



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SMA
Title : CRYSTAL STRUCTURE OF A MALTOGENIC AMYLASE
Authors : Kim, J.S.; Cha, S.S.; Oh, B.H.
Deposited on : 1999-04-21
Resolution : 2.80 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

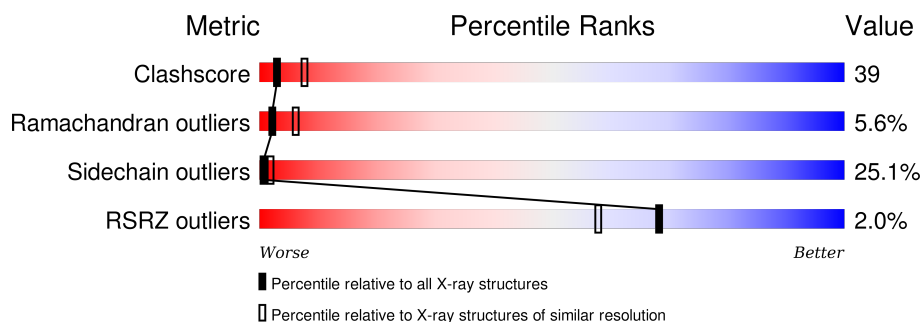
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	588	 2% 37% 46% 17%
1	B	588	 2% 37% 45% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9683 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 MALTOGENIC AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4746	3062	804	859	21			
1	B	588	Total	C	N	O	S	0	0	0
			4746	3062	804	859	21			

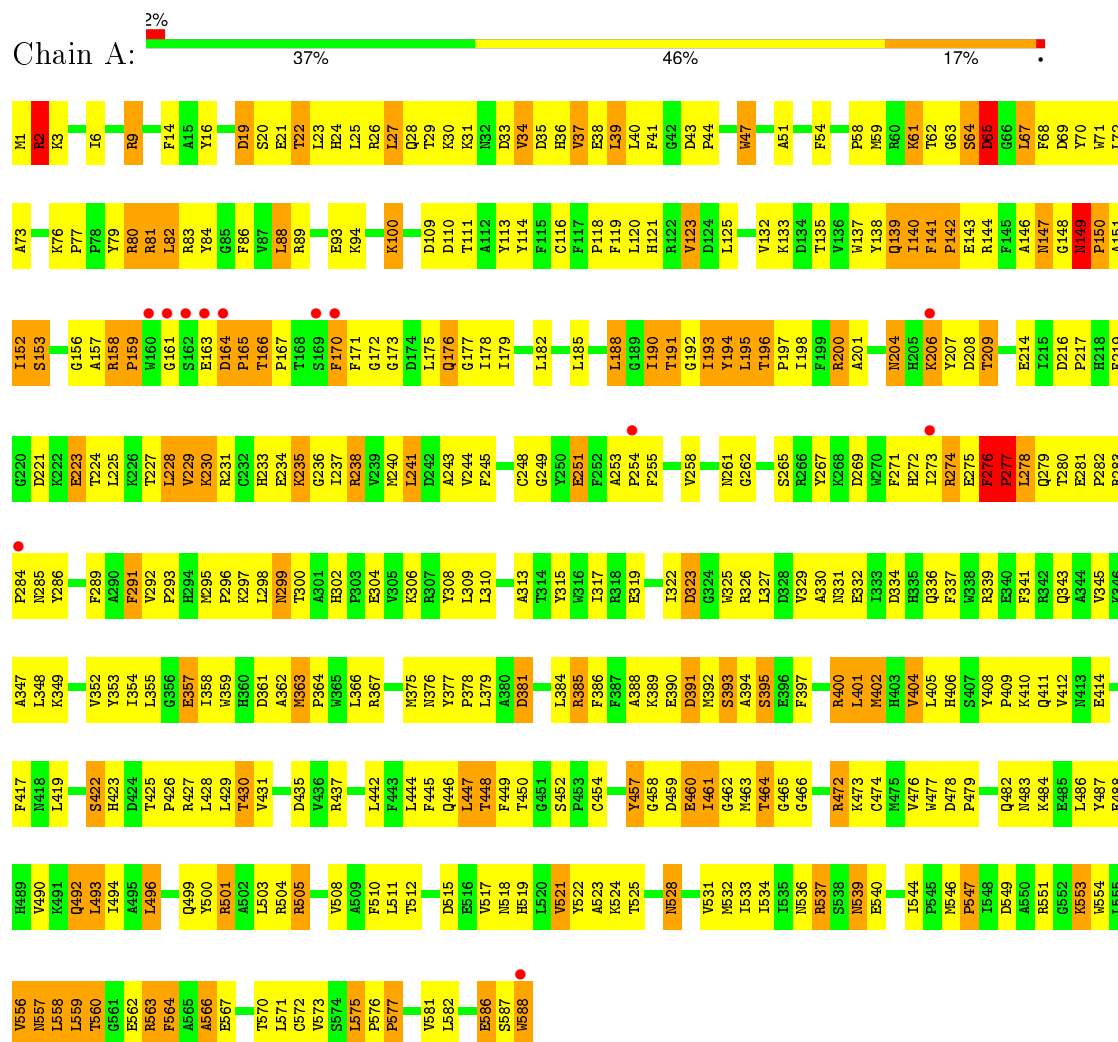
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		
2	B	98	Total	O	0	0
			98	98		

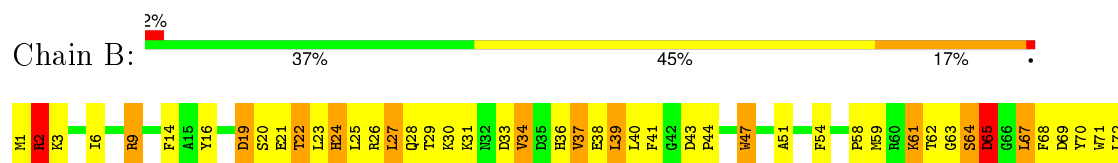
3 Residue-property plots

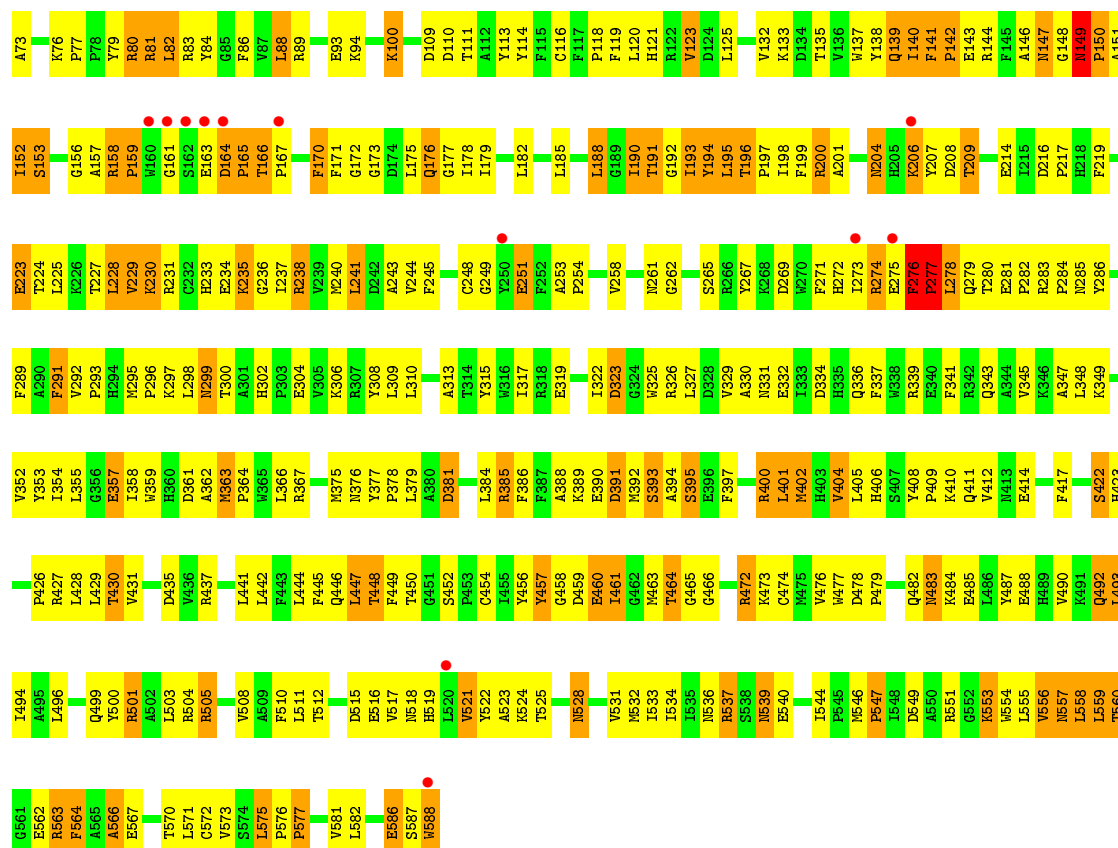
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MALTOGENIC AMYLASE



• Molecule 1: MALTOGENIC AMYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	118.37Å 118.37Å 266.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 29.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (8.00-2.80) 93.8 (29.59-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.267 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 48795 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/4895	0.56	2/6661 (0.0%)
1	B	0.31	0/4895	0.56	2/6661 (0.0%)
All	All	0.32	0/9790	0.56	4/13322 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	PRO	N-CA-CB	6.16	110.70	103.30
1	A	277	PRO	N-CA-CB	6.14	110.67	103.30
1	B	282	PRO	N-CA-CB	5.63	110.06	103.30
1	A	282	PRO	N-CA-CB	5.60	110.02	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4746	0	4458	362	0
1	B	4746	0	4458	367	0
2	A	93	0	0	2	0
2	B	98	0	0	1	0
All	All	9683	0	8916	717	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 39.

All (717) 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:158:ARG:HD3	1:B:159:PRO:HD2	1.35	1.04
1:A:158:ARG:HD3	1:A:159:PRO:HD2	1.35	1.04
1:B:27:LEU:HD12	1:B:37:VAL:HG21	1.49	0.95
1:A:27:LEU:HD12	1:A:37:VAL:HG21	1.49	0.92
1:B:201:ALA:HB3	1:B:206:LYS:HG3	1.52	0.90
1:B:331:ASN:HB3	1:B:358:ILE:HG12	1.54	0.90
1:A:201:ALA:HB3	1:A:206:LYS:HG3	1.53	0.89
1:A:140:ILE:HD12	1:A:178:ILE:HG12	1.55	0.89
1:B:140:ILE:HD12	1:B:178:ILE:HG12	1.54	0.89
1:A:326:ARG:HG2	1:A:355:LEU:HD23	1.55	0.88
1:A:196:THR:HG23	1:A:197:PRO:HD2	1.55	0.88
1:B:326:ARG:HG2	1:B:355:LEU:HD23	1.55	0.87
1:A:331:ASN:HB3	1:A:358:ILE:HG12	1.54	0.87
1:B:196:THR:HG23	1:B:197:PRO:HD2	1.56	0.87
1:B:446:GLN:HG2	1:B:447:LEU:HD23	1.55	0.87
1:A:446:GLN:HG2	1:A:447:LEU:HD23	1.56	0.86
1:B:428:LEU:HD11	1:B:442:LEU:HD13	1.58	0.85
1:A:492:GLN:HB2	2:A:1640:HOH:O	1.77	0.84
1:B:435:ASP:OD1	1:B:437:ARG:HB2	1.77	0.83
1:A:428:LEU:HD11	1:A:442:LEU:HD13	1.58	0.83
1:A:435:ASP:OD1	1:A:437:ARG:HB2	1.78	0.82
1:A:393:SER:HB2	1:A:517:VAL:HG13	1.63	0.79
1:A:158:ARG:CD	1:A:159:PRO:HD2	2.12	0.79
1:B:393:SER:HB2	1:B:517:VAL:HG13	1.63	0.79
1:B:253:ALA:HB3	1:B:254:PRO:HD3	1.64	0.79
1:B:158:ARG:CD	1:B:159:PRO:HD2	2.13	0.78
1:A:148:GLY:HA3	1:A:176:GLN:HB3	1.66	0.78
1:B:148:GLY:HA3	1:B:176:GLN:HB3	1.66	0.78
1:A:248:CYS:SG	1:A:296:PRO:HG2	2.24	0.77
1:A:158:ARG:HD3	1:A:159:PRO:CD	2.14	0.77
1:B:158:ARG:HD3	1:B:159:PRO:CD	2.14	0.77
1:B:363:MET:HE2	1:B:409:PRO:HD3	1.65	0.76
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.64	0.76
1:B:248:CYS:SG	1:B:296:PRO:HG2	2.25	0.76
1:B:450:THR:HG23	1:B:505:ARG:HA	1.68	0.76
1:B:132:VAL:HG11	1:B:353:TYR:CD1	2.21	0.76
1:A:34:VAL:HG11	1:A:88:LEU:HB2	1.67	0.75
1:A:450:THR:HG23	1:A:505:ARG:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG11	1:A:353:TYR:CD1	2.21	0.75
1:B:508:VAL:HG12	1:B:524:LYS:HE3	1.68	0.75
1:A:558:LEU:O	1:A:559:LEU:HD12	1.87	0.75
1:A:363:MET:HE2	1:A:409:PRO:HD3	1.67	0.75
1:B:34:VAL:HG11	1:B:88:LEU:HB2	1.67	0.75
1:B:558:LEU:O	1:B:559:LEU:HD12	1.87	0.74
1:A:508:VAL:HG12	1:A:524:LYS:HE3	1.68	0.74
1:B:444:LEU:O	1:B:448:THR:HB	1.88	0.74
1:A:377:TYR:N	1:A:378:PRO:HD2	2.02	0.74
1:B:143:GLU:OE1	1:B:170:PHE:HA	1.86	0.74
1:A:143:GLU:OE1	1:A:170:PHE:HA	1.87	0.74
1:A:444:LEU:O	1:A:448:THR:HB	1.88	0.74
1:B:377:TYR:N	1:B:378:PRO:HD2	2.03	0.73
1:B:401:LEU:HD23	1:B:510:PHE:CZ	2.23	0.73
1:A:158:ARG:NH1	1:A:474:CYS:HB3	2.04	0.73
1:B:158:ARG:NH1	1:B:474:CYS:HB3	2.04	0.73
1:A:164:ASP:N	1:A:165:PRO:HD3	2.04	0.73
1:B:395:SER:HA	1:B:512:THR:HG21	1.71	0.73
1:B:137:TRP:HB2	1:B:454:CYS:HB2	1.69	0.72
1:A:401:LEU:HD23	1:A:510:PHE:CZ	2.24	0.72
1:B:158:ARG:HB3	1:B:159:PRO:HD2	1.71	0.72
1:A:395:SER:HA	1:A:512:THR:HG21	1.71	0.72
1:A:158:ARG:HB3	1:A:159:PRO:HD2	1.71	0.72
1:A:137:TRP:HB2	1:A:454:CYS:HB2	1.70	0.72
1:B:488:GLU:O	1:B:492:GLN:HG2	1.89	0.72
1:B:164:ASP:N	1:B:165:PRO:HD3	2.04	0.72
1:A:158:ARG:CB	1:A:159:PRO:HD2	2.19	0.71
1:A:196:THR:HG23	1:A:197:PRO:CD	2.20	0.71
1:B:158:ARG:CB	1:B:159:PRO:HD2	2.20	0.71
1:A:488:GLU:O	1:A:492:GLN:HG2	1.90	0.71
1:B:196:THR:HG23	1:B:197:PRO:CD	2.21	0.70
1:B:557:ASN:HD22	1:B:558:LEU:N	1.89	0.70
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.56	0.70
1:B:559:LEU:HD12	1:B:560:THR:HG22	1.74	0.70
1:A:557:ASN:HD22	1:A:558:LEU:N	1.89	0.70
1:A:559:LEU:HD12	1:A:560:THR:HG22	1.74	0.70
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.56	0.69
1:A:29:THR:HG1	1:A:71:TRP:HZ3	1.41	0.69
1:B:16:TYR:CD2	1:B:409:PRO:HB3	2.28	0.68
1:A:16:TYR:CD2	1:A:409:PRO:HB3	2.28	0.68
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:O	1:A:114:TYR:HB3	1.94	0.67
1:A:423:HIS:HB2	1:A:472:ARG:NH1	2.11	0.66
1:A:366:LEU:HD12	1:A:408:TYR:CE1	2.31	0.66
1:A:327:LEU:HB2	1:A:330:ALA:HB2	1.77	0.66
1:A:80:ARG:NH1	1:A:80:ARG:HG2	2.09	0.66
1:B:245:PHE:HB3	1:B:309:LEU:HD13	1.78	0.66
1:A:245:PHE:HB3	1:A:309:LEU:HD13	1.77	0.65
1:A:393:SER:HB2	1:A:517:VAL:CG1	2.27	0.65
1:B:423:HIS:HB2	1:B:472:ARG:NH1	2.11	0.65
1:A:317:ILE:HD13	1:A:352:VAL:HG21	1.79	0.65
1:B:393:SER:HB2	1:B:517:VAL:CG1	2.27	0.65
1:B:366:LEU:HD12	1:B:408:TYR:CE1	2.31	0.64
1:B:84:TYR:O	1:B:114:TYR:HB3	1.96	0.64
1:A:147:ASN:HD22	1:A:148:GLY:N	1.95	0.64
1:B:317:ILE:HD13	1:B:352:VAL:HG21	1.80	0.64
1:B:147:ASN:HD22	1:B:148:GLY:N	1.96	0.64
1:A:450:THR:HG23	1:A:504:ARG:O	1.98	0.64
1:A:566:ALA:O	1:A:567:GLU:HG2	1.97	0.64
1:B:566:ALA:O	1:B:567:GLU:HG2	1.97	0.64
1:A:289:PHE:HB2	1:A:295:MET:HG2	1.80	0.64
1:A:385:ARG:HB3	1:A:392:MET:HE3	1.80	0.64
1:B:450:THR:HG23	1:B:504:ARG:O	1.98	0.64
1:A:146:ALA:O	1:A:177:GLY:HA3	1.97	0.64
1:A:206:LYS:HE2	1:A:219:PHE:CZ	2.33	0.64
1:B:41:PHE:CD2	1:B:82:LEU:HD11	2.33	0.63
1:B:206:LYS:HE2	1:B:219:PHE:CZ	2.33	0.63
1:B:327:LEU:HB2	1:B:330:ALA:HB2	1.78	0.63
1:B:559:LEU:HD12	1:B:560:THR:CG2	2.28	0.63
1:A:557:ASN:ND2	1:A:558:LEU:O	2.32	0.63
1:A:302:HIS:HD2	1:A:304:GLU:H	1.45	0.63
1:A:225:LEU:O	1:A:229:VAL:HG23	1.99	0.63
1:A:559:LEU:HD12	1:A:560:THR:CG2	2.29	0.63
1:A:238:ARG:HD2	1:A:323:ASP:CG	2.19	0.63
1:B:225:LEU:O	1:B:229:VAL:HG23	1.98	0.63
1:A:41:PHE:CD2	1:A:82:LEU:HD11	2.34	0.63
1:B:143:GLU:C	1:B:144:ARG:HG2	2.19	0.63
1:B:385:ARG:HB3	1:B:392:MET:HE3	1.80	0.63
1:A:141:PHE:CE2	1:A:472:ARG:HD2	2.34	0.62
1:B:289:PHE:HB2	1:B:295:MET:HG2	1.80	0.62
1:B:557:ASN:ND2	1:B:558:LEU:O	2.32	0.62
1:A:59:MET:SD	1:A:73:ALA:HB2	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:HD2	1:B:304:GLU:H	1.45	0.62
1:B:146:ALA:O	1:B:177:GLY:HA3	1.98	0.62
1:A:490:VAL:O	1:A:494:ILE:HG13	1.99	0.62
1:A:401:LEU:HD21	1:A:445:PHE:CZ	2.34	0.62
1:B:490:VAL:O	1:B:494:ILE:HG13	2.00	0.62
1:B:29:THR:HG1	1:B:71:TRP:HZ3	1.46	0.62
1:A:88:LEU:HD23	1:A:88:LEU:H	1.65	0.62
1:B:401:LEU:HD21	1:B:445:PHE:CZ	2.34	0.62
1:A:143:GLU:C	1:A:144:ARG:HG2	2.19	0.62
1:A:243:ALA:HB2	1:A:325:TRP:CE3	2.35	0.62
1:B:238:ARG:HD2	1:B:323:ASP:CG	2.20	0.62
1:A:557:ASN:ND2	1:A:560:THR:HG23	2.15	0.62
1:B:557:ASN:ND2	1:B:560:THR:HG23	2.15	0.62
1:B:139:GLN:OE1	1:B:423:HIS:HD2	1.83	0.62
1:A:40:LEU:HD11	1:A:54:PHE:CE1	2.35	0.62
1:B:138:TYR:CZ	1:B:457:TYR:HA	2.35	0.62
1:A:329:VAL:HG12	1:A:332:GLU:HB2	1.81	0.62
1:B:243:ALA:HB2	1:B:325:TRP:CE3	2.35	0.61
1:B:59:MET:SD	1:B:73:ALA:HB2	2.40	0.61
1:B:141:PHE:CE2	1:B:472:ARG:HD2	2.35	0.61
1:B:88:LEU:H	1:B:88:LEU:HD23	1.65	0.61
1:B:329:VAL:HG12	1:B:332:GLU:HB2	1.81	0.61
1:B:40:LEU:HD11	1:B:54:PHE:CE1	2.35	0.61
1:B:544:ILE:HD12	1:B:575:LEU:HD13	1.82	0.61
1:A:139:GLN:OE1	1:A:423:HIS:HD2	1.83	0.61
1:A:138:TYR:CZ	1:A:457:TYR:HA	2.34	0.61
1:B:400:ARG:O	1:B:404:VAL:HG22	2.00	0.60
1:B:461:ILE:HB	1:B:482:GLN:HB2	1.83	0.60
1:B:553:LYS:HB2	1:B:588:TRP:HB3	1.84	0.60
1:B:195:LEU:H	1:B:195:LEU:HD23	1.67	0.60
1:B:80:ARG:CG	1:B:80:ARG:HH11	2.14	0.60
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.14	0.60
1:A:357:GLU:HA	1:A:375:MET:HG3	1.83	0.60
1:B:478:ASP:O	1:B:482:GLN:HG2	2.01	0.60
1:A:461:ILE:HB	1:A:482:GLN:HB2	1.82	0.60
1:A:553:LYS:HB2	1:A:588:TRP:HB3	1.83	0.60
1:B:357:GLU:HA	1:B:375:MET:HG3	1.83	0.60
1:B:193:ILE:HD12	1:B:195:LEU:HD22	1.84	0.60
1:A:401:LEU:O	1:A:405:LEU:HB2	2.02	0.60
1:B:401:LEU:O	1:B:405:LEU:HB2	2.01	0.60
1:A:544:ILE:HD12	1:A:575:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:HD2	1:B:82:LEU:HD11	1.66	0.59
1:B:175:LEU:HB2	1:B:219:PHE:O	2.02	0.59
1:A:400:ARG:O	1:A:404:VAL:HG22	2.01	0.59
1:A:553:LYS:HD3	1:A:588:TRP:CE3	2.38	0.59
1:A:195:LEU:H	1:A:195:LEU:HD23	1.67	0.59
1:A:334:ASP:OD1	1:A:336:GLN:HB3	2.02	0.59
1:A:175:LEU:HB2	1:A:219:PHE:O	2.03	0.59
1:A:164:ASP:N	1:A:165:PRO:CD	2.65	0.59
1:B:559:LEU:CD1	1:B:560:THR:HG22	2.33	0.59
1:A:478:ASP:O	1:A:482:GLN:HG2	2.02	0.59
1:A:559:LEU:CD1	1:A:560:THR:HG22	2.33	0.59
1:B:164:ASP:N	1:B:165:PRO:CD	2.65	0.59
1:B:208:ASP:O	1:B:249:GLY:HA3	2.03	0.59
1:B:334:ASP:OD1	1:B:336:GLN:HB3	2.02	0.59
1:A:193:ILE:HD12	1:A:195:LEU:HD22	1.85	0.58
1:A:208:ASP:O	1:A:249:GLY:HA3	2.03	0.58
1:B:427:ARG:HB2	1:B:430:THR:HG23	1.85	0.58
1:A:427:ARG:HB2	1:A:430:THR:HG23	1.85	0.58
1:B:553:LYS:HD3	1:B:588:TRP:CE3	2.38	0.58
1:A:392:MET:SD	1:A:397:PHE:HA	2.43	0.58
1:A:41:PHE:HD2	1:A:82:LEU:HD11	1.67	0.58
1:A:100:LYS:HD2	1:B:400:ARG:HH21	1.67	0.58
1:B:426:PRO:HA	1:B:466:GLY:C	2.24	0.58
1:A:336:GLN:OE1	1:A:336:GLN:HA	2.03	0.58
1:A:426:PRO:HA	1:A:466:GLY:C	2.23	0.58
1:B:392:MET:SD	1:B:397:PHE:HA	2.44	0.58
1:A:400:ARG:HH21	1:B:100:LYS:HD2	1.67	0.58
1:B:245:PHE:HE2	1:B:341:PHE:HE1	1.52	0.58
1:B:534:ILE:CD1	1:B:546:MET:HB2	2.34	0.58
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.03	0.57
1:A:534:ILE:CD1	1:A:546:MET:HB2	2.34	0.57
1:A:377:TYR:N	1:A:378:PRO:CD	2.67	0.57
1:A:245:PHE:HE2	1:A:341:PHE:HE1	1.52	0.57
1:B:377:TYR:N	1:B:378:PRO:CD	2.67	0.57
1:B:1:MET:HE3	1:B:88:LEU:HD12	1.86	0.57
1:A:557:ASN:HD22	1:A:557:ASN:C	2.08	0.57
1:A:349:LYS:HD3	1:A:352:VAL:CG2	2.35	0.56
1:A:159:PRO:HD3	1:A:474:CYS:SG	2.45	0.56
1:B:349:LYS:HD3	1:B:352:VAL:CG2	2.35	0.56
1:A:185:LEU:HB3	1:A:190:ILE:HG12	1.86	0.56
1:A:519:HIS:CG	1:A:544:ILE:HG12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD11	1:A:546:MET:HB2	1.87	0.56
1:A:37:VAL:HA	1:A:88:LEU:HA	1.88	0.56
1:B:518:ASN:ND2	1:B:537:ARG:HH12	2.03	0.56
1:B:191:THR:HG22	1:B:236:GLY:O	2.06	0.56
1:B:557:ASN:C	1:B:557:ASN:HD22	2.09	0.56
1:A:148:GLY:O	1:A:149:ASN:C	2.44	0.56
1:B:532:MET:C	1:B:533:ILE:HD12	2.26	0.56
1:B:539:ASN:ND2	1:B:540:GLU:HG3	2.21	0.56
1:A:64:SER:HB3	1:A:69:ASP:HA	1.86	0.56
1:A:532:MET:C	1:A:533:ILE:HD12	2.26	0.56
1:B:159:PRO:HD3	1:B:474:CYS:SG	2.46	0.56
1:B:185:LEU:HB3	1:B:190:ILE:HG12	1.87	0.56
1:B:64:SER:HB3	1:B:69:ASP:HA	1.87	0.56
1:A:539:ASN:ND2	1:A:540:GLU:HG3	2.21	0.56
1:B:558:LEU:O	1:B:560:THR:HG23	2.06	0.56
1:A:523:ALA:HB2	1:A:532:MET:SD	2.46	0.56
1:B:88:LEU:N	1:B:88:LEU:HD23	2.20	0.56
1:A:558:LEU:O	1:A:560:THR:HG23	2.06	0.56
1:B:148:GLY:O	1:B:149:ASN:C	2.44	0.55
1:A:163:GLU:O	1:A:164:ASP:CB	2.54	0.55
1:B:193:ILE:CD1	1:B:195:LEU:HD22	2.36	0.55
1:B:30:LYS:HB3	1:B:33:ASP:HB2	1.88	0.55
1:B:519:HIS:CG	1:B:544:ILE:HG12	2.41	0.55
1:A:501:ARG:HA	1:A:504:ARG:NH1	2.22	0.55
1:B:523:ALA:HB2	1:B:532:MET:SD	2.47	0.55
1:A:191:THR:HG22	1:A:236:GLY:O	2.06	0.55
1:A:518:ASN:ND2	1:A:537:ARG:HH12	2.03	0.55
1:A:88:LEU:HD23	1:A:88:LEU:N	2.21	0.55
1:B:575:LEU:HD12	1:B:575:LEU:N	2.22	0.55
1:A:193:ILE:CD1	1:A:195:LEU:HD22	2.36	0.55
1:A:204:ASN:ND2	1:A:204:ASN:H	2.05	0.55
1:B:163:GLU:O	1:B:164:ASP:CB	2.54	0.55
1:B:534:ILE:HD11	1:B:546:MET:HB2	1.87	0.55
1:B:133:LYS:HG2	1:B:414:GLU:O	2.07	0.55
1:A:30:LYS:HB3	1:A:33:ASP:HB2	1.89	0.55
1:A:133:LYS:HG2	1:A:414:GLU:O	2.07	0.55
1:A:575:LEU:N	1:A:575:LEU:HD12	2.22	0.54
1:B:385:ARG:HD3	1:B:392:MET:HG2	1.89	0.54
1:B:37:VAL:HA	1:B:88:LEU:HA	1.88	0.54
1:A:286:TYR:HE2	1:A:296:PRO:HB3	1.73	0.54
1:B:1:MET:HE1	1:B:88:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HD3	1:A:375:MET:SD	2.48	0.54
1:A:385:ARG:HG3	1:A:385:ARG:HH11	1.72	0.54
1:B:280:THR:HA	1:B:284:PRO:HA	1.90	0.54
1:B:306:LYS:HG3	1:B:337:PHE:HD1	1.73	0.54
1:A:1:MET:HE3	1:A:88:LEU:HD12	1.90	0.54
1:B:254:PRO:O	1:B:258:VAL:HG23	2.08	0.54
1:A:280:THR:HA	1:A:284:PRO:HA	1.90	0.54
1:A:44:PRO:O	1:A:47:TRP:HZ3	1.91	0.53
1:A:549:ASP:OD2	1:A:551:ARG:HB2	2.08	0.53
1:A:291:PHE:O	1:A:293:PRO:HD3	2.09	0.53
1:A:385:ARG:HD3	1:A:392:MET:HG2	1.90	0.53
1:B:245:PHE:HE2	1:B:341:PHE:CE1	2.26	0.53
1:A:553:LYS:HD3	1:A:588:TRP:CD2	2.43	0.53
1:B:286:TYR:HE2	1:B:296:PRO:HB3	1.73	0.53
1:A:254:PRO:O	1:A:258:VAL:HG23	2.08	0.53
1:B:501:ARG:HA	1:B:504:ARG:NH1	2.22	0.53
1:A:132:VAL:O	1:A:452:SER:HB2	2.09	0.53
1:B:553:LYS:HD3	1:B:588:TRP:CD2	2.44	0.53
1:B:204:ASN:H	1:B:204:ASN:ND2	2.05	0.53
1:A:306:LYS:HG3	1:A:337:PHE:HD1	1.73	0.53
1:B:27:LEU:HD22	1:B:28:GLN:N	2.24	0.53
1:B:401:LEU:HD21	1:B:445:PHE:HZ	1.72	0.53
1:A:29:THR:OG1	1:A:71:TRP:HZ3	1.91	0.53
1:B:385:ARG:HG3	1:B:385:ARG:HH11	1.72	0.53
1:B:291:PHE:O	1:B:293:PRO:HD3	2.08	0.53
1:B:132:VAL:O	1:B:452:SER:HB2	2.09	0.53
1:B:429:LEU:HD23	1:B:464:THR:HB	1.91	0.53
1:B:326:ARG:HD3	1:B:375:MET:SD	2.49	0.53
1:B:430:THR:HG21	1:B:466:GLY:N	2.24	0.53
1:A:245:PHE:HE2	1:A:341:PHE:CE1	2.27	0.52
1:A:41:PHE:O	1:A:54:PHE:HB2	2.09	0.52
1:B:549:ASP:OD2	1:B:551:ARG:HB2	2.08	0.52
1:B:402:MET:O	1:B:406:HIS:HD2	1.92	0.52
1:A:427:ARG:O	1:A:431:VAL:HG23	2.10	0.52
1:B:72:LEU:HD12	1:B:73:ALA:H	1.74	0.52
1:B:306:LYS:O	1:B:310:LEU:HB2	2.09	0.52
1:A:564:PHE:CD1	1:A:564:PHE:N	2.78	0.52
1:B:564:PHE:CD1	1:B:564:PHE:N	2.78	0.52
1:B:44:PRO:O	1:B:47:TRP:HZ3	1.92	0.52
1:A:27:LEU:HD22	1:A:28:GLN:N	2.24	0.52
1:A:144:ARG:NH1	1:A:166:THR:HG22	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HD23	1:A:464:THR:HB	1.91	0.52
1:B:29:THR:OG1	1:B:71:TRP:HZ3	1.91	0.52
1:B:144:ARG:NH1	1:B:166:THR:HG22	2.24	0.52
1:A:72:LEU:HD12	1:A:73:ALA:H	1.75	0.52
1:B:461:ILE:CD1	1:B:476:VAL:HB	2.40	0.52
1:B:355:LEU:CD1	1:B:417:PHE:HB2	2.40	0.52
1:A:349:LYS:HD3	1:A:352:VAL:HG22	1.91	0.52
1:B:457:TYR:CD1	1:B:458:GLY:N	2.78	0.52
1:A:63:GLY:O	1:A:64:SER:HB3	2.10	0.52
1:A:306:LYS:O	1:A:310:LEU:HB2	2.09	0.52
1:B:41:PHE:O	1:B:54:PHE:HB2	2.10	0.52
1:B:427:ARG:O	1:B:431:VAL:HG23	2.10	0.52
1:B:63:GLY:O	1:B:64:SER:HB3	2.10	0.52
1:A:402:MET:O	1:A:406:HIS:HD2	1.93	0.52
1:A:401:LEU:HD21	1:A:445:PHE:HZ	1.72	0.52
1:A:430:THR:HG21	1:A:466:GLY:N	2.24	0.52
1:B:175:LEU:O	1:B:179:ILE:HG13	2.10	0.51
1:A:461:ILE:CD1	1:A:476:VAL:HB	2.40	0.51
1:B:133:LYS:CE	1:B:414:GLU:HB3	2.40	0.51
1:A:3:LYS:HB2	1:B:67:LEU:CD2	2.40	0.51
1:B:223:GLU:OE1	1:B:223:GLU:HA	2.10	0.51
1:B:152:ILE:HD12	1:B:153:SER:O	2.10	0.51
1:A:355:LEU:CD1	1:A:417:PHE:HB2	2.40	0.51
1:A:231:ARG:O	1:A:235:LYS:HD2	2.10	0.51
1:A:119:PHE:CE2	1:B:297:LYS:HE2	2.46	0.51
1:A:231:ARG:NH2	2:A:696:HOH:O	2.41	0.51
1:A:152:ILE:HD13	1:A:172:GLY:HA2	1.93	0.51
1:A:14:PHE:HD1	1:A:26:ARG:O	1.93	0.51
1:B:349:LYS:HD3	1:B:352:VAL:HG22	1.91	0.51
1:A:188:LEU:HD22	1:A:494:ILE:HD12	1.92	0.51
1:B:231:ARG:O	1:B:235:LYS:HD2	2.10	0.51
1:A:457:TYR:CD1	1:A:458:GLY:N	2.78	0.51
1:B:152:ILE:HD13	1:B:172:GLY:HA2	1.93	0.51
1:A:193:ILE:O	1:A:193:ILE:HG13	2.10	0.51
1:A:133:LYS:CE	1:A:414:GLU:HB3	2.40	0.51
1:A:241:LEU:HD12	1:A:322:ILE:HG21	1.93	0.51
1:A:175:LEU:O	1:A:179:ILE:HG13	2.11	0.51
1:A:152:ILE:HD12	1:A:153:SER:O	2.10	0.51
1:B:61:LYS:HE3	1:B:69:ASP:OD2	2.11	0.51
1:A:386:PHE:O	1:A:390:GLU:HA	2.11	0.50
1:A:144:ARG:HH12	1:A:166:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:OD1	1:A:81:ARG:HG2	2.12	0.50
1:A:447:LEU:HD12	1:A:493:LEU:HB3	1.94	0.50
1:A:192:GLY:HA2	1:A:237:ILE:HG23	1.94	0.50
1:B:193:ILE:O	1:B:193:ILE:HG13	2.10	0.50
1:A:67:LEU:CD2	1:B:3:LYS:HB2	2.41	0.50
1:B:386:PHE:O	1:B:390:GLU:HA	2.11	0.50
1:A:64:SER:HB2	1:A:68:PHE:O	2.11	0.50
1:A:110:ASP:O	1:A:113:TYR:HD2	1.95	0.50
1:B:576:PRO:HB2	1:B:577:PRO:HD2	1.94	0.50
1:B:158:ARG:HB3	1:B:159:PRO:CD	2.40	0.50
1:B:1:MET:HE1	1:B:34:VAL:HG13	1.93	0.50
1:B:554:TRP:H	1:B:586:GLU:HB2	1.77	0.50
1:A:158:ARG:HB3	1:A:159:PRO:CD	2.40	0.50
1:B:144:ARG:HH12	1:B:166:THR:HG22	1.76	0.50
1:B:64:SER:HB2	1:B:68:PHE:O	2.11	0.50
1:B:14:PHE:HD1	1:B:26:ARG:O	1.94	0.50
1:A:553:LYS:HB2	1:A:588:TRP:CE3	2.47	0.50
1:A:297:LYS:HE2	1:B:119:PHE:CE2	2.47	0.50
1:B:447:LEU:HD12	1:B:493:LEU:HB3	1.94	0.50
1:B:553:LYS:HB2	1:B:588:TRP:CE3	2.47	0.50
1:A:61:LYS:HE3	1:A:69:ASP:OD2	2.12	0.50
1:B:83:ARG:HD3	1:B:116:CYS:HB2	1.94	0.50
1:B:241:LEU:HD12	1:B:322:ILE:HG21	1.94	0.50
1:A:358:ILE:HG21	1:A:362:ALA:HB2	1.93	0.49
1:B:192:GLY:HA2	1:B:237:ILE:HG23	1.94	0.49
1:B:204:ASN:HD22	1:B:204:ASN:H	1.60	0.49
1:A:83:ARG:HD3	1:A:116:CYS:HB2	1.94	0.49
1:B:188:LEU:HD22	1:B:494:ILE:HD12	1.93	0.49
1:B:427:ARG:NH2	1:B:458:GLY:HA3	2.27	0.49
1:B:503:LEU:HD21	1:B:531:VAL:HG11	1.94	0.49
1:A:274:ARG:HG3	1:A:285:ASN:O	2.12	0.49
1:B:43:ASP:OD1	1:B:81:ARG:HG2	2.11	0.49
1:B:358:ILE:HG21	1:B:362:ALA:HB2	1.93	0.49
1:B:274:ARG:HG3	1:B:285:ASN:O	2.12	0.49
1:B:110:ASP:O	1:B:113:TYR:HD2	1.94	0.49
1:B:158:ARG:O	1:B:159:PRO:O	2.30	0.49
1:A:223:GLU:OE1	1:A:223:GLU:HA	2.10	0.49
1:A:41:PHE:HB2	1:A:82:LEU:HD11	1.95	0.49
1:A:503:LEU:HD21	1:A:531:VAL:HG11	1.95	0.49
1:A:158:ARG:O	1:A:159:PRO:O	2.30	0.49
1:A:576:PRO:HB2	1:A:577:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:HD22	1:A:204:ASN:H	1.59	0.49
1:B:152:ILE:HD13	1:B:172:GLY:CA	2.43	0.49
1:A:79:TYR:O	1:A:81:ARG:HD3	2.13	0.49
1:A:299:ASN:C	1:A:299:ASN:HD22	2.16	0.49
1:B:141:PHE:HE2	1:B:472:ARG:HD2	1.77	0.49
1:A:427:ARG:NH2	1:A:458:GLY:HA3	2.27	0.49
1:A:361:ASP:OD2	1:B:9:ARG:NH1	2.43	0.49
1:B:274:ARG:HG3	1:B:274:ARG:NH1	2.28	0.49
1:A:175:LEU:HD13	1:A:219:PHE:HB3	1.95	0.48
1:B:558:LEU:O	1:B:560:THR:N	2.46	0.48
1:A:9:ARG:NH1	1:B:361:ASP:OD2	2.44	0.48
1:B:355:LEU:HD11	1:B:417:PHE:HB2	1.94	0.48
1:A:558:LEU:O	1:A:560:THR:N	2.46	0.48
1:A:463:MET:CE	1:A:473:LYS:HB2	2.43	0.48
1:B:175:LEU:HB3	1:B:224:THR:CG2	2.43	0.48
1:B:41:PHE:HB2	1:B:82:LEU:HD11	1.94	0.48
1:A:141:PHE:CD2	1:A:472:ARG:HD2	2.49	0.48
1:B:299:ASN:HD22	1:B:299:ASN:C	2.16	0.48
1:A:355:LEU:HD11	1:A:417:PHE:CB	2.43	0.48
1:B:313:ALA:HB2	1:B:341:PHE:CE1	2.48	0.48
1:A:554:TRP:H	1:A:586:GLU:HB2	1.77	0.48
1:A:1:MET:HE1	1:A:88:LEU:HB2	1.95	0.48
1:B:175:LEU:HD13	1:B:219:PHE:HB3	1.96	0.48
1:B:355:LEU:HD11	1:B:417:PHE:CB	2.43	0.48
1:A:47:TRP:CD1	1:A:51:ALA:C	2.87	0.48
1:A:175:LEU:HB3	1:A:224:THR:CG2	2.44	0.48
1:B:137:TRP:O	1:B:454:CYS:HA	2.14	0.48
1:A:141:PHE:HE2	1:A:472:ARG:HD2	1.77	0.48
1:A:274:ARG:HG3	1:A:274:ARG:NH1	2.28	0.48
1:B:79:TYR:O	1:B:81:ARG:HD3	2.14	0.48
1:B:47:TRP:CD1	1:B:51:ALA:C	2.87	0.48
1:A:137:TRP:O	1:A:454:CYS:HA	2.14	0.48
1:A:182:LEU:HD23	1:A:235:LYS:HD3	1.95	0.48
1:B:63:GLY:O	1:B:64:SER:CB	2.62	0.48
1:A:62:THR:O	1:A:402:MET:HE1	2.13	0.48
1:A:401:LEU:HD23	1:A:510:PHE:CE2	2.49	0.47
1:B:119:PHE:HB3	1:B:121:HIS:NE2	2.29	0.47
1:A:355:LEU:HD11	1:A:417:PHE:HB2	1.95	0.47
1:A:313:ALA:HB2	1:A:341:PHE:CE1	2.48	0.47
1:A:63:GLY:O	1:A:64:SER:CB	2.62	0.47
1:B:463:MET:CE	1:B:473:LYS:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD23	1:B:235:LYS:HD3	1.96	0.47
1:A:286:TYR:CE2	1:A:296:PRO:HB3	2.50	0.47
1:A:119:PHE:HB3	1:A:121:HIS:NE2	2.30	0.47
1:B:1:MET:CE	1:B:34:VAL:HG13	2.45	0.47
1:A:289:PHE:CB	1:A:295:MET:HG2	2.44	0.47
1:A:229:VAL:HG12	1:A:233:HIS:NE2	2.30	0.47
1:B:286:TYR:CE2	1:B:296:PRO:HB3	2.50	0.47
1:A:327:LEU:HG	1:A:355:LEU:O	2.15	0.47
1:A:308:TYR:HD2	1:A:309:LEU:HD23	1.80	0.47
1:A:152:ILE:HD13	1:A:172:GLY:CA	2.43	0.47
1:B:327:LEU:HG	1:B:355:LEU:O	2.15	0.47
1:B:447:LEU:CD1	1:B:494:ILE:HG12	2.44	0.47
1:B:401:LEU:HD23	1:B:510:PHE:CE2	2.49	0.47
1:B:229:VAL:HG12	1:B:233:HIS:NE2	2.30	0.47
1:B:1:MET:HB2	1:B:93:GLU:CD	2.35	0.47
1:B:308:TYR:HD2	1:B:309:LEU:HD23	1.79	0.47
1:B:62:THR:O	1:B:402:MET:HE1	2.15	0.47
1:A:1:MET:CE	1:A:34:VAL:HG13	2.45	0.47
1:A:447:LEU:CD1	1:A:494:ILE:HG12	2.44	0.47
1:B:401:LEU:HD23	1:B:510:PHE:HZ	1.79	0.46
1:B:139:GLN:O	1:B:139:GLN:HG2	2.15	0.46
1:B:141:PHE:CD2	1:B:472:ARG:HD2	2.49	0.46
1:B:536:ASN:ND2	1:B:577:PRO:O	2.48	0.46
1:A:1:MET:HB2	1:A:93:GLU:CD	2.35	0.46
1:A:34:VAL:HG12	1:A:36:HIS:O	2.16	0.46
1:B:81:ARG:CG	1:B:81:ARG:HH11	2.27	0.46
1:B:22:THR:OG1	1:B:76:LYS:HE2	2.15	0.46
1:B:200:ARG:HG2	1:B:217:PRO:HD2	1.97	0.46
1:B:289:PHE:CB	1:B:295:MET:HG2	2.44	0.46
1:A:207:TYR:C	1:A:209:THR:H	2.17	0.46
1:A:178:ILE:HG22	1:A:228:LEU:HD21	1.96	0.46
1:B:447:LEU:HD11	1:B:494:ILE:HG12	1.97	0.46
1:A:397:PHE:O	1:A:401:LEU:HB2	2.16	0.46
1:A:139:GLN:O	1:A:139:GLN:HG2	2.15	0.46
1:A:536:ASN:ND2	1:A:577:PRO:O	2.48	0.46
1:A:315:TYR:CE1	1:A:319:GLU:HG3	2.50	0.46
1:A:178:ILE:CG2	1:A:228:LEU:HD21	2.45	0.46
1:A:139:GLN:HA	1:A:194:TYR:O	2.16	0.46
1:B:34:VAL:HG12	1:B:36:HIS:O	2.15	0.46
1:B:363:MET:N	1:B:364:PRO:CD	2.78	0.46
1:B:23:LEU:HD11	1:B:77:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:CG2	1:B:228:LEU:HD21	2.45	0.46
1:B:178:ILE:HG22	1:B:228:LEU:HD21	1.96	0.46
1:B:16:TYR:CE2	1:B:409:PRO:HB3	2.51	0.46
1:B:397:PHE:O	1:B:401:LEU:HB2	2.16	0.46
1:A:487:TYR:CD1	1:A:487:TYR:C	2.89	0.46
1:B:375:MET:O	1:B:377:TYR:N	2.49	0.46
1:A:447:LEU:HD11	1:A:494:ILE:HG12	1.97	0.46
1:B:363:MET:CE	1:B:409:PRO:HD3	2.40	0.46
1:A:363:MET:CE	1:A:409:PRO:HD3	2.41	0.46
1:B:274:ARG:HG3	1:B:274:ARG:HH11	1.81	0.46
1:B:487:TYR:CD1	1:B:487:TYR:C	2.89	0.46
1:A:34:VAL:HG11	1:A:88:LEU:CB	2.42	0.46
1:A:197:PRO:HB2	1:A:206:LYS:CB	2.46	0.46
1:A:22:THR:OG1	1:A:76:LYS:HE2	2.16	0.46
1:A:457:TYR:CG	1:A:458:GLY:N	2.84	0.46
1:B:198:ILE:HB	1:B:219:PHE:HD2	1.81	0.46
1:A:16:TYR:CE2	1:A:409:PRO:HB3	2.51	0.46
1:B:457:TYR:CG	1:B:458:GLY:N	2.84	0.46
1:A:496:LEU:HA	1:A:496:LEU:HD12	1.84	0.46
1:A:1:MET:O	1:A:2:ARG:C	2.55	0.45
1:B:501:ARG:NH1	1:B:505:ARG:HD2	2.31	0.45
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.28	0.45
1:B:315:TYR:CE1	1:B:319:GLU:HG3	2.50	0.45
1:A:23:LEU:HD11	1:A:77:PRO:HG3	1.99	0.45
1:A:363:MET:N	1:A:364:PRO:CD	2.78	0.45
1:B:144:ARG:NH1	1:B:166:THR:CG2	2.79	0.45
1:A:37:VAL:HG11	1:A:71:TRP:CD2	2.52	0.45
1:B:197:PRO:HB2	1:B:206:LYS:CB	2.46	0.45
1:A:501:ARG:NH1	1:A:505:ARG:HD2	2.31	0.45
1:B:573:VAL:HG12	1:B:575:LEU:HD11	1.99	0.45
1:A:375:MET:O	1:A:377:TYR:N	2.50	0.45
1:A:144:ARG:NH1	1:A:166:THR:CG2	2.80	0.45
1:A:588:TRP:CE3	1:A:588:TRP:C	2.89	0.45
1:B:37:VAL:HG11	1:B:71:TRP:CD2	2.52	0.45
1:B:292:VAL:HB	1:B:295:MET:HB3	1.99	0.45
1:B:457:TYR:O	1:B:460:GLU:HG3	2.16	0.45
1:B:588:TRP:CE3	1:B:588:TRP:C	2.89	0.45
1:B:152:ILE:HG21	1:B:172:GLY:O	2.17	0.45
1:B:207:TYR:C	1:B:209:THR:H	2.18	0.45
1:A:198:ILE:HB	1:A:219:PHE:HD2	1.82	0.45
1:A:292:VAL:HB	1:A:295:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CZ	1:B:297:LYS:HE2	2.51	0.45
1:A:200:ARG:HG2	1:A:217:PRO:HD2	1.97	0.45
1:B:313:ALA:HB2	1:B:341:PHE:HE1	1.82	0.45
1:B:1:MET:O	1:B:2:ARG:C	2.55	0.45
1:B:148:GLY:O	1:B:150:PRO:N	2.50	0.45
1:B:209:THR:HG23	1:B:248:CYS:HA	1.99	0.45
1:A:401:LEU:HD23	1:A:510:PHE:HZ	1.80	0.45
1:B:139:GLN:HE22	1:B:422:SER:HB2	1.81	0.45
1:A:152:ILE:HG21	1:A:172:GLY:O	2.17	0.45
1:B:6:ILE:HA	1:B:28:GLN:O	2.17	0.45
1:B:149:ASN:O	1:B:151:ALA:N	2.50	0.45
1:A:148:GLY:O	1:A:150:PRO:N	2.50	0.45
1:B:139:GLN:HA	1:B:194:TYR:O	2.16	0.45
1:A:457:TYR:O	1:A:460:GLU:HG3	2.16	0.45
1:A:123:VAL:CG1	1:B:334:ASP:HB2	2.47	0.45
1:B:34:VAL:HG11	1:B:88:LEU:CB	2.42	0.45
1:A:149:ASN:O	1:A:151:ALA:N	2.50	0.45
1:A:197:PRO:HG3	1:A:207:TYR:CE1	2.52	0.45
1:A:393:SER:OG	1:A:394:ALA:N	2.49	0.45
1:A:334:ASP:HB2	1:B:123:VAL:CG1	2.47	0.45
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.81	0.45
1:B:556:VAL:HA	1:B:563:ARG:HA	1.99	0.45
1:B:137:TRP:HB2	1:B:454:CYS:CB	2.42	0.44
1:B:448:THR:CG2	1:B:522:TYR:HE2	2.30	0.44
1:A:139:GLN:HE22	1:A:422:SER:HB2	1.82	0.44
1:A:573:VAL:HG12	1:A:575:LEU:HD11	1.99	0.44
1:A:209:THR:HG23	1:A:248:CYS:HA	2.00	0.44
1:A:448:THR:CG2	1:A:522:TYR:HE2	2.30	0.44
1:A:1:MET:HE1	1:A:88:LEU:O	2.17	0.44
1:A:197:PRO:HG3	1:A:207:TYR:CD1	2.53	0.44
1:A:534:ILE:HD11	1:A:546:MET:SD	2.58	0.44
1:A:6:ILE:HA	1:A:28:GLN:O	2.18	0.44
1:B:39:LEU:HD23	1:B:86:PHE:CE2	2.53	0.44
1:B:534:ILE:HD11	1:B:546:MET:SD	2.58	0.44
1:B:109:ASP:OD1	1:B:113:TYR:HE2	2.01	0.44
1:A:200:ARG:HE	1:A:214:GLU:CD	2.21	0.44
1:B:200:ARG:HE	1:B:214:GLU:CD	2.21	0.44
1:B:588:TRP:C	1:B:588:TRP:CD2	2.91	0.44
1:A:297:LYS:HE2	1:B:119:PHE:CZ	2.53	0.44
1:A:39:LEU:HD23	1:A:86:PHE:CE2	2.52	0.44
1:B:171:PHE:CD2	1:B:474:CYS:SG	3.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:HG3	1:B:357:GLU:O	2.15	0.44
1:A:62:THR:OG1	1:A:406:HIS:HE1	2.01	0.44
1:A:556:VAL:HA	1:A:563:ARG:HA	1.99	0.44
1:A:511:LEU:O	1:A:521:VAL:HG13	2.18	0.44
1:B:511:LEU:O	1:B:521:VAL:HG13	2.18	0.44
1:A:6:ILE:HG23	1:A:27:LEU:HD21	2.00	0.44
1:B:292:VAL:HG11	1:B:295:MET:CE	2.48	0.44
1:A:292:VAL:HG11	1:A:295:MET:CE	2.48	0.44
1:B:393:SER:OG	1:B:394:ALA:N	2.49	0.44
1:B:163:GLU:C	1:B:165:PRO:HD3	2.38	0.44
1:A:357:GLU:HG3	1:A:357:GLU:O	2.15	0.43
1:A:34:VAL:CG1	1:A:88:LEU:HB2	2.43	0.43
1:B:197:PRO:HG3	1:B:207:TYR:CE1	2.53	0.43
1:B:197:PRO:HG3	1:B:207:TYR:CD1	2.53	0.43
1:B:409:PRO:O	1:B:412:VAL:HB	2.18	0.43
1:B:427:ARG:NH1	1:B:459:ASP:N	2.66	0.43
1:B:6:ILE:HD13	1:B:88:LEU:HD11	1.99	0.43
1:A:588:TRP:C	1:A:588:TRP:CD2	2.90	0.43
1:B:277:PRO:O	1:B:278:LEU:C	2.57	0.43
1:A:271:PHE:HB2	1:A:273:ILE:CD1	2.49	0.43
1:A:230:LYS:HD3	1:A:231:ARG:HE	1.84	0.43
1:A:59:MET:HB2	1:A:59:MET:HE2	1.84	0.43
1:A:138:TYR:HB2	1:A:190:ILE:HG21	2.00	0.43
1:A:277:PRO:O	1:A:278:LEU:C	2.57	0.43
1:B:518:ASN:ND2	1:B:537:ARG:NH1	2.67	0.43
1:B:539:ASN:H	1:B:539:ASN:HD22	1.67	0.43
1:B:110:ASP:HB3	1:B:113:TYR:CE2	2.54	0.43
1:B:19:ASP:OD1	1:B:22:THR:N	2.51	0.43
1:A:171:PHE:CD2	1:A:474:CYS:SG	3.12	0.43
1:B:176:GLN:HA	1:B:179:ILE:HD12	2.00	0.43
1:B:62:THR:OG1	1:B:406:HIS:HE1	2.01	0.43
1:B:528:ASN:HD22	1:B:528:ASN:HA	1.61	0.43
1:A:345:VAL:CG2	1:A:354:ILE:HD11	2.49	0.43
1:B:59:MET:HE3	1:B:71:TRP:HB3	2.01	0.43
1:B:248:CYS:O	1:B:295:MET:HA	2.19	0.43
1:A:313:ALA:HB2	1:A:341:PHE:HE1	1.82	0.43
1:B:230:LYS:HD3	1:B:231:ARG:HE	1.84	0.43
1:B:427:ARG:NH1	1:B:459:ASP:H	2.17	0.43
1:A:427:ARG:NH1	1:A:459:ASP:N	2.67	0.43
1:A:546:MET:HA	1:A:547:PRO:HD3	1.90	0.43
1:A:109:ASP:OD1	1:A:113:TYR:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:OD1	1:A:22:THR:N	2.51	0.43
1:B:158:ARG:CB	1:B:159:PRO:CD	2.95	0.43
1:B:143:GLU:CD	1:B:170:PHE:HA	2.39	0.43
1:A:539:ASN:C	1:A:539:ASN:ND2	2.72	0.43
1:B:23:LEU:HG	1:B:120:LEU:HD12	2.00	0.43
1:B:147:ASN:C	1:B:147:ASN:HD22	2.21	0.43
1:A:137:TRP:NE1	1:A:452:SER:OG	2.51	0.43
1:A:65:ASP:OD1	1:A:65:ASP:N	2.49	0.43
1:A:163:GLU:C	1:A:165:PRO:HD3	2.38	0.42
1:A:185:LEU:HB3	1:A:190:ILE:CG1	2.49	0.42
1:B:271:PHE:HB2	1:B:273:ILE:CD1	2.49	0.42
1:B:206:LYS:NZ	1:B:216:ASP:OD2	2.51	0.42
1:B:345:VAL:CG2	1:B:354:ILE:HD11	2.49	0.42
1:B:450:THR:CG2	1:B:505:ARG:HA	2.45	0.42
1:B:539:ASN:C	1:B:540:GLU:HG3	2.39	0.42
1:A:539:ASN:HD22	1:A:539:ASN:H	1.67	0.42
1:A:137:TRP:HB2	1:A:454:CYS:CB	2.43	0.42
1:A:409:PRO:O	1:A:412:VAL:HB	2.18	0.42
1:A:553:LYS:HG2	1:A:554:TRP:CD1	2.54	0.42
1:A:110:ASP:HB3	1:A:113:TYR:CE2	2.54	0.42
1:A:345:VAL:HG21	1:A:354:ILE:HD11	2.01	0.42
1:A:244:VAL:O	1:A:244:VAL:HG12	2.19	0.42
1:A:158:ARG:CB	1:A:159:PRO:CD	2.94	0.42
1:B:200:ARG:HG3	1:B:214:GLU:OE2	2.20	0.42
1:B:185:LEU:HB3	1:B:190:ILE:CG1	2.48	0.42
1:A:427:ARG:NH1	1:A:459:ASP:H	2.17	0.42
1:B:588:TRP:OXT	1:B:588:TRP:CD2	2.72	0.42
1:A:23:LEU:HG	1:A:120:LEU:HD12	2.00	0.42
1:B:6:ILE:HG23	1:B:27:LEU:HD21	2.00	0.42
1:A:147:ASN:C	1:A:147:ASN:HD22	2.21	0.42
1:B:137:TRP:NE1	1:B:452:SER:OG	2.52	0.42
1:A:518:ASN:ND2	1:A:537:ARG:NH1	2.67	0.42
1:A:19:ASP:HA	1:A:125:LEU:HD21	2.02	0.42
1:A:477:TRP:O	1:A:479:PRO:HD3	2.20	0.42
1:B:477:TRP:O	1:B:479:PRO:HD3	2.20	0.42
1:A:248:CYS:O	1:A:295:MET:HA	2.19	0.42
1:A:143:GLU:CD	1:A:170:PHE:HA	2.40	0.42
1:A:141:PHE:CE2	1:A:472:ARG:NH1	2.87	0.42
1:A:235:LYS:HB3	1:A:237:ILE:HD12	2.01	0.42
1:B:553:LYS:HG2	1:B:554:TRP:CD1	2.54	0.42
1:B:576:PRO:O	1:B:577:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:VAL:O	1:B:230:LYS:C	2.57	0.42
1:B:138:TYR:HB2	1:B:190:ILE:HG21	2.02	0.42
1:A:539:ASN:C	1:A:540:GLU:HG3	2.40	0.42
1:B:140:ILE:HG13	1:B:142:PRO:HD3	2.02	0.42
1:B:141:PHE:CE2	1:B:472:ARG:NH1	2.88	0.42
1:B:460:GLU:HG3	1:B:460:GLU:H	1.44	0.42
1:B:539:ASN:ND2	1:B:539:ASN:C	2.72	0.42
1:B:279:GLN:H	1:B:285:ASN:ND2	2.18	0.42
1:A:253:ALA:HB3	1:A:254:PRO:CD	2.43	0.42
1:B:349:LYS:HD3	1:B:352:VAL:HG23	2.02	0.42
1:A:426:PRO:HA	1:A:466:GLY:O	2.20	0.42
1:A:448:THR:HG21	1:A:522:TYR:OH	2.20	0.42
1:B:381:ASP:O	1:B:385:ARG:HB2	2.19	0.42
1:A:381:ASP:O	1:A:385:ARG:HB2	2.19	0.42
1:A:229:VAL:O	1:A:230:LYS:C	2.57	0.42
1:A:576:PRO:O	1:A:577:PRO:C	2.58	0.42
1:A:39:LEU:HD23	1:A:86:PHE:CD2	2.55	0.42
1:A:343:GLN:O	1:A:347:ALA:HB2	2.20	0.42
1:B:216:ASP:HA	1:B:217:PRO:HD2	1.95	0.41
1:A:200:ARG:HG3	1:A:214:GLU:OE2	2.20	0.41
1:B:389:LYS:HD2	1:B:391:ASP:OD2	2.20	0.41
1:B:448:THR:HG21	1:B:522:TYR:OH	2.20	0.41
1:A:588:TRP:OXT	1:A:588:TRP:CD2	2.72	0.41
1:B:546:MET:HA	1:B:547:PRO:HD3	1.90	0.41
1:A:279:GLN:H	1:A:285:ASN:ND2	2.17	0.41
1:B:343:GLN:O	1:B:347:ALA:HB2	2.20	0.41
1:A:6:ILE:HD13	1:A:88:LEU:HD11	2.00	0.41
1:A:349:LYS:HD3	1:A:352:VAL:HG23	2.02	0.41
1:B:427:ARG:CZ	1:B:458:GLY:HA3	2.50	0.41
1:B:249:GLY:C	1:B:251:GLU:H	2.24	0.41
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.91	0.41
1:B:34:VAL:CG1	1:B:36:HIS:O	2.69	0.41
1:B:426:PRO:HA	1:B:466:GLY:O	2.21	0.41
1:A:249:GLY:C	1:A:251:GLU:H	2.24	0.41
1:B:547:PRO:HG3	2:B:1661:HOH:O	2.21	0.41
1:B:500:TYR:HB2	1:B:503:LEU:HD12	2.02	0.41
1:B:65:ASP:N	1:B:65:ASP:OD1	2.49	0.41
1:A:528:ASN:HA	1:A:528:ASN:HD22	1.61	0.41
1:B:244:VAL:HG12	1:B:244:VAL:O	2.20	0.41
1:A:265:SER:C	1:A:267:TYR:H	2.24	0.41
1:A:140:ILE:HG13	1:A:142:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASP:C	1:A:437:ARG:N	2.74	0.41
1:A:389:LYS:HD2	1:A:391:ASP:OD2	2.21	0.41
1:A:176:GLN:HA	1:A:179:ILE:HD12	2.01	0.41
1:B:435:ASP:C	1:B:437:ARG:H	2.23	0.41
1:B:235:LYS:HB3	1:B:237:ILE:HD12	2.02	0.41
1:A:44:PRO:O	1:A:47:TRP:CZ3	2.73	0.41
1:B:39:LEU:HD23	1:B:86:PHE:CD2	2.56	0.41
1:A:221:ASP:N	1:A:221:ASP:OD1	2.54	0.41
1:B:435:ASP:C	1:B:437:ARG:N	2.74	0.41
1:B:423:HIS:HB2	1:B:472:ARG:HH11	1.84	0.41
1:B:81:ARG:CG	1:B:81:ARG:NH1	2.83	0.41
1:B:555:LEU:HA	1:B:555:LEU:HD12	1.94	0.41
1:B:34:VAL:CG1	1:B:88:LEU:HB2	2.43	0.41
1:A:35:ASP:O	1:A:36:HIS:ND1	2.54	0.41
1:B:345:VAL:HG21	1:B:354:ILE:HD11	2.01	0.41
1:B:327:LEU:HD11	1:B:354:ILE:HG23	2.02	0.41
1:B:385:ARG:HG3	1:B:385:ARG:NH1	2.36	0.41
1:B:161:GLY:C	1:B:163:GLU:N	2.75	0.41
1:B:231:ARG:HD3	1:B:231:ARG:HA	1.93	0.41
1:A:427:ARG:CZ	1:A:458:GLY:HA3	2.51	0.41
1:A:384:LEU:O	1:A:388:ALA:HB3	2.21	0.41
1:B:274:ARG:HG2	1:B:274:ARG:H	1.56	0.41
1:B:265:SER:C	1:B:267:TYR:H	2.24	0.41
1:B:384:LEU:O	1:B:388:ALA:HB3	2.21	0.41
1:B:516:GLU:OE1	1:B:516:GLU:HA	2.21	0.41
1:A:262:GLY:C	1:A:276:PHE:HE2	2.24	0.41
1:A:255:PHE:HA	1:A:258:VAL:HG23	2.03	0.41
1:A:388:ALA:HB1	1:A:431:VAL:HG12	2.02	0.41
1:A:419:LEU:HD23	1:A:419:LEU:H	1.86	0.41
1:A:1:MET:CE	1:A:88:LEU:HB2	2.51	0.40
1:A:435:ASP:C	1:A:437:ARG:H	2.24	0.40
1:B:558:LEU:HD22	1:B:582:LEU:HB3	2.03	0.40
1:B:195:LEU:HD23	1:B:195:LEU:N	2.35	0.40
1:B:1:MET:CE	1:B:88:LEU:HB2	2.50	0.40
1:A:286:TYR:CD1	1:A:286:TYR:N	2.89	0.40
1:A:359:TRP:CZ2	1:A:377:TYR:CZ	3.09	0.40
1:B:375:MET:HE2	1:B:377:TYR:HE2	1.86	0.40
1:A:558:LEU:C	1:A:560:THR:H	2.24	0.40
1:B:456:TYR:O	1:B:457:TYR:C	2.60	0.40
1:A:195:LEU:HD23	1:A:195:LEU:N	2.35	0.40
1:B:262:GLY:C	1:B:276:PHE:HE2	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:TYR:CE1	1:B:24:HIS:HB2	2.56	0.40
1:A:423:HIS:HB2	1:A:472:ARG:HH11	1.84	0.40
1:B:553:LYS:HB2	1:B:588:TRP:HE3	1.86	0.40
1:B:534:ILE:HD11	1:B:546:MET:CB	2.51	0.40
1:B:284:PRO:HG3	1:B:293:PRO:HG3	2.03	0.40
1:B:19:ASP:HA	1:B:125:LEU:HD21	2.02	0.40
1:A:22:THR:HG23	1:A:76:LYS:HG2	2.03	0.40
1:B:38:GLU:HG3	1:B:58:PRO:HA	2.02	0.40
1:A:38:GLU:HG3	1:A:58:PRO:HA	2.03	0.40
1:A:462:GLY:H	1:A:486:LEU:HD23	1.86	0.40
1:B:483:ASN:OD1	1:B:485:GLU:HB3	2.22	0.40
1:B:199:PHE:O	1:B:200:ARG:C	2.60	0.40
1:A:206:LYS:NZ	1:A:216:ASP:OD2	2.50	0.40
1:B:359:TRP:HA	1:B:377:TYR:HB2	2.03	0.40
1:B:558:LEU:C	1:B:560:THR:H	2.24	0.40
1:B:44:PRO:HB3	1:B:83:ARG:HG3	2.03	0.40
1:A:500:TYR:HB2	1:A:503:LEU:HD12	2.02	0.40
1:A:34:VAL:CG1	1:A:36:HIS:O	2.69	0.40
1:A:558:LEU:HD22	1:A:582:LEU:HB3	2.03	0.40
1:A:161:GLY:C	1:A:163:GLU:N	2.74	0.40
1:A:425:THR:HB	1:A:426:PRO:HD2	2.04	0.40
1:A:553:LYS:HB2	1:A:588:TRP:HE3	1.87	0.40
1:A:81:ARG:NH1	1:A:81:ARG:CG	2.83	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	586/588 (100%)	461 (79%)	92 (16%)	33 (6%)	2 6
1	B	586/588 (100%)	460 (78%)	93 (16%)	33 (6%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1172/1176 (100%)	921 (79%)	185 (16%)	66 (6%)	2 6

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	37	VAL
1	A	64	SER
1	A	156	GLY
1	A	159	PRO
1	A	164	ASP
1	A	277	PRO
1	A	281	GLU
1	A	376	ASN
1	A	457	TYR
1	A	559	LEU
1	A	566	ALA
1	A	577	PRO
1	B	31	LYS
1	B	37	VAL
1	B	64	SER
1	B	156	GLY
1	B	159	PRO
1	B	164	ASP
1	B	277	PRO
1	B	281	GLU
1	B	376	ASN
1	B	457	TYR
1	B	559	LEU
1	B	566	ALA
1	B	577	PRO
1	A	2	ARG
1	A	150	PRO
1	A	278	LEU
1	B	2	ARG
1	B	150	PRO
1	B	278	LEU
1	A	65	ASP
1	A	142	PRO
1	A	209	THR
1	A	572	CYS
1	B	65	ASP

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Mol	Chain	Res	Type
1	B	142	PRO
1	B	209	THR
1	B	572	CYS
1	A	70	TYR
1	A	157	ALA
1	B	70	TYR
1	B	157	ALA
1	A	149	ASN
1	A	261	ASN
1	A	465	GLY
1	A	483	ASN
1	B	149	ASN
1	B	261	ASN
1	B	465	GLY
1	B	483	ASN
1	A	118	PRO
1	A	276	PHE
1	A	291	PHE
1	A	562	GLU
1	B	118	PRO
1	B	165	PRO
1	B	276	PHE
1	B	291	PHE
1	B	562	GLU
1	A	165	PRO
1	A	173	GLY
1	B	173	GLY
1	A	167	PRO
1	B	167	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	482/505 (95%)	361 (75%)	121 (25%)	1	2
1	B	482/505 (95%)	361 (75%)	121 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	964/1010 (95%)	722 (75%)	242 (25%)	1 2

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	ARG
1	A	19	ASP
1	A	20	SER
1	A	21	GLU
1	A	22	THR
1	A	24	HIS
1	A	25	LEU
1	A	27	LEU
1	A	34	VAL
1	A	39	LEU
1	A	47	TRP
1	A	61	LYS
1	A	65	ASP
1	A	67	LEU
1	A	80	ARG
1	A	81	ARG
1	A	82	LEU
1	A	88	LEU
1	A	89	ARG
1	A	94	LYS
1	A	100	LYS
1	A	111	THR
1	A	123	VAL
1	A	135	THR
1	A	139	GLN
1	A	140	ILE
1	A	141	PHE
1	A	147	ASN
1	A	149	ASN
1	A	152	ILE
1	A	153	SER
1	A	158	ARG
1	A	166	THR
1	A	170	PHE
1	A	176	GLN
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	190	ILE
1	A	191	THR
1	A	193	ILE
1	A	194	TYR
1	A	195	LEU
1	A	196	THR
1	A	200	ARG
1	A	204	ASN
1	A	206	LYS
1	A	223	GLU
1	A	227	THR
1	A	228	LEU
1	A	229	VAL
1	A	230	LYS
1	A	234	GLU
1	A	235	LYS
1	A	238	ARG
1	A	240	MET
1	A	241	LEU
1	A	251	GLU
1	A	269	ASP
1	A	272	HIS
1	A	274	ARG
1	A	275	GLU
1	A	276	PHE
1	A	283	ARG
1	A	298	LEU
1	A	299	ASN
1	A	300	THR
1	A	323	ASP
1	A	339	ARG
1	A	348	LEU
1	A	357	GLU
1	A	363	MET
1	A	367	ARG
1	A	379	LEU
1	A	381	ASP
1	A	385	ARG
1	A	391	ASP
1	A	393	SER
1	A	395	SER
1	A	400	ARG

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Mol	Chain	Res	Type
1	A	401	LEU
1	A	402	MET
1	A	404	VAL
1	A	410	LYS
1	A	411	GLN
1	A	422	SER
1	A	430	THR
1	A	447	LEU
1	A	448	THR
1	A	449	PHE
1	A	460	GLU
1	A	461	ILE
1	A	464	THR
1	A	472	ARG
1	A	484	LYS
1	A	492	GLN
1	A	493	LEU
1	A	496	LEU
1	A	499	GLN
1	A	501	ARG
1	A	505	ARG
1	A	515	ASP
1	A	521	VAL
1	A	525	THR
1	A	528	ASN
1	A	537	ARG
1	A	539	ASN
1	A	547	PRO
1	A	553	LYS
1	A	556	VAL
1	A	557	ASN
1	A	558	LEU
1	A	560	THR
1	A	563	ARG
1	A	564	PHE
1	A	570	THR
1	A	571	LEU
1	A	575	LEU
1	A	581	VAL
1	A	586	GLU
1	A	587	SER
1	A	588	TRP

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Mol	Chain	Res	Type
1	B	2	ARG
1	B	9	ARG
1	B	19	ASP
1	B	20	SER
1	B	21	GLU
1	B	22	THR
1	B	24	HIS
1	B	25	LEU
1	B	27	LEU
1	B	34	VAL
1	B	39	LEU
1	B	47	TRP
1	B	61	LYS
1	B	65	ASP
1	B	67	LEU
1	B	80	ARG
1	B	81	ARG
1	B	82	LEU
1	B	88	LEU
1	B	89	ARG
1	B	94	LYS
1	B	100	LYS
1	B	111	THR
1	B	123	VAL
1	B	135	THR
1	B	139	GLN
1	B	140	ILE
1	B	141	PHE
1	B	147	ASN
1	B	149	ASN
1	B	152	ILE
1	B	153	SER
1	B	158	ARG
1	B	166	THR
1	B	170	PHE
1	B	176	GLN
1	B	188	LEU
1	B	190	ILE
1	B	191	THR
1	B	193	ILE
1	B	194	TYR
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	196	THR
1	B	200	ARG
1	B	204	ASN
1	B	206	LYS
1	B	223	GLU
1	B	227	THR
1	B	228	LEU
1	B	229	VAL
1	B	230	LYS
1	B	234	GLU
1	B	235	LYS
1	B	238	ARG
1	B	240	MET
1	B	241	LEU
1	B	251	GLU
1	B	269	ASP
1	B	272	HIS
1	B	274	ARG
1	B	275	GLU
1	B	276	PHE
1	B	283	ARG
1	B	298	LEU
1	B	299	ASN
1	B	300	THR
1	B	323	ASP
1	B	339	ARG
1	B	348	LEU
1	B	357	GLU
1	B	363	MET
1	B	367	ARG
1	B	379	LEU
1	B	381	ASP
1	B	385	ARG
1	B	391	ASP
1	B	393	SER
1	B	395	SER
1	B	400	ARG
1	B	401	LEU
1	B	402	MET
1	B	404	VAL
1	B	410	LYS
1	B	411	GLN

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Mol	Chain	Res	Type
1	B	422	SER
1	B	430	THR
1	B	447	LEU
1	B	448	THR
1	B	449	PHE
1	B	460	GLU
1	B	461	ILE
1	B	464	THR
1	B	472	ARG
1	B	484	LYS
1	B	492	GLN
1	B	493	LEU
1	B	496	LEU
1	B	499	GLN
1	B	501	ARG
1	B	505	ARG
1	B	515	ASP
1	B	521	VAL
1	B	525	THR
1	B	528	ASN
1	B	537	ARG
1	B	539	ASN
1	B	547	PRO
1	B	553	LYS
1	B	556	VAL
1	B	557	ASN
1	B	558	LEU
1	B	560	THR
1	B	563	ARG
1	B	564	PHE
1	B	570	THR
1	B	571	LEU
1	B	575	LEU
1	B	581	VAL
1	B	586	GLU
1	B	587	SER
1	B	588	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS

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Mol	Chain	Res	Type
1	A	24	HIS
1	A	147	ASN
1	A	204	ASN
1	A	299	ASN
1	A	302	HIS
1	A	335	HIS
1	A	343	GLN
1	A	370	GLN
1	A	406	HIS
1	A	423	HIS
1	A	499	GLN
1	A	518	ASN
1	A	519	HIS
1	A	528	ASN
1	A	539	ASN
1	A	557	ASN
1	B	7	HIS
1	B	24	HIS
1	B	147	ASN
1	B	204	ASN
1	B	299	ASN
1	B	302	HIS
1	B	335	HIS
1	B	343	GLN
1	B	370	GLN
1	B	406	HIS
1	B	423	HIS
1	B	499	GLN
1	B	518	ASN
1	B	519	HIS
1	B	528	ASN
1	B	539	ASN
1	B	557	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	588/588 (100%)	0.21	12 (2%) 68 58	13, 39, 84, 100	0
1	B	588/588 (100%)	0.19	12 (2%) 68 58	12, 39, 85, 100	0
All	All	1176/1176 (100%)	0.20	24 (2%) 68 58	12, 39, 85, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	GLY	14.6
1	A	162	SER	8.7
1	B	161	GLY	8.1
1	B	162	SER	6.4
1	B	160	TRP	5.1
1	A	160	TRP	5.0
1	A	163	GLU	4.5
1	B	588	TRP	4.4
1	B	164	ASP	4.4
1	A	164	ASP	4.2
1	A	588	TRP	4.0
1	B	163	GLU	3.6
1	B	250	TYR	2.7
1	A	254	PRO	2.7
1	A	273	ILE	2.6
1	A	284	PRO	2.6
1	B	273	ILE	2.4
1	A	206	LYS	2.3
1	B	206	LYS	2.3
1	A	170	PHE	2.3
1	A	169	SER	2.2
1	B	520	LEU	2.1
1	B	275	GLU	2.1
1	B	167	PRO	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 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.