



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 01:41 AM UTC

PDB ID : 2VNC / pdb_00002vnc
Title : Crystal structure of Glycogen Debranching enzyme TreX from *Sulfolobus solfataricus*
Authors : Song, H.-N.; Yoon, S.-M.; Cha, H.; Park, K.-T.; Woo, E.-J.
Deposited on : 2008-02-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

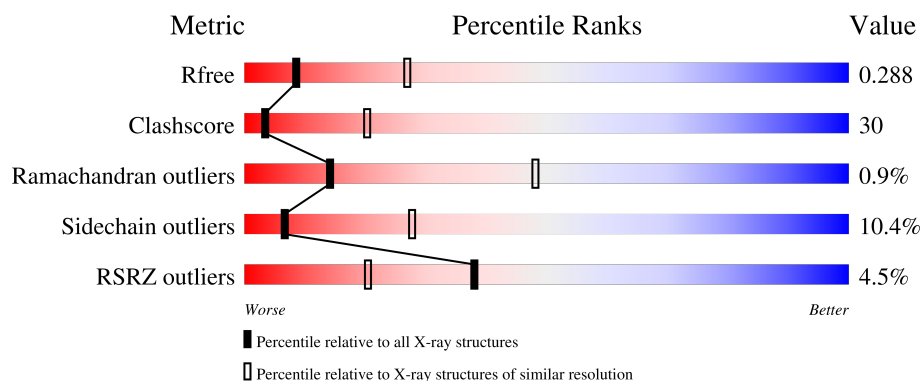
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	718	2% 65% 28% • •
1	B	718	7% 46% 36% 10% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11284 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 GLYCOGEN OPERON PROTEIN GLGX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5711	3661	959	1073	18			
1	B	666	Total	C	N	O	S	0	0	0
			5443	3490	919	1018	16			

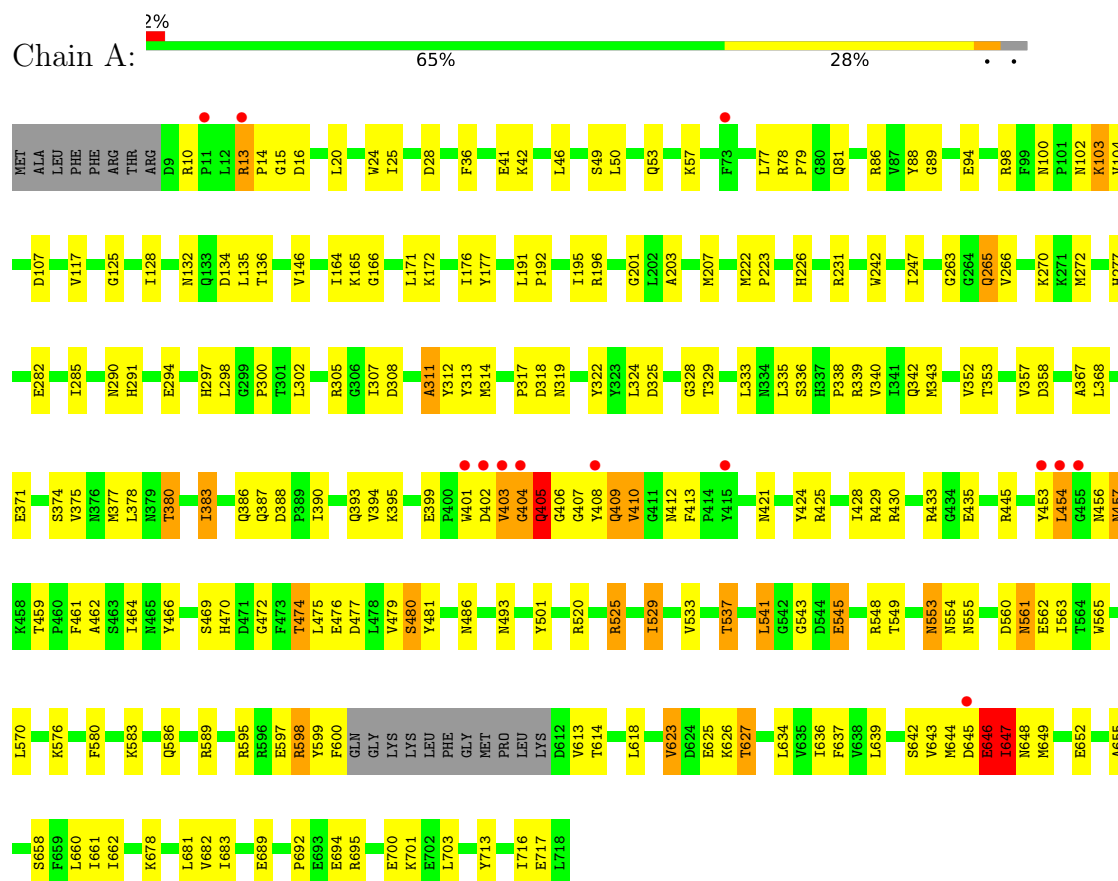
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	30	Total	O	0	0
			30	30		

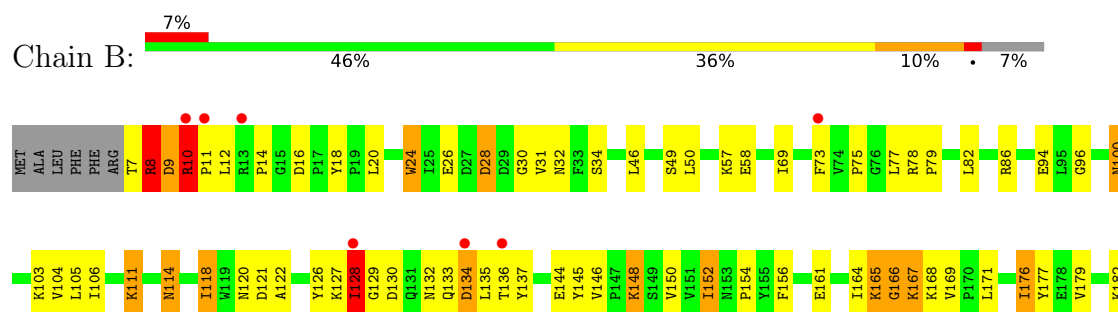
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: GLYCOGEN OPERON PROTEIN GLGX



• Molecule 1: GLYCOGEN OPERON PROTEIN GLGX





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.08Å 136.08Å 173.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 3.00 29.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-3.00) 99.7 (29.91-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.287 0.221 , 0.288	Depositor DCC
R_{free} test set	1909 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0.61	0/5860	0.93	14/7948 (0.2%)
1	B	0.58	1/5582 (0.0%)	0.89	15/7566 (0.2%)
All	All	0.60	1/11442 (0.0%)	0.91	29/15514 (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	3
1	B	0	23
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	ILE	CA-CB	5.33	1.59	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	THR	CA-C-N	6.85	128.41	119.84
1	B	459	THR	C-N-CA	6.85	128.41	119.84
1	A	388	ASP	CA-C-N	6.72	126.51	119.05
1	A	388	ASP	C-N-CA	6.72	126.51	119.05
1	A	646	GLU	CA-C-N	6.71	133.78	121.70
1	A	646	GLU	C-N-CA	6.71	133.78	121.70
1	B	514	GLN	N-CA-C	-6.45	106.62	114.75
1	A	128	ILE	N-CA-C	6.37	122.59	109.34
1	A	16	ASP	CA-C-N	6.18	125.40	118.97
1	A	16	ASP	C-N-CA	6.18	125.40	118.97
1	A	107	ASP	CA-C-N	6.10	125.99	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	C-N-CA	6.10	125.99	119.28
1	A	311	ALA	N-CA-C	-6.09	102.64	110.19
1	B	459	THR	N-CA-C	-5.98	96.91	108.45
1	B	437	LEU	CA-C-N	5.85	127.15	119.84
1	B	437	LEU	C-N-CA	5.85	127.15	119.84
1	A	313	TYR	N-CA-C	5.82	118.95	109.59
1	B	457	ASN	N-CA-C	-5.71	105.65	113.30
1	B	179	VAL	N-CA-C	5.62	115.97	108.27
1	B	690	ILE	N-CA-C	5.54	115.30	106.88
1	A	13	ARG	CA-C-N	5.48	125.57	119.32
1	A	13	ARG	C-N-CA	5.48	125.57	119.32
1	B	152	ILE	N-CA-C	5.40	116.96	109.29
1	A	623	VAL	N-CA-C	5.40	114.52	106.85
1	B	222	MET	CA-C-N	5.22	126.36	119.84
1	B	222	MET	C-N-CA	5.22	126.36	119.84
1	B	100	ASN	CA-C-N	5.21	124.83	119.05
1	B	100	ASN	C-N-CA	5.21	124.83	119.05
1	B	297	HIS	N-CA-C	-5.01	103.87	110.43

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	VAL	Peptide
1	A	404	GLY	Peptide
1	A	405	GLN	Peptide
1	B	10	ARG	Peptide
1	B	166	GLY	Peptide
1	B	231	ARG	Peptide
1	B	232	PHE	Peptide
1	B	474	THR	Peptide
1	B	475	LEU	Peptide
1	B	476	GLU	Peptide
1	B	477	ASP	Peptide
1	B	478	LEU	Peptide
1	B	480	SER	Peptide
1	B	481	TYR	Peptide
1	B	540	ILE	Peptide
1	B	571	ASP	Peptide
1	B	573	ARG	Peptide
1	B	574	LYS	Peptide
1	B	614	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	625	GLU	Peptide
1	B	626	LYS	Peptide
1	B	664	ASN	Peptide
1	B	665	ALA	Peptide
1	B	708	ARG	Peptide
1	B	710	ALA	Peptide
1	B	8	ARG	Peptide

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	5711	0	5508	164	1
1	B	5443	0	5242	502	12
2	A	100	0	0	5	0
2	B	30	0	0	6	0
All	All	11284	0	10750	656	13

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (656) 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:473:PHE:HB3	1:B:478:LEU:CD2	1.54	1.35
1:B:476:GLU:CG	1:B:479:VAL:HG13	1.58	1.31
1:B:9:ASP:CB	1:B:10:ARG:HA	1.63	1.25
1:B:475:LEU:H	1:B:476:GLU:C	1.48	1.20
1:B:476:GLU:HG2	1:B:479:VAL:CG1	1.72	1.18
1:B:9:ASP:HB3	1:B:10:ARG:CA	1.71	1.18
1:B:614:THR:OG1	1:B:637:PHE:HA	1.44	1.16
1:B:691:LYS:HG2	1:B:692:PRO:CD	1.75	1.15
1:B:231:ARG:CB	1:B:232:PHE:HB2	1.76	1.14
1:B:472:GLY:HA2	1:B:554:ASN:HA	1.24	1.14
1:B:543:GLY:O	1:B:548:ARG:HB2	1.47	1.14
1:B:473:PHE:O	1:B:474:THR:HG22	1.46	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HH21	1:B:10:ARG:HG3	1.03	1.12
1:B:691:LYS:HG2	1:B:692:PRO:HD3	1.17	1.11
1:B:559:GLN:HE21	1:B:563:ILE:HD12	1.11	1.11
1:B:231:ARG:HB3	1:B:232:PHE:HB2	1.15	1.10
1:B:473:PHE:HB3	1:B:478:LEU:HD21	1.25	1.10
1:B:482:ASN:OD1	1:B:502:SER:O	1.70	1.09
1:B:615:PHE:CD1	1:B:636:ILE:O	2.06	1.08
1:B:7:THR:HG22	1:B:8:ARG:H	1.12	1.07
1:B:458:LYS:O	1:B:458:LYS:HG3	1.54	1.07
1:B:665:ALA:HB3	1:B:666:ASN:HB3	1.34	1.07
1:B:473:PHE:HB3	1:B:478:LEU:HD22	1.29	1.05
1:B:574:LYS:HD3	1:B:574:LYS:N	1.59	1.05
1:B:614:THR:HG1	1:B:637:PHE:HA	1.12	1.05
1:B:10:ARG:HG3	1:B:10:ARG:O	1.57	1.04
1:B:7:THR:HG22	1:B:8:ARG:N	1.67	1.04
1:B:476:GLU:OE1	1:B:520:ARG:HG3	1.56	1.04
1:B:231:ARG:HB3	1:B:232:PHE:CB	1.86	1.04
1:B:476:GLU:CG	1:B:479:VAL:CG1	2.30	1.03
1:B:710:ALA:O	1:B:711:LEU:HD13	1.59	1.02
1:B:10:ARG:H	1:B:11:PRO:HA	1.23	1.02
1:B:476:GLU:OE2	1:B:479:VAL:HG11	1.60	1.01
1:B:471:ASP:O	1:B:554:ASN:O	1.80	0.99
1:B:476:GLU:HG2	1:B:479:VAL:HG13	1.33	0.99
1:B:615:PHE:HE1	1:B:636:ILE:H	1.00	0.98
1:B:230:GLN:O	1:B:233:LEU:N	1.97	0.98
1:B:481:TYR:H	1:B:482:ASN:HB2	1.30	0.96
1:B:559:GLN:NE2	1:B:563:ILE:HD12	1.80	0.96
1:B:231:ARG:CA	1:B:232:PHE:HB2	1.94	0.96
1:B:476:GLU:CD	1:B:479:VAL:HG13	1.91	0.94
1:B:231:ARG:N	1:B:232:PHE:HB2	1.83	0.94
1:B:618:LEU:HD13	1:B:618:LEU:O	1.68	0.93
1:B:614:THR:OG1	1:B:637:PHE:CA	2.16	0.93
1:B:480:SER:HG	1:B:481:TYR:HD1	0.94	0.93
1:B:473:PHE:HD2	1:B:474:THR:H	1.09	0.92
1:B:468:THR:CB	1:B:473:PHE:HE2	1.82	0.92
1:B:473:PHE:HA	1:B:478:LEU:HD13	1.49	0.91
1:B:468:THR:HB	1:B:473:PHE:HE2	1.31	0.91
1:B:473:PHE:CB	1:B:478:LEU:HD22	1.99	0.91
1:B:476:GLU:CD	1:B:479:VAL:CG1	2.43	0.91
1:B:708:ARG:N	1:B:709:THR:HG22	1.86	0.91
1:B:573:ARG:C	1:B:574:LYS:HD3	1.96	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ARG:N	1:B:709:THR:CG2	2.34	0.90
1:B:479:VAL:HG22	1:B:479:VAL:O	1.71	0.89
1:B:476:GLU:CB	1:B:479:VAL:HG13	2.03	0.89
1:B:475:LEU:N	1:B:476:GLU:C	2.31	0.89
1:B:480:SER:OG	1:B:481:TYR:HD1	1.55	0.88
1:B:571:ASP:HB3	1:B:574:LYS:HE3	1.55	0.88
1:B:473:PHE:CB	1:B:478:LEU:CD2	2.48	0.88
1:B:529:ILE:CD1	1:B:710:ALA:CB	2.50	0.88
1:B:10:ARG:HH21	1:B:10:ARG:CG	1.85	0.87
1:B:10:ARG:HG3	1:B:10:ARG:NH2	1.84	0.86
1:B:476:GLU:OE2	1:B:523:GLN:HB2	1.75	0.86
1:B:475:LEU:N	1:B:476:GLU:O	2.07	0.86
1:B:482:ASN:CG	1:B:502:SER:C	2.43	0.86
1:B:26:GLU:O	1:B:26:GLU:HG2	1.74	0.85
1:B:10:ARG:N	1:B:11:PRO:HA	1.92	0.85
1:B:503:TRP:HD1	1:B:504:ASN:H	1.23	0.84
1:B:615:PHE:CD1	1:B:616:TYR:N	2.44	0.84
1:B:472:GLY:HA2	1:B:554:ASN:CA	2.07	0.83
1:B:665:ALA:HB3	1:B:666:ASN:CB	2.08	0.83
1:A:380:THR:HG22	1:B:380:THR:HG22	1.59	0.83
1:B:529:ILE:HD11	1:B:710:ALA:CB	2.08	0.83
1:B:482:ASN:ND2	1:B:502:SER:C	2.34	0.83
1:B:9:ASP:CB	1:B:10:ARG:CA	2.41	0.83
1:B:476:GLU:HA	1:B:479:VAL:H	1.42	0.83
1:B:478:LEU:HD13	1:B:478:LEU:N	1.93	0.83
1:B:615:PHE:O	1:B:616:TYR:CD2	2.32	0.83
1:B:529:ILE:HD13	1:B:710:ALA:HB1	1.60	0.83
1:B:478:LEU:HD13	1:B:478:LEU:H	1.42	0.82
1:B:473:PHE:O	1:B:474:THR:CG2	2.27	0.82
1:A:265:GLN:H	1:A:265:GLN:HE21	1.26	0.81
1:B:626:LYS:CB	1:B:627:THR:HB	2.11	0.81
1:B:529:ILE:HD13	1:B:710:ALA:CB	2.12	0.80
1:B:574:LYS:N	1:B:574:LYS:CD	2.41	0.80
1:B:476:GLU:OE2	1:B:479:VAL:CG1	2.30	0.80
1:B:297:HIS:O	1:B:298:LEU:HB2	1.81	0.80
1:B:468:THR:HG22	1:B:473:PHE:CE2	2.17	0.79
1:B:529:ILE:CD1	1:B:710:ALA:HB3	2.10	0.79
1:B:674:PHE:HZ	1:B:703:LEU:HD12	1.48	0.79
1:B:684:SER:HB2	1:B:711:LEU:CD1	2.12	0.79
1:B:78:ARG:HB2	1:B:79:PRO:HD2	1.64	0.79
1:B:529:ILE:HD11	1:B:710:ALA:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HB3	1:B:12:LEU:HG	1.63	0.78
1:B:472:GLY:O	1:B:473:PHE:CG	2.36	0.78
1:B:691:LYS:HG3	1:B:692:PRO:HG3	1.65	0.78
1:B:478:LEU:HA	1:B:480:SER:H	1.49	0.78
1:B:707:GLY:C	1:B:709:THR:HG23	2.09	0.78
1:B:480:SER:OG	1:B:481:TYR:CD1	2.35	0.78
1:B:231:ARG:HB3	1:B:232:PHE:CG	2.18	0.78
1:B:321:ARG:HD3	1:B:322:TYR:HE2	1.49	0.77
1:B:473:PHE:CD2	1:B:474:THR:N	2.51	0.77
1:A:560:ASP:OD1	1:A:565:TRP:HH2	1.66	0.77
1:B:231:ARG:N	1:B:232:PHE:CB	2.48	0.77
1:A:297:HIS:O	1:A:298:LEU:HB2	1.85	0.77
1:B:458:LYS:O	1:B:458:LYS:CG	2.32	0.77
1:B:292:THR:H	1:B:331:ASN:HD21	1.31	0.76
1:B:16:ASP:H	1:B:32:ASN:HD21	1.33	0.76
1:B:626:LYS:H	1:B:627:THR:HB	1.50	0.76
1:B:191:LEU:HD21	1:B:206:GLN:NE2	2.01	0.76
1:B:168:LYS:HB3	1:B:282:GLU:OE2	1.86	0.76
1:B:10:ARG:H	1:B:11:PRO:CA	1.96	0.75
1:B:671:LYS:HA	1:B:704:GLU:HG3	1.67	0.75
1:A:560:ASP:OD1	1:A:565:TRP:CH2	2.40	0.75
1:A:265:GLN:H	1:A:265:GLN:NE2	1.84	0.74
1:B:472:GLY:C	1:B:473:PHE:CD1	2.66	0.74
1:B:49:SER:HB3	1:B:57:LYS:HD3	1.67	0.74
1:B:691:LYS:CG	1:B:692:PRO:HD3	2.10	0.74
1:B:134:ASP:HB3	1:B:298:LEU:HD12	1.68	0.74
1:B:482:ASN:CG	1:B:502:SER:O	2.30	0.74
1:B:708:ARG:H	1:B:709:THR:HG22	1.49	0.74
1:A:405:GLN:C	1:A:405:GLN:OE1	2.31	0.73
1:B:9:ASP:HB3	1:B:10:ARG:HA	0.79	0.73
1:B:468:THR:CB	1:B:473:PHE:CE2	2.70	0.73
1:B:133:GLN:O	1:B:134:ASP:CG	2.30	0.73
1:B:472:GLY:C	1:B:473:PHE:CG	2.66	0.73
1:A:476:GLU:O	1:A:480:SER:OG	2.06	0.73
1:B:674:PHE:CZ	1:B:703:LEU:HD12	2.23	0.73
1:B:710:ALA:O	1:B:711:LEU:CD1	2.36	0.73
1:B:612:ASP:OD2	1:B:641:GLY:CA	2.37	0.72
1:B:468:THR:HB	1:B:473:PHE:CE2	2.22	0.72
1:B:503:TRP:CD1	1:B:504:ASN:H	2.07	0.72
1:B:321:ARG:HD3	1:B:322:TYR:CE2	2.24	0.72
1:A:77:LEU:HD22	1:A:81:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:TYR:O	1:B:636:ILE:HD12	1.89	0.72
1:B:127:LYS:H	1:B:136:THR:HG23	1.55	0.71
1:B:570:LEU:H	1:B:570:LEU:HD23	1.54	0.71
1:B:223:PRO:HB2	1:B:243:GLY:HA3	1.73	0.71
1:B:230:GLN:H	1:B:230:GLN:NE2	1.87	0.71
1:B:479:VAL:O	1:B:479:VAL:CG2	2.39	0.70
1:B:703:LEU:HB3	1:B:704:GLU:HA	1.74	0.70
1:B:626:LYS:H	1:B:627:THR:CG2	2.04	0.70
1:B:193:GLU:HA	1:B:196:ARG:HH11	1.56	0.70
1:B:626:LYS:N	1:B:627:THR:HB	2.07	0.69
1:B:615:PHE:CE1	1:B:636:ILE:O	2.45	0.69
1:B:684:SER:CB	1:B:711:LEU:HD12	2.23	0.69
1:B:7:THR:CG2	1:B:8:ARG:H	1.88	0.69
1:B:478:LEU:HA	1:B:480:SER:N	2.07	0.69
1:B:193:GLU:HA	1:B:196:ARG:NH1	2.07	0.68
1:B:290:ASN:OD1	1:B:291:HIS:HD2	1.75	0.68
1:A:561:ASN:HD22	1:A:563:ILE:H	1.40	0.68
1:A:403:VAL:O	1:A:406:GLY:CA	2.41	0.68
1:B:615:PHE:HD1	1:B:636:ILE:O	1.72	0.68
1:A:371:GLU:O	1:A:374:SER:HB3	1.93	0.68
1:B:476:GLU:HA	1:B:479:VAL:N	2.09	0.68
1:B:626:LYS:H	1:B:627:THR:CB	2.06	0.68
1:B:222:MET:HE2	2:B:2013:HOH:O	1.94	0.68
1:B:708:ARG:N	1:B:709:THR:HG23	2.08	0.68
1:B:614:THR:OG1	1:B:637:PHE:CB	2.41	0.67
1:A:380:THR:HG22	1:B:380:THR:CG2	2.25	0.67
1:B:626:LYS:CA	1:B:627:THR:HB	2.23	0.67
1:A:380:THR:HB	1:B:380:THR:HB	1.77	0.67
1:B:684:SER:HB2	1:B:711:LEU:HD12	1.74	0.67
1:B:468:THR:HG22	1:B:473:PHE:CD2	2.29	0.67
1:B:618:LEU:O	1:B:618:LEU:HD22	1.92	0.67
1:B:712:VAL:O	1:B:713:TYR:CG	2.47	0.67
1:A:403:VAL:O	1:A:406:GLY:HA2	1.95	0.67
1:B:478:LEU:CD2	1:B:478:LEU:O	2.43	0.67
1:B:712:VAL:O	1:B:713:TYR:CD1	2.47	0.67
1:B:7:THR:CG2	1:B:8:ARG:N	2.42	0.66
1:B:191:LEU:HD22	1:B:195:ILE:HD11	1.77	0.66
1:B:430:ARG:HB3	1:B:437:LEU:HD21	1.77	0.66
1:B:468:THR:CG2	1:B:473:PHE:CE2	2.78	0.66
1:B:541:LEU:HD13	1:B:542:GLY:N	2.10	0.66
1:A:192:PRO:HG2	1:A:195:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:OD2	1:B:134:ASP:C	2.38	0.66
1:B:336:SER:HB3	1:B:375:VAL:HB	1.78	0.66
1:B:475:LEU:CD1	1:B:544:ASP:HB3	2.26	0.66
1:B:691:LYS:CG	1:B:692:PRO:CD	2.64	0.66
1:A:649:MET:HA	1:B:14:PRO:HG2	1.77	0.66
1:B:474:THR:HG23	1:B:474:THR:O	1.94	0.66
1:B:710:ALA:C	1:B:711:LEU:HD13	2.21	0.65
1:B:691:LYS:CG	1:B:692:PRO:HG3	2.27	0.65
1:B:247:ILE:HD13	1:B:247:ILE:O	1.96	0.65
1:A:486:ASN:H	1:A:493:ASN:ND2	1.94	0.65
1:B:221:LEU:O	1:B:286:ASP:HB2	1.96	0.65
1:B:242:TRP:HA	2:B:2013:HOH:O	1.96	0.65
1:B:285:ILE:HG12	1:B:357:VAL:HG11	1.79	0.65
1:A:649:MET:HA	1:B:14:PRO:CG	2.27	0.65
1:B:540:ILE:HG22	1:B:541:LEU:O	1.97	0.65
1:B:666:ASN:O	1:B:708:ARG:NH2	2.07	0.65
1:B:365:ALA:CB	1:B:398:ALA:HB1	2.27	0.64
1:B:389:PRO:O	1:B:393:GLN:NE2	2.30	0.64
1:B:473:PHE:HA	1:B:478:LEU:CD1	2.26	0.64
1:B:478:LEU:HD22	1:B:478:LEU:O	1.97	0.64
1:B:665:ALA:O	1:B:708:ARG:HD3	1.97	0.64
1:A:407:GLY:O	1:A:409:GLN:N	2.30	0.64
1:B:188:ARG:HG3	1:B:188:ARG:HH11	1.63	0.64
1:B:614:THR:HG23	1:B:638:VAL:O	1.97	0.64
1:A:291:HIS:ND1	1:A:329:THR:HG21	2.12	0.64
1:B:440:SER:HB3	1:B:628:TRP:CD1	2.33	0.64
1:B:233:LEU:O	1:B:235:ASP:N	2.30	0.64
1:B:615:PHE:HE1	1:B:636:ILE:N	1.84	0.64
1:B:633:GLN:HB3	1:B:665:ALA:CB	2.28	0.64
1:B:705:ILE:HG22	1:B:706:GLU:H	1.63	0.64
1:A:36:PHE:CE1	1:A:339:ARG:HG3	2.33	0.63
1:B:134:ASP:HB3	1:B:298:LEU:CD1	2.28	0.63
1:A:472:GLY:HA2	1:A:554:ASN:O	1.99	0.63
1:B:571:ASP:O	1:B:573:ARG:N	2.32	0.63
1:A:525:ARG:HG2	1:A:580:PHE:CE2	2.34	0.63
1:B:674:PHE:HE2	1:B:713:TYR:CE1	2.16	0.63
1:B:615:PHE:HD1	1:B:616:TYR:H	1.40	0.62
1:B:429:ARG:NH2	1:B:473:PHE:CZ	2.68	0.62
1:B:466:TYR:CE2	1:B:469:SER:HB3	2.34	0.62
1:B:633:GLN:HG2	1:B:665:ALA:CB	2.28	0.62
1:A:477:ASP:O	1:A:481:TYR:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:TYR:HB2	1:A:600:PHE:CE1	2.34	0.62
1:B:529:ILE:CD1	1:B:710:ALA:HB1	2.23	0.62
1:A:692:PRO:HA	1:A:695:ARG:HD2	1.82	0.61
2:A:2010:HOH:O	1:B:415:TYR:HE1	1.83	0.61
1:B:475:LEU:H	1:B:477:ASP:N	1.95	0.61
1:B:706:GLU:HG2	1:B:707:GLY:N	2.14	0.61
1:B:230:GLN:H	1:B:230:GLN:HE21	1.48	0.61
1:B:439:TYR:OH	1:B:634:LEU:N	2.34	0.61
1:B:473:PHE:HA	1:B:478:LEU:H	1.66	0.61
1:B:10:ARG:HB3	1:B:12:LEU:CG	2.30	0.61
1:B:188:ARG:HH11	1:B:188:ARG:CG	2.14	0.61
1:B:263:GLY:H	1:B:265:GLN:NE2	1.98	0.61
1:B:636:ILE:HG12	1:B:662:ILE:HG23	1.83	0.61
1:A:623:VAL:HG13	1:A:627:THR:HB	1.83	0.61
1:B:476:GLU:HG2	1:B:479:VAL:HG12	1.80	0.61
1:A:474:THR:O	1:A:477:ASP:N	2.34	0.61
1:A:561:ASN:ND2	1:A:563:ILE:H	1.99	0.61
1:B:190:ASP:O	1:B:191:LEU:HG	2.01	0.61
1:B:233:LEU:HD23	1:B:234:THR:H	1.66	0.61
1:B:476:GLU:OE2	1:B:523:GLN:CB	2.48	0.60
1:B:616:TYR:HB2	1:B:636:ILE:HB	1.81	0.60
1:A:425:ARG:HB3	1:A:466:TYR:O	2.01	0.60
1:B:127:LYS:O	1:B:129:GLY:N	2.34	0.60
1:B:684:SER:HB2	1:B:711:LEU:HD11	1.82	0.60
1:B:310:THR:CG2	2:B:2004:HOH:O	2.49	0.60
1:B:666:ASN:N	1:B:708:ARG:HE	1.99	0.60
1:B:26:GLU:O	1:B:26:GLU:CG	2.44	0.60
1:B:573:ARG:O	1:B:574:LYS:HD3	2.01	0.60
1:B:222:MET:HB3	1:B:223:PRO:HD2	1.83	0.60
1:A:285:ILE:HG12	1:A:357:VAL:HG11	1.83	0.60
1:B:111:LYS:HB2	1:B:152:ILE:HG12	1.83	0.60
1:B:126:TYR:HA	1:B:136:THR:O	2.02	0.60
1:B:171:LEU:HD12	1:B:171:LEU:H	1.66	0.60
1:B:335:LEU:HG	1:B:372:LEU:CD1	2.30	0.60
1:B:352:VAL:HG21	1:B:394:VAL:HG11	1.84	0.60
1:B:627:THR:HG22	1:B:628:TRP:N	2.17	0.59
1:A:353:THR:HG23	1:A:390:ILE:HD12	1.83	0.59
1:B:230:GLN:HE21	1:B:233:LEU:HD22	1.66	0.59
1:B:146:VAL:O	1:B:148:LYS:HE2	2.02	0.59
1:B:78:ARG:HB2	1:B:79:PRO:CD	2.32	0.59
1:A:642:SER:HB3	1:A:655:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HA	1:B:238:LEU:O	2.03	0.59
1:B:421:ASN:C	1:B:421:ASN:HD22	2.09	0.59
1:B:535:GLN:HE22	1:B:594:PHE:HA	1.67	0.59
1:A:317:PRO:O	1:A:318:ASP:HB2	2.03	0.58
1:A:265:GLN:HE21	1:A:265:GLN:N	1.99	0.58
1:B:503:TRP:CD1	1:B:505:CYS:H	2.22	0.58
1:A:410:VAL:CG1	1:A:413:PHE:CE1	2.85	0.58
1:B:10:ARG:N	1:B:11:PRO:CA	2.57	0.58
1:B:335:LEU:HG	1:B:372:LEU:HD12	1.86	0.58
1:B:596:ARG:HH22	1:B:639:LEU:HD21	1.68	0.58
1:B:472:GLY:O	1:B:473:PHE:CD2	2.56	0.58
1:B:222:MET:HE1	1:B:242:TRP:CD1	2.38	0.58
1:B:665:ALA:HB3	1:B:666:ASN:CA	2.33	0.58
1:A:290:ASN:OD1	1:A:291:HIS:HD2	1.87	0.58
1:A:297:HIS:CD2	1:A:298:LEU:HD13	2.39	0.58
1:B:10:ARG:NE	1:B:58:GLU:OE1	2.36	0.58
1:A:454:LEU:H	1:A:454:LEU:HD22	1.68	0.58
1:B:618:LEU:O	1:B:618:LEU:CD1	2.47	0.58
1:B:618:LEU:H	1:B:618:LEU:HD12	1.69	0.57
1:A:339:ARG:NH1	1:A:342:GLN:HE22	2.02	0.57
1:B:525:ARG:O	1:B:529:ILE:HG13	2.04	0.57
1:B:82:LEU:HD23	1:B:150:VAL:HG22	1.85	0.57
1:B:215:GLY:HA3	1:B:585:ILE:HD11	1.85	0.57
1:A:410:VAL:HG11	1:A:413:PHE:CE1	2.39	0.57
1:A:561:ASN:HD21	1:A:563:ILE:HB	1.69	0.57
1:B:625:GLU:O	1:B:625:GLU:HG3	2.04	0.57
1:A:399:GLU:O	1:A:401:TRP:CD1	2.57	0.57
1:A:405:GLN:OE1	1:A:405:GLN:CA	2.53	0.57
1:A:410:VAL:HG12	1:A:410:VAL:O	2.04	0.57
1:A:647:ILE:HG23	1:A:648:ASN:N	2.20	0.57
1:B:614:THR:OG1	1:B:615:PHE:HA	2.05	0.57
1:A:453:TYR:HB2	1:A:600:PHE:HE1	1.70	0.56
1:A:263:GLY:H	1:A:265:GLN:HE22	1.52	0.56
1:B:176:ILE:HG13	1:B:539:MET:HG3	1.87	0.56
1:B:633:GLN:HB3	1:B:665:ALA:HB2	1.85	0.56
1:B:513:ASP:HB3	1:B:516:VAL:H	1.71	0.56
1:A:380:THR:CG2	1:B:380:THR:HG22	2.35	0.56
1:B:692:PRO:O	1:B:693:GLU:C	2.48	0.56
1:B:705:ILE:HG22	1:B:706:GLU:N	2.20	0.56
1:A:100:ASN:HD21	1:A:102:ASN:HD22	1.54	0.56
1:B:691:LYS:HG2	1:B:692:PRO:CG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:SER:O	1:B:213:ASP:HB2	2.05	0.56
1:A:678:LYS:NZ	2:A:2097:HOH:O	2.39	0.55
1:B:473:PHE:CA	1:B:478:LEU:HD13	2.31	0.55
1:A:646:GLU:HB3	1:A:652:GLU:O	2.06	0.55
1:B:234:THR:O	1:B:237:GLY:N	2.31	0.55
1:B:311:ALA:O	1:B:312:TYR:HB2	2.05	0.55
1:B:691:LYS:CG	1:B:692:PRO:CG	2.84	0.55
1:A:694:GLU:HG2	1:A:703:LEU:HD11	1.89	0.55
1:B:231:ARG:H	1:B:232:PHE:HB2	1.71	0.55
1:B:478:LEU:N	1:B:478:LEU:CD1	2.66	0.55
1:A:424:TYR:HA	1:A:445:ARG:HD2	1.87	0.55
1:B:401:TRP:HZ3	1:B:408:TYR:O	1.89	0.55
1:B:618:LEU:CD1	1:B:618:LEU:H	2.20	0.55
1:A:13:ARG:HH11	1:A:14:PRO:HD2	1.72	0.55
1:B:50:LEU:HD23	1:B:50:LEU:H	1.72	0.55
1:B:24:TRP:CD2	1:B:79:PRO:HD3	2.42	0.55
1:B:365:ALA:HB3	1:B:399:GLU:HG2	1.88	0.55
1:B:473:PHE:HD2	1:B:474:THR:N	1.92	0.55
1:B:615:PHE:HD1	1:B:616:TYR:N	2.00	0.55
1:A:525:ARG:HG2	1:A:580:PHE:CD2	2.42	0.55
1:B:470:HIS:CD2	1:B:470:HIS:O	2.61	0.54
1:B:634:LEU:HD22	1:B:664:ASN:OD1	2.06	0.54
1:A:525:ARG:O	1:A:529:ILE:HG23	2.07	0.54
1:A:103:LYS:NZ	1:A:125:GLY:H	2.06	0.54
1:A:689:GLU:CD	1:A:689:GLU:H	2.16	0.54
1:B:82:LEU:CD2	1:B:150:VAL:HG22	2.37	0.54
1:B:265:GLN:H	1:B:265:GLN:HE21	1.55	0.54
1:B:469:SER:H	1:B:473:PHE:HZ	1.56	0.54
1:A:403:VAL:O	1:A:406:GLY:HA3	2.06	0.54
1:A:336:SER:HB3	1:A:375:VAL:HB	1.88	0.54
1:B:24:TRP:CH2	1:B:26:GLU:HB2	2.43	0.54
1:B:121:ASP:CG	1:B:128:ILE:HG12	2.33	0.54
1:B:20:LEU:HD21	1:B:69:ILE:HD12	1.88	0.54
1:B:135:LEU:HD11	1:B:321:ARG:HH21	1.71	0.54
1:B:481:TYR:N	1:B:482:ASN:HB2	2.11	0.54
1:A:425:ARG:O	1:A:429:ARG:HG3	2.08	0.53
1:B:424:TYR:HA	1:B:445:ARG:HD2	1.90	0.53
1:B:482:ASN:CB	1:B:504:ASN:HA	2.39	0.53
1:B:230:GLN:C	1:B:232:PHE:C	2.77	0.53
1:B:242:TRP:CD1	1:B:557:PHE:HA	2.43	0.53
1:B:473:PHE:CA	1:B:478:LEU:CD1	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:SER:HA	1:B:520:ARG:NH2	2.23	0.53
1:B:505:CYS:HB2	1:B:520:ARG:HE	1.74	0.53
1:B:191:LEU:HD11	1:B:206:GLN:CG	2.38	0.53
1:B:526:ASN:CG	1:B:527:PHE:H	2.17	0.53
1:B:707:GLY:C	1:B:709:THR:CG2	2.75	0.53
1:B:118:ILE:O	1:B:145:TYR:HB3	2.09	0.53
1:B:310:THR:HG22	2:B:2004:HOH:O	2.07	0.53
1:A:46:LEU:HD21	1:A:86:ARG:HD2	1.89	0.53
1:A:98:ARG:NH2	1:A:134:ASP:O	2.42	0.52
1:B:626:LYS:HB2	1:B:627:THR:HB	1.88	0.52
1:A:297:HIS:O	1:A:298:LEU:CB	2.56	0.52
1:B:521:GLU:HG3	1:B:525:ARG:HE	1.74	0.52
1:B:103:LYS:N	1:B:103:LYS:HD2	2.24	0.52
1:B:486:ASN:HD21	1:B:555:ASN:HB3	1.74	0.52
1:B:666:ASN:C	1:B:708:ARG:CZ	2.63	0.52
1:B:524:LYS:NZ	1:B:547:SER:HB3	2.24	0.52
1:B:666:ASN:C	1:B:708:ARG:HE	2.16	0.52
1:B:20:LEU:HA	1:B:34:SER:OG	2.09	0.52
1:B:207:MET:HE3	1:B:207:MET:HA	1.92	0.52
1:B:627:THR:CG2	1:B:628:TRP:N	2.72	0.52
1:A:410:VAL:HG12	1:A:413:PHE:CE1	2.45	0.52
1:A:401:TRP:HZ3	1:A:408:TYR:O	1.92	0.52
1:B:495:ASP:OD2	1:B:555:ASN:ND2	2.42	0.51
1:B:612:ASP:OD2	1:B:641:GLY:C	2.53	0.51
1:B:666:ASN:C	1:B:708:ARG:NE	2.68	0.51
1:A:367:ALA:O	1:A:371:GLU:HG3	2.11	0.51
1:B:265:GLN:NE2	1:B:265:GLN:H	2.09	0.51
1:B:10:ARG:CG	1:B:10:ARG:NH2	2.52	0.51
1:B:243:GLY:N	2:B:2013:HOH:O	2.34	0.51
1:B:373:TYR:CE1	1:B:404:GLY:HA3	2.46	0.51
1:B:712:VAL:HG13	1:B:713:TYR:N	2.25	0.51
1:B:624:ASP:C	1:B:627:THR:HG21	2.35	0.51
1:A:480:SER:HB3	1:A:520:ARG:CZ	2.41	0.50
1:A:646:GLU:HB2	1:A:647:ILE:CA	2.41	0.50
1:A:410:VAL:CG1	1:A:410:VAL:O	2.58	0.50
1:B:349:ARG:HA	1:B:390:ILE:HD11	1.92	0.50
1:B:472:GLY:O	1:B:473:PHE:CD1	2.63	0.50
1:A:15:GLY:O	1:B:167:LYS:NZ	2.38	0.50
1:A:469:SER:HA	1:A:541:LEU:HG	1.92	0.50
1:A:682:VAL:HG23	1:A:683:ILE:HG22	1.93	0.50
1:B:126:TYR:CE2	1:B:298:LEU:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD22	1:B:281:ILE:HD11	1.93	0.50
1:A:294:GLU:O	1:A:305:ARG:NH2	2.45	0.50
1:A:36:PHE:CD1	1:A:339:ARG:HG3	2.47	0.50
1:A:430:ARG:HD2	1:A:435:GLU:OE2	2.12	0.50
1:B:135:LEU:HD11	1:B:321:ARG:NH2	2.26	0.50
1:B:468:THR:HA	1:B:473:PHE:CE2	2.47	0.50
1:A:553:ASN:HD22	1:A:555:ASN:H	1.60	0.50
1:B:619:GLU:CD	1:B:672:VAL:HA	2.37	0.50
1:A:401:TRP:CZ3	1:A:408:TYR:O	2.65	0.50
1:B:703:LEU:HB3	1:B:704:GLU:CA	2.42	0.49
1:B:476:GLU:HB3	1:B:479:VAL:HG13	1.89	0.49
1:B:541:LEU:CD1	1:B:542:GLY:O	2.60	0.49
1:A:598:ARG:HD2	1:A:598:ARG:O	2.11	0.49
1:B:231:ARG:HB3	1:B:232:PHE:CD2	2.47	0.49
1:B:300:PRO:HB2	1:B:302:LEU:HG	1.95	0.49
1:B:233:LEU:O	1:B:234:THR:C	2.55	0.49
1:B:473:PHE:C	1:B:474:THR:HG22	2.29	0.49
1:A:300:PRO:HB2	1:A:302:LEU:HG	1.95	0.49
1:A:42:LYS:HB3	1:A:88:TYR:HB2	1.95	0.49
1:B:134:ASP:OD2	1:B:134:ASP:O	2.30	0.49
1:B:327:THR:HG22	1:B:364:LEU:HD23	1.94	0.49
1:B:476:GLU:OE1	1:B:520:ARG:CG	2.44	0.49
1:B:674:PHE:CE2	1:B:713:TYR:CE1	2.99	0.49
1:B:473:PHE:N	1:B:478:LEU:HD11	2.27	0.49
1:B:494:GLN:O	1:B:494:GLN:HG2	2.13	0.49
1:B:106:ILE:HD12	1:B:302:LEU:O	2.13	0.49
1:B:619:GLU:OE1	1:B:673:LYS:N	2.39	0.48
1:B:127:LYS:N	1:B:136:THR:HG23	2.25	0.48
1:B:133:GLN:O	1:B:134:ASP:CB	2.59	0.48
1:B:614:THR:OG1	1:B:637:PHE:HB2	2.12	0.48
1:B:633:GLN:HB3	1:B:665:ALA:HB3	1.94	0.48
1:A:408:TYR:O	1:A:409:GLN:HB2	2.13	0.48
1:B:349:ARG:HD3	1:B:388:ASP:OD2	2.13	0.48
1:B:468:THR:CA	1:B:473:PHE:HE2	2.26	0.48
1:B:524:LYS:O	1:B:526:ASN:N	2.37	0.48
1:B:692:PRO:O	1:B:694:GLU:HG3	2.12	0.48
1:B:230:GLN:O	1:B:231:ARG:C	2.57	0.48
1:B:294:GLU:HB3	1:B:305:ARG:NH2	2.28	0.48
1:B:475:LEU:HD12	1:B:544:ASP:HB3	1.94	0.48
1:B:662:ILE:O	1:B:711:LEU:O	2.31	0.48
1:B:191:LEU:HD11	1:B:206:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:SER:HB3	1:B:628:TRP:NE1	2.29	0.48
1:B:10:ARG:O	1:B:10:ARG:NH2	2.44	0.48
1:B:195:ILE:HD12	1:B:201:GLY:HA2	1.96	0.48
1:B:219:VAL:HG23	1:B:281:ILE:HD13	1.95	0.48
1:B:612:ASP:OD2	1:B:641:GLY:HA2	2.13	0.48
1:B:681:LEU:HB2	1:B:713:TYR:CE2	2.48	0.48
1:B:708:ARG:C	1:B:709:THR:HG22	2.39	0.48
1:A:312:TYR:CE2	1:A:343:MET:HE1	2.49	0.48
1:A:543:GLY:HA3	1:A:548:ARG:HD3	1.95	0.48
1:A:561:ASN:HD22	1:A:563:ILE:N	2.10	0.48
1:B:229:ASP:OD1	1:B:255:ARG:NH2	2.47	0.48
1:B:708:ARG:H	1:B:709:THR:CG2	2.15	0.48
1:A:195:ILE:HD12	1:A:201:GLY:HA2	1.96	0.48
1:B:441:GLU:O	1:B:444:ASN:HB2	2.13	0.48
1:B:461:PHE:CZ	1:B:597:GLU:HB3	2.49	0.48
1:B:468:THR:CA	1:B:473:PHE:CE2	2.97	0.48
1:B:100:ASN:ND2	1:B:137:TYR:HE1	2.11	0.47
1:B:263:GLY:H	1:B:265:GLN:HE22	1.62	0.47
1:B:228:ILE:HG12	1:B:293:ALA:HB1	1.95	0.47
1:B:378:LEU:O	1:B:382:PHE:HD2	1.97	0.47
1:B:467:VAL:HG13	1:B:531:LEU:HD13	1.95	0.47
1:B:535:GLN:NE2	1:B:594:PHE:HA	2.29	0.47
1:B:543:GLY:HA2	1:B:545:GLU:OE2	2.14	0.47
1:B:666:ASN:O	1:B:708:ARG:CZ	2.60	0.47
1:B:203:ALA:HB2	1:B:272:MET:HG3	1.95	0.47
1:B:503:TRP:CD1	1:B:504:ASN:N	2.78	0.47
1:A:290:ASN:OD1	1:A:291:HIS:CD2	2.67	0.47
1:A:405:GLN:OE1	1:A:405:GLN:O	2.32	0.47
1:A:464:ILE:HD13	1:A:537:THR:HG23	1.95	0.47
1:B:540:ILE:H	1:B:540:ILE:HD12	1.80	0.47
1:B:694:GLU:HB3	1:B:703:LEU:HD21	1.95	0.47
1:A:242:TRP:CZ2	1:A:470:HIS:O	2.67	0.47
1:B:184:PHE:CE2	1:B:207:MET:HG3	2.49	0.47
1:B:465:ASN:O	1:B:538:PRO:HA	2.14	0.47
1:B:519:CYS:O	1:B:523:GLN:N	2.45	0.47
1:A:78:ARG:O	1:A:79:PRO:C	2.57	0.47
1:B:230:GLN:O	1:B:232:PHE:C	2.56	0.47
1:A:132:ASN:HB2	1:A:136:THR:HG23	1.96	0.47
1:B:467:VAL:HG22	1:B:531:LEU:HD22	1.97	0.47
1:A:433:ARG:CZ	1:A:501:TYR:HA	2.45	0.47
1:A:24:TRP:CD2	1:A:79:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HG	1:B:234:THR:N	2.29	0.46
1:A:49:SER:OG	1:A:57:LYS:HD2	2.15	0.46
1:A:266:VAL:HG12	1:A:270:LYS:HD2	1.97	0.46
1:A:649:MET:HA	1:B:14:PRO:HG3	1.95	0.46
1:B:241:TYR:CE2	1:B:564:THR:HG21	2.49	0.46
1:B:473:PHE:CB	1:B:478:LEU:HD21	2.18	0.46
1:B:526:ASN:CG	1:B:527:PHE:N	2.73	0.46
1:B:614:THR:HG1	1:B:615:PHE:HA	1.79	0.46
1:A:393:GLN:HG2	1:B:18:TYR:CD1	2.51	0.46
1:B:233:LEU:C	1:B:235:ASP:N	2.72	0.46
1:B:482:ASN:HB3	1:B:504:ASN:HA	1.96	0.46
1:B:614:THR:CG2	1:B:638:VAL:O	2.61	0.46
1:B:362:PHE:HE1	1:B:396:LEU:HD22	1.80	0.46
1:A:402:ASP:OD1	1:A:405:GLN:O	2.34	0.46
1:A:561:ASN:HD22	1:A:561:ASN:C	2.23	0.46
1:A:474:THR:O	1:A:475:LEU:C	2.58	0.46
1:B:127:LYS:O	1:B:128:ILE:C	2.58	0.46
1:B:161:GLU:HA	1:B:164:ILE:HD12	1.97	0.46
1:B:242:TRP:CG	1:B:557:PHE:HA	2.51	0.46
1:B:584:MET:HE2	1:B:584:MET:HA	1.97	0.46
1:B:705:ILE:CG2	1:B:706:GLU:H	2.26	0.46
1:B:120:ASN:HD22	1:B:122:ALA:H	1.64	0.46
1:B:230:GLN:HB3	1:B:232:PHE:O	2.16	0.46
1:B:444:ASN:HB3	1:B:445:ARG:NH1	2.30	0.46
1:A:553:ASN:HD22	1:A:553:ASN:C	2.24	0.46
1:B:152:ILE:O	1:B:154:PRO:HD3	2.16	0.46
1:B:219:VAL:HG12	1:B:221:LEU:HD12	1.98	0.46
1:B:225:PHE:CZ	1:B:287:VAL:HG12	2.51	0.46
1:B:331:ASN:C	1:B:331:ASN:HD22	2.24	0.46
1:A:41:GLU:HG2	1:A:89:GLY:HA2	1.97	0.45
1:A:104:VAL:O	1:A:146:VAL:HG11	2.16	0.45
1:B:626:LYS:H	1:B:627:THR:HG22	1.81	0.45
1:A:103:LYS:HD3	1:A:125:GLY:HA2	1.99	0.45
1:B:261:CYS:C	1:B:265:GLN:HE22	2.25	0.45
1:B:528:MET:HE2	1:B:581:VAL:HG13	1.99	0.45
1:B:574:LYS:O	1:B:576:LYS:N	2.49	0.45
1:B:537:THR:HA	1:B:538:PRO:HD3	1.85	0.45
1:A:402:ASP:OD1	1:A:406:GLY:CA	2.65	0.45
1:A:525:ARG:HG2	1:A:580:PHE:CZ	2.50	0.45
1:B:96:GLY:O	1:B:309:ASN:ND2	2.38	0.45
1:B:482:ASN:CB	1:B:504:ASN:CA	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:LYS:HZ1	1:B:547:SER:HB3	1.81	0.45
1:B:584:MET:HE3	1:B:683:ILE:HG21	1.98	0.45
1:B:165:LYS:HA	1:B:166:GLY:HA2	1.56	0.45
1:B:317:PRO:O	1:B:318:ASP:HB2	2.16	0.45
1:B:388:ASP:HB3	1:B:391:LEU:HB2	1.98	0.45
1:A:339:ARG:HH11	1:A:342:GLN:HE22	1.64	0.45
1:A:553:ASN:ND2	1:A:555:ASN:H	2.14	0.45
1:A:645:ASP:HA	1:A:646:GLU:HA	1.74	0.45
1:B:429:ARG:NH2	1:B:467:VAL:O	2.49	0.45
1:B:46:LEU:HD21	1:B:86:ARG:HH11	1.82	0.45
1:B:542:GLY:O	1:B:548:ARG:HD3	2.17	0.45
1:B:11:PRO:O	1:B:75:PRO:HG2	2.17	0.44
1:A:172:LYS:HB3	1:A:597:GLU:OE1	2.17	0.44
1:A:352:VAL:HG21	1:A:394:VAL:HG11	2.00	0.44
1:B:665:ALA:CB	1:B:666:ASN:CA	2.95	0.44
1:B:666:ASN:C	1:B:666:ASN:HD22	2.24	0.44
1:A:583:LYS:HD2	1:A:683:ILE:HD12	1.99	0.44
1:A:642:SER:O	1:A:644:MET:HE3	2.17	0.44
1:B:310:THR:HG21	2:B:2004:HOH:O	2.13	0.44
1:B:432:TRP:CZ3	1:B:664:ASN:O	2.70	0.44
1:B:593:ALA:HB1	1:B:639:LEU:HG	1.99	0.44
1:A:403:VAL:N	1:A:406:GLY:HA3	2.33	0.44
1:B:570:LEU:H	1:B:570:LEU:CD2	2.22	0.44
1:B:570:LEU:HD23	1:B:570:LEU:N	2.28	0.44
1:B:626:LYS:N	1:B:627:THR:CB	2.75	0.44
1:B:679:TRP:HZ3	1:B:694:GLU:O	2.00	0.44
1:B:708:ARG:HD3	1:B:708:ARG:HA	1.67	0.44
1:A:694:GLU:HG2	1:A:703:LEU:HD21	1.99	0.44
1:B:168:LYS:O	1:B:169:VAL:C	2.61	0.44
1:A:191:LEU:O	1:A:196:ARG:NE	2.51	0.44
1:A:314:MET:HB3	1:A:324:LEU:HD12	1.98	0.44
1:A:456:ASN:ND2	1:A:456:ASN:O	2.51	0.44
1:A:472:GLY:CA	1:A:554:ASN:O	2.65	0.44
1:A:479:VAL:O	1:A:520:ARG:HG2	2.18	0.44
1:B:182:LYS:HA	1:B:197:GLY:HA2	2.00	0.44
1:B:571:ASP:O	1:B:571:ASP:OD2	2.35	0.44
1:B:633:GLN:CG	1:B:665:ALA:HB2	2.48	0.44
1:B:662:ILE:C	1:B:663:LEU:HG	2.42	0.44
1:A:277:HIS:HE1	1:A:358:ASP:OD2	2.01	0.43
1:A:647:ILE:CG2	1:A:648:ASN:N	2.80	0.43
1:B:171:LEU:O	1:B:537:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:THR:HG22	1:B:638:VAL:HB	1.47	0.43
1:A:461:PHE:HZ	1:A:595:ARG:HA	1.83	0.43
1:B:195:ILE:O	1:B:201:GLY:HA3	2.17	0.43
1:B:430:ARG:HA	1:B:433:ARG:HB3	2.00	0.43
1:A:545:GLU:CD	1:A:545:GLU:H	2.25	0.43
1:B:28:ASP:OD2	1:B:28:ASP:N	2.50	0.43
1:B:191:LEU:HD11	1:B:206:GLN:HG2	2.00	0.43
1:A:171:LEU:HD22	1:A:537:THR:HG21	1.99	0.43
1:B:524:LYS:C	1:B:526:ASN:H	2.21	0.43
1:B:126:TYR:CZ	1:B:298:LEU:HA	2.53	0.43
1:B:559:GLN:O	1:B:564:THR:OG1	2.27	0.43
1:B:633:GLN:CG	1:B:665:ALA:CB	2.96	0.43
1:A:383:ILE:O	1:A:387:GLN:HG3	2.18	0.43
1:A:681:LEU:HD23	1:A:713:TYR:CE1	2.53	0.43
1:B:475:LEU:HD11	1:B:544:ASP:HB3	1.98	0.43
1:B:711:LEU:HD12	1:B:711:LEU:HA	1.81	0.43
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.86	0.43
1:B:638:VAL:HG12	1:B:639:LEU:N	2.34	0.43
1:A:222:MET:O	1:A:223:PRO:C	2.62	0.43
1:B:169:VAL:HG11	1:B:217:THR:HB	2.00	0.43
1:B:166:GLY:O	1:B:167:LYS:C	2.61	0.43
1:B:347:SER:O	1:B:351:TRP:HD1	2.02	0.43
1:B:591:HIS:HA	1:B:592:PRO:HD3	1.83	0.43
1:B:618:LEU:CD1	1:B:618:LEU:N	2.79	0.43
1:B:703:LEU:CB	1:B:704:GLU:HA	2.46	0.43
1:A:222:MET:HB3	1:A:223:PRO:HD2	2.00	0.42
1:A:625:GLU:O	1:A:626:LYS:HB3	2.20	0.42
1:A:637:PHE:CE1	1:A:661:ILE:HD13	2.54	0.42
1:B:132:ASN:O	1:B:133:GLN:C	2.62	0.42
1:B:444:ASN:HB3	1:B:445:ARG:HH12	1.83	0.42
1:B:612:ASP:OD2	1:B:641:GLY:HA3	2.18	0.42
1:A:226:HIS:O	1:A:247:ILE:HG22	2.19	0.42
1:A:333:LEU:HB3	1:A:340:VAL:HG11	2.01	0.42
1:A:410:VAL:HG11	1:A:413:PHE:CZ	2.55	0.42
1:B:232:PHE:HD1	1:B:232:PHE:HA	1.71	0.42
1:A:319:ASN:ND2	1:A:322:TYR:CE2	2.88	0.42
1:B:618:LEU:HA	1:B:619:GLU:HA	1.53	0.42
1:B:188:ARG:CG	1:B:188:ARG:NH1	2.77	0.42
1:B:424:TYR:CD1	1:B:445:ARG:HB3	2.55	0.42
1:B:514:GLN:HE21	1:B:514:GLN:HB3	1.74	0.42
1:B:541:LEU:CD1	1:B:548:ARG:HE	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:HA	1:A:166:GLY:HA2	1.74	0.42
1:B:156:PHE:CD2	1:B:156:PHE:C	2.98	0.42
1:B:666:ASN:O	1:B:708:ARG:NE	2.53	0.42
1:B:671:LYS:CA	1:B:704:GLU:HG3	2.44	0.42
1:A:311:ALA:O	1:A:312:TYR:HB2	2.20	0.42
1:A:405:GLN:HB2	2:A:2066:HOH:O	2.19	0.42
1:B:121:ASP:CB	1:B:128:ILE:HG12	2.50	0.42
1:B:530:THR:O	1:B:533:VAL:HG12	2.20	0.42
1:B:10:ARG:HG2	1:B:12:LEU:HD21	2.02	0.42
1:B:127:LYS:C	1:B:129:GLY:N	2.75	0.42
1:B:486:ASN:ND2	1:B:495:ASP:OD2	2.52	0.42
1:A:176:ILE:HG22	1:A:177:TYR:N	2.34	0.42
1:A:636:ILE:HG23	1:A:662:ILE:HG12	2.02	0.42
1:B:30:GLY:HA3	1:B:73:PHE:CZ	2.55	0.42
1:B:105:LEU:HA	1:B:302:LEU:O	2.20	0.42
1:B:680:GLU:HB2	1:B:714:ARG:HG2	2.02	0.42
1:A:377:MET:HE1	1:B:383:ILE:HG21	2.02	0.41
1:B:614:THR:HG21	1:B:638:VAL:HG23	2.02	0.41
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.79	0.41
1:B:618:LEU:O	1:B:618:LEU:CD2	2.64	0.41
1:A:10:ARG:HA	2:A:2001:HOH:O	2.20	0.41
1:A:46:LEU:HD21	1:A:86:ARG:HH11	1.86	0.41
1:A:282:GLU:OE1	1:A:395:LYS:HE3	2.20	0.41
1:A:462:ALA:HB1	2:A:2075:HOH:O	2.20	0.41
1:A:634:LEU:CD2	1:A:636:ILE:HD11	2.51	0.41
1:B:24:TRP:HA	1:B:31:VAL:HA	2.02	0.41
1:B:365:ALA:HB1	1:B:398:ALA:HB1	1.99	0.41
1:B:666:ASN:HB2	1:B:667:PRO:CD	2.50	0.41
1:A:421:ASN:ND2	1:A:424:TYR:H	2.19	0.41
1:B:188:ARG:NH1	1:B:190:ASP:OD2	2.54	0.41
1:B:312:TYR:O	1:B:333:LEU:HA	2.20	0.41
1:B:468:THR:CG2	1:B:473:PHE:CD2	3.01	0.41
1:A:263:GLY:H	1:A:265:GLN:NE2	2.16	0.41
1:B:128:ILE:HD12	1:B:129:GLY:N	2.36	0.41
1:B:31:VAL:HG23	1:B:77:LEU:HB2	2.02	0.41
1:B:233:LEU:CG	1:B:234:THR:N	2.83	0.41
1:B:290:ASN:OD1	1:B:291:HIS:CD2	2.64	0.41
1:B:700:GLU:O	1:B:701:LYS:HG3	2.21	0.41
1:A:10:ARG:HE	1:A:10:ARG:HB3	1.69	0.41
1:A:41:GLU:CG	1:A:89:GLY:HA2	2.51	0.41
1:A:325:ASP:OD1	1:A:328:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PRO:O	1:A:342:GLN:HB2	2.21	0.41
1:A:386:GLN:HE22	1:A:412:ASN:HB3	1.86	0.41
1:A:429:ARG:O	1:A:433:ARG:HB2	2.21	0.41
1:B:104:VAL:O	1:B:146:VAL:HG11	2.21	0.41
1:B:114:ASN:ND2	1:B:261:CYS:O	2.48	0.41
1:B:581:VAL:O	1:B:585:ILE:HG23	2.21	0.41
1:B:618:LEU:HD13	1:B:618:LEU:C	2.34	0.41
1:A:25:ILE:HG21	1:A:28:ASP:OD2	2.20	0.41
1:B:177:TYR:HD1	1:B:216:ILE:HG21	1.86	0.41
1:B:207:MET:O	1:B:208:ILE:HB	2.21	0.41
1:B:225:PHE:O	1:B:226:HIS:C	2.63	0.41
1:B:230:GLN:O	1:B:233:LEU:HD23	2.21	0.41
1:B:431:PHE:CE1	1:B:633:GLN:HA	2.56	0.41
1:B:612:ASP:OD1	1:B:612:ASP:O	2.38	0.41
1:B:233:LEU:O	1:B:236:LYS:N	2.30	0.40
1:B:421:ASN:C	1:B:423:LYS:H	2.28	0.40
1:B:559:GLN:NE2	1:B:561:ASN:HD22	2.19	0.40
1:B:624:ASP:CG	1:B:625:GLU:H	2.30	0.40
1:A:474:THR:O	1:A:476:GLU:N	2.54	0.40
1:B:349:ARG:HG2	1:B:390:ILE:HD11	2.04	0.40
1:B:478:LEU:O	1:B:478:LEU:HD23	2.18	0.40
1:B:672:VAL:N	1:B:704:GLU:HG3	2.36	0.40
1:A:716:ILE:O	1:A:717:GLU:HG3	2.21	0.40
1:A:203:ALA:HB2	1:A:272:MET:HG3	2.04	0.40
1:A:308:ASP:C	1:A:308:ASP:OD1	2.65	0.40
1:A:403:VAL:C	1:A:406:GLY:HA3	2.47	0.40
1:B:9:ASP:HB2	1:B:10:ARG:HB2	2.04	0.40
1:B:324:LEU:O	1:B:332:THR:HG22	2.20	0.40
1:B:663:LEU:C	1:B:664:ASN:CG	2.89	0.40

All (13) 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:569:ASN:C	1:B:572:GLU:OE2[5_554]	0.89	1.31
1:B:571:ASP:OD1	1:B:571:ASP:OD1[5_554]	1.34	0.86
1:B:569:ASN:CA	1:B:572:GLU:OE2[5_554]	1.47	0.73
1:B:569:ASN:ND2	1:B:572:GLU:OE1[5_554]	1.58	0.62
1:B:569:ASN:O	1:B:572:GLU:OE2[5_554]	1.61	0.59
1:A:336:SER:OG	1:A:404:GLY:O[6_554]	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:N	1:B:572:GLU:OE2[5_554]	1.75	0.45
1:B:569:ASN:CB	1:B:572:GLU:OE2[5_554]	1.91	0.29
1:B:569:ASN:C	1:B:572:GLU:CD[5_554]	2.05	0.15
1:B:569:ASN:CG	1:B:572:GLU:OE1[5_554]	2.09	0.11
1:B:571:ASP:CG	1:B:571:ASP:OD1[5_554]	2.09	0.11
1:B:569:ASN:CB	1:B:572:GLU:OE1[5_554]	2.10	0.10
1:B:569:ASN:CB	1:B:572:GLU:CD[5_554]	2.16	0.04

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	695/718 (97%)	629 (90%)	62 (9%)	4 (1%)	21	56
1	B	652/718 (91%)	531 (81%)	113 (17%)	8 (1%)	10	40
All	All	1347/1436 (94%)	1160 (86%)	175 (13%)	12 (1%)	14	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	ILE
1	B	517	VAL
1	B	234	THR
1	B	190	ASP
1	B	420	TRP
1	B	675	PRO
1	B	231	ARG
1	A	457	ASN
1	B	10	ARG
1	A	164	ILE
1	A	643	VAL
1	B	128	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	617/636 (97%)	566 (92%)	51 (8%)	10	37
1	B	589/636 (93%)	514 (87%)	75 (13%)	4	20
All	All	1206/1272 (95%)	1080 (90%)	126 (10%)	7	28

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	50	LEU
1	A	53	GLN
1	A	94	GLU
1	A	103	LYS
1	A	117	VAL
1	A	135	LEU
1	A	207	MET
1	A	231	ARG
1	A	265	GLN
1	A	307	ILE
1	A	335	LEU
1	A	368	LEU
1	A	378	LEU
1	A	380	THR
1	A	383	ILE
1	A	405	GLN
1	A	409	GLN
1	A	410	VAL
1	A	428	ILE
1	A	454	LEU
1	A	457	ASN
1	A	459	THR
1	A	474	THR
1	A	480	SER
1	A	525	ARG
1	A	529	ILE

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Mol	Chain	Res	Type
1	A	533	VAL
1	A	537	THR
1	A	541	LEU
1	A	545	GLU
1	A	549	THR
1	A	553	ASN
1	A	561	ASN
1	A	562	GLU
1	A	570	LEU
1	A	576	LYS
1	A	586	GLN
1	A	589	ARG
1	A	598	ARG
1	A	599	TYR
1	A	613	VAL
1	A	614	THR
1	A	618	LEU
1	A	627	THR
1	A	646	GLU
1	A	647	ILE
1	A	658	SER
1	A	660	LEU
1	A	700	GLU
1	A	701	LYS
1	B	8	ARG
1	B	9	ASP
1	B	10	ARG
1	B	24	TRP
1	B	28	ASP
1	B	94	GLU
1	B	111	LYS
1	B	114	ASN
1	B	128	ILE
1	B	130	ASP
1	B	134	ASP
1	B	144	GLU
1	B	148	LYS
1	B	165	LYS
1	B	167	LYS
1	B	176	ILE
1	B	188	ARG
1	B	193	GLU

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Mol	Chain	Res	Type
1	B	206	GLN
1	B	207	MET
1	B	217	THR
1	B	230	GLN
1	B	232	PHE
1	B	245	ASP
1	B	247	ILE
1	B	265	GLN
1	B	281	ILE
1	B	315	LEU
1	B	327	THR
1	B	331	ASN
1	B	335	LEU
1	B	372	LEU
1	B	380	THR
1	B	394	VAL
1	B	447	LEU
1	B	452	ILE
1	B	458	LYS
1	B	461	PHE
1	B	464	ILE
1	B	475	LEU
1	B	478	LEU
1	B	479	VAL
1	B	491	PHE
1	B	493	ASN
1	B	504	ASN
1	B	533	VAL
1	B	540	ILE
1	B	541	LEU
1	B	545	GLU
1	B	550	GLN
1	B	564	THR
1	B	570	LEU
1	B	572	GLU
1	B	573	ARG
1	B	574	LYS
1	B	583	LYS
1	B	584	MET
1	B	596	ARG
1	B	613	VAL
1	B	618	LEU

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Mol	Chain	Res	Type
1	B	619	GLU
1	B	626	LYS
1	B	627	THR
1	B	634	LEU
1	B	663	LEU
1	B	666	ASN
1	B	682	VAL
1	B	690	ILE
1	B	691	LYS
1	B	702	GLU
1	B	704	GLU
1	B	708	ARG
1	B	709	THR
1	B	711	LEU
1	B	712	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	52	ASN
1	A	64	ASN
1	A	71	HIS
1	A	81	GLN
1	A	102	ASN
1	A	114	ASN
1	A	133	GLN
1	A	240	ASN
1	A	265	GLN
1	A	274	ASN
1	A	291	HIS
1	A	297	HIS
1	A	319	ASN
1	A	342	GLN
1	A	376	ASN
1	A	456	ASN
1	A	465	ASN
1	A	489	ASN
1	A	493	ASN
1	A	494	GLN
1	A	553	ASN
1	A	559	GLN

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Mol	Chain	Res	Type
1	A	561	ASN
1	A	591	HIS
1	A	633	GLN
1	A	669	ASN
1	B	32	ASN
1	B	39	ASN
1	B	81	GLN
1	B	102	ASN
1	B	120	ASN
1	B	230	GLN
1	B	265	GLN
1	B	277	HIS
1	B	291	HIS
1	B	331	ASN
1	B	356	HIS
1	B	376	ASN
1	B	409	GLN
1	B	421	ASN
1	B	444	ASN
1	B	456	ASN
1	B	465	ASN
1	B	486	ASN
1	B	500	ASN
1	B	504	ASN
1	B	514	GLN
1	B	523	GLN
1	B	535	GLN
1	B	559	GLN
1	B	666	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	699/718 (97%)	-0.24	13 (1%)	66 43	21, 51, 83, 92	3 (0%)
1	B	666/718 (92%)	0.58	49 (7%)	20 10	24, 82, 122, 128	2 (0%)
All	All	1365/1436 (95%)	0.16	62 (4%)	38 20	21, 61, 118, 128	5 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	PHE	7.6
1	B	13	ARG	6.8
1	B	73	PHE	5.4
1	B	685	SER	4.7
1	B	475	LEU	4.6
1	A	13	ARG	4.5
1	B	707	GLY	4.2
1	B	687	LEU	4.0
1	B	570	LEU	3.2
1	B	478	LEU	3.2
1	B	710	ALA	3.1
1	B	232	PHE	3.1
1	A	408	TYR	3.1
1	B	615	PHE	3.0
1	A	415	TYR	3.0
1	B	500	ASN	3.0
1	B	482	ASN	2.8
1	B	660	LEU	2.8
1	B	11	PRO	2.8
1	B	703	LEU	2.7
1	B	572	GLU	2.7
1	B	670	VAL	2.7
1	B	636	ILE	2.7
1	B	488	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	569	ASN	2.7
1	A	11	PRO	2.6
1	A	404	GLY	2.6
1	B	461	PHE	2.6
1	B	699	GLY	2.6
1	B	518	ILE	2.6
1	A	645	ASP	2.6
1	A	455	GLY	2.6
1	B	233	LEU	2.6
1	B	476	GLU	2.5
1	B	667	PRO	2.4
1	B	136	THR	2.4
1	B	563	ILE	2.4
1	B	529	ILE	2.3
1	B	541	LEU	2.3
1	B	683	ILE	2.3
1	A	401	TRP	2.3
1	A	453	TYR	2.3
1	B	477	ASP	2.3
1	B	503	TRP	2.3
1	B	437	LEU	2.3
1	A	402	ASP	2.3
1	B	631	PRO	2.2
1	B	452	ILE	2.1
1	A	454	LEU	2.1
1	B	618	LEU	2.1
1	B	408	TYR	2.1
1	B	134	ASP	2.1
1	B	546	LEU	2.1
1	B	637	PHE	2.1
1	B	522	LYS	2.1
1	B	662	ILE	2.1
1	B	665	ALA	2.1
1	B	128	ILE	2.0
1	B	471	ASP	2.0
1	A	403	VAL	2.0
1	B	553	ASN	2.0
1	B	10	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.