS:HD2	1:B:717:LYS:C	2.37	0.43
1:B:928:GLY:HA2	1:B:966:ARG:NH1	2.33	0.43
1:A:143:LEU:HD23	1:A:143:LEU:O	2.18	0.43
1:A:66:TRP:O	1:A:109:PHE:HA	2.18	0.43
1:A:899:TYR:O	1:A:900:ARG:HB2	2.19	0.43
1:A:962:TYR:O	1:A:966:ARG:HG3	2.19	0.43
1:B:1084:ARG:HG3	1:B:1088:LEU:HD12	2.00	0.43
1:B:114:LYS:HE2	1:B:118:ASP:CA	2.45	0.43
1:B:425:ARG:CD	1:B:426:ILE:HD12	2.38	0.43
1:B:900:ARG:HD3	1:B:900:ARG:HA	1.74	0.43
1:A:1185:TYR:CE1	1:A:1189:ASN:HB2	2.53	0.43
1:A:1456:GLY:HA3	1:A:1460:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CE2	1:A:411:TYR:CD1	3.05	0.43
1:B:1050:SER:OG	1:B:1051:ILE:N	2.52	0.43
1:B:637:ASN:N	1:B:638:PRO:HD3	2.34	0.43
1:A:947:HIS:HD2	1:A:949:LEU:H	1.67	0.43
1:B:794:ARG:HH21	1:B:850:LEU:HD21	1.84	0.43
1:A:1201:ASN:HB2	1:A:1206:LEU:HD11	2.00	0.43
1:A:67:THR:HG21	1:A:99:LEU:HD22	2.00	0.43
1:B:414:ASP:O	1:B:417:GLU:HG2	2.19	0.43
1:B:835:GLY:HA3	1:B:852:PRO:HB3	2.00	0.43
1:A:1293:LYS:HD2	1:A:1294:PRO:HD2	1.99	0.43
1:A:1463:PRO:HD3	1:A:1526:TYR:CE1	2.54	0.43
1:B:1031:PHE:CD1	1:B:1479:ARG:HG3	2.54	0.43
1:B:327:TRP:CE3	1:B:388:TYR:CD1	3.07	0.43
1:B:422:LEU:CA	1:B:425:ARG:HD3	2.48	0.43
1:B:426:ILE:HD13	1:B:447:LEU:HD11	1.99	0.43
1:B:455:PHE:HE2	1:B:465:LEU:HG	1.82	0.43
1:A:302:VAL:HG23	1:A:303:ILE:N	2.34	0.43
1:A:594:SER:OG	1:A:597:GLU:HG3	2.19	0.43
1:B:106:THR:HG21	1:B:579:ARG:O	2.18	0.43
1:B:1108:LYS:HD3	1:B:1124:TYR:CE1	2.54	0.43
1:B:1160:PRO:HG2	1:B:1162:ASP:O	2.19	0.43
1:B:214:ASP:O	1:B:218:ARG:HB2	2.19	0.43
1:A:1337:ARG:HB2	1:A:1340:ILE:HD12	2.01	0.43
1:B:318:GLN:O	1:B:318:GLN:HG2	2.18	0.43
1:B:728:ILE:O	1:B:731:VAL:N	2.49	0.43
1:A:285:LEU:HD21	1:A:290:ASP:CB	2.48	0.42
1:A:868:LEU:O	1:A:994:PRO:HD3	2.18	0.42
1:B:1131:TRP:HA	1:B:1134:VAL:HG12	2.00	0.42
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.34	0.42
1:B:697:ILE:HD11	1:B:739:ARG:NE	2.35	0.42
1:A:1322:LYS:CD	1:A:1322:LYS:H	2.27	0.42
1:A:446:PRO:HG2	1:A:448:SER:O	2.19	0.42
1:B:493:VAL:HG12	1:B:495:VAL:HG22	2.01	0.42
1:A:451:TYR:CD1	1:A:495:VAL:HG11	2.55	0.42
1:A:77:PHE:O	1:A:554:ARG:NH1	2.52	0.42
1:B:1248:LYS:NZ	1:B:1414:ASP:HB3	2.34	0.42
1:B:1514:CYS:O	1:B:1517:ASP:HB2	2.19	0.42
1:B:350:PHE:O	1:B:353:ASP:CG	2.58	0.42
1:B:395:LEU:HA	1:B:398:LYS:HG2	2.00	0.42
1:A:611:GLY:N	1:A:753:GLU:OE1	2.52	0.42
1:B:520:LYS:HZ2	1:B:524:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:MET:HA	1:A:298:ILE:HB	2.02	0.42
1:A:447:LEU:HD12	1:A:448:SER:N	2.34	0.42
1:B:281:TYR:HA	1:B:282:PRO:HD3	1.60	0.42
1:B:69:CYS:HA	1:B:70:PRO:HD2	1.92	0.42
1:A:114:LYS:HZ3	1:A:118:ASP:HA	1.84	0.42
1:B:1174:PHE:CB	1:B:1174:PHE:CD2	2.93	0.42
1:B:966:ARG:CG	1:B:967:LEU:N	2.83	0.42
1:A:115:ASN:OD1	1:A:116:ASP:N	2.51	0.42
1:A:214:ASP:O	1:A:218:ARG:HB2	2.19	0.42
1:B:1306:ASP:O	1:B:1310:GLU:HG3	2.20	0.42
1:B:136:VAL:HG13	1:B:137:ASN:N	2.34	0.42
1:B:1240:MET:HA	1:B:1425:HIS:CE1	2.54	0.42
1:B:51:LEU:HD13	1:B:65:ILE:HD13	2.02	0.42
1:A:417:GLU:HG3	1:A:490:ARG:CZ	2.49	0.42
1:B:325:GLU:OE2	1:B:326:LYS:HG2	2.18	0.42
1:A:1120:ARG:O	1:A:1120:ARG:CG	2.66	0.42
1:A:1190:ARG:HG3	1:A:1195:ILE:CG2	2.49	0.42
1:A:547:TYR:O	1:A:551:VAL:HG23	2.19	0.42
1:B:149:GLN:HG2	1:B:175:TYR:CD1	2.55	0.42
1:B:153:SER:HA	1:B:156:MET:SD	2.60	0.42
1:B:541:PRO:HB2	1:B:543:HIS:HE1	1.85	0.42
1:B:682:ASP:O	1:B:683:THR:C	2.56	0.42
1:B:682:ASP:CB	1:B:783:LYS:CD	2.95	0.42
1:A:1195:ILE:O	1:A:1218:GLU:HB3	2.20	0.42
1:B:834:THR:HG22	1:B:835:GLY:N	2.35	0.42
1:A:1151:LEU:HD11	1:A:1280:LEU:HD21	2.01	0.41
1:A:1319:PRO:O	1:A:1338:ARG:HB2	2.20	0.41
1:A:51:LEU:HD13	1:A:65:ILE:HD13	2.01	0.41
1:B:891:LEU:HD13	1:B:1092:ARG:HD3	2.01	0.41
1:B:1196:LYS:HA	1:B:1218:GLU:CG	2.49	0.41
1:B:229:THR:OG1	1:B:230:ASP:O	2.34	0.41
1:B:426:ILE:HA	1:B:429:LEU:CB	2.43	0.41
1:B:490:ARG:NH2	1:B:492:GLU:OE2	2.53	0.41
1:B:742:ILE:HD13	1:B:767:ARG:HE	1.84	0.41
1:B:947:HIS:HD2	1:B:949:LEU:H	1.68	0.41
1:A:194:SER:HB3	1:A:498:ASP:HB3	2.01	0.41
1:A:573:ASP:O	1:A:577:VAL:HG23	2.20	0.41
1:B:1105:LYS:HG2	1:B:1155:VAL:HB	2.02	0.41
1:B:315:ASP:HB3	1:B:370:LYS:NZ	2.35	0.41
1:A:203:PRO:O	1:A:207:LYS:NZ	2.53	0.41
1:B:1077:ARG:NE	1:B:1128:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1395:THR:HB	1:B:1425:HIS:O	2.20	0.41
1:B:182:PRO:HD3	1:B:230:ASP:HB2	2.02	0.41
1:B:310:GLU:CD	1:B:310:GLU:H	2.23	0.41
1:B:313:VAL:HG21	1:B:408:TYR:CD1	2.55	0.41
1:B:194:SER:OG	1:B:498:ASP:OD2	2.31	0.41
1:B:989:ARG:HB2	1:B:989:ARG:HE	1.62	0.41
1:A:1107:LEU:HB3	1:A:1157:ARG:NH1	2.36	0.41
1:A:1218:GLU:HB3	1:A:1219:VAL:H	1.44	0.41
1:A:1264:VAL:HG23	1:A:1343:ASP:O	2.20	0.41
1:A:286:LYS:HG2	1:A:438:GLN:OE1	2.21	0.41
1:A:681:GLU:HB2	1:A:783:LYS:HG2	2.02	0.41
1:A:905:GLU:OE2	1:A:966:ARG:HD2	2.19	0.41
1:B:1198:ARG:HD3	1:B:1216:ASN:ND2	2.35	0.41
1:B:267:LYS:HD2	1:B:454:ARG:HD2	2.02	0.41
1:A:456:LYS:CD	1:A:456:LYS:N	2.83	0.41
1:A:466:ALA:C	1:A:501:LYS:HG3	2.40	0.41
1:B:1035:LEU:O	1:B:1038:THR:HB	2.20	0.41
1:B:1086:LEU:HD21	1:B:1512:THR:OG1	2.20	0.41
1:B:520:LYS:NZ	1:B:527:ARG:HH22	2.17	0.41
1:A:1107:LEU:HB3	1:A:1157:ARG:CZ	2.51	0.41
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.01	0.41
1:B:1396:LEU:HD12	1:B:1397:ASP:O	2.20	0.41
1:B:307:LYS:HB3	1:B:366:ARG:HH21	1.85	0.41
1:B:875:ASP:O	1:B:879:ARG:HG3	2.21	0.41
1:A:1199:GLU:O	1:A:1202:ALA:HB2	2.20	0.41
1:A:1198:ARG:HB2	1:A:1216:ASN:HB3	2.02	0.41
1:A:20:SER:HB2	1:A:656:THR:OG1	2.20	0.41
1:A:297:GLY:O	1:A:301:HIS:HB2	2.20	0.41
1:B:1317:TYR:CE2	1:B:1319:PRO:HA	2.56	0.41
1:B:350:PHE:O	1:B:351:VAL:C	2.59	0.41
1:B:547:TYR:O	1:B:551:VAL:HG23	2.20	0.41
1:B:635:ALA:C	1:B:636:TYR:HD1	2.24	0.41
1:A:152:VAL:HB	1:A:155:TRP:CE3	2.55	0.41
1:A:326:LYS:HZ3	1:A:331:LYS:NZ	2.18	0.41
1:B:636:TYR:N	1:B:636:TYR:CD1	2.87	0.41
1:B:679:THR:C	1:B:783:LYS:HZ3	2.07	0.41
1:B:794:ARG:HE	1:B:850:LEU:HD21	1.86	0.41
1:B:680:VAL:CG1	1:B:826:ILE:HD13	2.47	0.41
1:B:88:LYS:HE2	1:B:95:ASP:OD1	2.21	0.41
1:B:990:ILE:HG12	1:B:1001:PHE:HB3	2.03	0.41
1:B:1076:GLY:HA2	1:B:1103:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:ARG:O	1:B:1159:PHE:HD1	2.04	0.41
1:B:323:LEU:HD21	1:B:377:ALA:CB	2.40	0.41
1:B:340:SER:OG	1:B:383:LEU:HD21	2.21	0.41
1:B:697:ILE:HG22	1:B:698:GLY:N	2.35	0.41
1:A:1196:LYS:HD2	1:A:1218:GLU:HB2	2.03	0.41
1:A:180:PHE:HB3	1:A:183:LEU:HD13	2.02	0.41
1:A:285:LEU:CD2	1:A:290:ASP:OD2	2.69	0.41
1:A:772:ASN:HB3	1:A:872:ASP:OD1	2.21	0.41
1:B:1432:TRP:CB	1:B:1511:SER:OG	2.61	0.41
1:A:1131:TRP:HA	1:A:1134:VAL:HG12	2.01	0.41
1:A:319:THR:OG1	1:A:370:LYS:HE3	2.21	0.41
1:B:1460:LYS:HE2	1:B:1460:LYS:HB3	1.94	0.41
1:B:380:LEU:HD22	1:B:395:LEU:HD23	2.03	0.41
1:B:682:ASP:C	1:B:684:LEU:N	2.72	0.41
1:B:718:ARG:HH21	1:B:823:ILE:CG1	2.34	0.41
1:A:185:HIS:CD2	1:A:186:ARG:N	2.89	0.40
1:A:326:LYS:HZ3	1:A:331:LYS:HZ1	1.69	0.40
1:A:674:PRO:O	1:A:679:THR:N	2.54	0.40
1:B:160:ILE:O	1:B:163:TRP:HB2	2.21	0.40
1:B:303:ILE:HA	1:B:306:LEU:HD21	2.02	0.40
1:A:1236:CYS:HB3	1:A:1241:ASP:HB2	2.02	0.40
1:A:1384:ASP:OD1	1:A:1474:ARG:CZ	2.68	0.40
1:A:556:ASN:HA	1:A:557:PRO:HD2	1.89	0.40
1:B:293:LYS:HA	1:B:293:LYS:HD2	1.88	0.40
1:B:323:LEU:O	1:B:323:LEU:HD23	2.22	0.40
1:B:609:PRO:O	1:B:612:SER:HB2	2.19	0.40
1:A:1185:TYR:HE1	1:A:1290:GLU:O	2.05	0.40
1:A:878:ILE:HG21	1:A:1004:LEU:HD23	2.03	0.40
1:B:1277:VAL:HA	1:B:1280:LEU:HB2	2.04	0.40
1:B:1432:TRP:HA	1:B:1511:SER:CB	2.51	0.40
1:B:350:PHE:O	1:B:352:ARG:N	2.54	0.40
1:A:1108:LYS:CE	1:A:1159:PHE:HD1	2.33	0.40
1:A:370:LYS:CD	1:A:371:ILE:H	2.35	0.40
1:A:425:ARG:NH2	1:A:491:ARG:CB	2.84	0.40
1:A:612:SER:OG	1:A:943:ASN:ND2	2.55	0.40
1:A:777:TYR:CE1	1:A:795:ILE:HD13	2.57	0.40
1:B:1264:VAL:HG11	1:B:1360:PHE:HA	2.04	0.40
1:B:1407:TYR:CE1	1:B:1424:TYR:CD1	3.00	0.40
1:B:749:ILE:HG13	1:B:750:GLU:N	2.37	0.40
1:B:878:ILE:HG21	1:B:1004:LEU:HD23	2.04	0.40
1:A:1314:ARG:NH1	1:A:1329:GLU:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:ND2	1:A:375:LYS:HD2	2.37	0.40
1:A:284:ASP:OD2	1:A:438:GLN:HG3	2.22	0.40
1:B:1016:ARG:HD3	1:B:1016:ARG:HH11	1.76	0.40
1:B:1209:VAL:HG11	1:B:1245:GLU:CG	2.51	0.40
1:B:182:PRO:HB2	1:B:184:GLN:OE1	2.22	0.40
1:B:807:ALA:HB2	1:B:861:VAL:HG13	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:PHE:CG	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CD1	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CG	1:B:1174:PHE:CG[3_656]	1.91	0.29
1:B:116:ASP:O	1:B:390:ASN:ND2[4_567]	2.13	0.07

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	1524/1528 (100%)	1376 (90%)	133 (9%)	15 (1%)	18	57
1	B	1496/1528 (98%)	1337 (89%)	140 (9%)	19 (1%)	14	48
All	All	3020/3056 (99%)	2713 (90%)	273 (9%)	34 (1%)	17	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	437	LYS
1	A	440	PRO
1	A	1165	TYR

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Mol	Chain	Res	Type
1	A	1167	PRO
1	A	1455	GLU
1	A	1459	LYS
1	B	238	ASN
1	B	282	PRO
1	B	308	LEU
1	B	423	PHE
1	B	430	ARG
1	B	637	ASN
1	B	1167	PRO
1	B	1175	SER
1	A	124	ARG
1	A	238	ASN
1	A	501	LYS
1	B	1459	LYS
1	A	326	LYS
1	A	1162	ASP
1	B	37	GLN
1	B	422	LEU
1	B	729	SER
1	A	729	SER
1	B	124	ARG
1	B	165	LYS
1	A	321	SER
1	B	299	LYS
1	B	425	ARG
1	A	1168	TYR
1	B	294	VAL
1	B	350	PHE
1	B	749	ILE

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	1344/1346 (100%)	1309 (97%)	35 (3%)	51 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1327/1346 (99%)	1279 (96%)	48 (4%)	40	75
All	All	2671/2692 (99%)	2588 (97%)	83 (3%)	45	78

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	125	LYS
1	A	273	SER
1	A	274	GLU
1	A	284	ASP
1	A	325	GLU
1	A	334	SER
1	A	349	GLN
1	A	370	LYS
1	A	374	ASP
1	A	441	ILE
1	A	443	LYS
1	A	445	LEU
1	A	456	LYS
1	A	467	ASN
1	A	543	HIS
1	A	572	MET
1	A	616	VAL
1	A	628	LYS
1	A	671	ASN
1	A	709	GLN
1	A	767	ARG
1	A	905	GLU
1	A	1152	GLN
1	A	1162	ASP
1	A	1198	ARG
1	A	1206	LEU
1	A	1227	LEU
1	A	1321	ASN
1	A	1330	ILE
1	A	1338	ARG
1	A	1455	GLU
1	A	1459	LYS
1	A	1462	LYS
1	A	1527	GLU
1	B	4	HIS

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Mol	Chain	Res	Type
1	B	19	THR
1	B	43	ASP
1	B	86	ILE
1	B	114	LYS
1	B	117	LYS
1	B	148	MET
1	B	164	GLU
1	B	207	LYS
1	B	209	GLU
1	B	241	GLN
1	B	252	ASN
1	B	267	LYS
1	B	274	GLU
1	B	288	VAL
1	B	292	ILE
1	B	295	MET
1	B	305	GLU
1	B	306	LEU
1	B	323	LEU
1	B	425	ARG
1	B	429	LEU
1	B	543	HIS
1	B	570	GLU
1	B	616	VAL
1	B	618	LEU
1	B	637	ASN
1	B	644	LYS
1	B	653	LYS
1	B	716	GLU
1	B	749	ILE
1	B	751	ASP
1	B	886	THR
1	B	905	GLU
1	B	1123	ARG
1	B	1170	ASP
1	B	1174	PHE
1	B	1196	LYS
1	B	1272	SER
1	B	1324	ASP
1	B	1326	ASN
1	B	1396	LEU
1	B	1409	ASN

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Mol	Chain	Res	Type
1	B	1415	ASP
1	B	1459	LYS
1	B	1490	LEU
1	B	1492	GLU
1	B	1524	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	198	GLN
1	A	337	ASN
1	A	536	ASN
1	A	675	ASN
1	A	947	HIS
1	A	1070	ASN
1	A	1152	GLN
1	A	1409	ASN
1	B	185	HIS
1	B	354	ASN
1	B	421	GLN
1	B	424	ASN
1	B	661	HIS
1	B	669	HIS
1	B	675	ASN
1	B	876	HIS
1	B	947	HIS
1	B	1070	ASN
1	B	1109	HIS
1	B	1216	ASN
1	B	1235	ASN
1	B	1385	GLN
1	B	1402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1526/1528 (99%)	0.24	79 (5%) 28 12	52, 93, 140, 187	0
1	B	1506/1528 (98%)	0.34	109 (7%) 16 6	47, 87, 148, 190	0
All	All	3032/3056 (99%)	0.29	188 (6%) 21 8	47, 90, 146, 190	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	LEU	6.0
1	B	447	LEU	5.6
1	A	374	ASP	5.5
1	B	1354	TYR	5.0
1	B	289	ASP	4.9
1	B	288	VAL	4.9
1	B	314	VAL	4.8
1	B	375	LYS	4.6
1	A	303	ILE	4.6
1	A	1458	ALA	4.5
1	B	415	ILE	4.4
1	B	363	LEU	4.4
1	A	281	TYR	4.4
1	B	379	ILE	4.3
1	B	1510	TRP	4.2
1	A	1417	ALA	4.2
1	B	492	GLU	4.2
1	B	355	ALA	4.1
1	A	364	GLY	4.1
1	A	288	VAL	4.1
1	A	371	ILE	4.0
1	B	292	ILE	4.0
1	A	287	THR	4.0
1	A	309	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	337	ASN	3.9
1	A	289	ASP	3.9
1	A	419	LEU	3.9
1	B	399	ILE	3.8
1	A	270	LEU	3.8
1	B	395	LEU	3.8
1	B	486	LYS	3.7
1	B	404	ASN	3.7
1	A	1457	SER	3.7
1	B	371	ILE	3.7
1	A	363	LEU	3.6
1	B	489	LEU	3.6
1	B	423	PHE	3.6
1	B	1416	PHE	3.6
1	A	1208	ARG	3.6
1	B	638	PRO	3.6
1	B	296	ASP	3.6
1	B	419	LEU	3.4
1	B	400	LEU	3.4
1	B	336	ASP	3.4
1	B	416	ASN	3.4
1	B	403	ILE	3.3
1	A	292	ILE	3.3
1	B	354	ASN	3.3
1	A	282	PRO	3.2
1	A	313	VAL	3.2
1	B	284	ASP	3.2
1	B	290	ASP	3.2
1	A	295	MET	3.2
1	B	643	VAL	3.2
1	B	373	ILE	3.1
1	B	383	LEU	3.1
1	A	354	ASN	3.1
1	B	241	GLN	3.0
1	B	398	LYS	3.0
1	A	1334	ILE	3.0
1	B	1217	VAL	3.0
1	B	295	MET	3.0
1	B	364	GLY	3.0
1	B	316	VAL	3.0
1	A	280	GLY	3.0
1	B	372	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1458	ALA	2.9
1	B	370	LYS	2.9
1	B	640	ASP	2.9
1	B	1348	GLY	2.9
1	A	312	TYR	2.9
1	A	1224	GLU	2.9
1	A	314	VAL	2.9
1	A	286	LYS	2.9
1	A	355	ALA	2.8
1	B	409	LYS	2.8
1	B	280	GLY	2.8
1	A	422	LEU	2.8
1	B	412	ASP	2.8
1	A	378	ALA	2.8
1	B	396	ALA	2.8
1	B	411	TYR	2.8
1	B	301	HIS	2.8
1	A	265	LEU	2.8
1	B	374	ASP	2.8
1	B	426	ILE	2.7
1	A	1416	PHE	2.7
1	B	281	TYR	2.7
1	B	348	ALA	2.7
1	B	1291	VAL	2.7
1	B	377	ALA	2.7
1	A	201	PHE	2.7
1	B	1353	ASP	2.7
1	A	348	ALA	2.7
1	A	464	ALA	2.7
1	A	459	ASP	2.7
1	B	402	ASP	2.6
1	B	490	ARG	2.6
1	B	391	GLY	2.6
1	B	1417	ALA	2.6
1	A	501	LYS	2.6
1	A	291	LEU	2.6
1	A	1459	LYS	2.6
1	A	408	TYR	2.6
1	B	326	LYS	2.6
1	B	644	LYS	2.6
1	B	270	LEU	2.6
1	B	309	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	376	PHE	2.6
1	B	448	SER	2.5
1	B	303	ILE	2.5
1	A	409	LYS	2.5
1	B	1267	ASN	2.5
1	B	312	TYR	2.5
1	B	1342	LYS	2.5
1	A	370	LYS	2.5
1	A	1401	TYR	2.5
1	A	373	ILE	2.4
1	A	1165	TYR	2.4
1	B	297	GLY	2.4
1	A	376	PHE	2.4
1	A	489	LEU	2.4
1	A	351	VAL	2.4
1	B	352	ARG	2.4
1	A	304	GLY	2.4
1	B	639	ASP	2.4
1	A	425	ARG	2.3
1	B	275	GLN	2.3
1	B	273	SER	2.3
1	A	259	LEU	2.3
1	A	242	TRP	2.3
1	A	316	VAL	2.3
1	B	242	TRP	2.3
1	A	341	LYS	2.3
1	B	413	ASP	2.3
1	B	357	GLU	2.3
1	B	1345	TYR	2.3
1	A	1402	ASN	2.3
1	B	325	GLU	2.3
1	B	1251	SER	2.3
1	B	630	ASP	2.3
1	A	1403	TYR	2.3
1	B	425	ARG	2.3
1	A	356	THR	2.3
1	B	418	VAL	2.3
1	B	1328	PHE	2.3
1	A	276	MET	2.3
1	B	347	LEU	2.3
1	B	443	LYS	2.3
1	A	631	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1128	ASP	2.2
1	A	1418	THR	2.2
1	A	307	LYS	2.2
1	A	1202	ALA	2.2
1	B	422	LEU	2.2
1	A	372	ASN	2.2
1	A	1404	ARG	2.2
1	B	636	TYR	2.2
1	B	1422	ARG	2.2
1	A	160	ILE	2.2
1	A	283	VAL	2.2
1	A	639	ASP	2.2
1	B	243	LEU	2.1
1	A	407	PHE	2.1
1	A	305	GLU	2.1
1	B	254	LYS	2.1
1	B	307	LYS	2.1
1	B	369	ASN	2.1
1	B	261	SER	2.1
1	B	424	ASN	2.1
1	B	750	GLU	2.1
1	B	44	MET	2.1
1	A	1412	ASP	2.1
1	B	1257	THR	2.1
1	A	260	ILE	2.1
1	A	1422	ARG	2.1
1	A	1354	TYR	2.1
1	B	1255	PRO	2.1
1	B	265	LEU	2.1
1	B	748	ASP	2.1
1	A	297	GLY	2.0
1	A	1204	PRO	2.0
1	A	334	SER	2.0
1	B	191	SER	2.0
1	A	375	LYS	2.0
1	A	423	PHE	2.0
1	B	1356	PHE	2.0
1	B	394	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.