



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:33 AM UTC

PDB ID : 5CJ5 / pdb_00005cj5
Title : Structure of Mycobacterium thermoresistibile GlgE APO form at 3.13Å resolution
Authors : Mendes, V.; Blaszczyk, M.; Maranhã, A.; Empadinhas, N.; Blundell, T.L.
Deposited on : 2015-07-13
Resolution : 3.13 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

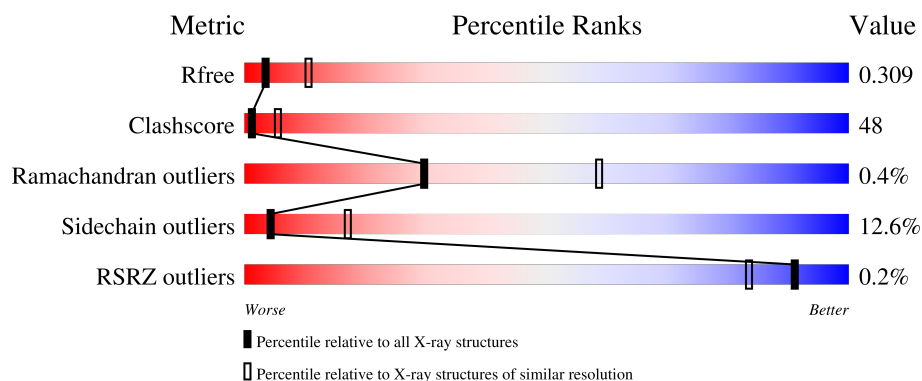
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

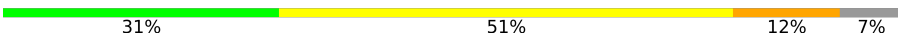
The reported resolution of this entry is 3.13 Å.

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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	698	
1	B	698	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10489 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 Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	1	0
			5104	3263	896	936	9			
1	B	678	Total	C	N	O	S	0	6	0
			5385	3443	948	985	9			

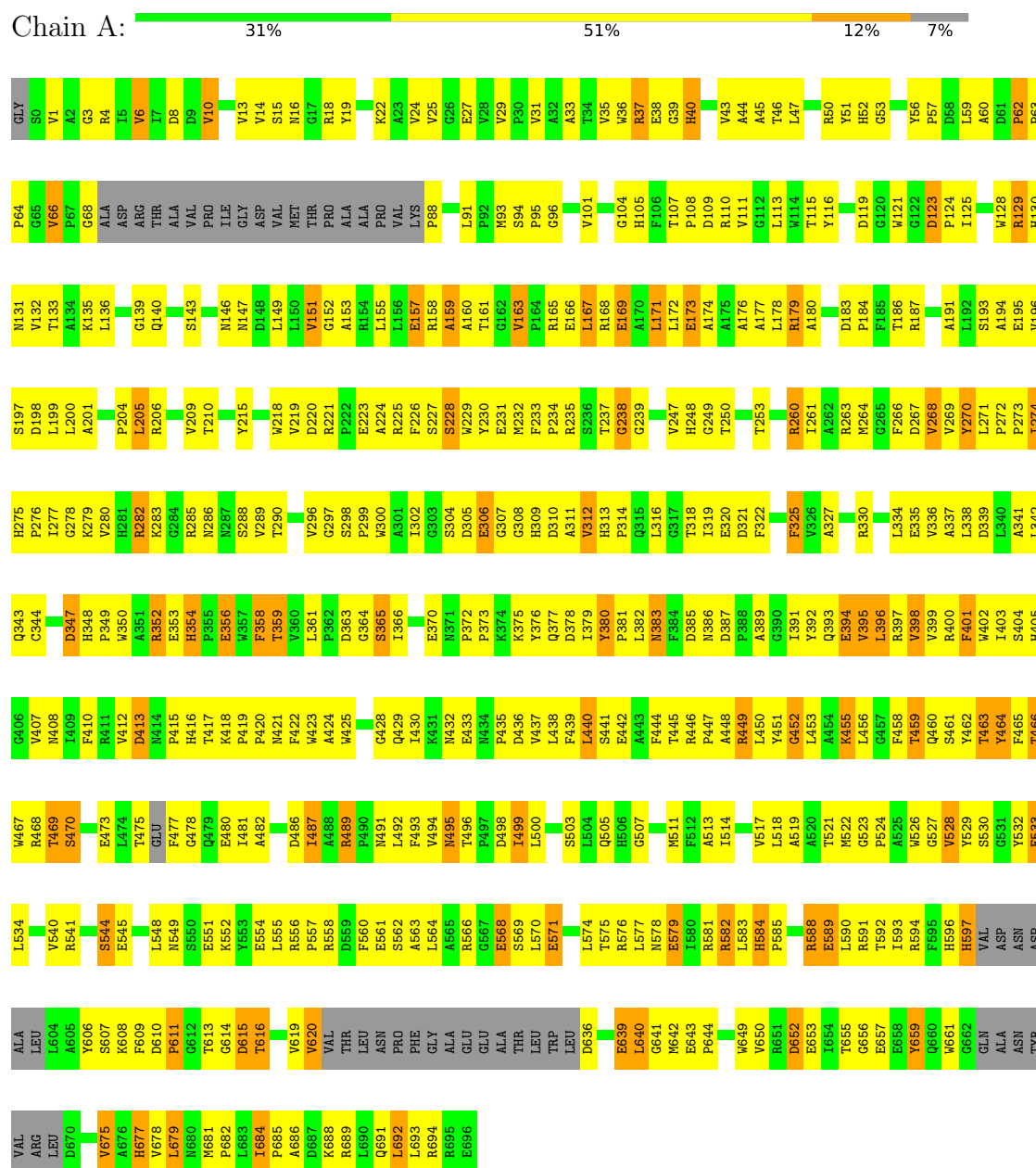
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G7CL00
A	0	SER	-	expression tag	UNP G7CL00
A	1	VAL	-	cloning artifact	UNP G7CL00
B	-1	GLY	-	expression tag	UNP G7CL00
B	0	SER	-	expression tag	UNP G7CL00
B	1	VAL	-	cloning artifact	UNP G7CL00

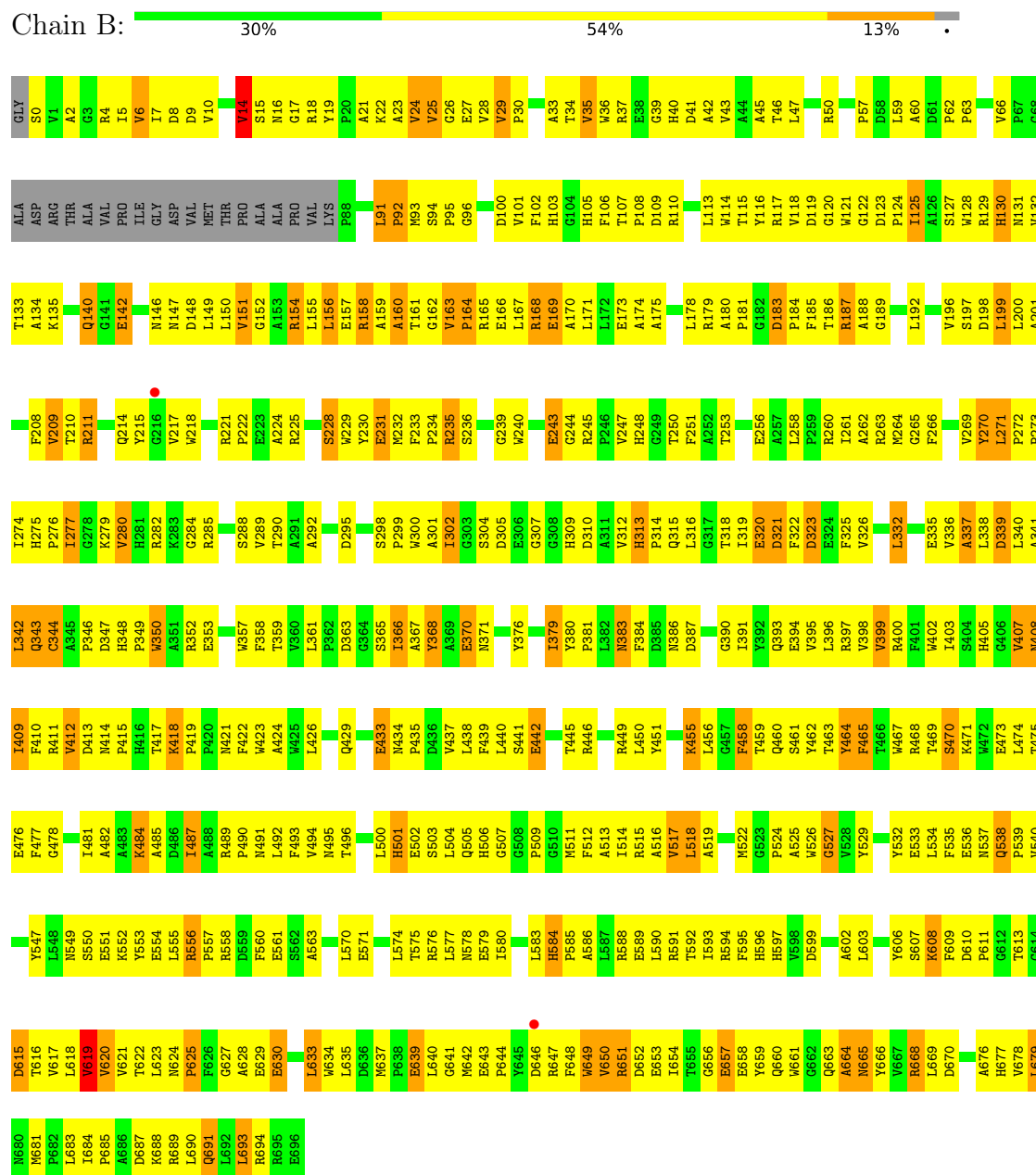
3 Residue-property plots

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: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



● Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	197.64Å 197.64Å 105.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	171.16 – 3.13 171.16 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (171.16-3.13) 100.0 (171.16-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.308 0.255 , 0.309	Depositor DCC
R_{free} test set	2093 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 269.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-h-k,-l	Depositor
Outliers	0 of 41621 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10489	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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	0.81	0/5262	1.34	60/7186 (0.8%)
1	B	0.80	3/5568 (0.1%)	1.32	55/7610 (0.7%)
All	All	0.80	3/10830 (0.0%)	1.33	115/14796 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	418	LYS	CA-C	6.87	1.58	1.52
1	B	63	PRO	CA-C	6.01	1.57	1.52
1	B	91	LEU	CA-C	5.51	1.57	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LEU	CA-C-N	10.96	131.67	120.38
1	B	271	LEU	C-N-CA	10.96	131.67	120.38
1	A	643	GLU	CA-C-N	10.13	132.51	119.84
1	A	643	GLU	C-N-CA	10.13	132.51	119.84
1	B	313	HIS	CA-C-N	9.34	130.30	119.47
1	B	313	HIS	C-N-CA	9.34	130.30	119.47
1	A	588	ARG	N-CA-C	-9.23	102.15	113.97
1	A	62	PRO	CA-C-N	8.99	129.63	120.38
1	A	62	PRO	C-N-CA	8.99	129.63	120.38
1	A	298	SER	CA-C-N	8.47	128.08	118.85
1	A	298	SER	C-N-CA	8.47	128.08	118.85
1	B	323	ASP	N-CA-C	8.34	120.45	111.36
1	A	123	ASP	CA-C-N	8.19	130.08	119.84
1	A	123	ASP	C-N-CA	8.19	130.08	119.84
1	B	160	ALA	N-CA-C	-8.04	102.47	111.07
1	B	693	LEU	N-CA-C	-7.85	103.70	113.28
1	B	158	ARG	CB-CA-C	-7.74	98.95	110.95
1	A	652	ASP	N-CA-C	7.64	122.79	109.96
1	B	332	LEU	N-CA-C	-7.62	103.52	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	N-CA-CB	7.42	120.74	109.98
1	B	584	HIS	CA-C-N	7.39	127.56	119.87
1	B	584	HIS	C-N-CA	7.39	127.56	119.87
1	A	385	ASP	N-CA-C	-7.38	104.31	113.38
1	A	147	ASN	N-CA-C	-7.25	103.46	111.36
1	A	692	LEU	N-CA-C	-7.20	103.65	113.30
1	B	646	ASP	N-CA-C	7.19	120.02	110.53
1	B	643	GLU	CA-C-N	6.93	128.50	119.84
1	B	643	GLU	C-N-CA	6.93	128.50	119.84
1	A	37	ARG	N-CA-C	6.89	116.41	108.49
1	A	401	PHE	N-CA-C	-6.88	103.71	111.07
1	B	633	LEU	N-CA-C	6.87	120.36	108.76
1	B	289	VAL	N-CA-C	-6.82	104.84	113.22
1	B	125	ILE	N-CA-C	6.79	116.88	110.30
1	A	417	THR	N-CA-C	-6.74	104.96	113.72
1	A	380	TYR	CA-C-N	6.72	128.24	119.84
1	A	380	TYR	C-N-CA	6.72	128.24	119.84
1	A	449	ARG	N-CA-C	-6.69	104.76	113.12
1	A	571	GLU	CA-C-N	-6.68	112.75	119.56
1	A	571	GLU	C-N-CA	-6.68	112.75	119.56
1	A	358	PHE	N-CA-C	6.49	119.04	109.24
1	B	45	ALA	N-CA-C	6.49	118.63	108.96
1	B	199	LEU	N-CA-C	-6.49	104.25	111.71
1	B	657	GLU	N-CA-C	6.46	119.32	108.02
1	A	455	LYS	N-CA-C	-6.45	103.37	111.11
1	B	418	LYS	CA-C-N	-6.43	113.76	120.38
1	B	418	LYS	C-N-CA	-6.43	113.76	120.38
1	B	154	ARG	N-CA-C	-6.42	105.44	113.20
1	A	584	HIS	CA-C-N	6.37	126.50	119.87
1	A	584	HIS	C-N-CA	6.37	126.50	119.87
1	A	201	ALA	N-CA-C	-6.36	105.55	113.38
1	B	169	GLU	N-CA-C	-6.35	103.65	111.33
1	B	168	ARG	N-CA-C	-6.20	104.42	112.23
1	B	40	HIS	N-CA-C	6.17	122.53	114.75
1	A	394	GLU	N-CA-C	-6.16	104.48	111.07
1	B	615	ASP	N-CA-C	6.13	119.50	110.30
1	A	66	VAL	CA-C-N	6.08	126.04	120.21
1	A	66	VAL	C-N-CA	6.08	126.04	120.21
1	B	320	GLU	N-CA-C	-6.07	104.77	111.82
1	A	282	ARG	N-CA-C	-5.97	102.66	110.53
1	B	343	GLN	N-CA-C	5.96	115.34	108.49
1	A	338	LEU	N-CA-C	5.88	118.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	LEU	CA-C-N	-5.77	115.10	122.77
1	A	440	LEU	C-N-CA	-5.77	115.10	122.77
1	B	339	ASP	CA-C-N	-5.75	114.63	123.14
1	B	339	ASP	C-N-CA	-5.75	114.63	123.14
1	B	556	ARG	CA-C-N	-5.74	113.87	119.78
1	B	556	ARG	C-N-CA	-5.74	113.87	119.78
1	A	159	ALA	N-CA-C	-5.70	105.15	111.71
1	B	350	TRP	N-CA-C	-5.70	106.95	114.31
1	A	151	VAL	N-CA-C	-5.70	104.79	111.00
1	A	344	CYS	N-CA-C	5.68	119.50	109.96
1	B	14	VAL	N-CA-C	5.66	115.95	107.51
1	A	307	GLY	N-CA-C	5.56	121.35	111.01
1	A	675	VAL	N-CA-C	-5.52	105.51	113.07
1	A	495	ASN	N-CA-C	5.51	118.17	108.75
1	B	337	ALA	N-CA-C	5.48	118.71	107.37
1	A	452	GLY	N-CA-C	5.45	119.75	112.77
1	B	92	PRO	N-CA-C	5.45	120.87	111.77
1	B	501	HIS	N-CA-C	5.41	118.49	110.48
1	A	570	LEU	N-CA-C	-5.41	106.85	113.50
1	B	164	PRO	N-CA-C	5.39	119.78	111.21
1	A	157	GLU	N-CA-C	5.36	118.04	111.82
1	B	535	PHE	N-CA-C	5.35	117.17	110.91
1	B	619	VAL	N-CA-C	5.33	115.54	107.75
1	B	639	GLU	N-CA-C	-5.28	106.10	112.54
1	B	243	GLU	N-CA-C	-5.28	107.01	113.50
1	B	342	LEU	N-CA-C	5.28	117.74	107.71
1	A	582	ARG	N-CA-C	-5.26	106.13	112.54
1	B	664	ALA	CA-C-N	-5.26	111.54	121.63
1	B	664	ALA	C-N-CA	-5.26	111.54	121.63
1	B	154	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	383	ASN	N-CA-C	5.22	117.31	108.02
1	B	115	THR	N-CA-C	5.21	117.92	109.06
1	A	167	LEU	N-CA-C	-5.21	105.39	112.26
1	B	187	ARG	N-CA-C	-5.20	105.30	111.69
1	A	480	GLU	N-CA-C	-5.18	105.08	111.40
1	A	179	ARG	N-CA-C	5.17	116.72	111.14
1	A	44	ALA	N-CA-C	5.16	116.83	109.14
1	A	496	THR	CA-C-N	5.16	126.28	119.84
1	A	496	THR	C-N-CA	5.16	126.28	119.84
1	A	615	ASP	N-CA-C	5.14	118.00	110.30
1	A	692	LEU	CB-CG-CD2	-5.14	95.29	110.70
1	A	45	ALA	N-CA-C	5.12	116.59	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLY	N-CA-C	5.12	119.32	112.77
1	A	352	ARG	N-CA-C	-5.12	106.73	113.12
1	B	110	ARG	N-CA-C	5.09	118.04	109.95
1	A	169	GLU	N-CA-C	-5.07	105.76	111.28
1	A	289	VAL	N-CA-C	-5.06	107.00	113.22
1	A	325	PHE	N-CA-C	5.04	116.46	111.07
1	B	154	ARG	CB-CG-CD	5.03	122.88	111.30
1	A	579	GLU	N-CA-C	-5.02	105.27	111.40
1	B	527	GLY	N-CA-C	5.02	118.44	110.96
1	A	334	LEU	N-CA-C	5.02	117.92	110.14
1	B	455	LYS	N-CA-C	5.01	116.43	111.07
1	B	23	ALA	N-CA-C	5.00	116.59	109.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5104	0	4910	452	2
1	B	5385	0	5209	557	2
All	All	10489	0	10119	979	2

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 48.

All (979) 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:221:ARG:HH22	1:B:408:ASN:HB3	1.16	1.04
1:A:264:MET:HA	1:A:575:THR:HG22	1.40	1.01
1:B:270:TYR:HE2	1:B:339:ASP:HB2	1.21	1.00
1:B:651:ARG:HG3	1:B:658:GLU:HG2	1.47	0.94
1:A:652:ASP:HB3	1:A:656:GLY:H	1.34	0.92
1:B:299:PRO:HD2	1:B:552:LYS:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ALA:C	1:B:665:ASN:HD22	1.80	0.90
1:B:607:SER:HB3	1:B:618:LEU:HD12	1.54	0.89
1:A:174:ALA:HA	1:A:177:ALA:HB3	1.55	0.88
1:A:109:ASP:OD2	1:A:110:ARG:NH1	2.07	0.88
1:B:121:TRP:HB3	1:B:209:VAL:HB	1.53	0.88
1:A:574:LEU:O	1:A:578:ASN:ND2	2.07	0.88
1:A:529:TYR:OH	1:A:551:GLU:OE1	1.92	0.87
1:A:239:GLY:O	1:A:247:VAL:N	2.08	0.86
1:A:151:VAL:O	1:A:155:LEU:N	2.09	0.86
1:A:299:PRO:HD2	1:A:552:LYS:HG3	1.57	0.86
1:B:270:TYR:CE2	1:B:339:ASP:HB2	2.11	0.85
1:A:263:ARG:NH2	1:A:571:GLU:OE1	2.08	0.84
1:A:442:GLU:HA	1:A:462:TYR:HB2	1.59	0.84
1:B:665:ASN:HD22	1:B:665:ASN:N	1.74	0.84
1:A:163:VAL:HG11	1:A:199:LEU:HD21	1.60	0.83
1:A:421:ASN:HD21	1:B:4:ARG:HA	1.41	0.83
1:B:121:TRP:HZ3	1:B:123:ASP:HB2	1.44	0.82
1:B:228:SER:HB3	1:B:266:PHE:HA	1.61	0.82
1:B:25:VAL:HG12	1:B:222:PRO:HG3	1.62	0.82
1:A:589:GLU:OE1	1:A:590:LEU:N	2.13	0.81
1:B:158:ARG:O	1:B:161:THR:OG1	1.99	0.81
1:A:394:GLU:OE2	1:A:397:ARG:NH2	2.10	0.81
1:B:464:TYR:HB3	1:B:467:TRP:HE3	1.45	0.81
1:B:619:VAL:HB	1:B:678:VAL:HG22	1.63	0.80
1:A:153:ALA:HB2	1:A:178:LEU:HD22	1.63	0.80
1:B:335:GLU:HB3	1:B:409:ILE:HD11	1.64	0.80
1:B:502:GLU:O	1:B:506:HIS:ND1	2.14	0.80
1:A:173:GLU:O	1:A:177:ALA:N	2.16	0.79
1:A:446:ARG:O	1:A:450:LEU:N	2.16	0.79
1:A:4:ARG:HA	1:B:421:ASN:HD21	1.48	0.78
1:A:19:TYR:HD1	1:A:59:LEU:HD23	1.49	0.78
1:B:24:VAL:HG23	1:B:489:ARG:HH22	1.47	0.78
1:A:39:GLY:H	1:B:417:THR:HA	1.50	0.77
1:B:304:SER:HA	1:B:347:ASP:HB3	1.66	0.76
1:B:461:SER:O	1:B:491:ASN:N	2.18	0.76
1:A:128:TRP:HA	1:A:131:ASN:HB2	1.68	0.76
1:B:536:GLU:OE1	1:B:556:ARG:NH2	2.20	0.75
1:A:157:GLU:OE1	1:A:179:ARG:NH1	2.14	0.75
1:B:160:ALA:HA	1:B:171:LEU:HD13	1.68	0.75
1:B:514:ILE:O	1:B:518:LEU:HD22	1.87	0.75
1:A:56:TYR:CD2	1:A:428:GLY:HA2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ILE:O	1:A:689:ARG:NH2	2.18	0.75
1:B:647:ARG:HA	1:B:661:TRP:O	1.87	0.75
1:A:228:SER:HB3	1:A:266:PHE:HA	1.68	0.74
1:A:393:GLN:HA	1:A:396:LEU:HD21	1.69	0.74
1:B:4:ARG:NH2	1:B:210:THR:OG1	2.20	0.74
1:B:368:TYR:HA	1:B:380:TYR:CD1	2.23	0.74
1:B:282:ARG:NH2	1:B:295:ASP:O	2.21	0.74
1:B:589:GLU:OE2	1:B:591:ARG:N	2.20	0.74
1:B:121:TRP:CZ3	1:B:123:ASP:HB2	2.23	0.73
1:A:261:ILE:HA	1:A:264:MET:HE2	1.71	0.73
1:A:50:ARG:HD3	1:A:88:PRO:HG3	1.70	0.73
1:B:165:ARG:HA	1:B:168:ARG:HD3	1.71	0.73
1:A:131:ASN:OD1	1:A:135:LYS:NZ	2.22	0.73
1:B:300:TRP:HB2	1:B:552:LYS:HZ3	1.52	0.73
1:A:125:ILE:HD11	1:A:205:LEU:HG	1.69	0.73
1:A:576:ARG:NH1	1:A:579:GLU:OE2	2.23	0.72
1:A:194:ALA:O	1:A:198:ASP:N	2.21	0.72
1:B:342:LEU:HD12	1:B:418:LYS:HD3	1.71	0.72
1:B:551:GLU:OE2	1:B:558:ARG:NH2	2.22	0.72
1:A:56:TYR:HB3	1:A:432:ASN:ND2	2.04	0.72
1:A:571:GLU:O	1:A:575:THR:HG23	1.90	0.72
1:B:276:PRO:HG2	1:B:307:GLY:HA3	1.72	0.72
1:A:37:ARG:HH11	1:A:38:GLU:C	1.97	0.72
1:B:178:LEU:HD13	1:B:187:ARG:HG2	1.70	0.72
1:A:350:TRP:HA	1:A:353:GLU:HB2	1.71	0.72
1:A:421:ASN:ND2	1:B:4:ARG:HA	2.05	0.72
1:B:10:VAL:HG13	1:B:33:ALA:HB2	1.72	0.72
1:B:495:ASN:CG	1:B:529:TYR:HB3	2.15	0.72
1:B:649:TRP:CD1	1:B:660:GLN:HB2	2.25	0.72
1:B:549:ASN:O	1:B:556:ARG:NH1	2.23	0.71
1:A:652:ASP:HA	1:A:679:LEU:HD22	1.71	0.71
1:B:515:ARG:HD2	1:B:518:LEU:HD23	1.72	0.71
1:A:589:GLU:O	1:A:608:LYS:NZ	2.14	0.71
1:A:500:LEU:N	1:A:545:GLU:O	2.23	0.71
1:A:176:ALA:O	1:A:187:ARG:NH1	2.24	0.71
1:A:416:HIS:O	1:B:39:GLY:N	2.20	0.71
1:B:652:ASP:HB3	1:B:657:GLU:H	1.55	0.71
1:A:363:ASP:OD1	1:A:365:SER:N	2.24	0.70
1:B:4:ARG:HH22	1:B:209:VAL:C	1.98	0.70
1:B:361:LEU:N	1:B:365:SER:O	2.21	0.70
1:B:599:ASP:OD2	1:B:634:TRP:NE1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:HB2	1:B:4:ARG:NH1	2.05	0.70
1:A:4:ARG:CA	1:B:421:ASN:HD21	2.04	0.70
1:B:300:TRP:H	1:B:552:LYS:NZ	1.89	0.70
1:B:240:TRP:CZ2	1:B:557:PRO:HB2	2.26	0.70
1:B:159:ALA:O	1:B:163:VAL:HG23	1.92	0.70
1:A:269:VAL:N	1:A:335:GLU:O	2.24	0.70
1:A:276:PRO:HD3	1:A:312:VAL:C	2.18	0.69
1:A:173:GLU:OE1	1:A:173:GLU:N	2.23	0.69
1:B:258:LEU:HA	1:B:261:ILE:HD12	1.74	0.69
1:A:279:LYS:NZ	1:A:305:ASP:OD1	2.26	0.69
1:B:411:ARG:NH1	1:B:413:ASP:OD2	2.26	0.69
1:B:464:TYR:HB3	1:B:467:TRP:CE3	2.27	0.69
1:A:226:PHE:HB2	1:A:588:ARG:HB3	1.75	0.69
1:B:439:PHE:O	1:B:459:THR:OG1	2.11	0.69
1:B:505:GLN:NE2	1:B:537:ASN:O	2.22	0.69
1:A:445:THR:H	1:A:450:LEU:HD12	1.58	0.69
1:B:484:LYS:NZ	1:B:484:LYS:HB2	2.08	0.69
1:A:96:GLY:HA2	1:A:694:ARG:NH1	2.08	0.68
1:B:18[B]:ARG:NH1	1:B:59:LEU:O	2.26	0.68
1:A:619:VAL:HG22	1:A:678:VAL:HG13	1.75	0.68
1:B:240:TRP:HB3	1:B:244:GLY:HA2	1.74	0.68
1:B:275:HIS:HB2	1:B:302:ILE:HD11	1.76	0.68
1:B:460:GLN:HG2	1:B:489:ARG:HB2	1.76	0.68
1:B:231:GLU:OE2	1:B:270:TYR:HD1	1.76	0.68
1:A:513:ALA:O	1:A:517:VAL:HG23	1.94	0.68
1:A:650:VAL:HG23	1:A:659:TYR:HD1	1.59	0.68
1:B:337:ALA:HB2	1:B:409:ILE:HB	1.76	0.68
1:B:243:GLU:O	1:B:245:ARG:NH1	2.27	0.68
1:B:414:ASN:ND2	1:B:442:GLU:O	2.26	0.68
1:B:7:ILE:HG23	1:B:35:VAL:HG12	1.76	0.67
1:B:350:TRP:HA	1:B:353:GLU:HB2	1.74	0.67
1:B:574:LEU:O	1:B:578:ASN:ND2	2.26	0.67
1:B:661:TRP:HB3	1:B:665:ASN:OD1	1.95	0.67
1:A:200:LEU:O	1:A:204:PRO:HG3	1.93	0.67
1:A:461:SER:N	1:A:489:ARG:O	2.28	0.67
1:B:370:GLU:HA	1:B:376:TYR:HD2	1.57	0.67
1:B:484:LYS:HB2	1:B:484:LYS:HZ2	1.60	0.67
1:A:221:ARG:NH1	1:A:436:ASP:O	2.27	0.67
1:A:652:ASP:OD2	1:A:677:HIS:CE1	2.48	0.67
1:B:156:LEU:O	1:B:160:ALA:N	2.26	0.67
1:B:312:VAL:HG21	1:B:318:THR:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:N	1:B:411:ARG:O	2.17	0.67
1:B:235:ARG:NH2	1:B:273:PRO:O	2.26	0.67
1:A:440:LEU:HA	1:A:460:GLN:HB3	1.76	0.67
1:B:224:ALA:HB1	1:B:489:ARG:HH12	1.59	0.67
1:B:189:GLY:HA2	1:B:192:LEU:HD12	1.77	0.66
1:A:304:SER:OG	1:A:306:GLU:OE2	2.11	0.66
1:B:368:TYR:HA	1:B:380:TYR:HD1	1.59	0.66
1:A:614:GLY:HA2	1:A:689:ARG:HD3	1.76	0.66
1:B:576:ARG:NH1	1:B:579:GLU:OE2	2.28	0.66
1:A:230:TYR:HE1	1:A:232:MET:HB3	1.61	0.66
1:B:596:HIS:HB3	1:B:635:LEU:HA	1.76	0.66
1:B:305:ASP:N	1:B:347:ASP:OD1	2.29	0.66
1:A:652:ASP:HB3	1:A:656:GLY:N	2.09	0.66
1:A:652:ASP:HB3	1:A:657:GLU:H	1.59	0.66
1:A:596:HIS:ND1	1:A:636:ASP:HB3	2.11	0.66
1:B:370:GLU:HA	1:B:376:TYR:CD2	2.31	0.66
1:A:267:ASP:O	1:A:335:GLU:HB2	1.96	0.65
1:A:302:ILE:HD12	1:A:343:GLN:O	1.95	0.65
1:A:4:ARG:HA	1:B:421:ASN:ND2	2.11	0.65
1:A:62:PRO:HG2	1:A:68:GLY:HA2	1.78	0.65
1:A:230:TYR:CE1	1:A:232:MET:HB3	2.30	0.65
1:B:106:PHE:HE1	1:B:108:PRO:HG3	1.61	0.65
1:A:3:GLY:C	1:B:421:ASN:HD21	2.05	0.65
1:A:37:ARG:HD2	1:A:38:GLU:N	2.11	0.65
1:B:348:HIS:HD2	1:B:349:PRO:HD2	1.61	0.65
1:A:684:ILE:HG13	1:A:688:LYS:HD2	1.78	0.65
1:B:94:SER:O	1:B:103:HIS:N	2.24	0.65
1:A:158:ARG:HA	1:A:161:THR:HG23	1.79	0.65
1:A:358:PHE:HB3	1:A:366:ILE:HG12	1.79	0.65
1:A:277:ILE:O	1:A:304:SER:HB3	1.96	0.64
1:B:340:LEU:HD11	1:B:410:PHE:CD1	2.32	0.64
1:A:309:HIS:O	1:A:402:TRP:HZ2	1.80	0.64
1:A:507:GLY:HA3	1:A:511:MET:HB2	1.78	0.64
1:B:130:HIS:O	1:B:130:HIS:ND1	2.29	0.64
1:A:393:GLN:OE1	1:A:393:GLN:N	2.30	0.64
1:B:117:ARG:HB2	1:B:214:GLN:HE21	1.63	0.64
1:B:42:ALA:HB3	1:B:127:SER:HB3	1.77	0.64
1:B:616:THR:OG1	1:B:681:MET:HB2	1.97	0.64
1:A:286:ASN:ND2	1:A:549:ASN:OD1	2.29	0.64
1:A:563:ALA:O	1:A:568:GLU:N	2.26	0.64
1:B:94:SER:OG	1:B:694:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:HD23	1:A:577:LEU:HD12	1.80	0.63
1:A:250:THR:HA	1:A:316:LEU:HA	1.80	0.63
1:A:447:PRO:HA	1:A:450:LEU:HB3	1.80	0.63
1:A:1:VAL:HA	1:B:18[B]:ARG:HG2	1.80	0.63
1:A:500:LEU:HG	1:A:505:GLN:NE2	2.13	0.63
1:B:627:GLY:O	1:B:629:GLU:HG2	1.98	0.63
1:A:464:TYR:HB3	1:A:467:TRP:HZ3	1.64	0.63
1:A:540:VAL:HG13	1:A:541:ARG:HE	1.63	0.62
1:B:106:PHE:CE1	1:B:108:PRO:HG3	2.34	0.62
1:A:495:ASN:HD21	1:A:532:TYR:HB2	1.63	0.62
1:A:541:ARG:O	1:A:544:SER:OG	2.16	0.62
1:A:160:ALA:HB1	1:A:171:LEU:HD22	1.81	0.62
1:A:524:PRO:O	1:A:581:ARG:NH2	2.30	0.62
1:A:233:PHE:HB2	1:A:551:GLU:OE2	1.99	0.62
1:B:15:SER:OG	1:B:455:LYS:NZ	2.26	0.62
1:B:338:LEU:HD12	1:B:339:ASP:H	1.63	0.62
1:B:504:LEU:HD21	1:B:512:PHE:CD1	2.35	0.62
1:A:234:PRO:O	1:A:237:THR:OG1	2.16	0.62
1:A:464:TYR:HB3	1:A:467:TRP:CZ3	2.34	0.62
1:B:19:TYR:HA	1:B:59:LEU:HD23	1.82	0.62
1:B:151:VAL:O	1:B:155:LEU:N	2.33	0.62
1:A:343:GLN:HB3	1:A:379:ILE:HG21	1.82	0.62
1:B:240:TRP:CH2	1:B:557:PRO:HB2	2.34	0.62
1:A:288:SER:OG	1:A:290:THR:N	2.32	0.61
1:B:4:ARG:NH2	1:B:209:VAL:O	2.33	0.61
1:A:441:SER:O	1:A:462:TYR:N	2.32	0.61
1:B:313:HIS:CD2	1:B:315:GLN:H	2.18	0.61
1:B:665:ASN:N	1:B:665:ASN:ND2	2.44	0.61
1:A:19:TYR:CD1	1:A:59:LEU:HD23	2.35	0.61
1:B:637:MET:HE2	1:B:663:GLN:HB2	1.82	0.61
1:A:493:PHE:CD1	1:A:527:GLY:HA3	2.35	0.61
1:A:116:TYR:N	1:A:215:TYR:O	2.33	0.61
1:A:439:PHE:HB2	1:A:459:THR:H	1.65	0.61
1:A:499:ILE:HG23	1:A:545:GLU:CD	2.26	0.61
1:B:24:VAL:HG23	1:B:489:ARG:NH2	2.15	0.61
1:B:37:ARG:NH2	1:B:41:ASP:HB2	2.15	0.61
1:B:596:HIS:HE2	1:B:607:SER:HG	1.47	0.61
1:A:639:GLU:HA	1:A:692:LEU:CD2	2.30	0.61
1:B:490:PRO:HB2	1:B:492:LEU:HD21	1.82	0.61
1:A:194:ALA:HA	1:A:197:SER:HB2	1.82	0.61
1:A:277:ILE:HB	1:A:282:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:HG22	1:A:321:ASP:CG	2.26	0.60
1:B:231:GLU:OE1	1:B:270:TYR:HB3	2.01	0.60
1:A:191:ALA:C	1:A:196:VAL:HG11	2.26	0.60
1:B:130:HIS:O	1:B:133:THR:OG1	2.11	0.60
1:A:39:GLY:N	1:B:417:THR:HA	2.16	0.60
1:A:428:GLY:C	1:A:432:ASN:HD22	2.09	0.60
1:A:521:THR:HG1	1:A:606:TYR:HH	1.47	0.60
1:B:157:GLU:OE2	1:B:179:ARG:NH2	2.34	0.60
1:B:161:THR:HA	1:B:168:ARG:NH2	2.16	0.60
1:B:471:LYS:HB2	1:B:623:LEU:HD11	1.84	0.60
1:B:29:VAL:HG13	1:B:106:PHE:O	2.00	0.60
1:A:24:VAL:HG11	1:A:225:ARG:HB2	1.83	0.60
1:A:40:HIS:CE1	1:B:371:ASN:HD21	2.19	0.60
1:A:313:HIS:HB3	1:A:316:LEU:HD12	1.84	0.60
1:A:393:GLN:HA	1:A:396:LEU:CD2	2.32	0.60
1:A:160:ALA:HB2	1:A:171:LEU:HD13	1.82	0.60
1:A:139:GLY:O	1:A:140:GLN:NE2	2.35	0.60
1:A:642:MET:SD	1:A:682:PRO:HB2	2.42	0.60
1:A:231:GLU:HB3	1:A:529:TYR:HA	1.84	0.60
1:A:652:ASP:CB	1:A:657:GLU:H	2.15	0.60
1:A:521:THR:OG1	1:A:606:TYR:OH	2.18	0.59
1:B:384:PHE:HA	1:B:391:ILE:HD12	1.83	0.59
1:B:641:GLY:HA3	1:B:684:ILE:HD12	1.82	0.59
1:A:419:PRO:O	1:A:422:PHE:HB3	2.02	0.59
1:A:53:GLY:O	1:A:113:LEU:N	2.27	0.59
1:A:60:ALA:O	1:A:62:PRO:HD3	2.02	0.59
1:A:639:GLU:OE2	1:A:692:LEU:HD21	2.02	0.59
1:B:168:ARG:O	1:B:171:LEU:N	2.27	0.59
1:A:38:GLU:HB2	1:B:418:LYS:N	2.17	0.59
1:A:342:LEU:N	1:A:343:GLN:OE1	2.36	0.59
1:A:238:GLY:HA3	1:A:247:VAL:O	2.03	0.59
1:B:664:ALA:C	1:B:665:ASN:ND2	2.56	0.59
1:B:503:SER:OG	1:B:504:LEU:N	2.36	0.59
1:A:260:ARG:HA	1:A:263:ARG:NH1	2.18	0.59
1:A:275:HIS:CD2	1:A:309:HIS:HA	2.38	0.59
1:B:396:LEU:HD12	1:B:426:LEU:HD12	1.84	0.59
1:B:117:ARG:CB	1:B:214:GLN:HE21	2.15	0.59
1:A:420:PRO:HA	1:A:423:TRP:HD1	1.66	0.59
1:B:441:SER:OG	1:B:460:GLN:O	2.19	0.58
1:A:18:ARG:HE	1:B:2:ALA:HB3	1.67	0.58
1:A:149:LEU:O	1:A:178:LEU:HD21	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLY:HA2	1:A:455:LYS:HD2	1.86	0.58
1:A:649:TRP:HA	1:A:659:TYR:O	2.04	0.58
1:A:37:ARG:NH1	1:A:39:GLY:C	2.62	0.58
1:A:136:LEU:HD12	1:A:140:GLN:O	2.04	0.58
1:B:30:PRO:HG3	1:B:693:LEU:HG	1.85	0.58
1:B:60:ALA:O	1:B:62:PRO:HD3	2.03	0.58
1:B:183:ASP:OD2	1:B:186:THR:N	2.19	0.58
1:B:285[A]:ARG:NH1	1:B:554:GLU:HG2	2.18	0.58
1:A:461:SER:O	1:A:491:ASN:N	2.32	0.58
1:B:117:ARG:HD3	1:B:214:GLN:HE21	1.69	0.58
1:B:408:ASN:C	1:B:409:ILE:HG13	2.29	0.58
1:B:348:HIS:HD2	1:B:349:PRO:CD	2.17	0.58
1:A:16:ASN:ND2	1:B:16:ASN:OD1	2.37	0.57
1:B:647:ARG:HE	1:B:660:GLN:HG2	1.67	0.57
1:B:402:TRP:HA	1:B:405:HIS:ND1	2.19	0.57
1:B:500:LEU:HD22	1:B:547:TYR:CE1	2.38	0.57
1:B:394:GLU:O	1:B:398:VAL:N	2.38	0.57
1:A:37:ARG:HH12	1:A:39:GLY:C	2.13	0.57
1:A:478:GLY:HA2	1:A:481:ILE:HG12	1.87	0.57
1:B:128:TRP:HZ2	1:B:149:LEU:HA	1.68	0.57
1:B:234:PRO:HD3	1:B:272:PRO:HG2	1.86	0.57
1:B:361:LEU:HD11	1:B:367:ALA:HB2	1.86	0.57
1:A:473:GLU:O	1:A:477:PHE:N	2.38	0.57
1:B:270:TYR:OH	1:B:411:ARG:NH2	2.37	0.57
1:B:348:HIS:CD2	1:B:349:PRO:HD2	2.39	0.57
1:A:564:LEU:HA	1:A:569:SER:OG	2.05	0.56
1:A:66:VAL:HG12	1:A:393:GLN:HE22	1.69	0.56
1:A:248:HIS:CD2	1:A:555:LEU:HD21	2.40	0.56
1:B:511:MET:HB2	1:B:625:PRO:HB3	1.87	0.56
1:A:152:GLY:HA2	1:A:155:LEU:HB3	1.86	0.56
1:A:541:ARG:HG2	1:A:544:SER:OG	2.04	0.56
1:B:240:TRP:HA	1:B:247:VAL:HG13	1.87	0.56
1:B:399:VAL:HA	1:B:402:TRP:HD1	1.69	0.56
1:B:602:ALA:O	1:B:623:LEU:N	2.35	0.56
1:A:659:TYR:HE1	1:A:679:LEU:HD11	1.69	0.56
1:B:258:LEU:O	1:B:262:ALA:N	2.30	0.56
1:B:323:ASP:O	1:B:326:VAL:HG22	2.05	0.56
1:B:224:ALA:O	1:B:489:ARG:NH1	2.39	0.56
1:B:299:PRO:HD2	1:B:552:LYS:HZ2	1.70	0.56
1:B:610:ASP:OD2	1:B:613:THR:N	2.33	0.56
1:A:551:GLU:OE1	1:A:558:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:HD11	1:A:681:MET:HE3	1.86	0.56
1:B:196:VAL:O	1:B:199:LEU:HB2	2.05	0.56
1:A:37:ARG:NH1	1:A:39:GLY:O	2.34	0.56
1:B:550:SER:OG	1:B:553:TYR:HD2	1.89	0.56
1:A:171:LEU:HG	1:A:172:LEU:HG	1.88	0.56
1:B:415:PRO:HB3	1:B:423:TRP:CZ2	2.40	0.56
1:A:4:ARG:N	1:B:421:ASN:HD21	2.04	0.55
1:A:450:LEU:HD13	1:A:464:TYR:CE2	2.41	0.55
1:B:94:SER:OG	1:B:103:HIS:O	2.22	0.55
1:B:185:PHE:O	1:B:189:GLY:N	2.28	0.55
1:B:276:PRO:O	1:B:302:ILE:HD12	2.06	0.55
1:B:370:GLU:HG3	1:B:371:ASN:N	2.20	0.55
1:B:470:SER:OG	1:B:473:GLU:N	2.39	0.55
1:B:490:PRO:HB2	1:B:492:LEU:CD2	2.35	0.55
1:B:534:LEU:HD21	1:B:560:PHE:HA	1.88	0.55
1:A:398:VAL:O	1:A:401:PHE:HB3	2.06	0.55
1:B:163:VAL:HG12	1:B:164:PRO:HD2	1.88	0.55
1:B:393:GLN:OE1	1:B:393:GLN:N	2.36	0.55
1:B:630:GLU:HB3	1:B:668:ARG:HB2	1.87	0.55
1:B:650:VAL:O	1:B:658:GLU:HA	2.06	0.55
1:B:95:PRO:HA	1:B:102:PHE:HA	1.87	0.55
1:B:117:ARG:HD3	1:B:214:GLN:NE2	2.20	0.55
1:B:445:THR:OG1	1:B:446:ARG:N	2.39	0.55
1:A:267:ASP:OD1	1:A:267:ASP:N	2.37	0.55
1:A:403:ILE:HD11	1:A:430:ILE:HD12	1.88	0.55
1:B:387:ASP:OD2	1:B:390:GLY:HA3	2.06	0.55
1:A:413:ASP:O	1:A:418:LYS:NZ	2.38	0.55
1:A:610:ASP:HB3	1:A:615:ASP:N	2.22	0.55
1:B:319:ILE:O	1:B:322:PHE:HB3	2.07	0.55
1:A:37:ARG:NH1	1:B:449:ARG:HH22	2.05	0.55
1:A:250:THR:HG23	1:A:316:LEU:C	2.32	0.55
1:B:131:ASN:HD21	1:B:135:LYS:NZ	2.04	0.55
1:A:128:TRP:CH2	1:A:152:GLY:HA3	2.42	0.55
1:A:363:ASP:OD1	1:A:364:GLY:N	2.40	0.55
1:A:444:PHE:CZ	1:A:462:TYR:HD2	2.24	0.55
1:A:125:ILE:HD12	1:A:125:ILE:H	1.72	0.54
1:A:421:ASN:HD22	1:A:421:ASN:H	1.55	0.54
1:A:350:TRP:HB3	1:A:354:HIS:ND1	2.22	0.54
1:A:540:VAL:HG11	1:A:541:ARG:HH11	1.72	0.54
1:B:264:MET:O	1:B:575:THR:HA	2.07	0.54
1:B:300:TRP:NE1	1:B:413:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:TRP:HB3	1:B:468:ARG:NH1	2.22	0.54
1:A:283:LYS:NZ	1:A:376:TYR:HA	2.22	0.54
1:A:579:GLU:HA	1:A:582:ARG:CZ	2.37	0.54
1:B:50:ARG:HH21	1:B:214:GLN:HE22	1.56	0.54
1:A:359:THR:HG23	1:A:383:ASN:ND2	2.22	0.54
1:B:161:THR:HA	1:B:168:ARG:HH22	1.73	0.54
1:A:167:LEU:HD13	1:A:167:LEU:O	2.08	0.54
1:A:173:GLU:CD	1:A:174:ALA:H	2.16	0.54
1:B:28:VAL:HG21	1:B:611:PRO:HB2	1.88	0.54
1:B:154:ARG:NH2	1:B:157:GLU:OE1	2.40	0.54
1:A:470:SER:N	1:A:473:GLU:OE1	2.26	0.54
1:B:209:VAL:HG22	1:B:211:ARG:NH2	2.23	0.54
1:B:262:ALA:HB2	1:B:332:LEU:HD13	1.88	0.54
1:B:481:ILE:HG13	1:B:482:ALA:N	2.22	0.54
1:B:585:PRO:O	1:B:588:ARG:HG3	2.08	0.54
1:B:630:GLU:HB3	1:B:668:ARG:HD3	1.89	0.54
1:A:235:ARG:HH11	1:A:277:ILE:HD11	1.73	0.54
1:B:117:ARG:NE	1:B:211:ARG:HB3	2.23	0.54
1:B:96:GLY:HA3	1:B:103:HIS:CE1	2.42	0.54
1:A:250:THR:HG23	1:A:316:LEU:O	2.08	0.54
1:A:370:GLU:HG3	1:A:375:LYS:HB3	1.89	0.54
1:A:446:ARG:NE	1:B:100:ASP:OD1	2.40	0.54
1:A:639:GLU:HA	1:A:692:LEU:HD23	1.90	0.54
1:B:36:TRP:HE3	1:B:37:ARG:O	1.89	0.54
1:A:235:ARG:O	1:A:249:GLY:N	2.41	0.53
1:B:109:ASP:OD1	1:B:109:ASP:N	2.33	0.53
1:B:230:TYR:HB2	1:B:266:PHE:CD1	2.42	0.53
1:B:620:VAL:HG13	1:B:677:HIS:HB2	1.90	0.53
1:A:350:TRP:O	1:A:354:HIS:N	2.41	0.53
1:A:650:VAL:HB	1:A:679:LEU:HD12	1.91	0.53
1:B:10:VAL:HG22	1:B:33:ALA:HB1	1.91	0.53
1:B:417:THR:OG1	1:B:418:LYS:HE3	2.07	0.53
1:B:463:THR:CG2	1:B:490:PRO:HB3	2.38	0.53
1:B:509:PRO:HA	1:B:512:PHE:CD1	2.43	0.53
1:A:121:TRP:HB3	1:A:209:VAL:HG22	1.90	0.53
1:A:415:PRO:HA	1:A:423:TRP:HZ2	1.74	0.53
1:B:250:THR:OG1	1:B:251:PHE:N	2.42	0.53
1:B:357:TRP:CD2	1:B:391:ILE:HG12	2.42	0.53
1:B:585:PRO:HA	1:B:588:ARG:HE	1.72	0.53
1:B:620:VAL:HG22	1:B:677:HIS:HB2	1.91	0.53
1:A:401:PHE:O	1:A:405:HIS:CD2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLY:O	1:A:456:LEU:HD12	2.06	0.53
1:B:276:PRO:HD3	1:B:312:VAL:O	2.08	0.53
1:B:504:LEU:HD21	1:B:512:PHE:CG	2.44	0.53
1:B:4:ARG:HB2	1:B:4:ARG:HH11	1.70	0.53
1:B:236:SER:HB3	1:B:556:ARG:O	2.08	0.53
1:B:275:HIS:C	1:B:313:HIS:HB2	2.33	0.53
1:B:398:VAL:HG12	1:B:402:TRP:HE1	1.73	0.53
1:B:461:SER:N	1:B:489:ARG:O	2.41	0.53
1:B:579:GLU:O	1:B:583:LEU:HG	2.09	0.53
1:A:554:GLU:HG2	1:A:555:LEU:N	2.24	0.53
1:B:105:HIS:CE1	1:B:690:LEU:HD13	2.44	0.53
1:B:421:ASN:N	1:B:421:ASN:HD22	2.05	0.53
1:B:633:LEU:HD21	1:B:635:LEU:HD21	1.90	0.53
1:A:453:LEU:O	1:A:456:LEU:N	2.41	0.53
1:B:130:HIS:ND1	1:B:130:HIS:C	2.62	0.53
1:A:124:PRO:HG2	1:A:205:LEU:HD11	1.91	0.53
1:A:460:GLN:OE1	1:A:491:ASN:HB2	2.09	0.53
1:A:678:VAL:C	1:A:679:LEU:HD23	2.33	0.53
1:B:22:LYS:HE2	1:B:459:THR:O	2.09	0.53
1:B:28:VAL:HA	1:B:107:THR:HG22	1.90	0.53
1:B:37:ARG:NH2	1:B:41:ASP:O	2.42	0.53
1:B:586:ALA:HB3	1:B:617:VAL:HG22	1.91	0.53
1:B:151:VAL:HG23	1:B:155:LEU:HG	1.89	0.53
1:B:156:LEU:HD22	1:B:159:ALA:HB3	1.91	0.53
1:B:224:ALA:HB2	1:B:438:LEU:HD13	1.90	0.53
1:B:265:GLY:HA3	1:B:578:ASN:CB	2.39	0.53
1:B:280:VAL:HG12	1:B:346:PRO:HG2	1.90	0.53
1:B:478:GLY:HA2	1:B:481:ILE:HG12	1.91	0.53
1:B:516:ALA:HB2	1:B:532:TYR:HE2	1.74	0.53
1:A:6:VAL:HG21	1:A:36:TRP:CE2	2.43	0.53
1:A:423:TRP:CG	1:A:458:PHE:HZ	2.28	0.52
1:B:628:ALA:HB2	1:B:670:ASP:OD2	2.09	0.52
1:B:128:TRP:NE1	1:B:148:ASP:O	2.38	0.52
1:A:129:ARG:HB3	1:A:129:ARG:HH21	1.75	0.52
1:A:224:ALA:HB1	1:A:489:ARG:HH12	1.75	0.52
1:B:47:LEU:HB2	1:B:93:MET:SD	2.49	0.52
1:B:181:PRO:HA	1:B:187:ARG:CZ	2.40	0.52
1:A:395:VAL:O	1:A:399:VAL:HG23	2.09	0.52
1:B:57:PRO:O	1:B:59:LEU:HD12	2.09	0.52
1:B:320:GLU:OE2	1:B:320:GLU:N	2.35	0.52
1:B:408:ASN:HA	1:B:437:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:PRO:C	1:A:581:ARG:HH12	2.17	0.52
1:B:4:ARG:NH1	1:B:208:PHE:O	2.42	0.52
1:B:14:VAL:O	1:B:17:GLY:N	2.40	0.52
1:A:153:ALA:O	1:A:157:GLU:HG3	2.10	0.52
1:A:395:VAL:O	1:A:398:VAL:HG22	2.10	0.52
1:B:43:VAL:HG23	1:B:122:GLY:HA2	1.92	0.52
1:B:595:PHE:CD1	1:B:606:TYR:HB3	2.45	0.52
1:B:156:LEU:HD11	1:B:171:LEU:HD22	1.92	0.52
1:B:236:SER:HB3	1:B:556:ARG:C	2.35	0.52
1:B:611:PRO:O	1:B:689:ARG:NE	2.42	0.52
1:A:272:PRO:HB3	1:A:300:TRP:CZ3	2.45	0.52
1:A:518:LEU:O	1:A:522:MET:N	2.27	0.52
1:A:585:PRO:HA	1:A:588:ARG:NE	2.24	0.52
1:B:276:PRO:HD3	1:B:312:VAL:C	2.34	0.52
1:A:349:PRO:O	1:A:350:TRP:HD1	1.93	0.52
1:B:495:ASN:HD21	1:B:532:TYR:HB2	1.73	0.52
1:A:56:TYR:HD2	1:A:428:GLY:HA2	1.74	0.52
1:A:415:PRO:HA	1:A:423:TRP:CZ2	2.45	0.52
1:B:620:VAL:O	1:B:677:HIS:N	2.39	0.52
1:B:651:ARG:CG	1:B:658:GLU:HG2	2.31	0.52
1:B:8:ASP:N	1:B:34:THR:O	2.43	0.51
1:A:620:VAL:HG13	1:A:677:HIS:O	2.11	0.51
1:B:14:VAL:C	1:B:17:GLY:H	2.17	0.51
1:B:29:VAL:O	1:B:105:HIS:HA	2.10	0.51
1:B:173:GLU:HG3	1:B:174:ALA:H	1.74	0.51
1:B:264:MET:O	1:B:578:ASN:ND2	2.28	0.51
1:B:341:ALA:C	1:B:342:LEU:HD23	2.36	0.51
1:B:493:PHE:CE1	1:B:527:GLY:HA3	2.45	0.51
1:A:611:PRO:O	1:A:689:ARG:HD2	2.11	0.51
1:A:66:VAL:HG12	1:A:393:GLN:NE2	2.26	0.51
1:A:168:ARG:HA	1:A:171:LEU:HD23	1.93	0.51
1:A:492:LEU:HD12	1:A:519:ALA:HA	1.91	0.51
1:A:498:ASP:C	1:A:499:ILE:HD12	2.36	0.51
1:B:159:ALA:C	1:B:162:GLY:H	2.18	0.51
1:B:357:TRP:O	1:B:383:ASN:N	2.43	0.51
1:B:570:LEU:O	1:B:574:LEU:HD12	2.10	0.51
1:B:596:HIS:CE1	1:B:640:LEU:HG	2.45	0.51
1:A:320:GLU:OE1	1:A:320:GLU:N	2.43	0.51
1:A:446:ARG:HE	1:B:100:ASP:CG	2.17	0.51
1:B:125:ILE:HD12	1:B:125:ILE:H	1.74	0.51
1:B:260:ARG:HH22	1:B:533:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:O	1:B:35:VAL:HA	2.11	0.51
1:B:124:PRO:HD2	1:B:125:ILE:HD12	1.93	0.51
1:B:231:GLU:OE2	1:B:493:PHE:CZ	2.64	0.51
1:B:593:ILE:C	1:B:594:ARG:HG2	2.34	0.51
1:A:424:ALA:HB2	1:A:456:LEU:HD23	1.93	0.51
1:A:563:ALA:HB1	1:A:568:GLU:O	2.11	0.51
1:B:260:ARG:HA	1:B:263:ARG:NH1	2.26	0.51
1:B:19:TYR:CE2	1:B:456:LEU:HG	2.46	0.51
1:B:276:PRO:CG	1:B:307:GLY:HA3	2.40	0.51
1:B:277:ILE:HG21	1:B:299:PRO:HA	1.93	0.51
1:A:420:PRO:HA	1:A:423:TRP:CD1	2.45	0.51
1:B:129:ARG:O	1:B:132:VAL:HG22	2.10	0.51
1:A:14:VAL:HG23	1:A:19:TYR:HB2	1.93	0.50
1:B:277:ILE:O	1:B:304:SER:HB3	2.11	0.50
1:B:465:PHE:HB2	1:B:477:PHE:CE2	2.46	0.50
1:B:616:THR:OG1	1:B:681:MET:O	2.29	0.50
1:A:686:ALA:HA	1:A:689:ARG:NE	2.27	0.50
1:B:50:ARG:O	1:B:114:TRP:HA	2.10	0.50
1:B:288:SER:OG	1:B:290:THR:OG1	2.27	0.50
1:B:585:PRO:HA	1:B:588:ARG:NE	2.25	0.50
1:B:621:VAL:HG23	1:B:676:ALA:HB2	1.93	0.50
1:A:318:THR:OG1	1:A:319:ILE:N	2.39	0.50
1:B:116:TYR:CE2	1:B:215:TYR:HB2	2.46	0.50
1:B:131:ASN:HD21	1:B:135:LYS:CE	2.24	0.50
1:B:165:ARG:HA	1:B:168:ARG:CD	2.39	0.50
1:B:337:ALA:CB	1:B:409:ILE:HB	2.40	0.50
1:B:580:ILE:HA	1:B:583:LEU:HB2	1.93	0.50
1:B:691:GLN:OE1	1:B:694:ARG:HD2	2.12	0.50
1:A:481:ILE:HG13	1:A:482:ALA:N	2.26	0.50
1:A:579:GLU:HA	1:A:582:ARG:NH1	2.27	0.50
1:A:396:LEU:HD23	1:A:396:LEU:H	1.77	0.50
1:A:442:GLU:HA	1:A:462:TYR:CB	2.38	0.50
1:A:452:GLY:O	1:A:455:LYS:HB2	2.11	0.50
1:A:433:GLU:O	1:A:435:PRO:HD3	2.12	0.50
1:A:616:THR:HB	1:A:681:MET:HB2	1.94	0.50
1:B:165:ARG:HA	1:B:168:ARG:CG	2.41	0.50
1:B:650:VAL:CG1	1:B:679:LEU:HD22	2.42	0.50
1:A:260:ARG:NH1	1:A:533:GLU:OE1	2.45	0.50
1:A:534:LEU:HD12	1:A:558:ARG:HD2	1.94	0.50
1:B:357:TRP:CD1	1:B:387:ASP:HB3	2.46	0.50
1:A:445:THR:OG1	1:A:449:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:NH1	1:B:208:PHE:C	2.70	0.50
1:B:197:SER:HA	1:B:200:LEU:HD13	1.94	0.50
1:B:493:PHE:CZ	1:B:527:GLY:HA3	2.47	0.50
1:A:18:ARG:HE	1:B:2:ALA:CB	2.24	0.49
1:A:304:SER:HA	1:A:347:ASP:OD2	2.12	0.49
1:A:348:HIS:HE1	1:A:350:TRP:CD2	2.30	0.49
1:A:460:GLN:HG2	1:A:461:SER:H	1.76	0.49
1:B:394:GLU:O	1:B:398:VAL:HG23	2.11	0.49
1:A:327:ALA:O	1:A:330:ARG:HB2	2.12	0.49
1:A:596:HIS:HD1	1:A:636:ASP:HB3	1.77	0.49
1:B:274:ILE:HG22	1:B:316:LEU:HD13	1.95	0.49
1:A:47:LEU:HB3	1:A:91:LEU:HB2	1.94	0.49
1:A:589:GLU:OE1	1:A:591:ARG:HG2	2.12	0.49
1:A:685:PRO:HD2	1:A:688:LYS:HD2	1.95	0.49
1:B:7:ILE:HG23	1:B:35:VAL:CG1	2.42	0.49
1:B:493:PHE:CD1	1:B:527:GLY:HA3	2.47	0.49
1:B:592:THR:HB	1:B:609:PHE:CE2	2.47	0.49
1:B:687:ASP:OD1	1:B:688:LYS:N	2.45	0.49
1:A:36:TRP:HB2	1:B:449:ARG:HG2	1.94	0.49
1:B:250:THR:HG22	1:B:253:THR:HG23	1.94	0.49
1:B:465:PHE:HB2	1:B:477:PHE:CZ	2.48	0.49
1:B:470:SER:HB3	1:B:473:GLU:OE1	2.12	0.49
1:A:46:THR:HB	1:A:119:ASP:HB2	1.94	0.49
1:A:171:LEU:HG	1:A:172:LEU:N	2.27	0.49
1:A:302:ILE:HD11	1:A:341:ALA:HB3	1.95	0.49
1:A:322:PHE:O	1:A:325:PHE:HB3	2.12	0.49
1:A:466:THR:HG1	1:A:467:TRP:CD1	2.30	0.49
1:A:650:VAL:HG23	1:A:659:TYR:CD1	2.43	0.49
1:A:392:TYR:O	1:A:395:VAL:HG22	2.12	0.49
1:A:421:ASN:ND2	1:A:421:ASN:H	2.11	0.49
1:B:25:VAL:CG1	1:B:222:PRO:HG3	2.40	0.49
1:B:690:LEU:O	1:B:694:ARG:HG3	2.11	0.49
1:A:3:GLY:C	1:B:421:ASN:ND2	2.71	0.49
1:A:180:ALA:HB3	1:A:187:ARG:NH2	2.28	0.49
1:A:225:ARG:HH22	1:A:589:GLU:HG2	1.77	0.49
1:B:163:VAL:HB	1:B:171:LEU:HD11	1.95	0.49
1:B:346:PRO:HG3	1:B:380:TYR:CE2	2.47	0.49
1:B:414:ASN:ND2	1:B:442:GLU:OE2	2.46	0.49
1:A:37:ARG:HD2	1:A:37:ARG:C	2.38	0.49
1:A:56:TYR:HB3	1:A:432:ASN:CG	2.38	0.49
1:A:231:GLU:N	1:A:528:VAL:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:HG23	1:A:320:GLU:H	1.78	0.49
1:B:4:ARG:HB2	1:B:4:ARG:CZ	2.43	0.49
1:B:239:GLY:C	1:B:247:VAL:HG22	2.38	0.49
1:B:628:ALA:HB1	1:B:668:ARG:CZ	2.43	0.49
1:B:637:MET:HG3	1:B:644:PRO:HA	1.95	0.49
1:A:52:HIS:CE1	1:A:115:THR:HG22	2.48	0.49
1:A:163:VAL:HG11	1:A:199:LEU:CD2	2.38	0.49
1:B:410:PHE:HE2	1:B:437:VAL:HG11	1.78	0.49
1:A:609:PHE:HA	1:A:616:THR:HA	1.95	0.48
1:A:684:ILE:HD12	1:A:684:ILE:HA	1.64	0.48
1:A:193:SER:OG	1:A:196:VAL:HG12	2.13	0.48
1:B:198:ASP:HA	1:B:201:ALA:HB3	1.93	0.48
1:B:251:PHE:CD2	1:B:321:ASP:HB2	2.47	0.48
1:B:495:ASN:OD1	1:B:529:TYR:HB3	2.12	0.48
1:B:640:LEU:HD23	1:B:640:LEU:HA	1.71	0.48
1:A:540:VAL:CG1	1:A:541:ARG:HH11	2.27	0.48
1:A:25:VAL:HG12	1:A:219:VAL:HG12	1.95	0.48
1:A:52:HIS:O	1:A:113:LEU:HB3	2.13	0.48
1:B:168:ARG:HA	1:B:171:LEU:HD12	1.94	0.48
1:B:240:TRP:HD1	1:B:245:ARG:C	2.22	0.48
1:B:318:THR:HG23	1:B:320:GLU:OE2	2.13	0.48
1:B:422:PHE:CE2	1:B:426:LEU:HD22	2.49	0.48
1:A:579:GLU:HA	1:A:582:ARG:NH2	2.29	0.48
1:B:275:HIS:HB3	1:B:276:PRO:HD2	1.93	0.48
1:B:399:VAL:HA	1:B:402:TRP:CD1	2.48	0.48
1:B:439:PHE:HB3	1:B:458:PHE:HE1	1.78	0.48
1:A:270:TYR:HA	1:A:337:ALA:O	2.14	0.48
1:A:495:ASN:ND2	1:A:532:TYR:HB2	2.26	0.48
1:B:14:VAL:HB	1:B:19:TYR:O	2.14	0.48
1:B:224:ALA:CB	1:B:489:ARG:HH12	2.26	0.48
1:B:403:ILE:HG23	1:B:407:VAL:O	2.13	0.48
1:A:444:PHE:CE1	1:A:462:TYR:HB3	2.49	0.48
1:B:46:THR:HB	1:B:119:ASP:HB2	1.95	0.48
1:B:340:LEU:HD21	1:B:410:PHE:HD1	1.79	0.48
1:A:593:ILE:O	1:A:594:ARG:NH2	2.47	0.48
1:B:196:VAL:O	1:B:200:LEU:HD12	2.14	0.48
1:B:313:HIS:HD2	1:B:315:GLN:H	1.61	0.48
1:B:468:ARG:HB3	1:B:473:GLU:HB3	1.96	0.48
1:B:129:ARG:O	1:B:129:ARG:HG2	2.13	0.48
1:A:300:TRP:NE1	1:A:339:ASP:OD2	2.47	0.48
1:B:463:THR:C	1:B:465:PHE:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:HIS:ND1	1:B:371:ASN:ND2	2.58	0.47
1:B:152:GLY:HA2	1:B:155:LEU:HB2	1.95	0.47
1:B:394:GLU:CD	1:B:397:ARG:HH21	2.22	0.47
1:A:10:VAL:HG12	1:A:10:VAL:O	2.14	0.47
1:A:130:HIS:ND1	1:A:133:THR:OG1	2.46	0.47
1:A:195:GLU:HA	1:A:198:ASP:OD1	2.13	0.47
1:B:116:TYR:CE1	1:B:215:TYR:HD1	2.31	0.47
1:B:300:TRP:H	1:B:552:LYS:HZ3	1.61	0.47
1:B:494:VAL:HG12	1:B:519:ALA:HB3	1.94	0.47
1:B:529:TYR:HE1	1:B:547:TYR:CZ	2.31	0.47
1:A:10:VAL:HG22	1:A:33:ALA:HB2	1.97	0.47
1:A:273:PRO:HG2	1:A:300:TRP:HA	1.95	0.47
1:A:440:LEU:HD11	1:A:462:TYR:CD1	2.49	0.47
1:B:50:ARG:CZ	1:B:214:GLN:OE1	2.63	0.47
1:B:429:GLN:O	1:B:433:GLU:HG3	2.13	0.47
1:B:524:PRO:HG2	1:B:590:LEU:HD23	1.96	0.47
1:A:556:ARG:HH11	1:A:556:ARG:HA	1.79	0.47
1:B:363:ASP:OD1	1:B:365:SER:OG	2.25	0.47
1:B:586:ALA:HB2	1:B:615:ASP:O	2.13	0.47
1:A:239:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
1:A:639:GLU:HA	1:A:692:LEU:HD21	1.97	0.47
1:A:652:ASP:OD1	1:A:653:GLU:N	2.48	0.47
1:A:183:ASP:HB3	1:A:186:THR:OG1	2.15	0.47
1:A:276:PRO:HD3	1:A:312:VAL:O	2.14	0.47
1:A:610:ASP:OD2	1:A:613:THR:OG1	2.19	0.47
1:B:175:ALA:O	1:B:179:ARG:HG3	2.14	0.47
1:B:637:MET:HB3	1:B:642:MET:O	2.15	0.47
1:A:129:ARG:O	1:A:132:VAL:HG12	2.13	0.47
1:A:223:GLU:O	1:A:227:SER:HB3	2.15	0.47
1:A:322:PHE:HE1	1:A:405:HIS:HB3	1.80	0.47
1:A:579:GLU:O	1:A:583:LEU:HG	2.15	0.47
1:A:596:HIS:NE2	1:A:607:SER:OG	2.47	0.47
1:B:439:PHE:HB3	1:B:458:PHE:CE1	2.49	0.47
1:B:513:ALA:O	1:B:517:VAL:HG13	2.15	0.47
1:B:596:HIS:HE1	1:B:640:LEU:HG	1.80	0.47
1:A:50:ARG:HB2	1:A:88:PRO:HA	1.96	0.47
1:A:160:ALA:CB	1:A:171:LEU:HD22	2.44	0.47
1:A:271:LEU:O	1:A:339:ASP:HB2	2.15	0.47
1:B:341:ALA:HB1	1:B:343:GLN:HE22	1.80	0.47
1:A:686:ALA:HA	1:A:689:ARG:HE	1.80	0.47
1:B:413:ASP:O	1:B:418:LYS:NZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:SER:HB3	1:B:618:LEU:CD1	2.35	0.47
1:A:27:GLU:C	1:A:107:THR:HG23	2.40	0.47
1:A:549:ASN:HB3	1:A:554:GLU:OE1	2.15	0.47
1:A:14:VAL:CG2	1:A:19:TYR:HB2	2.45	0.46
1:A:264:MET:O	1:A:575:THR:HA	2.15	0.46
1:A:296:VAL:HG11	1:A:555:LEU:HD21	1.97	0.46
1:A:440:LEU:HD21	1:A:462:TYR:CE1	2.50	0.46
1:B:60:ALA:HB3	1:B:424:ALA:HB3	1.96	0.46
1:B:183:ASP:OD1	1:B:184:PRO:HD2	2.15	0.46
1:A:562:SER:O	1:A:566:ARG:N	2.30	0.46
1:A:657:GLU:HB3	1:A:659:TYR:CE2	2.50	0.46
1:B:91:LEU:HB3	1:B:92:PRO:CD	2.45	0.46
1:B:264:MET:HA	1:B:575:THR:OG1	2.15	0.46
1:B:551:GLU:HB3	1:B:556:ARG:CG	2.45	0.46
1:A:327:ALA:HA	1:A:330:ARG:HB2	1.95	0.46
1:A:500:LEU:H	1:A:545:GLU:HB2	1.81	0.46
1:B:652:ASP:CB	1:B:657:GLU:H	2.26	0.46
1:A:14:VAL:HG11	1:A:487:ILE:HG23	1.97	0.46
1:A:274:ILE:HD12	1:A:275:HIS:CE1	2.51	0.46
1:A:358:PHE:CD2	1:A:366:ILE:HD13	2.50	0.46
1:A:394:GLU:O	1:A:398:VAL:HG13	2.15	0.46
1:A:514:ILE:O	1:A:518:LEU:HD22	2.15	0.46
1:B:534:LEU:HD22	1:B:563:ALA:HB3	1.97	0.46
1:A:522:MET:O	1:A:524:PRO:HD3	2.16	0.46
1:B:264:MET:C	1:B:578:ASN:HD22	2.17	0.46
1:B:421:ASN:ND2	1:B:421:ASN:N	2.64	0.46
1:B:607:SER:C	1:B:608:LYS:HG3	2.40	0.46
1:B:648:PHE:HD2	1:B:650:VAL:HG23	1.81	0.46
1:A:66:VAL:HG13	1:A:389:ALA:HA	1.96	0.46
1:A:129:ARG:O	1:A:133:THR:HG23	2.16	0.46
1:A:283:LYS:HE2	1:A:377:GLN:OE1	2.15	0.46
1:A:596:HIS:HE1	1:A:639:GLU:HG3	1.80	0.46
1:B:152:GLY:O	1:B:155:LEU:HB2	2.16	0.46
1:B:322:PHE:O	1:B:325:PHE:HB3	2.15	0.46
1:B:398:VAL:O	1:B:402:TRP:NE1	2.48	0.46
1:B:597:HIS:O	1:B:634:TRP:HB2	2.16	0.46
1:A:50:ARG:HG2	1:A:51:TYR:N	2.31	0.46
1:A:402:TRP:HB2	1:A:410:PHE:HZ	1.80	0.46
1:A:444:PHE:CE1	1:A:463:THR:O	2.69	0.46
1:A:500:LEU:HB3	1:A:545:GLU:C	2.41	0.46
1:B:516:ALA:HB2	1:B:532:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:HG13	1:B:336:VAL:HA	1.97	0.46
1:B:551:GLU:HA	1:B:554:GLU:O	2.15	0.46
1:B:584:HIS:HA	1:B:585:PRO:HD3	1.62	0.46
1:A:269:VAL:O	1:A:336:VAL:HA	2.15	0.46
1:A:318:THR:HG23	1:A:321:ASP:H	1.81	0.46
1:B:593:ILE:HG13	1:B:608:LYS:HG2	1.97	0.46
1:B:684:ILE:O	1:B:689:ARG:HD3	2.15	0.46
1:A:146:ASN:OD1	1:A:146:ASN:O	2.34	0.46
1:A:448:ALA:HB1	1:B:34:THR:HG21	1.98	0.46
1:B:19:TYR:HD2	1:B:59:LEU:HD23	1.80	0.46
1:B:147:ASN:HA	1:B:150:LEU:HB2	1.98	0.46
1:A:108:PRO:HB2	1:A:219:VAL:HG11	1.97	0.45
1:A:358:PHE:CB	1:A:366:ILE:HG12	2.46	0.45
1:B:302:ILE:HG21	1:B:309:HIS:CE1	2.51	0.45
1:B:336:VAL:O	1:B:409:ILE:HD12	2.16	0.45
1:B:515:ARG:HD2	1:B:515:ARG:HA	1.74	0.45
1:B:463:THR:HG21	1:B:490:PRO:HB3	1.97	0.45
1:B:471:LYS:O	1:B:475:THR:HG23	2.17	0.45
1:B:507:GLY:O	1:B:625:PRO:HB2	2.16	0.45
1:B:594:ARG:HD2	1:B:639:GLU:HB3	1.99	0.45
1:A:180:ALA:O	1:A:187:ARG:HD2	2.16	0.45
1:A:503:SER:HB2	1:A:511:MET:HE3	1.99	0.45
1:A:584:HIS:HA	1:A:585:PRO:HD3	1.61	0.45
1:B:10:VAL:HA	1:B:33:ALA:HA	1.98	0.45
1:B:163:VAL:O	1:B:168:ARG:NH1	2.49	0.45
1:B:233:PHE:HE2	1:B:299:PRO:HG2	1.81	0.45
1:B:574:LEU:HA	1:B:577:LEU:HB2	1.97	0.45
1:B:628:ALA:HA	1:B:670:ASP:HA	1.97	0.45
1:B:383:ASN:O	1:B:391:ILE:HD11	2.16	0.45
1:A:177:ALA:O	1:A:187:ARG:HD3	2.16	0.45
1:A:260:ARG:HD2	1:A:560:PHE:CD2	2.51	0.45
1:A:361:LEU:HD12	1:A:365:SER:OG	2.16	0.45
1:A:492:LEU:HG	1:A:523:GLY:HA3	1.97	0.45
1:A:576:ARG:HD2	1:A:576:ARG:HA	1.79	0.45
1:B:265:GLY:HA3	1:B:578:ASN:HB3	1.97	0.45
1:B:509:PRO:HA	1:B:512:PHE:CE1	2.52	0.45
1:A:378:ASP:OD1	1:A:379:ILE:HG13	2.17	0.45
1:B:232:MET:O	1:B:271:LEU:HD23	2.16	0.45
1:B:368:TYR:HB3	1:B:380:TYR:HE1	1.82	0.45
1:A:37:ARG:NH1	1:B:449:ARG:NH2	2.65	0.45
1:A:37:ARG:NH2	1:A:40:HIS:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLY:HA3	1:A:248:HIS:C	2.41	0.45
1:A:238:GLY:O	1:A:247:VAL:HB	2.16	0.45
1:A:540:VAL:HA	1:A:548:LEU:HD13	1.98	0.45
1:A:575:THR:O	1:A:579:GLU:N	2.49	0.45
1:B:275:HIS:HB2	1:B:302:ILE:CD1	2.46	0.45
1:B:277:ILE:H	1:B:277:ILE:HG12	1.59	0.45
1:B:292:ALA:HB3	1:B:295:ASP:OD1	2.16	0.45
1:B:340:LEU:HG	1:B:410:PHE:HB3	1.97	0.45
1:B:481:ILE:HG13	1:B:482:ALA:H	1.82	0.45
1:A:341:ALA:C	1:A:342:LEU:HD23	2.41	0.45
1:A:348:HIS:CE1	1:A:350:TRP:CD2	3.05	0.45
1:B:116:TYR:O	1:B:214:GLN:HA	2.15	0.45
1:B:142:GLU:O	1:B:146:ASN:HB2	2.16	0.45
1:B:157:GLU:O	1:B:161:THR:HG23	2.16	0.45
1:B:450:LEU:HD22	1:B:451:TYR:CE1	2.52	0.45
1:B:594:ARG:HD2	1:B:639:GLU:CD	2.41	0.45
1:A:206:ARG:NH1	1:A:206:ARG:HB2	2.32	0.45
1:B:250:THR:N	1:B:253:THR:OG1	2.50	0.45
1:B:262:ALA:HB1	1:B:332:LEU:HD22	1.98	0.45
1:A:36:TRP:CG	1:B:449:ARG:HG2	2.51	0.45
1:A:47:LEU:HB2	1:A:93:MET:SD	2.57	0.45
1:A:273:PRO:HG3	1:A:339:ASP:OD2	2.17	0.45
1:A:396:LEU:HD12	1:A:400:ARG:HE	1.82	0.45
1:B:576:ARG:NE	1:B:580:ILE:HD11	2.32	0.45
1:A:159:ALA:O	1:A:163:VAL:HG13	2.17	0.44
1:A:684:ILE:HA	1:A:685:PRO:HD3	1.77	0.44
1:B:440:LEU:HD12	1:B:441:SER:N	2.31	0.44
1:B:589:GLU:OE2	1:B:590:LEU:N	2.50	0.44
1:B:273:PRO:HG2	1:B:299:PRO:C	2.41	0.44
1:B:414:ASN:N	1:B:442:GLU:OE2	2.49	0.44
1:A:650:VAL:HG21	1:A:661:TRP:CD2	2.52	0.44
1:B:19:TYR:CD1	1:B:455:LYS:HB3	2.53	0.44
1:B:59:LEU:HD12	1:B:59:LEU:N	2.32	0.44
1:A:62:PRO:HG3	1:A:425:TRP:HD1	1.82	0.44
1:A:268:VAL:HA	1:A:335:GLU:O	2.17	0.44
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.69	0.44
1:B:515:ARG:HD2	1:B:518:LEU:CD2	2.45	0.44
1:B:558:ARG:HD2	1:B:558:ARG:N	2.33	0.44
1:B:593:ILE:HG12	1:B:608:LYS:NZ	2.32	0.44
1:A:178:LEU:HD23	1:A:178:LEU:C	2.43	0.44
1:B:235:ARG:HB3	1:B:555:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ASN:OD1	1:B:495:ASN:N	2.51	0.44
1:B:251:PHE:CE1	1:B:322:PHE:HB2	2.52	0.44
1:B:275:HIS:CB	1:B:302:ILE:HD11	2.46	0.44
1:B:683:LEU:O	1:B:684:ILE:HD13	2.17	0.44
1:A:460:GLN:HA	1:A:489:ARG:O	2.18	0.44
1:B:485:ALA:CB	1:B:590:LEU:HB2	2.48	0.44
1:A:183:ASP:CG	1:A:184:PRO:HD2	2.42	0.44
1:A:350:TRP:CD1	1:A:354:HIS:HE1	2.35	0.44
1:A:402:TRP:HB2	1:A:410:PHE:CZ	2.53	0.44
1:B:221:ARG:HE	1:B:438:LEU:HD11	1.83	0.44
1:B:589:GLU:CD	1:B:590:LEU:H	2.25	0.44
1:B:358:PHE:HD2	1:B:381:PRO:O	2.00	0.44
1:B:371:ASN:H	1:B:376:TYR:HE2	1.64	0.44
1:B:398:VAL:O	1:B:402:TRP:CD1	2.71	0.44
1:B:650:VAL:O	1:B:659:TYR:N	2.43	0.44
1:A:396:LEU:HD22	1:A:425:TRP:CZ3	2.53	0.43
1:A:500:LEU:N	1:A:545:GLU:HB2	2.33	0.43
1:A:514:ILE:HD11	1:A:675:VAL:HG21	2.00	0.43
1:B:196:VAL:HA	1:B:199:LEU:HD23	2.00	0.43
1:B:263:ARG:NH2	1:B:263:ARG:HB2	2.33	0.43
1:B:270:TYR:HA	1:B:337:ALA:O	2.17	0.43
1:A:38:GLU:HB2	1:B:417:THR:C	2.43	0.43
1:A:115:THR:HG1	1:A:215:TYR:C	2.20	0.43
1:A:224:ALA:HB2	1:A:438:LEU:HD13	1.99	0.43
1:A:300:TRP:CZ2	1:A:339:ASP:OD1	2.71	0.43
1:A:399:VAL:HA	1:A:402:TRP:HD1	1.83	0.43
1:A:440:LEU:HD11	1:A:462:TYR:HD1	1.83	0.43
1:A:487:ILE:H	1:A:487:ILE:HG13	1.67	0.43
1:A:650:VAL:HG21	1:A:661:TRP:CE3	2.52	0.43
1:B:156:LEU:HD21	1:B:171:LEU:HD22	1.99	0.43
1:B:359:THR:N	1:B:366:ILE:HD13	2.33	0.43
1:A:169:GLU:HA	1:A:172:LEU:HD12	1.99	0.43
1:A:641:GLY:HA3	1:A:684:ILE:HG12	1.99	0.43
1:B:120:GLY:O	1:B:209:VAL:HA	2.18	0.43
1:B:556:ARG:O	1:B:558:ARG:HD2	2.19	0.43
1:A:121:TRP:HZ3	1:A:123:ASP:OD1	2.02	0.43
1:B:0:SER:OG	1:B:9:ASP:N	2.41	0.43
1:B:27:GLU:O	1:B:108:PRO:HD2	2.18	0.43
1:B:107:THR:HA	1:B:108:PRO:HD3	1.78	0.43
1:B:300:TRP:HB2	1:B:552:LYS:NZ	2.26	0.43
1:B:313:HIS:CD2	1:B:313:HIS:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD21	1:B:515:ARG:HH12	1.82	0.43
1:B:180:ALA:HA	1:B:181:PRO:HD3	1.81	0.43
1:B:229:TRP:HE1	1:B:525:ALA:HB1	1.83	0.43
1:B:402:TRP:O	1:B:407:VAL:HG13	2.19	0.43
1:B:589:GLU:CD	1:B:591:ARG:H	2.26	0.43
1:A:278:GLY:HA2	1:A:304:SER:HA	1.99	0.43
1:A:308:GLY:H	1:A:311:ALA:HB3	1.83	0.43
1:A:396:LEU:HD22	1:A:425:TRP:HZ3	1.82	0.43
1:A:442:GLU:HB2	1:A:462:TYR:CD2	2.53	0.43
1:A:451:TYR:O	1:A:455:LYS:HG3	2.18	0.43
1:B:154:ARG:NH1	1:B:157:GLU:HB3	2.33	0.43
1:A:153:ALA:CB	1:A:178:LEU:HD22	2.41	0.43
1:B:47:LEU:HD13	1:B:93:MET:SD	2.59	0.43
1:B:121:TRP:HB3	1:B:209:VAL:CB	2.37	0.43
1:B:158:ARG:O	1:B:161:THR:N	2.51	0.43
1:B:301:ALA:HB2	1:B:379:ILE:HD11	2.00	0.43
1:B:358:PHE:HB3	1:B:366:ILE:HG12	1.99	0.43
1:B:390:GLY:O	1:B:393:GLN:NE2	2.52	0.43
1:A:448:ALA:HB3	1:B:100:ASP:OD2	2.18	0.43
1:B:224:ALA:CB	1:B:438:LEU:HD13	2.49	0.43
1:B:225:ARG:O	1:B:525:ALA:HB2	2.17	0.43
1:B:300:TRP:CD1	1:B:341:ALA:HB2	2.54	0.43
1:B:637:MET:HG2	1:B:663:GLN:OE1	2.19	0.43
1:A:94:SER:HA	1:A:95:PRO:HD2	1.91	0.43
1:A:306:GLU:O	1:A:306:GLU:HG2	2.19	0.43
1:A:318:THR:HG23	1:A:320:GLU:N	2.34	0.43
1:A:401:PHE:O	1:A:404:SER:OG	2.33	0.43
1:A:592:THR:HB	1:A:609:PHE:CD2	2.53	0.43
1:A:652:ASP:O	1:A:656:GLY:HA2	2.19	0.43
1:B:260:ARG:NH1	1:B:571:GLU:OE1	2.52	0.43
1:B:441:SER:OG	1:B:461:SER:HA	2.19	0.43
1:B:522:MET:O	1:B:524:PRO:HD3	2.18	0.43
1:B:610:ASP:HB3	1:B:615:ASP:N	2.33	0.43
1:A:354:HIS:HB3	1:A:356:GLU:OE1	2.19	0.43
1:A:518:LEU:O	1:A:522:MET:HB2	2.18	0.43
1:A:594:ARG:HB3	1:A:596:HIS:CE1	2.54	0.43
1:B:170:ALA:HA	1:B:173:GLU:CD	2.44	0.43
1:B:178:LEU:HA	1:B:187:ARG:CG	2.49	0.43
1:B:313:HIS:HA	1:B:314:PRO:HD2	1.61	0.43
1:B:666:TYR:OH	1:B:668:ARG:HB3	2.19	0.43
1:A:399:VAL:HG13	1:A:410:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:TRP:CD1	1:B:526:TRP:O	2.72	0.42
1:A:260:ARG:NH2	1:A:560:PHE:HB3	2.35	0.42
1:A:310:ASP:HA	1:A:402:TRP:CZ2	2.54	0.42
1:A:343:GLN:HE22	1:A:413:ASP:CG	2.27	0.42
1:A:468:ARG:HA	1:A:473:GLU:OE2	2.18	0.42
1:B:125:ILE:HG21	1:B:200:LEU:HD21	2.01	0.42
1:B:229:TRP:CD1	1:B:229:TRP:N	2.87	0.42
1:B:493:PHE:CE2	1:B:527:GLY:HA3	2.54	0.42
1:B:501:HIS:ND1	1:B:503:SER:HB3	2.35	0.42
1:B:504:LEU:HD11	1:B:512:PHE:CE2	2.54	0.42
1:A:168:ARG:CA	1:A:171:LEU:HD23	2.49	0.42
1:B:166:GLU:CD	1:B:166:GLU:H	2.28	0.42
1:A:596:HIS:CE1	1:A:636:ASP:HB3	2.54	0.42
1:A:499:ILE:HG23	1:A:545:GLU:OE2	2.20	0.42
1:A:597:HIS:N	1:A:597:HIS:ND1	2.67	0.42
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.85	0.42
1:B:168:ARG:H	1:B:168:ARG:HG2	1.63	0.42
1:B:394:GLU:OE1	1:B:397:ARG:NH2	2.48	0.42
1:B:475:THR:OG1	1:B:476:GLU:N	2.52	0.42
1:A:93:MET:SD	1:A:104:GLY:HA3	2.59	0.42
1:A:296:VAL:HG23	1:A:297:GLY:H	1.85	0.42
1:A:387:ASP:O	1:A:391:ILE:HG22	2.19	0.42
1:A:445:THR:OG1	1:A:446:ARG:N	2.53	0.42
1:B:26:GLY:N	1:B:108:PRO:O	2.37	0.42
1:B:135:LYS:O	1:B:140:GLN:HG2	2.19	0.42
1:B:276:PRO:HG2	1:B:307:GLY:CA	2.46	0.42
1:B:470:SER:O	1:B:473:GLU:N	2.49	0.42
1:A:113:LEU:HB2	1:A:218:TRP:CZ3	2.55	0.42
1:B:248:HIS:HE1	1:B:316:LEU:HG	1.84	0.42
1:B:685:PRO:HB2	1:B:687:ASP:OD1	2.18	0.42
1:A:10:VAL:HG22	1:A:33:ALA:CB	2.49	0.42
1:A:372:PRO:HA	1:A:373:PRO:HA	1.73	0.42
1:A:469:THR:N	1:A:473:GLU:OE1	2.42	0.42
1:B:24:VAL:HG13	1:B:222:PRO:HA	2.02	0.42
1:B:142:GLU:O	1:B:142:GLU:HG2	2.19	0.42
1:B:277:ILE:HG21	1:B:298:SER:O	2.19	0.42
1:A:22:LYS:N	1:A:486:ASP:O	2.37	0.42
1:A:37:ARG:NH1	1:A:38:GLU:C	2.73	0.42
1:A:105:HIS:O	1:A:105:HIS:CG	2.72	0.42
1:A:220:ASP:HB2	1:A:489:ARG:HH22	1.85	0.42
1:A:225:ARG:NH1	1:A:588:ARG:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:HA	1:A:234:PRO:HD3	1.87	0.42
1:A:693:LEU:O	1:A:693:LEU:HD13	2.20	0.42
1:B:284:GLY:O	1:B:553:TYR:HB3	2.20	0.42
1:B:652:ASP:CA	1:B:679:LEU:HD23	2.50	0.42
1:A:206:ARG:HB2	1:A:206:ARG:CZ	2.50	0.42
1:A:335:GLU:OE1	1:A:408:ASN:HB2	2.20	0.42
1:B:4:ARG:O	1:B:5:ILE:HD13	2.20	0.42
1:B:24:VAL:HG22	1:B:221:ARG:O	2.20	0.42
1:B:168:ARG:O	1:B:169:GLU:C	2.62	0.42
1:B:514:ILE:HD13	1:B:622:THR:O	2.20	0.42
1:B:618:LEU:O	1:B:678:VAL:HA	2.20	0.42
1:A:63:PRO:HB3	1:A:64:PRO:HD2	2.02	0.41
1:A:296:VAL:HG23	1:A:297:GLY:N	2.35	0.41
1:A:402:TRP:O	1:A:407:VAL:HG23	2.20	0.41
1:B:188:ALA:O	1:B:192:LEU:HG	2.20	0.41
1:B:250:THR:O	1:B:253:THR:OG1	2.36	0.41
1:B:647:ARG:HB3	1:B:660:GLN:HG3	2.01	0.41
1:B:648:PHE:O	1:B:660:GLN:HA	2.20	0.41
1:B:651:ARG:NH2	1:B:656:GLY:HA2	2.35	0.41
1:B:492:LEU:O	1:B:519:ALA:HB1	2.20	0.41
1:A:36:TRP:HB2	1:B:449:ARG:CG	2.50	0.41
1:A:36:TRP:CD2	1:B:449:ARG:HG2	2.55	0.41
1:A:237:THR:HB	1:A:253:THR:HG22	2.02	0.41
1:A:313:HIS:HA	1:A:314:PRO:HD2	1.80	0.41
1:A:358:PHE:CG	1:A:366:ILE:HG21	2.55	0.41
1:B:130:HIS:CE1	1:B:134:ALA:HB2	2.56	0.41
1:B:221:ARG:NH2	1:B:408:ASN:O	2.53	0.41
1:B:301:ALA:HA	1:B:379:ILE:HD11	2.01	0.41
1:B:301:ALA:CB	1:B:379:ILE:HD11	2.50	0.41
1:B:538:GLN:HA	1:B:539:PRO:HD3	1.90	0.41
1:B:271:LEU:HA	1:B:272:PRO:HD2	1.67	0.41
1:B:418:LYS:O	1:B:419:PRO:C	2.63	0.41
1:B:440:LEU:HD13	1:B:460:GLN:HB3	2.02	0.41
1:B:464:TYR:O	1:B:467:TRP:N	2.53	0.41
1:A:57:PRO:O	1:A:59:LEU:HD12	2.19	0.41
1:B:37:ARG:HH22	1:B:41:ASP:HB2	1.84	0.41
1:B:234:PRO:HG3	1:B:274:ILE:HD12	2.02	0.41
1:B:434:ASN:HA	1:B:435:PRO:HD3	1.78	0.41
1:B:661:TRP:CB	1:B:665:ASN:OD1	2.67	0.41
1:A:158:ARG:O	1:A:158:ARG:HG2	2.19	0.41
1:A:165:ARG:NH2	1:A:166:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:C	1:A:475:THR:N	2.79	0.41
1:A:652:ASP:OD2	1:A:677:HIS:ND1	2.53	0.41
1:B:96:GLY:HA3	1:B:103:HIS:ND1	2.36	0.41
1:B:166:GLU:C	1:B:167:LEU:HD23	2.45	0.41
1:B:196:VAL:O	1:B:199:LEU:N	2.54	0.41
1:B:288:SER:OG	1:B:290:THR:N	2.46	0.41
1:B:313:HIS:HD2	1:B:314:PRO:N	2.17	0.41
1:B:576:ARG:HA	1:B:576:ARG:HD2	1.89	0.41
1:B:684:ILE:HA	1:B:685:PRO:HD3	1.87	0.41
1:A:3:GLY:HA3	1:A:210:THR:CG2	2.51	0.41
1:A:380:TYR:HA	1:A:381:PRO:HD3	1.82	0.41
1:B:412:VAL:HG21	1:B:439:PHE:HD2	1.84	0.41
1:A:279:LYS:NZ	1:A:306:GLU:OE2	2.54	0.41
1:A:398:VAL:O	1:A:402:TRP:CD1	2.74	0.41
1:A:412:VAL:O	1:A:442:GLU:HG3	2.20	0.41
1:A:441:SER:O	1:A:461:SER:HA	2.20	0.41
1:B:180:ALA:O	1:B:187:ARG:NE	2.49	0.41
1:B:504:LEU:HD11	1:B:512:PHE:CZ	2.56	0.41
1:B:593:ILE:HG12	1:B:608:LYS:HZ2	1.86	0.41
1:A:248:HIS:HA	1:A:555:LEU:HD13	2.02	0.41
1:A:283:LYS:HZ3	1:A:376:TYR:HA	1.86	0.41
1:A:356:GLU:C	1:A:358:PHE:H	2.29	0.41
1:A:444:PHE:HZ	1:A:462:TYR:HD2	1.64	0.41
1:A:460:GLN:CG	1:A:461:SER:H	2.34	0.41
1:A:493:PHE:HA	1:A:527:GLY:O	2.20	0.41
1:A:500:LEU:HG	1:A:505:GLN:CD	2.46	0.41
1:A:691:GLN:O	1:A:691:GLN:NE2	2.54	0.41
1:B:113:LEU:HB2	1:B:218:TRP:CE3	2.56	0.41
1:B:173:GLU:HG3	1:B:174:ALA:N	2.35	0.41
1:B:184:PRO:O	1:B:188:ALA:N	2.51	0.41
1:B:349:PRO:C	1:B:350:TRP:CD1	2.98	0.41
1:B:442:GLU:HA	1:B:462:TYR:CD2	2.55	0.41
1:A:15:SER:HB3	1:B:0:SER:HB3	2.03	0.41
1:A:299:PRO:CD	1:A:552:LYS:HG3	2.38	0.41
1:B:168:ARG:C	1:B:171:LEU:H	2.22	0.41
1:B:183:ASP:O	1:B:187:ARG:N	2.44	0.41
1:B:229:TRP:HB2	1:B:527:GLY:HA2	2.02	0.41
1:B:239:GLY:O	1:B:247:VAL:HG22	2.20	0.41
1:B:290:THR:H	1:B:290:THR:HG1	1.63	0.41
1:B:299:PRO:CD	1:B:552:LYS:HZ2	2.34	0.41
1:B:668:ARG:C	1:B:669:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:O	1:A:107:THR:HA	2.21	0.40
1:A:392:TYR:HB2	1:A:393:GLN:OE1	2.20	0.40
1:A:473:GLU:C	1:A:475:THR:H	2.28	0.40
1:B:225:ARG:NH1	1:B:588:ARG:HB2	2.35	0.40
1:B:279:LYS:HE2	1:B:279:LYS:HB3	1.79	0.40
1:B:302:ILE:HD12	1:B:302:ILE:HA	1.69	0.40
1:B:463:THR:HG23	1:B:490:PRO:HB3	2.02	0.40
1:B:596:HIS:N	1:B:596:HIS:CD2	2.89	0.40
1:A:493:PHE:CG	1:A:527:GLY:HA3	2.56	0.40
1:A:498:ASP:HB3	1:A:499:ILE:HD12	2.02	0.40
1:B:383:ASN:HD22	1:B:386:ASN:H	1.69	0.40
1:B:574:LEU:O	1:B:578:ASN:CG	2.65	0.40
1:B:650:VAL:HG12	1:B:679:LEU:HD22	2.02	0.40
1:A:229:TRP:HB2	1:A:526:TRP:O	2.22	0.40
1:A:493:PHE:HA	1:A:527:GLY:C	2.47	0.40
1:A:541:ARG:HH21	1:A:541:ARG:HD3	1.74	0.40
1:B:116:TYR:CZ	1:B:215:TYR:HD1	2.39	0.40
1:B:124:PRO:HG2	1:B:125:ILE:HD12	2.03	0.40
1:B:344:CYS:SG	1:B:348:HIS:HB2	2.61	0.40
1:A:350:TRP:CD1	1:A:354:HIS:CE1	3.10	0.40
1:A:397:ARG:O	1:A:397:ARG:HG2	2.21	0.40
1:A:402:TRP:O	1:A:403:ILE:C	2.64	0.40
1:B:21:ALA:HB3	1:B:217:VAL:HG22	2.04	0.40
1:B:230:TYR:O	1:B:231:GLU:OE1	2.39	0.40
1:A:383:ASN:CG	1:A:386:ASN:HD22	2.30	0.40
1:A:464:TYR:O	1:A:466:THR:N	2.54	0.40
1:B:253:THR:O	1:B:256:GLU:HB2	2.22	0.40
1:B:484:LYS:HB3	1:B:487:ILE:HG13	2.04	0.40
1:B:504:LEU:HD13	1:B:504:LEU:C	2.47	0.40

All (2) 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:A:248:HIS:O	1:B:165:ARG:NH1[2_775]	2.04	0.16
1:A:143:SER:OG	1:B:142:GLU:OE1[1_554]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	638/698 (91%)	575 (90%)	60 (9%)	3 (0%)	24	54
1	B	680/698 (97%)	616 (91%)	62 (9%)	2 (0%)	36	64
All	All	1318/1396 (94%)	1191 (90%)	122 (9%)	5 (0%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	PHE
1	B	433	GLU
1	A	611	PRO
1	B	625	PRO
1	A	644	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	525/566 (93%)	459 (87%)	66 (13%)	4	17
1	B	556/566 (98%)	486 (87%)	70 (13%)	4	17
All	All	1081/1132 (96%)	945 (87%)	136 (13%)	4	17

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL

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Mol	Chain	Res	Type
1	A	8	ASP
1	A	10	VAL
1	A	13	VAL
1	A	29	VAL
1	A	31	VAL
1	A	35	VAL
1	A	40	HIS
1	A	43	VAL
1	A	101	VAL
1	A	111	VAL
1	A	129	ARG
1	A	163	VAL
1	A	171	LEU
1	A	173	GLU
1	A	205	LEU
1	A	228	SER
1	A	260	ARG
1	A	268	VAL
1	A	270	TYR
1	A	274	ILE
1	A	280	VAL
1	A	285	ARG
1	A	306	GLU
1	A	312	VAL
1	A	347	ASP
1	A	352	ARG
1	A	354	HIS
1	A	356	GLU
1	A	359	THR
1	A	365	SER
1	A	382	LEU
1	A	395	VAL
1	A	396	LEU
1	A	398	VAL
1	A	413	ASP
1	A	429	GLN
1	A	437	VAL
1	A	459	THR
1	A	463	THR
1	A	464	TYR
1	A	466	THR
1	A	469	THR

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Mol	Chain	Res	Type
1	A	470	SER
1	A	487	ILE
1	A	489	ARG
1	A	494	VAL
1	A	499	ILE
1	A	528	VAL
1	A	530[A]	SER
1	A	530[B]	SER
1	A	533	GLU
1	A	544	SER
1	A	561	GLU
1	A	568	GLU
1	A	589	GLU
1	A	597	HIS
1	A	616	THR
1	A	620	VAL
1	A	639	GLU
1	A	640	LEU
1	A	655	THR
1	A	659	TYR
1	A	677	HIS
1	A	679	LEU
1	A	684	ILE
1	B	6	VAL
1	B	14	VAL
1	B	24	VAL
1	B	25	VAL
1	B	29	VAL
1	B	35	VAL
1	B	66	VAL
1	B	101	VAL
1	B	118	VAL
1	B	130	HIS
1	B	140	GLN
1	B	142	GLU
1	B	151	VAL
1	B	156	LEU
1	B	163	VAL
1	B	183	ASP
1	B	209	VAL
1	B	211	ARG
1	B	228	SER

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Mol	Chain	Res	Type
1	B	231	GLU
1	B	235	ARG
1	B	270	TYR
1	B	277	ILE
1	B	280	VAL
1	B	302	ILE
1	B	310	ASP
1	B	321	ASP
1	B	344	CYS
1	B	352	ARG
1	B	366	ILE
1	B	368	TYR
1	B	370	GLU
1	B	379	ILE
1	B	383	ASN
1	B	395	VAL
1	B	399	VAL
1	B	400	ARG
1	B	407	VAL
1	B	408	ASN
1	B	409	ILE
1	B	412	VAL
1	B	442	GLU
1	B	458	PHE
1	B	464	TYR
1	B	465	PHE
1	B	469	THR
1	B	470	SER
1	B	484	LYS
1	B	487	ILE
1	B	496	THR
1	B	517	VAL
1	B	518	LEU
1	B	538	GLN
1	B	540	VAL
1	B	561	GLU
1	B	603	LEU
1	B	608	LYS
1	B	619	VAL
1	B	620	VAL
1	B	624	ASN
1	B	630	GLU

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Mol	Chain	Res	Type
1	B	649	TRP
1	B	650	VAL
1	B	651	ARG
1	B	653	GLU
1	B	654	ILE
1	B	665	ASN
1	B	668	ARG
1	B	679	LEU
1	B	691	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	214	GLN
1	A	313	HIS
1	A	386	ASN
1	A	429	GLN
1	A	578	ASN
1	A	677	HIS
1	B	40	HIS
1	B	131	ASN
1	B	214	GLN
1	B	248	HIS
1	B	313	HIS
1	B	348	HIS
1	B	371	ASN
1	B	377	GLN
1	B	414	ASN
1	B	421	ASN
1	B	665	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	649/698 (92%)	-1.10	0	100 100	33, 58, 140, 186	1 (0%)
1	B	678/698 (97%)	-1.01	2 (0%)	90 80	36, 75, 117, 164	6 (0%)
All	All	1327/1396 (95%)	-1.05	2 (0%)	91 83	33, 68, 130, 186	7 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	GLY	2.3
1	B	646	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.