



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:57 PM UTC

PDB ID : 3FN9 / pdb_00003fn9
Title : Crystal structure of putative beta-galactosidase from bacteroides fragilis
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-12-23
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

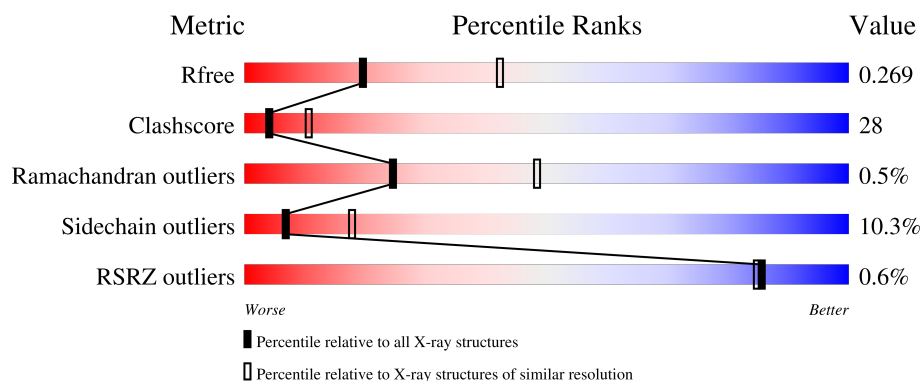
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	692	58% 34% 5% .
1	B	692	48% 41% 8% .
1	C	692	61% 31% 5% .
1	D	692	57% 34% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21740 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 Putative beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5426	3469	926	1013	18			
1	B	672	Total	C	N	O	S	0	0	0
			5410	3463	923	1006	18			
1	C	673	Total	C	N	O	S	0	0	0
			5431	3471	927	1015	18			
1	D	666	Total	C	N	O	S	0	0	0
			5374	3439	916	1001	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP Q5LJ68
A	21	SER	-	expression tag	UNP Q5LJ68
A	22	LEU	-	expression tag	UNP Q5LJ68
A	704	GLU	-	expression tag	UNP Q5LJ68
A	705	GLY	-	expression tag	UNP Q5LJ68
A	706	HIS	-	expression tag	UNP Q5LJ68
A	707	HIS	-	expression tag	UNP Q5LJ68
A	708	HIS	-	expression tag	UNP Q5LJ68
A	709	HIS	-	expression tag	UNP Q5LJ68
A	710	HIS	-	expression tag	UNP Q5LJ68
A	711	HIS	-	expression tag	UNP Q5LJ68
B	20	MET	-	expression tag	UNP Q5LJ68
B	21	SER	-	expression tag	UNP Q5LJ68
B	22	LEU	-	expression tag	UNP Q5LJ68
B	704	GLU	-	expression tag	UNP Q5LJ68
B	705	GLY	-	expression tag	UNP Q5LJ68
B	706	HIS	-	expression tag	UNP Q5LJ68
B	707	HIS	-	expression tag	UNP Q5LJ68
B	708	HIS	-	expression tag	UNP Q5LJ68
B	709	HIS	-	expression tag	UNP Q5LJ68
B	710	HIS	-	expression tag	UNP Q5LJ68

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Chain	Residue	Modelled	Actual	Comment	Reference
B	711	HIS	-	expression tag	UNP Q5LJ68
C	20	MET	-	expression tag	UNP Q5LJ68
C	21	SER	-	expression tag	UNP Q5LJ68
C	22	LEU	-	expression tag	UNP Q5LJ68
C	704	GLU	-	expression tag	UNP Q5LJ68
C	705	GLY	-	expression tag	UNP Q5LJ68
C	706	HIS	-	expression tag	UNP Q5LJ68
C	707	HIS	-	expression tag	UNP Q5LJ68
C	708	HIS	-	expression tag	UNP Q5LJ68
C	709	HIS	-	expression tag	UNP Q5LJ68
C	710	HIS	-	expression tag	UNP Q5LJ68
C	711	HIS	-	expression tag	UNP Q5LJ68
D	20	MET	-	expression tag	UNP Q5LJ68
D	21	SER	-	expression tag	UNP Q5LJ68
D	22	LEU	-	expression tag	UNP Q5LJ68
D	704	GLU	-	expression tag	UNP Q5LJ68
D	705	GLY	-	expression tag	UNP Q5LJ68
D	706	HIS	-	expression tag	UNP Q5LJ68
D	707	HIS	-	expression tag	UNP Q5LJ68
D	708	HIS	-	expression tag	UNP Q5LJ68
D	709	HIS	-	expression tag	UNP Q5LJ68
D	710	HIS	-	expression tag	UNP Q5LJ68
D	711	HIS	-	expression tag	UNP Q5LJ68

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	C	1	Total Cl 1 1	0	0
2	D	3	Total Cl 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	B	18	Total O 18 18	0	0

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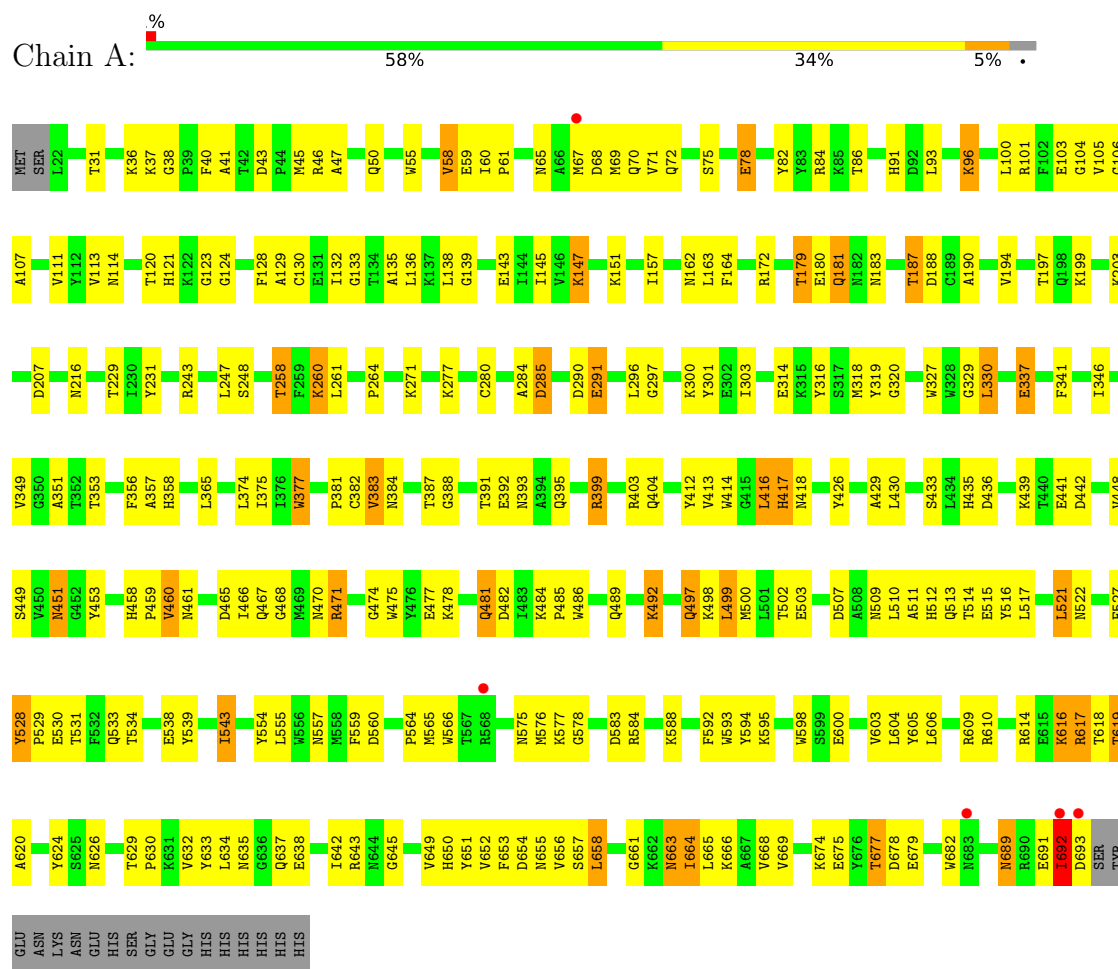
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	23	Total	O	0	0
			23	23		
3	D	20	Total	O	0	0
			20	20		

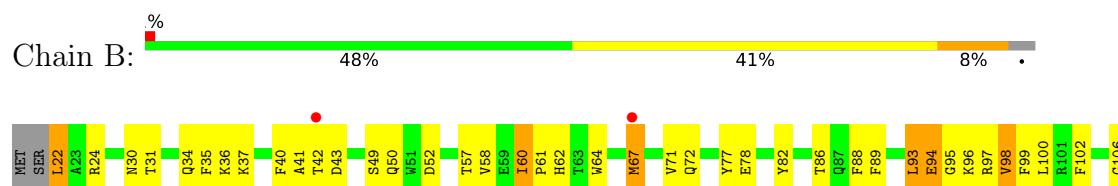
3 Residue-property plots

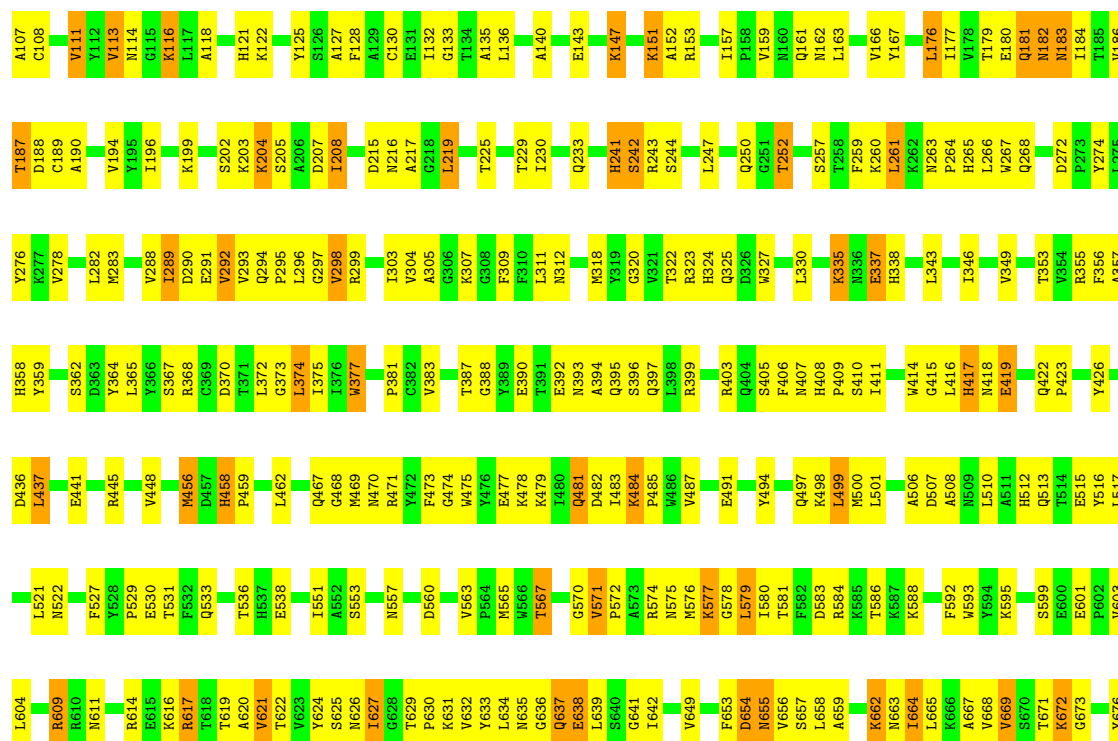
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative beta-galactosidase

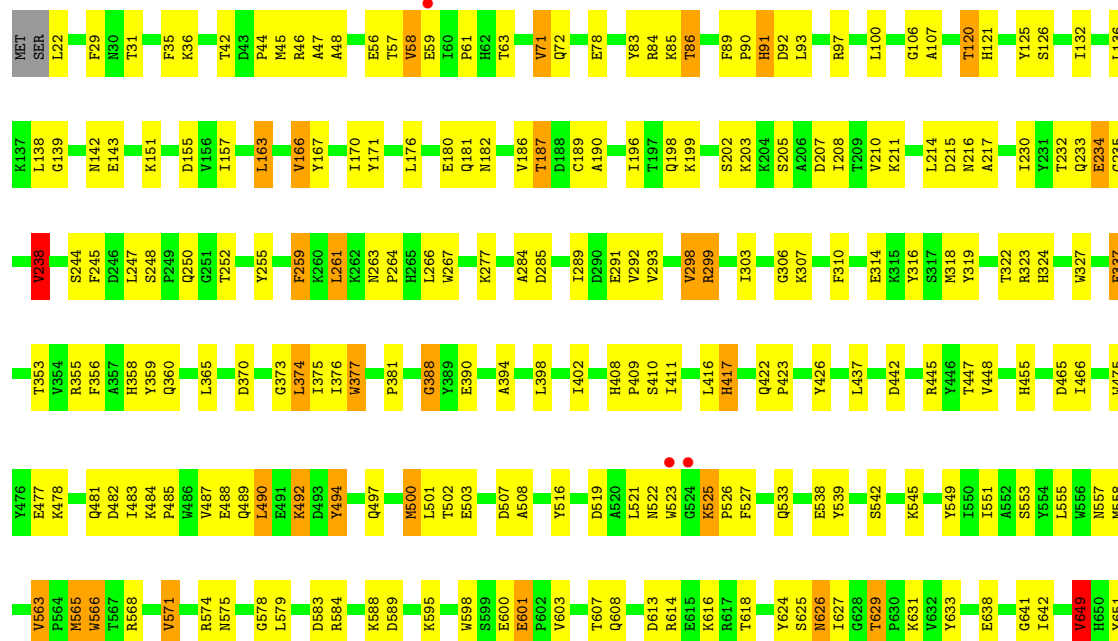


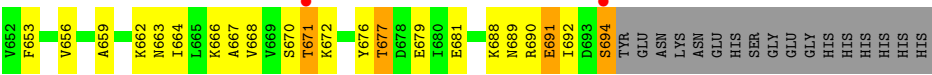
• Molecule 1: Putative beta-galactosidase



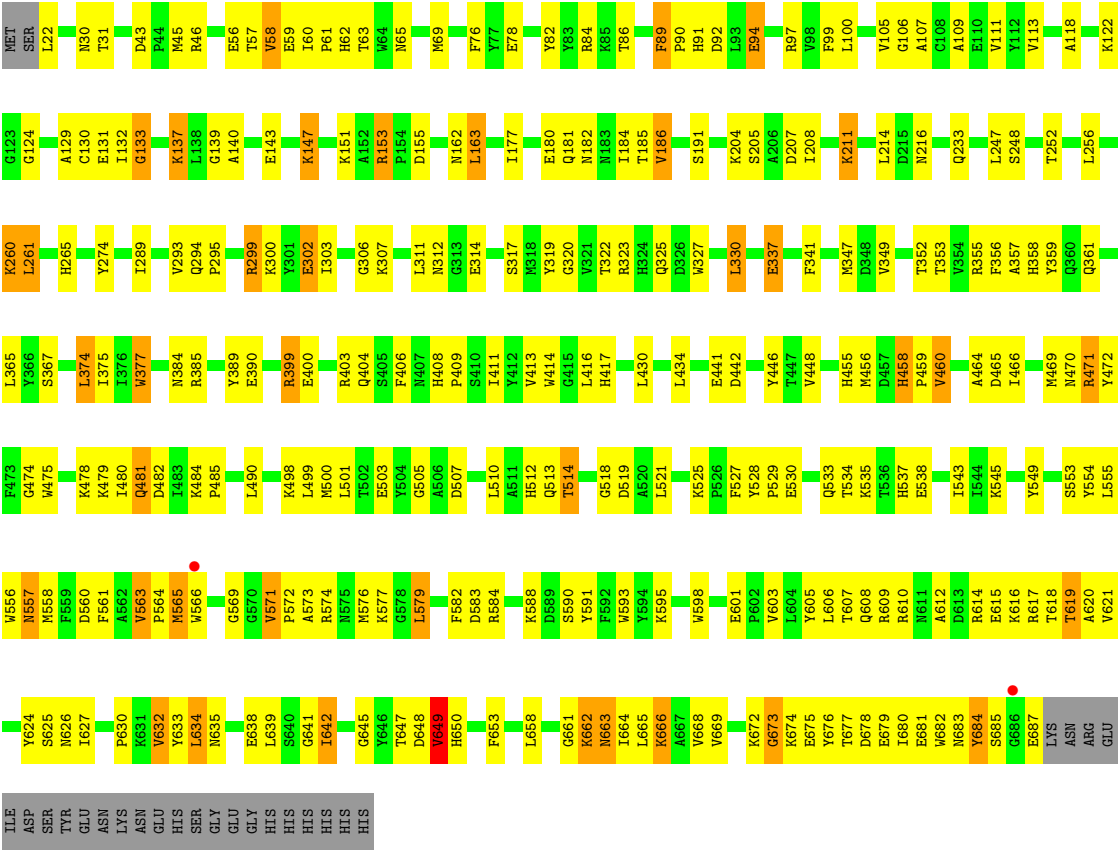


• Molecule 1: Putative beta-galactosidase





● Molecule 1: Putative beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.45Å 133.07Å 221.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.70 49.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.39-2.70) 99.9 (49.39-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.270 0.205 , 0.269	Depositor DCC
R_{free} test set	4414 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21740	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.68	0/5577	0.95	8/7579 (0.1%)
1	B	0.67	0/5561	0.96	6/7558 (0.1%)
1	C	0.69	0/5582	0.97	14/7586 (0.2%)
1	D	0.68	0/5525	0.98	13/7509 (0.2%)
All	All	0.68	0/22245	0.97	41/30232 (0.1%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	600	GLU	N-CA-C	-8.91	103.52	114.75
1	D	89	PHE	CA-C-N	8.58	128.44	120.21
1	D	89	PHE	C-N-CA	8.58	128.44	120.21
1	A	248	SER	CA-C-N	-7.58	113.09	120.83
1	A	248	SER	C-N-CA	-7.58	113.09	120.83
1	D	579	LEU	N-CA-C	-7.31	104.36	113.28
1	A	383	VAL	N-CA-C	7.26	117.91	107.88
1	B	437	LEU	N-CA-C	-7.23	103.48	111.36
1	C	494	TYR	CA-C-N	7.22	126.93	119.56
1	C	494	TYR	C-N-CA	7.22	126.93	119.56
1	C	388	GLY	N-CA-C	-7.02	105.40	115.64
1	C	566	TRP	N-CA-C	6.81	118.86	109.18
1	D	525	LYS	CA-C-N	6.73	128.25	119.84
1	D	525	LYS	C-N-CA	6.73	128.25	119.84
1	D	563	VAL	CA-C-N	6.63	126.26	119.56
1	D	563	VAL	C-N-CA	6.63	126.26	119.56
1	A	383	VAL	CB-CA-C	-6.42	102.87	111.80
1	B	458	HIS	CA-C-N	6.12	126.57	119.47
1	B	458	HIS	C-N-CA	6.12	126.57	119.47
1	C	626	ASN	N-CA-C	-5.95	106.64	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	THR	N-CA-C	-5.74	106.91	114.31
1	A	164	PHE	CA-C-N	-5.61	117.52	122.73
1	A	164	PHE	C-N-CA	-5.61	117.52	122.73
1	C	376	ILE	N-CA-C	5.55	116.90	108.80
1	C	563	VAL	CA-C-N	5.53	125.36	119.28
1	C	563	VAL	C-N-CA	5.53	125.36	119.28
1	C	166	VAL	N-CA-C	5.49	112.08	106.21
1	C	649	VAL	N-CA-C	-5.44	107.68	112.90
1	D	458	HIS	CA-C-N	5.43	126.63	119.84
1	D	458	HIS	C-N-CA	5.43	126.63	119.84
1	C	626	ASN	N-CA-CB	-5.43	103.67	110.90
1	C	91	HIS	N-CA-C	-5.42	106.36	112.87
1	B	183	ASN	N-CA-C	5.40	116.19	108.74
1	D	191	SER	CA-C-N	-5.37	114.28	119.87
1	D	191	SER	C-N-CA	-5.37	114.28	119.87
1	B	276	TYR	N-CA-C	-5.32	103.59	110.19
1	B	364	TYR	N-CA-C	-5.26	105.46	111.14
1	D	302	GLU	N-CA-C	5.22	117.32	109.23
1	C	411	ILE	N-CA-C	5.21	116.26	108.54
1	A	429	ALA	N-CA-C	-5.13	105.38	110.97
1	D	649	VAL	N-CA-C	-5.06	108.19	113.10

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	5426	0	5216	284	0
1	B	5410	0	5189	386	0
1	C	5431	0	5219	218	0
1	D	5374	0	5167	298	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	1	0
3	A	31	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	1	0
3	C	23	0	0	2	0
3	D	20	0	0	5	0
All	All	21740	0	20791	1173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1173) 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:630:PRO:HA	1:B:669:VAL:CG2	1.65	1.26
1:D:347:MET:HE1	1:D:374:LEU:CD1	1.70	1.22
1:D:347:MET:CE	1:D:374:LEU:HD13	1.69	1.20
1:D:347:MET:CE	1:D:374:LEU:CD1	2.24	1.15
1:B:208:ILE:CD1	1:B:259:PHE:HB2	1.76	1.15
1:D:607:THR:HG22	1:D:608:GLN:HG3	1.20	1.13
1:A:157:ILE:HG13	1:A:381:PRO:HG2	1.14	1.13
1:A:481:GLN:H	1:A:481:GLN:NE2	1.49	1.10
1:B:617:ARG:HG2	1:B:617:ARG:HH11	0.98	1.10
1:B:37:LYS:HD2	1:B:77:TYR:CD2	1.86	1.10
1:D:481:GLN:H	1:D:481:GLN:NE2	1.48	1.10
1:B:67:MET:HA	1:B:67:MET:CE	1.82	1.09
1:B:630:PRO:HA	1:B:669:VAL:HG23	1.27	1.07
1:A:617:ARG:HH11	1:A:617:ARG:CG	1.66	1.07
1:D:630:PRO:HA	1:D:669:VAL:HG12	1.37	1.06
1:A:617:ARG:HG3	1:A:617:ARG:NH1	1.51	1.06
1:B:67:MET:HE2	1:B:67:MET:CA	1.86	1.04
1:D:642:ILE:HB	1:D:653:PHE:CE2	1.92	1.03
1:C:642:ILE:HD13	1:C:653:PHE:CZ	1.92	1.03
1:D:565:MET:HE3	1:D:565:MET:HA	1.41	1.02
1:B:633:TYR:CD1	1:B:638:GLU:HA	1.94	1.01
1:C:307:LYS:HE3	1:C:310:PHE:CZ	1.95	1.01
1:B:67:MET:HA	1:B:67:MET:HE2	1.02	1.00
1:D:630:PRO:HA	1:D:669:VAL:CG1	1.91	1.00
1:C:629:THR:HG22	3:C:1:HOH:O	1.59	1.00
1:D:662:LYS:C	1:D:663:ASN:HD22	1.67	1.00
1:B:202:SER:OG	1:B:204:LYS:HG3	1.62	0.99
1:A:78:GLU:HG3	1:A:151:LYS:HA	1.45	0.98
1:A:179:THR:HG22	1:A:180:GLU:O	1.63	0.98
1:B:630:PRO:CA	1:B:669:VAL:CG2	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:HB2	1:A:655:ASN:ND2	1.79	0.97
1:B:97:ARG:NH1	1:B:217:ALA:HB2	1.79	0.97
1:D:99:PHE:CE2	1:D:131:GLU:HG3	2.00	0.97
1:B:41:ALA:H	1:B:50:GLN:HE22	1.11	0.97
1:B:689:ASN:ND2	1:B:692:ILE:HG13	1.79	0.97
1:A:692:ILE:O	1:A:692:ILE:CG2	2.13	0.97
1:A:41:ALA:H	1:A:50:GLN:HE22	1.13	0.96
1:A:661:GLY:HA3	3:A:737:HOH:O	1.63	0.96
1:C:187:THR:CG2	1:C:187:THR:O	2.12	0.96
1:B:659:ALA:N	1:B:663:ASN:HD21	1.64	0.95
1:D:684:TYR:CD2	1:D:685:SER:N	2.33	0.95
1:A:498:LYS:H	1:B:250:GLN:HE22	1.04	0.95
1:D:662:LYS:HE2	1:D:681:GLU:OE2	1.67	0.95
1:B:595:LYS:HG2	1:B:603:VAL:HG21	1.45	0.94
1:B:617:ARG:HH11	1:B:617:ARG:CG	1.80	0.94
1:C:662:LYS:HE3	1:C:681:GLU:OE2	1.67	0.94
1:B:659:ALA:H	1:B:663:ASN:ND2	1.65	0.94
1:B:356:PHE:CE2	1:B:365:LEU:HD21	2.02	0.94
1:B:456:MET:HE1	1:B:467:GLN:HG2	1.48	0.94
1:B:456:MET:HE3	1:B:469:MET:HE2	1.48	0.93
1:B:633:TYR:HD1	1:B:638:GLU:HA	1.30	0.93
1:B:179:THR:HG21	1:B:183:ASN:HB3	1.49	0.93
1:B:633:TYR:HE1	1:B:638:GLU:HB2	1.31	0.93
1:B:630:PRO:CA	1:B:669:VAL:HG23	1.97	0.93
1:B:659:ALA:H	1:B:663:ASN:HD21	0.95	0.93
1:D:111:VAL:HG23	1:D:118:ALA:HB3	1.51	0.92
1:A:133:GLY:HA2	1:A:136:LEU:HD23	1.47	0.92
1:A:179:THR:CG2	1:A:180:GLU:N	2.33	0.92
1:B:181:GLN:HA	1:B:181:GLN:HE21	1.35	0.92
1:D:607:THR:HG22	1:D:608:GLN:CG	1.98	0.92
1:D:347:MET:HE3	1:D:374:LEU:HD22	1.50	0.92
1:D:510:LEU:HD21	1:D:588:LYS:HG2	1.51	0.92
1:B:208:ILE:HD13	1:B:259:PHE:HB2	1.50	0.91
1:B:179:THR:HG22	1:B:180:GLU:N	1.86	0.91
1:C:583:ASP:O	1:C:584:ARG:HB2	1.71	0.91
1:A:481:GLN:H	1:A:481:GLN:HE21	1.12	0.90
1:B:684:TYR:OH	1:B:687:GLU:HG2	1.71	0.90
1:A:629:THR:HG22	1:A:651:TYR:HE2	1.33	0.90
1:A:633:TYR:HD2	1:A:638:GLU:HA	1.33	0.90
1:A:470:ASN:OD1	1:A:503:GLU:HB2	1.70	0.90
1:B:395:GLN:HG2	1:B:437:LEU:CD1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ILE:HG22	1:B:681:GLU:HG3	1.54	0.89
1:D:633:TYR:CE1	1:D:638:GLU:HB2	2.07	0.89
1:A:654:ASP:HB2	1:A:655:ASN:HD22	1.33	0.89
1:B:41:ALA:N	1:B:50:GLN:HE22	1.71	0.89
1:D:478:LYS:HB3	1:D:482:ASP:OD2	1.73	0.89
1:B:680:ILE:HD12	1:B:682:TRP:NE1	1.87	0.89
1:D:565:MET:HA	1:D:565:MET:CE	2.02	0.88
1:D:557:ASN:HD22	1:D:558:MET:N	1.71	0.88
1:B:512:HIS:CD2	1:B:527:PHE:CE1	2.60	0.88
1:D:632:VAL:CG2	1:D:653:PHE:CE1	2.57	0.88
1:A:179:THR:HG22	1:A:180:GLU:N	1.88	0.87
1:B:680:ILE:HD12	1:B:682:TRP:HE1	1.38	0.87
1:A:507:ASP:OD1	1:A:577:LYS:HE2	1.75	0.87
1:D:557:ASN:HD22	1:D:558:MET:H	1.22	0.86
1:B:181:GLN:HA	1:B:181:GLN:NE2	1.88	0.86
1:D:347:MET:HE1	1:D:374:LEU:HD13	0.87	0.86
1:D:632:VAL:HG21	1:D:653:PHE:HE1	1.41	0.86
1:A:629:THR:HG22	1:A:651:TYR:CE2	2.11	0.86
1:B:97:ARG:HH11	1:B:217:ALA:HB2	1.38	0.86
1:B:617:ARG:HG2	1:B:617:ARG:NH1	1.80	0.86
1:B:309:PHE:CE1	1:B:318:MET:HE3	2.10	0.85
1:A:477:GLU:HG2	1:A:478:LYS:HD3	1.55	0.85
1:A:692:ILE:O	1:A:692:ILE:HG22	1.75	0.85
1:D:684:TYR:HD2	1:D:685:SER:N	1.73	0.85
1:C:356:PHE:CE2	1:C:365:LEU:HD21	2.11	0.85
1:D:632:VAL:HG21	1:D:653:PHE:CE1	2.12	0.85
1:D:635:ASN:HD21	1:D:663:ASN:HA	1.41	0.84
1:A:481:GLN:NE2	1:A:481:GLN:N	2.26	0.84
1:B:309:PHE:CD1	1:B:318:MET:HE3	2.13	0.84
1:A:181:GLN:HA	1:A:181:GLN:HE21	1.42	0.84
1:B:456:MET:CE	1:B:467:GLN:HG2	2.07	0.84
1:D:481:GLN:H	1:D:481:GLN:HE21	1.22	0.83
1:B:487:VAL:O	1:B:491:GLU:HG2	1.78	0.83
1:B:34:GLN:HE21	1:B:57:THR:HG22	1.42	0.83
1:C:307:LYS:HE3	1:C:310:PHE:HZ	1.37	0.83
1:D:560:ASP:O	1:D:582:PHE:CD1	2.33	0.82
1:B:609:ARG:HG2	1:B:609:ARG:HH21	1.44	0.82
1:B:621:VAL:HG21	1:B:665:LEU:HD13	1.62	0.82
1:B:41:ALA:H	1:B:50:GLN:NE2	1.77	0.82
1:C:608:GLN:OE1	1:C:614:ARG:NH2	2.11	0.82
1:A:157:ILE:CG1	1:A:381:PRO:HG2	2.04	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ALA:H	1:C:663:ASN:HD21	1.27	0.82
1:A:489:GLN:HA	1:A:489:GLN:NE2	1.94	0.82
1:C:78:GLU:HG3	1:C:151:LYS:HA	1.62	0.82
1:A:284:ALA:O	1:A:285:ASP:HB2	1.78	0.81
1:D:684:TYR:CD2	1:D:684:TYR:C	2.57	0.81
1:D:684:TYR:HD2	1:D:684:TYR:C	1.88	0.81
1:D:377:TRP:HZ3	1:D:500:MET:CE	1.94	0.81
1:D:632:VAL:CG2	1:D:653:PHE:HE1	1.93	0.81
1:B:456:MET:HE3	1:B:469:MET:CE	2.10	0.81
1:A:633:TYR:HD2	1:A:638:GLU:CA	1.94	0.80
1:A:489:GLN:HA	1:A:489:GLN:HE21	1.46	0.80
1:B:621:VAL:HG21	1:B:665:LEU:CD1	2.12	0.80
1:C:187:THR:O	1:C:187:THR:HG22	1.80	0.80
1:B:383:VAL:HG12	1:B:418:ASN:HB3	1.62	0.80
1:A:451:ASN:ND2	1:A:453:TYR:H	1.80	0.80
1:D:131:GLU:HG2	3:D:723:HOH:O	1.81	0.80
1:B:181:GLN:HE21	1:B:181:GLN:CA	1.93	0.79
1:B:494:TYR:HB3	1:B:497:GLN:HG3	1.64	0.79
1:D:471:ARG:HG3	1:D:471:ARG:HH11	1.46	0.79
1:D:618:THR:HG23	1:D:618:THR:O	1.82	0.79
1:A:510:LEU:HD11	1:A:588:LYS:HG2	1.63	0.79
1:B:267:TRP:CZ2	1:B:373:GLY:HA2	2.17	0.79
1:C:29:PHE:CZ	1:C:85:LYS:HE2	2.17	0.79
1:C:484:LYS:HB3	1:C:485:PRO:CD	2.13	0.79
1:C:595:LYS:HG2	1:C:603:VAL:HG21	1.64	0.78
1:B:205:SER:OG	1:B:260:LYS:HE3	1.83	0.78
1:D:400:GLU:O	1:D:404:GLN:HG3	1.83	0.78
1:B:475:TRP:CH2	1:B:507:ASP:HB2	2.19	0.78
1:D:664:ILE:HG13	1:D:679:GLU:OE1	1.82	0.78
1:C:337:GLU:CD	1:C:337:GLU:H	1.91	0.78
1:A:663:ASN:C	1:A:664:ILE:HD12	2.09	0.78
1:A:41:ALA:N	1:A:50:GLN:HE22	1.80	0.78
1:C:565:MET:HA	1:C:565:MET:HE3	1.66	0.78
1:C:448:VAL:HG23	1:C:466:ILE:HB	1.66	0.78
1:D:94:GLU:HA	1:D:94:GLU:OE1	1.84	0.78
1:B:296:LEU:HA	3:B:725:HOH:O	1.85	0.77
1:A:498:LYS:N	1:B:250:GLN:HE22	1.80	0.77
1:B:456:MET:CE	1:B:469:MET:HE2	2.14	0.77
1:D:481:GLN:NE2	1:D:481:GLN:N	2.30	0.77
1:B:67:MET:CE	1:B:67:MET:CA	2.51	0.77
1:D:577:LYS:HE2	3:D:718:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TRP:CD1	1:C:377:TRP:C	2.63	0.77
1:D:111:VAL:CG2	1:D:118:ALA:HB3	2.14	0.77
1:A:41:ALA:H	1:A:50:GLN:NE2	1.82	0.76
1:B:179:THR:CG2	1:B:183:ASN:HB3	2.14	0.76
1:A:632:VAL:HG21	1:A:653:PHE:CE1	2.21	0.76
1:A:179:THR:CG2	1:A:180:GLU:O	2.33	0.76
1:B:680:ILE:CD1	1:B:682:TRP:HE1	1.99	0.76
1:A:633:TYR:CD2	1:A:638:GLU:HA	2.20	0.76
1:D:30:ASN:HB3	1:D:60:ILE:HB	1.65	0.76
1:D:347:MET:HE2	1:D:374:LEU:HD11	1.68	0.76
1:D:663:ASN:HD22	1:D:663:ASN:N	1.82	0.76
1:B:208:ILE:HD11	1:B:259:PHE:HB2	1.67	0.75
1:A:634:LEU:HD22	1:A:656:VAL:CG1	2.15	0.75
1:A:477:GLU:HG2	1:A:478:LYS:CD	2.17	0.75
1:D:635:ASN:HA	1:D:664:ILE:HG22	1.69	0.75
1:B:82:TYR:CE1	1:B:147:LYS:HG2	2.21	0.75
1:A:475:TRP:CZ3	1:A:521:LEU:HD22	2.21	0.75
1:D:347:MET:HE2	1:D:374:LEU:CD1	2.15	0.75
1:B:654:ASP:OD2	1:B:654:ASP:N	2.20	0.74
1:D:632:VAL:HG23	1:D:653:PHE:CE1	2.21	0.74
1:A:43:ASP:OD2	1:A:45:MET:HB3	1.87	0.74
1:C:642:ILE:HD13	1:C:653:PHE:CE1	2.21	0.74
1:D:182:ASN:ND2	1:D:216:ASN:HB2	2.02	0.74
1:D:322:THR:HG22	1:D:355:ARG:HB3	1.68	0.74
1:D:347:MET:HE3	1:D:374:LEU:CD2	2.17	0.74
1:D:561:PHE:HA	1:D:582:PHE:CE1	2.22	0.74
1:B:512:HIS:CD2	1:B:527:PHE:CD1	2.75	0.74
1:C:494:TYR:HB3	1:C:497:GLN:HG3	1.69	0.74
1:B:179:THR:HG21	1:B:183:ASN:CB	2.17	0.73
1:D:43:ASP:HB2	1:D:46:ARG:HH12	1.54	0.73
1:C:187:THR:O	1:C:187:THR:HG23	1.88	0.73
1:A:46:ARG:O	1:A:50:GLN:HG3	1.88	0.73
1:B:521:LEU:HD23	1:B:522:ASN:C	2.13	0.73
1:B:179:THR:HG21	1:B:183:ASN:HD22	1.54	0.73
1:B:157:ILE:HD12	1:B:381:PRO:HD2	1.69	0.73
1:A:296:LEU:HD12	1:A:297:GLY:N	2.04	0.72
1:D:347:MET:CE	1:D:374:LEU:HD11	2.18	0.72
1:D:634:LEU:HB3	1:D:639:LEU:HD21	1.71	0.72
1:B:377:TRP:CD1	1:B:377:TRP:C	2.65	0.72
1:B:417:HIS:C	1:B:417:HIS:CD2	2.67	0.72
1:C:46:ARG:HB2	1:C:46:ARG:CZ	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:TRP:CZ3	1:D:500:MET:CE	2.72	0.72
1:B:680:ILE:CD1	1:B:682:TRP:NE1	2.52	0.72
1:A:132:ILE:O	1:A:136:LEU:HD22	1.89	0.72
1:B:208:ILE:HD11	1:B:230:ILE:HD11	1.72	0.72
1:D:82:TYR:CE1	1:D:147:LYS:HG2	2.24	0.72
1:B:515:GLU:OE1	1:B:616:LYS:HB2	1.88	0.72
1:B:633:TYR:CD1	1:B:638:GLU:CA	2.71	0.72
1:D:377:TRP:CD1	1:D:377:TRP:C	2.66	0.72
1:D:634:LEU:C	1:D:634:LEU:HD12	2.15	0.71
1:B:208:ILE:HD11	1:B:259:PHE:CD2	2.25	0.71
1:C:521:LEU:HG	1:C:522:ASN:N	2.04	0.71
1:C:579:LEU:O	1:C:588:LYS:HG3	1.90	0.71
1:C:641:GLY:O	1:C:642:ILE:C	2.32	0.71
1:B:395:GLN:HG2	1:B:437:LEU:HD12	1.71	0.71
1:D:616:LYS:HA	1:D:687:GLU:OE2	1.91	0.71
1:A:617:ARG:HH11	1:A:617:ARG:HG3	0.71	0.71
1:B:268:GLN:HG3	1:B:268:GLN:O	1.89	0.70
1:A:132:ILE:HG13	1:A:136:LEU:HD21	1.73	0.70
1:B:609:ARG:HH21	1:B:609:ARG:CG	2.04	0.70
1:D:322:THR:O	1:D:557:ASN:ND2	2.23	0.70
1:B:179:THR:CG2	1:B:180:GLU:N	2.55	0.70
1:B:633:TYR:HD1	1:B:638:GLU:CA	2.04	0.70
1:C:90:PRO:HB2	1:C:92:ASP:HB2	1.73	0.70
1:D:472:TYR:CE1	1:D:577:LYS:HE3	2.27	0.70
1:A:481:GLN:HE21	1:A:481:GLN:N	1.88	0.70
1:D:619:THR:HB	1:D:658:LEU:HD11	1.73	0.70
1:D:630:PRO:CA	1:D:669:VAL:CG1	2.69	0.70
1:A:172:ARG:HA	3:A:716:HOH:O	1.91	0.69
1:B:162:ASN:HD22	1:B:565:MET:HE3	1.57	0.69
1:A:530:GLU:OE2	1:A:610:ARG:NH2	2.23	0.69
1:D:347:MET:CE	1:D:374:LEU:CD2	2.70	0.69
1:B:662:LYS:HA	1:B:683:ASN:HB3	1.73	0.69
1:C:78:GLU:CG	1:C:151:LYS:HA	2.21	0.69
1:D:662:LYS:C	1:D:663:ASN:ND2	2.47	0.69
1:B:377:TRP:C	1:B:377:TRP:HD1	2.00	0.69
1:C:83:TYR:CE2	1:C:170:ILE:HG13	2.26	0.69
1:A:555:LEU:C	1:A:555:LEU:HD12	2.18	0.69
1:D:182:ASN:ND2	1:D:216:ASN:CB	2.55	0.69
1:B:377:TRP:CZ3	1:B:500:MET:HE1	2.27	0.69
1:B:626:ASN:HA	1:B:649:VAL:HG12	1.75	0.69
1:D:668:VAL:HG13	1:D:675:GLU:OE2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG21	1:A:183:ASN:HD22	1.58	0.69
1:D:627:ILE:HG13	1:D:669:VAL:HG21	1.75	0.69
1:D:634:LEU:CB	1:D:639:LEU:HD21	2.23	0.69
1:A:474:GLY:HA2	1:A:478:LYS:O	1.93	0.68
1:A:604:LEU:HD22	1:A:669:VAL:HG12	1.74	0.68
1:B:377:TRP:HZ3	1:B:500:MET:CE	2.06	0.68
1:A:692:ILE:O	1:A:692:ILE:HG23	1.92	0.68
1:C:322:THR:HG22	1:C:355:ARG:HB3	1.74	0.68
1:C:388:GLY:HA2	1:C:426:TYR:CZ	2.28	0.68
1:C:557:ASN:O	1:C:578:GLY:HA2	1.92	0.68
1:A:689:ASN:OD1	1:A:692:ILE:HB	1.94	0.68
1:B:633:TYR:CE1	1:B:638:GLU:HB2	2.22	0.68
1:C:266:LEU:HD23	1:C:298:VAL:CG2	2.22	0.68
1:D:337:GLU:OE2	1:D:337:GLU:N	2.26	0.68
1:D:43:ASP:CB	1:D:46:ARG:NH1	2.57	0.68
1:D:471:ARG:HG3	1:D:471:ARG:NH1	2.03	0.68
1:D:182:ASN:HD21	1:D:216:ASN:CG	2.01	0.68
1:D:377:TRP:C	1:D:377:TRP:HD1	2.02	0.68
1:D:642:ILE:HB	1:D:653:PHE:HE2	1.56	0.68
1:C:180:GLU:HG3	1:C:289:ILE:HB	1.75	0.68
1:C:494:TYR:HB3	1:C:497:GLN:CG	2.24	0.68
1:D:182:ASN:HD21	1:D:216:ASN:CB	2.06	0.67
1:D:399:ARG:O	1:D:399:ARG:HG3	1.83	0.67
1:B:395:GLN:HG2	1:B:437:LEU:HD13	1.76	0.67
1:C:84:ARG:HD2	1:C:143:GLU:OE2	1.93	0.67
1:A:632:VAL:CG2	1:A:653:PHE:CE1	2.77	0.67
1:C:659:ALA:N	1:C:663:ASN:HD21	1.93	0.67
1:A:383:VAL:HG12	1:A:418:ASN:HB3	1.76	0.67
1:C:377:TRP:C	1:C:377:TRP:HD1	2.02	0.67
1:D:43:ASP:OD2	1:D:45:MET:HB3	1.93	0.67
1:A:512:HIS:CD2	1:A:527:PHE:HA	2.30	0.67
1:C:477:GLU:HG2	1:C:478:LYS:HG3	1.75	0.67
1:A:527:PHE:O	1:A:529:PRO:HD3	1.95	0.67
1:B:187:THR:HG23	1:B:187:THR:O	1.93	0.67
1:C:327:TRP:CZ2	1:C:584:ARG:HG2	2.29	0.67
1:B:108:CYS:SG	1:B:122:LYS:HG2	2.35	0.67
1:C:299:ARG:NH2	1:C:409:PRO:HA	2.09	0.67
1:D:617:ARG:O	1:D:658:LEU:HD12	1.95	0.67
1:D:635:ASN:ND2	1:D:663:ASN:HA	2.10	0.67
1:A:187:THR:O	1:A:187:THR:CG2	2.43	0.67
1:A:575:ASN:OD1	1:A:577:LYS:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:GLN:OE1	1:C:423:PRO:HA	1.94	0.66
1:A:516:TYR:OH	1:A:616:LYS:HD3	1.95	0.66
1:B:633:TYR:HE1	1:B:638:GLU:CB	2.07	0.66
1:D:634:LEU:HD12	1:D:635:ASN:N	2.11	0.66
1:A:484:LYS:HB3	1:A:485:PRO:CD	2.26	0.66
1:B:322:THR:HG22	1:B:355:ARG:HB3	1.77	0.66
1:D:560:ASP:O	1:D:582:PHE:HD1	1.76	0.66
1:B:182:ASN:N	1:B:182:ASN:HD22	1.93	0.66
1:B:506:ALA:O	1:B:533:GLN:NE2	2.26	0.66
1:B:609:ARG:HB3	1:B:609:ARG:NH2	2.11	0.66
1:B:78:GLU:OE1	1:B:161:GLN:NE2	2.29	0.66
1:B:642:ILE:HG23	1:B:642:ILE:O	1.95	0.66
1:B:668:VAL:O	1:B:669:VAL:HG23	1.95	0.66
1:A:478:LYS:HB3	1:A:482:ASP:OD2	1.95	0.65
1:B:337:GLU:H	1:B:337:GLU:CD	2.03	0.65
1:D:469:MET:HE3	1:D:499:LEU:HD11	1.77	0.65
1:A:353:THR:HA	1:A:375:ILE:O	1.97	0.65
1:B:114:ASN:ND2	1:B:143:GLU:H	1.93	0.65
1:A:203:LYS:O	1:A:264:PRO:HD2	1.97	0.65
1:B:184:ILE:HD13	1:B:292:VAL:HG13	1.79	0.65
1:B:299:ARG:HD2	1:B:299:ARG:C	2.21	0.65
1:B:634:LEU:HD22	1:B:656:VAL:CG1	2.26	0.65
1:A:618:THR:HA	1:A:656:VAL:O	1.97	0.65
1:D:619:THR:HG23	1:D:620:ALA:N	2.10	0.65
1:D:105:VAL:O	1:D:124:GLY:HA2	1.97	0.65
1:A:663:ASN:O	1:A:664:ILE:HD12	1.97	0.65
1:B:357:ALA:HB1	1:B:358:HIS:ND1	2.13	0.64
1:A:451:ASN:HD22	1:A:453:TYR:H	1.43	0.64
1:B:630:PRO:HA	1:B:669:VAL:HG22	1.72	0.64
1:A:475:TRP:CZ3	1:A:521:LEU:CD2	2.80	0.64
1:B:93:LEU:O	1:B:96:LYS:HB2	1.98	0.64
1:B:583:ASP:O	1:B:584:ARG:HB2	1.98	0.64
1:D:557:ASN:ND2	1:D:558:MET:H	1.94	0.64
1:A:133:GLY:HA2	1:A:136:LEU:CD2	2.24	0.64
1:A:689:ASN:OD1	1:A:689:ASN:O	2.16	0.64
1:C:629:THR:CG2	3:C:1:HOH:O	2.31	0.64
1:D:299:ARG:HD2	1:D:299:ARG:C	2.23	0.64
1:B:58:VAL:HG21	1:B:62:HIS:CD2	2.33	0.64
1:B:283:MET:HG2	1:B:288:VAL:HG22	1.80	0.64
1:B:563:VAL:HG21	1:B:575:ASN:HB2	1.79	0.63
1:C:327:TRP:CH2	1:C:584:ARG:HG2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:GLU:HG3	1:B:478:LYS:CG	2.27	0.63
1:D:470:ASN:OD1	1:D:503:GLU:HB2	1.98	0.63
1:D:680:ILE:HD12	1:D:682:TRP:NE1	2.13	0.63
1:C:671:THR:HG23	1:C:672:LYS:N	2.12	0.63
1:D:469:MET:HE3	1:D:499:LEU:CD1	2.28	0.63
1:D:353:THR:HA	1:D:375:ILE:O	1.99	0.63
1:B:182:ASN:N	1:B:182:ASN:ND2	2.46	0.63
1:B:631:LYS:O	1:B:667:ALA:HA	1.99	0.63
1:C:377:TRP:HZ3	1:C:500:MET:CE	2.10	0.62
1:B:422:GLN:HA	1:B:422:GLN:OE1	1.99	0.62
1:D:163:LEU:HD22	1:D:384:ASN:HB2	1.80	0.62
1:D:665:LEU:O	1:D:679:GLU:HA	1.99	0.62
1:A:626:ASN:HA	1:A:649:VAL:HG12	1.81	0.62
1:D:475:TRP:CH2	1:D:507:ASP:HB2	2.34	0.62
1:D:481:GLN:HE21	1:D:481:GLN:N	1.96	0.62
1:A:618:THR:HG22	1:A:657:SER:OG	1.99	0.62
1:B:182:ASN:HD22	1:B:182:ASN:H	1.47	0.62
1:A:642:ILE:HG23	1:A:642:ILE:O	1.97	0.62
1:B:82:TYR:CE1	1:B:147:LYS:CG	2.83	0.62
1:A:632:VAL:HG21	1:A:653:PHE:HE1	1.63	0.62
1:B:374:LEU:O	1:B:410:SER:HB2	2.00	0.62
1:B:595:LYS:HG2	1:B:603:VAL:CG2	2.24	0.62
1:B:617:ARG:CG	1:B:617:ARG:NH1	2.50	0.62
1:C:633:TYR:CE1	1:C:638:GLU:HB2	2.35	0.62
1:D:233:GLN:NE2	1:D:274:TYR:CD1	2.68	0.62
1:B:567:THR:CG2	1:B:567:THR:O	2.47	0.61
1:A:668:VAL:HG11	1:A:675:GLU:OE2	1.99	0.61
1:B:567:THR:O	1:B:567:THR:HG23	1.99	0.61
1:C:522:ASN:HD22	1:C:522:ASN:C	2.08	0.61
1:D:186:VAL:HG23	1:D:186:VAL:O	2.00	0.61
1:D:207:ASP:OD2	1:D:260:LYS:HG2	2.01	0.61
1:A:633:TYR:CD2	1:A:638:GLU:CA	2.80	0.61
1:B:299:ARG:HD2	1:B:299:ARG:O	2.00	0.61
1:B:658:LEU:CD2	1:B:663:ASN:ND2	2.64	0.61
1:C:502:THR:O	1:C:503:GLU:HG3	2.00	0.61
1:B:630:PRO:CA	1:B:669:VAL:HG21	2.28	0.61
1:B:634:LEU:HD13	1:B:665:LEU:HD21	1.81	0.61
1:A:377:TRP:CD1	1:A:377:TRP:C	2.78	0.61
1:A:512:HIS:HB2	1:A:529:PRO:HA	1.82	0.61
3:A:728:HOH:O	1:B:252:THR:HG22	2.01	0.61
1:A:451:ASN:HD22	1:A:453:TYR:N	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASN:O	1:A:578:GLY:HA2	1.99	0.61
1:D:527:PHE:CE2	1:D:529:PRO:HG3	2.35	0.61
1:D:614:ARG:HD3	1:D:682:TRP:CG	2.36	0.61
1:A:399:ARG:HH21	1:B:399:ARG:NH2	1.98	0.61
1:B:484:LYS:H	1:B:485:PRO:HD2	1.65	0.61
1:D:642:ILE:HD12	1:D:653:PHE:CZ	2.36	0.61
1:D:647:THR:C	1:D:649:VAL:H	2.08	0.61
1:B:179:THR:HG21	1:B:183:ASN:ND2	2.15	0.61
1:C:90:PRO:HG2	1:C:92:ASP:HB3	1.83	0.61
1:C:625:SER:O	1:C:649:VAL:HG22	2.01	0.60
1:A:512:HIS:HD2	1:A:528:TYR:N	1.99	0.60
1:D:607:THR:CG2	1:D:608:GLN:HG3	2.13	0.60
1:D:609:ARG:HB2	1:D:680:ILE:HG22	1.84	0.60
1:B:346:ILE:O	1:B:349:VAL:HG12	2.02	0.60
1:B:633:TYR:CE1	1:B:638:GLU:HA	2.34	0.60
1:D:43:ASP:HB3	1:D:46:ARG:NH1	2.16	0.60
1:B:37:LYS:HD2	1:B:77:TYR:CE2	2.34	0.60
1:C:516:TYR:CZ	1:C:616:LYS:HE2	2.37	0.60
1:D:182:ASN:HD22	1:D:247:LEU:HD23	1.67	0.60
1:B:689:ASN:HD21	1:B:692:ILE:HG13	1.60	0.60
1:D:78:GLU:HG3	1:D:151:LYS:HA	1.84	0.60
1:B:113:VAL:HG11	1:B:132:ILE:HB	1.83	0.60
1:B:512:HIS:CG	1:B:527:PHE:CE1	2.90	0.60
1:C:437:LEU:C	1:C:437:LEU:HD23	2.26	0.60
1:C:523:TRP:CZ3	1:C:568:ARG:NH2	2.69	0.60
1:A:284:ALA:O	1:A:285:ASP:CB	2.48	0.60
1:A:498:LYS:H	1:B:250:GLN:NE2	1.87	0.60
1:B:367:SER:O	1:B:370:ASP:HB2	2.02	0.60
1:C:538:GLU:OE2	1:C:624:TYR:OH	2.15	0.60
1:D:574:ARG:HG2	1:D:576:MET:HG3	1.84	0.59
1:A:595:LYS:HG2	1:A:603:VAL:HG21	1.84	0.59
1:B:377:TRP:CZ3	1:B:500:MET:CE	2.85	0.59
1:D:614:ARG:HD3	1:D:682:TRP:HB3	1.83	0.59
1:D:642:ILE:CB	1:D:653:PHE:CE2	2.79	0.59
1:B:30:ASN:HB3	1:B:60:ILE:HB	1.84	0.59
1:B:241:HIS:ND1	1:B:241:HIS:C	2.60	0.59
1:A:448:VAL:HG22	1:A:449:SER:N	2.17	0.59
1:B:202:SER:HG	1:B:204:LYS:HG3	1.67	0.59
1:B:494:TYR:HB3	1:B:497:GLN:CG	2.32	0.59
1:C:323:ARG:HD3	1:C:324:HIS:O	2.02	0.59
1:D:180:GLU:HG3	1:D:289:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG21	1:A:183:ASN:ND2	2.16	0.59
1:B:418:ASN:ND2	1:B:419:GLU:HG3	2.17	0.59
1:C:642:ILE:HD11	1:C:651:TYR:HB3	1.83	0.59
1:D:664:ILE:O	1:D:664:ILE:CG2	2.50	0.59
1:A:448:VAL:HG23	1:A:466:ILE:O	2.02	0.59
1:B:282:LEU:CD2	1:B:289:ILE:HD11	2.32	0.59
1:B:521:LEU:HD23	1:B:521:LEU:C	2.28	0.59
1:C:316:TYR:HD2	1:C:318:MET:HE3	1.67	0.59
1:C:563:VAL:HG21	1:C:575:ASN:HB2	1.83	0.59
1:A:82:TYR:CE1	1:A:147:LYS:HG2	2.38	0.59
1:A:521:LEU:O	1:A:522:ASN:C	2.45	0.59
1:C:484:LYS:HB3	1:C:485:PRO:HD2	1.85	0.59
1:C:571:VAL:CG2	1:C:574:ARG:HB3	2.33	0.59
1:D:182:ASN:ND2	1:D:247:LEU:HD23	2.18	0.59
1:D:664:ILE:CG1	1:D:679:GLU:OE1	2.50	0.59
1:A:417:HIS:C	1:A:417:HIS:CD2	2.80	0.59
1:C:316:TYR:CD2	1:C:318:MET:HE3	2.37	0.59
1:C:671:THR:CG2	1:C:672:LYS:N	2.65	0.59
1:A:71:VAL:HG12	1:A:71:VAL:O	2.02	0.58
1:B:187:THR:O	1:B:187:THR:CG2	2.51	0.58
1:B:512:HIS:CD2	1:B:527:PHE:HE1	2.15	0.58
1:B:617:ARG:NE	1:B:658:LEU:O	2.32	0.58
1:B:668:VAL:HA	1:B:676:TYR:O	2.03	0.58
1:C:525:LYS:CD	1:C:694:SER:HB2	2.33	0.58
1:A:114:ASN:ND2	1:A:143:GLU:H	2.02	0.58
1:A:630:PRO:HD2	1:A:642:ILE:HD11	1.85	0.58
1:D:583:ASP:O	1:D:584:ARG:HB2	2.03	0.58
1:A:515:GLU:OE1	1:A:619:THR:OG1	2.20	0.58
1:B:34:GLN:NE2	1:B:57:THR:HG22	2.15	0.58
1:B:318:MET:HE1	1:B:375:ILE:HD13	1.85	0.58
1:B:658:LEU:HD22	1:B:663:ASN:ND2	2.18	0.58
1:B:630:PRO:CB	1:B:669:VAL:CG2	2.82	0.58
1:A:346:ILE:O	1:A:349:VAL:HG12	2.04	0.58
1:B:477:GLU:HG3	1:B:478:LYS:HG2	1.84	0.58
1:D:43:ASP:HB2	1:D:46:ARG:NH1	2.16	0.58
1:D:634:LEU:HB3	1:D:639:LEU:CD2	2.33	0.58
1:D:632:VAL:HG23	1:D:653:PHE:CZ	2.38	0.58
1:C:234:GLU:CD	1:C:234:GLU:H	2.12	0.57
1:D:406:PHE:HE1	1:D:442:ASP:HB2	1.68	0.57
1:A:663:ASN:C	1:A:664:ILE:CD1	2.76	0.57
1:B:609:ARG:CG	1:B:609:ARG:NH2	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LYS:CB	1:C:492:LYS:NZ	2.66	0.57
1:D:484:LYS:HB3	1:D:485:PRO:CD	2.33	0.57
1:D:514:THR:HA	1:D:615:GLU:OE2	2.03	0.57
1:A:58:VAL:HG13	1:A:59:GLU:N	2.19	0.57
1:B:567:THR:OG1	1:B:572:PRO:HA	2.03	0.57
1:B:621:VAL:CG2	1:B:665:LEU:CD1	2.80	0.57
1:D:417:HIS:C	1:D:417:HIS:CD2	2.82	0.57
1:A:179:THR:HG23	1:A:180:GLU:N	2.18	0.57
1:B:478:LYS:HB3	1:B:482:ASP:OD2	2.05	0.57
1:A:530:GLU:CD	1:A:610:ARG:HH21	2.12	0.57
1:A:555:LEU:HD12	1:A:555:LEU:O	2.05	0.57
1:A:471:ARG:HD2	1:A:486:TRP:CZ2	2.39	0.57
1:B:456:MET:HE1	1:B:467:GLN:CG	2.27	0.57
1:B:609:ARG:HB3	1:B:609:ARG:CZ	2.35	0.57
1:B:671:THR:O	1:B:672:LYS:C	2.48	0.57
1:C:595:LYS:HG2	1:C:603:VAL:CG2	2.35	0.57
1:D:645:GLY:HA3	1:D:650:HIS:ND1	2.19	0.57
1:B:176:LEU:HD23	1:B:177:ILE:N	2.20	0.57
1:B:662:LYS:HA	1:B:683:ASN:CB	2.35	0.57
1:C:58:VAL:CG1	1:C:59:GLU:N	2.67	0.57
1:C:455:HIS:CD2	1:C:455:HIS:H	2.22	0.57
1:A:229:THR:CG2	1:A:231:TYR:CE2	2.88	0.57
1:A:296:LEU:HD12	1:A:296:LEU:C	2.29	0.57
1:A:388:GLY:HA2	1:A:426:TYR:CZ	2.40	0.57
1:B:97:ARG:HD3	1:B:180:GLU:O	2.05	0.57
1:B:417:HIS:C	1:B:417:HIS:HD2	2.13	0.57
1:B:642:ILE:O	1:B:642:ILE:CG2	2.53	0.57
1:A:72:GLN:NE2	1:A:75:SER:O	2.38	0.56
1:A:489:GLN:HE21	1:A:489:GLN:CA	2.11	0.56
1:A:677:THR:HG22	1:A:677:THR:O	2.03	0.56
1:B:179:THR:HG22	1:B:180:GLU:H	1.65	0.56
1:B:422:GLN:OE1	1:B:423:PRO:HA	2.05	0.56
1:D:182:ASN:HD21	1:D:216:ASN:HB2	1.68	0.56
1:A:216:ASN:HB2	1:A:247:LEU:HG	1.87	0.56
1:B:303:ILE:CG2	1:B:498:LYS:HD3	2.35	0.56
1:D:78:GLU:CG	1:D:151:LYS:HA	2.35	0.56
1:C:126:SER:HB3	1:C:360:GLN:OE1	2.06	0.56
1:D:356:PHE:CE2	1:D:365:LEU:HD21	2.41	0.56
1:A:179:THR:HG22	1:A:180:GLU:C	2.28	0.56
1:A:557:ASN:HD22	1:A:559:PHE:H	1.54	0.56
1:A:632:VAL:HG23	1:A:653:PHE:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ASP:OD1	1:B:576:MET:HA	2.06	0.56
1:C:478:LYS:HB3	1:C:482:ASP:OD2	2.05	0.56
1:B:114:ASN:HD21	1:B:143:GLU:H	1.51	0.56
1:B:162:ASN:ND2	1:B:565:MET:HE3	2.20	0.56
1:B:407:ASN:O	1:B:409:PRO:HD3	2.06	0.56
1:C:22:LEU:HA	1:C:291:GLU:OE2	2.04	0.56
1:C:481:GLN:HE22	1:C:519:ASP:HB3	1.71	0.56
1:D:668:VAL:CG1	1:D:675:GLU:OE2	2.54	0.56
1:A:492:LYS:HB3	1:A:492:LYS:HZ2	1.70	0.56
1:C:388:GLY:HA2	1:C:426:TYR:CE1	2.41	0.56
1:A:382:CYS:C	1:A:383:VAL:HG13	2.30	0.56
1:B:664:ILE:HD12	1:B:664:ILE:C	2.31	0.56
1:B:512:HIS:HD2	1:B:527:PHE:HE1	1.52	0.56
1:B:630:PRO:CB	1:B:669:VAL:HG23	2.36	0.56
1:D:303:ILE:O	1:D:498:LYS:NZ	2.39	0.56
1:A:179:THR:HG23	1:A:180:GLU:H	1.69	0.55
1:A:516:TYR:CZ	1:A:616:LYS:HD3	2.41	0.55
1:A:538:GLU:HA	1:A:593:TRP:CZ2	2.42	0.55
1:B:633:TYR:CE1	1:B:638:GLU:CA	2.89	0.55
1:B:677:THR:CG2	1:B:677:THR:O	2.54	0.55
1:C:89:PHE:O	1:C:139:GLY:N	2.37	0.55
1:C:525:LYS:O	1:C:527:PHE:N	2.32	0.55
1:D:137:LYS:O	1:D:140:ALA:HB3	2.06	0.55
1:A:316:TYR:HD2	1:A:318:MET:HE3	1.70	0.55
1:B:303:ILE:HG21	1:B:498:LYS:HD3	1.88	0.55
1:B:370:ASP:CG	1:B:409:PRO:HD2	2.31	0.55
1:A:642:ILE:HB	1:A:653:PHE:CE2	2.42	0.55
1:B:469:MET:HE3	1:B:499:LEU:CD1	2.37	0.55
1:C:90:PRO:C	1:C:92:ASP:N	2.61	0.55
1:D:527:PHE:O	1:D:529:PRO:HD3	2.05	0.55
1:A:179:THR:CG2	1:A:180:GLU:H	2.19	0.55
1:B:356:PHE:CZ	1:B:365:LEU:HD21	2.42	0.55
1:C:205:SER:HA	1:C:261:LEU:O	2.06	0.55
1:C:319:TYR:HB3	1:C:598:TRP:CE2	2.41	0.55
1:D:503:GLU:HG2	1:D:556:TRP:HB2	1.89	0.55
1:C:299:ARG:HD2	1:C:299:ARG:C	2.32	0.55
1:D:565:MET:HE3	1:D:565:MET:CA	2.24	0.55
1:D:647:THR:O	1:D:649:VAL:N	2.40	0.55
1:A:460:VAL:O	1:A:460:VAL:CG1	2.55	0.55
1:C:205:SER:HA	1:C:264:PRO:HD3	1.89	0.55
1:D:325:GLN:HG2	1:D:359:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLN:O	1:A:638:GLU:C	2.50	0.54
1:B:456:MET:HE3	1:B:456:MET:HA	1.89	0.54
1:C:492:LYS:NZ	1:C:492:LYS:HB3	2.22	0.54
1:D:512:HIS:CE1	1:D:527:PHE:HA	2.42	0.54
1:A:179:THR:CG2	1:A:183:ASN:HB3	2.37	0.54
1:B:100:LEU:HG	1:B:132:ILE:HD13	1.89	0.54
1:C:266:LEU:CD2	1:C:298:VAL:CG2	2.85	0.54
1:A:538:GLU:HA	1:A:593:TRP:CE2	2.42	0.54
1:C:484:LYS:HB3	1:C:485:PRO:HD3	1.88	0.54
1:D:484:LYS:HG3	1:D:543:ILE:HD12	1.88	0.54
1:A:633:TYR:CE2	1:A:638:GLU:HG3	2.43	0.54
1:A:356:PHE:CE2	1:A:365:LEU:HD21	2.41	0.54
1:B:580:ILE:HG22	1:B:581:THR:N	2.22	0.54
1:C:90:PRO:HB2	1:C:92:ASP:CB	2.36	0.54
1:C:442:ASP:OD2	1:C:445:ARG:HD2	2.07	0.54
1:A:377:TRP:C	1:A:377:TRP:HD1	2.16	0.54
1:D:78:GLU:O	1:D:78:GLU:HG2	2.08	0.54
1:A:458:HIS:ND1	1:A:459:PRO:HD2	2.22	0.54
1:B:219:LEU:N	1:B:219:LEU:HD13	2.23	0.54
1:C:299:ARG:HH21	1:C:409:PRO:HA	1.71	0.54
1:C:502:THR:O	1:C:503:GLU:CG	2.55	0.54
1:C:626:ASN:HB3	1:C:627:ILE:HG23	1.89	0.54
1:A:69:MET:HG2	1:A:564:PRO:HG2	1.89	0.54
1:D:377:TRP:HZ3	1:D:500:MET:HE2	1.70	0.54
1:C:516:TYR:OH	1:C:616:LYS:HE2	2.07	0.53
1:D:614:ARG:NH1	1:D:682:TRP:CE2	2.77	0.53
1:A:69:MET:HG2	1:A:564:PRO:CG	2.38	0.53
1:A:392:GLU:OE2	1:B:122:LYS:CE	2.56	0.53
1:A:436:ASP:OD1	1:A:436:ASP:C	2.50	0.53
1:B:484:LYS:N	1:B:485:PRO:HD2	2.23	0.53
1:C:492:LYS:HB3	1:C:492:LYS:HZ1	1.72	0.53
1:C:555:LEU:HD12	1:C:555:LEU:C	2.33	0.53
1:C:157:ILE:HD13	1:C:394:ALA:HA	1.89	0.53
1:C:216:ASN:HB2	1:C:247:LEU:HG	1.91	0.53
1:C:377:TRP:CZ3	1:C:500:MET:HE1	2.43	0.53
1:C:649:VAL:O	1:C:649:VAL:CG1	2.56	0.53
1:D:162:ASN:ND2	1:D:565:MET:HG2	2.23	0.53
1:B:626:ASN:O	1:B:627:ILE:HG23	2.08	0.53
1:B:630:PRO:HB3	1:B:669:VAL:HG21	1.89	0.53
1:B:368:ARG:O	1:B:372:LEU:HG	2.09	0.53
1:B:393:ASN:OD1	1:B:397:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ASP:OD1	1:A:576:MET:HA	2.09	0.53
1:A:654:ASP:CB	1:A:655:ASN:HD22	2.15	0.53
1:A:162:ASN:HD22	1:A:565:MET:HG2	1.73	0.53
1:B:481:GLN:H	1:B:481:GLN:NE2	2.06	0.53
1:D:484:LYS:N	1:D:485:PRO:HD2	2.24	0.53
1:A:187:THR:O	1:A:187:THR:HG23	2.08	0.53
1:A:393:ASN:HA	1:B:392:GLU:OE1	2.09	0.53
1:C:203:LYS:O	1:C:263:ASN:HA	2.08	0.53
1:A:91:HIS:CE1	1:A:139:GLY:HA3	2.43	0.52
1:A:181:GLN:HA	1:A:181:GLN:NE2	2.19	0.52
1:A:634:LEU:HD22	1:A:656:VAL:HG11	1.88	0.52
1:B:188:ASP:O	1:B:189:CYS:HB2	2.08	0.52
1:C:97:ARG:NH2	1:C:215:ASP:OD2	2.38	0.52
1:B:196:ILE:HD13	1:B:278:VAL:HG21	1.91	0.52
1:C:91:HIS:CE1	1:C:139:GLY:HA3	2.44	0.52
1:B:22:LEU:HA	1:B:291:GLU:CD	2.34	0.52
1:B:34:GLN:HG2	1:B:57:THR:HG22	1.90	0.52
1:B:116:LYS:HE2	1:B:135:ALA:HB1	1.90	0.52
1:B:406:PHE:O	1:B:445:ARG:NH1	2.37	0.52
1:C:484:LYS:CB	1:C:485:PRO:CD	2.85	0.52
1:A:617:ARG:CG	1:A:617:ARG:NH1	2.38	0.52
1:B:639:LEU:HD13	1:B:656:VAL:CG2	2.39	0.52
1:C:196:ILE:HG12	1:C:210:VAL:HG22	1.91	0.52
1:D:60:ILE:CG2	1:D:61:PRO:HA	2.39	0.52
1:D:529:PRO:O	1:D:530:GLU:C	2.50	0.52
1:D:672:LYS:O	1:D:674:LYS:N	2.42	0.52
1:C:71:VAL:HG13	1:C:71:VAL:O	2.09	0.52
1:C:565:MET:HB3	1:C:566:TRP:CD1	2.43	0.52
1:B:166:VAL:O	1:B:167:TYR:C	2.52	0.52
1:B:419:GLU:OE1	1:B:470:ASN:ND2	2.36	0.52
1:B:689:ASN:CG	1:B:692:ILE:HG13	2.35	0.52
1:C:662:LYS:HE3	1:C:681:GLU:CD	2.35	0.52
1:D:327:TRP:CZ2	1:D:584:ARG:HG2	2.44	0.52
1:A:470:ASN:CG	1:A:503:GLU:HB2	2.35	0.52
1:A:664:ILE:CD1	1:A:664:ILE:N	2.73	0.52
1:B:579:LEU:O	1:B:588:LYS:HG3	2.10	0.52
1:D:633:TYR:CD1	1:D:638:GLU:HB2	2.45	0.52
1:A:383:VAL:O	1:A:384:ASN:CB	2.58	0.52
1:A:392:GLU:OE1	1:B:393:ASN:HA	2.09	0.52
1:C:578:GLY:O	1:C:588:LYS:HD2	2.09	0.52
1:D:99:PHE:CZ	1:D:131:GLU:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:HIS:HD2	1:A:528:TYR:H	1.58	0.51
1:B:318:MET:HE1	1:B:375:ILE:HG21	1.92	0.51
1:B:604:LEU:HA	1:B:624:TYR:O	2.10	0.51
1:C:589:ASP:OD2	1:C:607:THR:HB	2.10	0.51
1:D:320:GLY:HA2	1:D:353:THR:HG23	1.93	0.51
1:A:190:ALA:HB3	1:A:404:GLN:NE2	2.25	0.51
1:B:517:LEU:HD11	1:B:531:THR:HB	1.92	0.51
1:B:639:LEU:HD13	1:B:656:VAL:HG21	1.91	0.51
1:B:655:ASN:OD1	1:B:655:ASN:N	2.44	0.51
1:C:299:ARG:HD2	1:C:299:ARG:O	2.10	0.51
1:D:367:SER:OG	1:D:408:HIS:HE1	1.93	0.51
1:D:413:VAL:HG21	1:D:448:VAL:HB	1.92	0.51
1:B:475:TRP:CZ2	1:B:507:ASP:HB2	2.46	0.51
1:C:90:PRO:C	1:C:92:ASP:H	2.17	0.51
1:C:93:LEU:HB2	1:C:138:LEU:CD2	2.39	0.51
1:C:417:HIS:CD2	1:C:417:HIS:C	2.88	0.51
1:C:525:LYS:HG2	1:C:526:PRO:CD	2.41	0.51
1:C:525:LYS:HD3	1:C:694:SER:HB2	1.92	0.51
1:D:641:GLY:O	1:D:642:ILE:C	2.52	0.51
1:D:618:THR:O	1:D:618:THR:CG2	2.52	0.51
1:D:208:ILE:HD13	1:D:208:ILE:N	2.24	0.51
1:D:377:TRP:CZ3	1:D:500:MET:HE1	2.44	0.51
1:D:430:LEU:O	1:D:434:LEU:HG	2.11	0.51
1:A:341:PHE:C	1:A:341:PHE:CD2	2.89	0.51
1:C:603:VAL:HB	1:C:626:ASN:HD22	1.76	0.51
1:A:475:TRP:CH2	1:A:507:ASP:HB2	2.46	0.51
1:B:179:THR:CG2	1:B:180:GLU:H	2.22	0.51
1:B:311:LEU:O	1:B:312:ASN:C	2.54	0.51
1:D:456:MET:HE1	1:D:499:LEU:HD12	1.92	0.51
1:A:642:ILE:O	1:A:642:ILE:CG2	2.58	0.51
1:B:267:TRP:HZ2	1:B:373:GLY:HA2	1.75	0.51
1:D:545:LYS:O	1:D:545:LYS:HG3	2.10	0.51
1:D:666:LYS:HG3	1:D:679:GLU:HB2	1.93	0.51
1:A:412:TYR:OH	1:A:500:MET:HE1	2.10	0.51
1:D:319:TYR:HB3	1:D:598:TRP:CE2	2.46	0.51
1:D:638:GLU:HG2	1:D:639:LEU:O	2.11	0.51
1:A:517:LEU:HD11	1:A:531:THR:HB	1.92	0.50
1:B:208:ILE:HD11	1:B:259:PHE:HD2	1.75	0.50
1:D:672:LYS:O	1:D:673:GLY:C	2.54	0.50
1:A:183:ASN:HB2	1:A:290:ASP:OD2	2.11	0.50
1:B:501:LEU:O	1:B:553:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ILE:HG23	1:C:551:ILE:HG12	1.93	0.50
1:D:484:LYS:HB3	1:D:485:PRO:HD3	1.93	0.50
1:B:630:PRO:HB3	1:B:669:VAL:CG2	2.42	0.50
1:A:451:ASN:ND2	1:A:453:TYR:N	2.54	0.50
1:A:630:PRO:HD2	1:A:642:ILE:CD1	2.41	0.50
1:B:34:GLN:HE21	1:B:57:THR:CG2	2.19	0.50
1:B:405:SER:HB2	1:B:414:TRP:HH2	1.76	0.50
1:A:416:LEU:HD21	1:A:435:HIS:HA	1.93	0.50
1:A:509:ASN:O	1:A:510:LEU:C	2.55	0.50
1:B:98:VAL:HG13	1:B:133:GLY:HA2	1.93	0.50
1:B:323:ARG:HD3	1:B:324:HIS:O	2.12	0.50
1:B:477:GLU:HG3	1:B:478:LYS:HG3	1.92	0.50
1:A:392:GLU:OE2	1:B:122:LYS:HE3	2.11	0.50
1:A:484:LYS:HB3	1:A:485:PRO:HD2	1.93	0.50
1:B:484:LYS:HG2	1:B:485:PRO:HD3	1.94	0.50
1:C:522:ASN:C	1:C:522:ASN:ND2	2.69	0.50
1:C:631:LYS:HG2	1:C:638:GLU:OE2	2.11	0.50
1:D:341:PHE:C	1:D:341:PHE:CD2	2.89	0.50
1:B:61:PRO:HD2	1:B:335:LYS:NZ	2.26	0.50
1:B:634:LEU:HD22	1:B:656:VAL:HG13	1.94	0.50
1:C:398:LEU:O	1:C:402:ILE:HG13	2.11	0.50
1:B:89:PHE:CD2	1:B:136:LEU:HD22	2.47	0.50
1:B:216:ASN:HB2	1:B:247:LEU:HG	1.94	0.50
1:D:303:ILE:HB	1:D:498:LYS:HZ2	1.76	0.50
1:D:627:ILE:CD1	1:D:676:TYR:CD2	2.94	0.50
1:A:357:ALA:HB1	1:A:358:HIS:ND1	2.27	0.50
1:A:629:THR:HA	1:A:651:TYR:CZ	2.47	0.50
1:B:671:THR:O	1:B:673:GLY:N	2.45	0.50
1:C:539:TYR:O	1:C:542:SER:OG	2.25	0.50
1:C:233:GLN:HB3	1:C:234:GLU:OE2	2.11	0.49
1:A:512:HIS:HD2	1:A:527:PHE:HA	1.76	0.49
1:B:473:PHE:HB3	1:B:479:LYS:O	2.11	0.49
1:A:633:TYR:HE2	1:A:638:GLU:HG3	1.77	0.49
1:B:637:GLN:O	1:B:638:GLU:C	2.54	0.49
1:C:489:GLN:HA	1:C:492:LYS:HE3	1.93	0.49
1:D:512:HIS:ND1	1:D:528:TYR:N	2.57	0.49
1:D:595:LYS:HG2	1:D:603:VAL:HG21	1.94	0.49
1:A:78:GLU:O	1:A:78:GLU:HG2	2.12	0.49
1:A:538:GLU:OE2	1:A:624:TYR:OH	2.13	0.49
1:C:266:LEU:CD2	1:C:298:VAL:HG23	2.43	0.49
1:D:377:TRP:CE3	1:D:500:MET:HE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:MET:CE	1:B:456:MET:HA	2.43	0.49
1:B:665:LEU:O	1:B:679:GLU:HA	2.13	0.49
1:D:563:VAL:O	1:D:573:ALA:HA	2.12	0.49
1:A:391:THR:OG1	1:A:430:LEU:HD13	2.12	0.49
1:A:512:HIS:CD2	1:A:528:TYR:H	2.31	0.49
1:C:198:GLN:OE1	1:C:298:VAL:HA	2.13	0.49
1:C:671:THR:CG2	1:C:672:LYS:H	2.25	0.49
1:D:406:PHE:CE1	1:D:442:ASP:HB2	2.48	0.49
1:B:233:GLN:HB3	1:B:274:TYR:CE1	2.48	0.49
1:C:299:ARG:HH21	1:C:409:PRO:C	2.21	0.49
1:D:530:GLU:OE2	1:D:610:ARG:NH2	2.45	0.49
1:D:565:MET:O	1:D:566:TRP:CD2	2.65	0.49
1:B:632:VAL:CB	1:B:653:PHE:CE1	2.96	0.49
1:D:662:LYS:O	1:D:663:ASN:ND2	2.44	0.49
1:B:266:LEU:HD23	1:B:298:VAL:HG22	1.95	0.49
1:D:403:ARG:NE	1:D:441:GLU:OE2	2.39	0.49
1:A:318:MET:HE2	1:A:318:MET:HA	1.95	0.49
1:B:294:GLN:HB3	1:B:295:PRO:HD2	1.95	0.49
1:C:97:ARG:CZ	1:C:217:ALA:HB2	2.43	0.49
1:C:155:ASP:OD1	1:C:155:ASP:N	2.45	0.49
1:B:157:ILE:CD1	1:B:381:PRO:HD2	2.38	0.48
1:B:282:LEU:HD23	1:B:289:ILE:HD11	1.95	0.48
1:B:512:HIS:HB3	1:B:527:PHE:CE1	2.48	0.48
1:C:318:MET:HE2	1:C:318:MET:HA	1.95	0.48
1:D:91:HIS:CE1	1:D:139:GLY:HA3	2.48	0.48
1:D:626:ASN:OD1	1:D:627:ILE:HG23	2.13	0.48
1:B:35:PHE:CG	1:B:36:LYS:N	2.81	0.48
1:B:97:ARG:HH21	1:B:99:PHE:HZ	1.59	0.48
1:C:232:THR:O	1:C:233:GLN:C	2.56	0.48
1:C:565:MET:HB3	1:C:566:TRP:NE1	2.28	0.48
1:D:347:MET:CE	1:D:374:LEU:CG	2.89	0.48
1:A:67:MET:O	1:A:71:VAL:HG23	2.13	0.48
1:A:383:VAL:CG1	1:A:418:ASN:HB3	2.43	0.48
1:B:357:ALA:HB1	1:B:358:HIS:CG	2.48	0.48
1:B:508:ALA:HB2	1:B:533:GLN:HB2	1.95	0.48
1:C:238:VAL:HG13	1:C:238:VAL:O	2.13	0.48
3:A:735:HOH:O	1:B:462:LEU:HA	2.13	0.48
1:B:116:LYS:CE	1:B:135:ALA:HB1	2.44	0.48
1:D:647:THR:C	1:D:649:VAL:N	2.71	0.48
1:A:121:HIS:HE1	1:A:123:GLY:O	1.96	0.48
1:A:319:TYR:HB3	1:A:598:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLY:HA3	1:A:502:THR:CG2	2.44	0.48
1:B:630:PRO:CB	1:B:669:VAL:HG21	2.44	0.48
1:C:61:PRO:HB3	1:C:171:TYR:O	2.14	0.48
1:C:475:TRP:CH2	1:C:507:ASP:HB2	2.49	0.48
1:D:565:MET:HB2	3:D:727:HOH:O	2.12	0.48
1:A:448:VAL:HG22	1:A:449:SER:H	1.79	0.48
1:B:641:GLY:O	1:B:642:ILE:C	2.55	0.48
1:A:128:PHE:HA	1:A:190:ALA:HB2	1.95	0.48
1:B:37:LYS:CG	1:B:77:TYR:CE2	2.96	0.48
1:C:58:VAL:HG13	1:C:59:GLU:N	2.29	0.48
1:D:664:ILE:O	1:D:664:ILE:HG23	2.12	0.48
1:A:101:ARG:NH2	1:A:190:ALA:O	2.32	0.48
1:B:658:LEU:HD23	1:B:663:ASN:ND2	2.29	0.48
1:D:265:HIS:HB3	1:D:274:TYR:CD2	2.49	0.48
1:D:530:GLU:OE1	1:D:610:ARG:NH2	2.46	0.48
1:A:357:ALA:HB1	1:A:358:HIS:CG	2.49	0.48
1:A:468:GLY:HA3	1:A:502:THR:HG21	1.95	0.48
1:A:632:VAL:CG2	1:A:653:PHE:CZ	2.97	0.48
1:B:22:LEU:HD12	1:B:291:GLU:OE1	2.14	0.48
1:B:403:ARG:NE	1:B:441:GLU:OE2	2.40	0.48
1:C:377:TRP:CZ3	1:C:500:MET:CE	2.95	0.48
1:A:565:MET:HB3	1:A:566:TRP:CD1	2.48	0.48
1:B:469:MET:HE3	1:B:499:LEU:HD11	1.95	0.48
1:D:574:ARG:CG	1:D:576:MET:HG3	2.43	0.48
1:D:377:TRP:CZ3	1:D:500:MET:HE2	2.47	0.47
1:B:377:TRP:HZ3	1:B:500:MET:HE3	1.79	0.47
1:B:484:LYS:CB	1:B:485:PRO:CD	2.92	0.47
1:D:299:ARG:HD2	1:D:299:ARG:O	2.13	0.47
1:D:479:LYS:HD3	1:D:519:ASP:HB2	1.95	0.47
1:A:162:ASN:ND2	1:A:565:MET:HG2	2.29	0.47
1:B:395:GLN:O	1:B:396:SER:C	2.56	0.47
1:D:317:SER:O	1:D:352:THR:OG1	2.29	0.47
1:A:229:THR:HG21	1:A:231:TYR:CE2	2.48	0.47
1:A:258:THR:HG22	1:A:258:THR:O	2.14	0.47
1:A:330:LEU:N	1:A:330:LEU:CD1	2.77	0.47
1:A:337:GLU:CD	1:A:337:GLU:H	2.20	0.47
1:A:527:PHE:O	1:A:529:PRO:CD	2.62	0.47
1:B:633:TYR:CE1	1:B:638:GLU:CB	2.90	0.47
1:C:35:PHE:CG	1:C:36:LYS:N	2.82	0.47
1:C:266:LEU:HD23	1:C:298:VAL:HG22	1.95	0.47
1:C:337:GLU:CD	1:C:337:GLU:N	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:CG	1:A:151:LYS:HA	2.31	0.47
1:A:106:GLY:HA2	1:A:107:ALA:HA	1.65	0.47
1:A:382:CYS:C	1:A:383:VAL:CG1	2.88	0.47
1:B:241:HIS:ND1	1:B:242:SER:N	2.63	0.47
1:B:654:ASP:HA	1:B:655:ASN:HA	1.56	0.47
1:C:163:LEU:HD12	1:C:163:LEU:HA	1.72	0.47
1:D:455:HIS:H	1:D:455:HIS:CD2	2.33	0.47
1:A:70:GLN:OE1	1:A:329:GLY:N	2.29	0.47
1:D:137:LYS:HE2	1:D:137:LYS:HB2	1.64	0.47
1:D:684:TYR:OH	1:D:687:GLU:HG2	2.15	0.47
1:A:84:ARG:HG3	1:A:145:ILE:HG12	1.96	0.47
1:A:330:LEU:N	1:A:330:LEU:HD13	2.30	0.47
1:B:22:LEU:HG	1:B:291:GLU:OE2	2.15	0.47
1:D:605:TYR:O	1:D:624:TYR:N	2.36	0.47
1:D:634:LEU:HB2	1:D:639:LEU:HD21	1.97	0.47
1:B:181:GLN:HB3	1:B:182:ASN:ND2	2.30	0.47
1:B:626:ASN:O	1:B:627:ILE:CG2	2.63	0.47
1:D:513:GLN:HE22	1:D:530:GLU:HB3	1.79	0.47
1:B:689:ASN:ND2	1:B:692:ILE:CG1	2.65	0.46
1:D:614:ARG:CD	1:D:682:TRP:HB3	2.45	0.46
1:B:304:VAL:O	1:B:305:ALA:C	2.57	0.46
1:C:259:PHE:N	1:C:259:PHE:CD2	2.83	0.46
1:D:614:ARG:HD3	1:D:682:TRP:CB	2.45	0.46
1:A:179:THR:HG23	1:A:183:ASN:HB3	1.96	0.46
1:B:58:VAL:CG2	1:B:62:HIS:CD2	2.97	0.46
1:B:106:GLY:HA2	1:B:107:ALA:HA	1.65	0.46
1:D:100:LEU:O	1:D:129:ALA:HA	2.16	0.46
1:D:182:ASN:ND2	1:D:216:ASN:HA	2.30	0.46
1:A:229:THR:HG21	1:A:231:TYR:CZ	2.50	0.46
1:B:299:ARG:HA	1:B:312:ASN:OD1	2.15	0.46
1:B:456:MET:CE	1:B:469:MET:CE	2.83	0.46
1:B:609:ARG:NH2	1:B:609:ARG:CB	2.77	0.46
1:B:621:VAL:HG12	1:B:653:PHE:HD1	1.80	0.46
1:B:658:LEU:HA	1:B:663:ASN:ND2	2.30	0.46
1:B:665:LEU:HD23	1:B:665:LEU:HA	1.57	0.46
1:D:92:ASP:OD1	1:D:92:ASP:N	2.49	0.46
1:A:207:ASP:OD2	1:A:260:LYS:HE3	2.16	0.46
1:B:297:GLY:H	1:B:409:PRO:HG3	1.80	0.46
1:B:303:ILE:HG23	1:B:551:ILE:HG12	1.97	0.46
1:D:513:GLN:HE22	1:D:530:GLU:CB	2.28	0.46
1:A:133:GLY:CA	1:A:136:LEU:HD23	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLY:HA2	1:B:478:LYS:O	2.16	0.46
1:D:384:ASN:C	1:D:385:ARG:HG2	2.41	0.46
1:D:591:TYR:CD1	1:D:591:TYR:C	2.93	0.46
1:A:301:TYR:CD2	1:A:412:TYR:HB2	2.51	0.46
1:B:512:HIS:HB3	1:B:527:PHE:CZ	2.50	0.46
1:C:666:LYS:HD2	1:C:679:GLU:OE1	2.16	0.46
1:A:527:PHE:C	1:A:529:PRO:HD3	2.41	0.46
1:B:617:ARG:O	1:B:617:ARG:HD3	2.15	0.46
1:D:214:LEU:O	1:D:252:THR:HG23	2.16	0.46
1:A:460:VAL:O	1:A:460:VAL:HG13	2.16	0.46
1:B:208:ILE:CD1	1:B:230:ILE:HD11	2.43	0.46
1:C:250:GLN:HB3	1:D:464:ALA:O	2.15	0.46
1:C:642:ILE:CD1	1:C:653:PHE:CE1	2.95	0.46
1:B:94:GLU:HG3	1:B:95:GLY:N	2.31	0.46
1:C:358:HIS:O	1:C:381:PRO:HA	2.16	0.46
1:D:60:ILE:HG22	1:D:61:PRO:HA	1.97	0.46
1:D:99:PHE:HB2	1:D:177:ILE:HB	1.97	0.46
1:D:320:GLY:HA2	1:D:353:THR:CG2	2.45	0.46
1:D:661:GLY:N	1:D:684:TYR:O	2.48	0.46
1:A:555:LEU:C	1:A:555:LEU:CD1	2.89	0.45
1:B:639:LEU:CD1	1:B:656:VAL:HG21	2.45	0.45
1:C:86:THR:HA	1:C:142:ASN:O	2.16	0.45
1:C:176:LEU:HD12	1:C:176:LEU:HA	1.74	0.45
1:D:501:LEU:O	1:D:553:SER:HA	2.15	0.45
1:A:203:LYS:HE3	1:A:203:LYS:HB3	1.63	0.45
1:A:399:ARG:HH21	1:B:399:ARG:HH22	1.64	0.45
1:A:512:HIS:CB	1:A:529:PRO:HA	2.46	0.45
1:B:111:VAL:CG2	1:B:118:ALA:HB3	2.45	0.45
1:C:132:ILE:HD12	1:C:136:LEU:HD21	1.97	0.45
1:A:395:GLN:HE21	1:A:433:SER:HB2	1.81	0.45
1:A:399:ARG:NH2	1:B:399:ARG:NH2	2.65	0.45
1:A:477:GLU:CG	1:A:478:LYS:CD	2.92	0.45
1:C:230:ILE:O	1:C:238:VAL:HG12	2.16	0.45
1:D:60:ILE:HA	1:D:61:PRO:C	2.42	0.45
1:A:467:GLN:O	1:A:499:LEU:HA	2.17	0.45
1:A:533:GLN:O	1:A:534:THR:C	2.60	0.45
1:B:394:ALA:O	1:B:395:GLN:C	2.59	0.45
1:B:458:HIS:CG	1:B:459:PRO:HD2	2.51	0.45
1:B:482:ASP:C	1:B:484:LYS:H	2.24	0.45
1:B:570:GLY:C	1:B:571:VAL:HG12	2.42	0.45
1:C:181:GLN:CA	1:C:181:GLN:HE21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ARG:HE	1:D:399:ARG:HB2	1.60	0.45
1:D:614:ARG:HG2	1:D:683:ASN:O	2.15	0.45
1:A:229:THR:HG22	1:A:231:TYR:CE2	2.50	0.45
1:B:203:LYS:O	1:B:263:ASN:HA	2.15	0.45
1:B:325:GLN:HG2	1:B:359:TYR:CE1	2.52	0.45
1:B:563:VAL:CG2	1:B:575:ASN:HB2	2.44	0.45
1:B:580:ILE:CG2	1:B:581:THR:N	2.80	0.45
1:B:595:LYS:O	1:B:599:SER:CB	2.65	0.45
1:D:89:PHE:O	1:D:139:GLY:N	2.50	0.45
1:D:474:GLY:HA2	1:D:479:LYS:HA	1.99	0.45
1:A:618:THR:CG2	1:A:657:SER:OG	2.65	0.45
1:A:645:GLY:HA3	1:A:650:HIS:ND1	2.31	0.45
1:B:225:THR:HA	1:B:243:ARG:O	2.17	0.45
1:B:619:THR:HG21	1:B:682:TRP:HZ3	1.81	0.45
1:D:630:PRO:CA	1:D:669:VAL:HG12	2.25	0.45
1:B:208:ILE:HD11	1:B:259:PHE:CB	2.41	0.45
1:B:512:HIS:CG	1:B:527:PHE:CD1	3.05	0.45
1:D:446:TYR:HA	1:D:465:ASP:OD2	2.16	0.45
1:A:157:ILE:HD11	1:A:381:PRO:HD2	1.98	0.45
1:A:461:ASN:HB3	1:A:467:GLN:OE1	2.17	0.45
1:A:543:ILE:HD13	1:A:543:ILE:N	2.32	0.45
1:C:267:TRP:CZ2	1:C:373:GLY:HA2	2.52	0.45
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.75	0.45
1:B:335:LYS:HB3	1:B:337:GLU:OE2	2.17	0.45
1:B:516:TYR:O	1:B:517:LEU:HD23	2.17	0.45
1:B:580:ILE:HG22	1:B:581:THR:H	1.82	0.45
1:C:501:LEU:O	1:C:553:SER:HA	2.17	0.45
1:D:94:GLU:OE1	1:D:94:GLU:CA	2.61	0.45
1:A:416:LEU:N	1:A:416:LEU:CD1	2.79	0.45
1:C:125:TYR:CG	1:C:359:TYR:HB2	2.52	0.45
1:A:327:TRP:CZ2	1:A:584:ARG:HG2	2.52	0.44
1:B:372:LEU:N	1:B:372:LEU:HD23	2.31	0.44
1:D:106:GLY:HA2	1:D:107:ALA:HA	1.59	0.44
1:A:105:VAL:O	1:A:124:GLY:HA2	2.16	0.44
1:D:528:TYR:CD2	1:D:569:GLY:HA3	2.52	0.44
1:D:627:ILE:HG13	1:D:669:VAL:CG2	2.43	0.44
1:A:439:LYS:NZ	1:A:465:ASP:OD2	2.37	0.44
1:A:517:LEU:HD21	1:A:531:THR:OG1	2.17	0.44
1:A:617:ARG:NH1	1:A:658:LEU:O	2.50	0.44
1:C:408:HIS:HA	1:C:409:PRO:HD2	1.86	0.44
1:C:565:MET:HA	1:C:565:MET:CE	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:HA	1:B:250:GLN:NE2	2.32	0.44
1:B:64:TRP:CD1	1:B:64:TRP:C	2.96	0.44
1:B:296:LEU:HD12	1:B:296:LEU:C	2.43	0.44
1:B:358:HIS:O	1:B:381:PRO:HA	2.17	0.44
1:C:106:GLY:HA2	1:C:107:ALA:HA	1.55	0.44
1:C:689:ASN:OD1	1:C:691:GLU:N	2.49	0.44
1:D:319:TYR:HB3	1:D:598:TRP:CD2	2.53	0.44
1:D:323:ARG:HA	1:D:557:ASN:HD21	1.82	0.44
1:B:88:PHE:CD2	1:B:140:ALA:O	2.71	0.44
1:B:121:HIS:CD2	1:B:128:PHE:HB3	2.52	0.44
1:B:529:PRO:O	1:B:530:GLU:C	2.59	0.44
1:C:120:THR:HG23	1:C:121:HIS:N	2.31	0.44
1:C:437:LEU:HD23	1:C:437:LEU:O	2.18	0.44
1:C:601:GLU:H	1:C:601:GLU:HG2	1.58	0.44
1:D:512:HIS:O	1:D:529:PRO:HA	2.16	0.44
1:C:46:ARG:HB2	1:C:46:ARG:NH1	2.33	0.44
1:C:353:THR:HA	1:C:375:ILE:O	2.18	0.44
1:C:484:LYS:O	1:C:488:GLU:HG3	2.17	0.44
1:D:505:GLY:HA2	1:D:537:HIS:CE1	2.52	0.44
1:B:132:ILE:O	1:B:133:GLY:C	2.61	0.44
1:B:176:LEU:HD23	1:B:176:LEU:C	2.42	0.44
1:B:580:ILE:CG2	1:B:581:THR:H	2.31	0.44
1:C:508:ALA:HB2	1:C:533:GLN:HB2	1.99	0.44
1:C:557:ASN:OD1	1:C:558:MET:N	2.50	0.44
1:D:155:ASP:HA	1:D:389:TYR:O	2.18	0.44
1:D:306:GLY:HA2	1:D:549:TYR:HA	1.99	0.44
1:A:179:THR:CG2	1:A:183:ASN:HD22	2.28	0.44
1:A:645:GLY:HA3	1:A:650:HIS:CG	2.53	0.44
1:B:111:VAL:HG23	1:B:118:ALA:HB3	1.99	0.44
1:B:456:MET:HE2	1:B:467:GLN:HG2	1.97	0.44
1:B:667:ALA:O	1:B:677:THR:HA	2.18	0.44
1:C:374:LEU:O	1:C:410:SER:HB2	2.18	0.44
1:C:416:LEU:N	1:C:416:LEU:HD23	2.32	0.44
1:A:413:VAL:HG22	1:A:414:TRP:N	2.32	0.43
1:A:592:PHE:CD2	1:A:605:TYR:CE1	3.06	0.43
1:B:512:HIS:CB	1:B:527:PHE:CE1	3.01	0.43
1:B:72:GLN:HA	1:B:572:PRO:HB2	2.00	0.43
1:B:512:HIS:C	1:B:513:GLN:HG2	2.43	0.43
1:D:320:GLY:HA2	1:D:353:THR:O	2.18	0.43
1:D:448:VAL:HG23	1:D:466:ILE:HB	2.00	0.43
1:A:188:ASP:OD1	1:A:403:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ILE:HD13	1:B:292:VAL:CG1	2.47	0.43
1:B:483:ILE:O	1:B:483:ILE:HG12	2.16	0.43
1:C:613:ASP:O	1:C:690:ARG:NH2	2.48	0.43
1:C:692:ILE:O	1:C:692:ILE:HG22	2.19	0.43
1:D:109:ALA:HA	1:D:147:LYS:O	2.18	0.43
1:A:60:ILE:CG2	1:A:61:PRO:HA	2.49	0.43
1:B:603:VAL:O	1:B:625:SER:HA	2.18	0.43
1:B:634:LEU:O	1:B:635:ASN:HB2	2.17	0.43
1:C:181:GLN:HA	1:C:181:GLN:NE2	2.33	0.43
1:C:199:LYS:HB3	1:C:207:ASP:HB2	2.00	0.43
1:D:593:TRP:HE3	1:D:624:TYR:CE2	2.36	0.43
1:A:179:THR:HG21	1:A:183:ASN:HB3	2.00	0.43
1:D:205:SER:HA	1:D:261:LEU:O	2.18	0.43
1:D:300:LYS:HE3	2:D:803:CL:CL	2.56	0.43
1:D:571:VAL:HG23	1:D:572:PRO:HD2	2.00	0.43
1:B:102:PHE:O	1:B:127:ALA:HA	2.19	0.43
1:C:525:LYS:CD	1:C:694:SER:CB	2.96	0.43
1:C:649:VAL:O	1:C:649:VAL:HG13	2.18	0.43
1:D:614:ARG:CG	1:D:682:TRP:HB3	2.48	0.43
1:A:36:LYS:HB2	1:A:55:TRP:CD2	2.54	0.43
1:A:104:GLY:HA3	1:A:172:ARG:HD2	1.99	0.43
1:A:320:GLY:CA	1:A:353:THR:HG23	2.47	0.43
1:A:619:THR:HG23	1:A:620:ALA:O	2.17	0.43
1:B:265:HIS:NE2	1:B:272:ASP:OD2	2.33	0.43
1:B:510:LEU:HD22	1:B:530:GLU:OE1	2.18	0.43
1:B:611:ASN:CG	1:B:611:ASN:O	2.59	0.43
1:B:617:ARG:HD3	1:B:617:ARG:C	2.44	0.43
1:C:214:LEU:HD12	1:C:255:TYR:CE2	2.53	0.43
1:C:377:TRP:HZ3	1:C:500:MET:HE3	1.81	0.43
1:C:563:VAL:CG2	1:C:575:ASN:HB2	2.46	0.43
1:D:84:ARG:HD2	1:D:143:GLU:OE2	2.19	0.43
1:D:208:ILE:HG12	1:D:261:LEU:HD22	2.00	0.43
1:D:530:GLU:CD	1:D:610:ARG:NH2	2.77	0.43
1:A:82:TYR:CE1	1:A:147:LYS:CG	3.01	0.43
1:B:620:ALA:HA	1:B:653:PHE:O	2.19	0.43
1:C:125:TYR:HB3	1:C:360:GLN:O	2.19	0.43
1:C:667:ALA:O	1:C:677:THR:HA	2.17	0.43
1:D:111:VAL:HG23	1:D:111:VAL:O	2.17	0.43
1:D:211:LYS:HB2	1:D:256:LEU:CD2	2.48	0.43
1:D:481:GLN:H	1:D:481:GLN:CD	2.21	0.43
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASN:HB3	1:D:69:MET:HB2	2.01	0.43
1:D:294:GLN:HB3	1:D:295:PRO:HD2	2.00	0.43
1:B:133:GLY:HA2	1:B:136:LEU:HD12	2.00	0.43
1:B:320:GLY:HA2	1:B:353:THR:O	2.19	0.43
1:B:614:ARG:HG2	1:B:682:TRP:HB3	2.01	0.43
1:C:244:SER:O	1:C:245:PHE:HB3	2.18	0.43
1:D:609:ARG:CB	1:D:680:ILE:CG2	2.97	0.43
1:D:619:THR:HG21	1:D:682:TRP:HZ3	1.84	0.43
1:A:121:HIS:CE1	1:A:123:GLY:O	2.72	0.42
1:A:383:VAL:O	1:A:383:VAL:HG23	2.19	0.42
1:A:634:LEU:O	1:A:635:ASN:C	2.62	0.42
1:B:189:CYS:O	1:B:190:ALA:HB3	2.19	0.42
1:B:471:ARG:HB2	1:B:501:LEU:HD11	2.01	0.42
1:C:487:VAL:HG13	1:C:488:GLU:N	2.34	0.42
1:D:56:GLU:HG2	1:D:58:VAL:HG23	2.01	0.42
1:D:97:ARG:HH21	1:D:131:GLU:CD	2.26	0.42
1:D:153:ARG:HB2	1:D:155:ASP:OD1	2.18	0.42
1:D:672:LYS:C	1:D:674:LYS:N	2.76	0.42
1:A:93:LEU:O	1:A:96:LYS:HB2	2.18	0.42
1:A:103:GLU:HB2	1:A:172:ARG:HB3	2.01	0.42
1:B:468:GLY:HA2	1:B:500:MET:O	2.19	0.42
1:B:664:ILE:HD12	1:B:665:LEU:N	2.34	0.42
1:C:44:PRO:O	1:C:45:MET:C	2.62	0.42
1:C:492:LYS:CB	1:C:492:LYS:HZ1	2.28	0.42
1:D:90:PRO:HB2	1:D:92:ASP:OD1	2.18	0.42
1:D:330:LEU:HD12	1:D:330:LEU:HA	1.64	0.42
1:D:475:TRP:CZ3	1:D:521:LEU:HD22	2.54	0.42
1:D:684:TYR:CD2	1:D:685:SER:CA	3.01	0.42
1:A:187:THR:O	1:A:187:THR:HG22	2.20	0.42
1:A:383:VAL:O	1:A:384:ASN:HB3	2.19	0.42
1:A:642:ILE:HD12	1:A:653:PHE:CZ	2.54	0.42
1:C:545:LYS:O	1:C:545:LYS:HG3	2.17	0.42
1:D:533:GLN:O	1:D:534:THR:C	2.63	0.42
1:D:560:ASP:HB2	1:D:582:PHE:HB2	2.00	0.42
1:D:565:MET:CB	3:D:727:HOH:O	2.66	0.42
1:A:691:GLU:C	1:A:693:ASP:H	2.27	0.42
1:B:24:ARG:HH21	1:B:290:ASP:CG	2.25	0.42
1:C:120:THR:CG2	1:C:121:HIS:N	2.79	0.42
1:C:377:TRP:CD1	1:C:377:TRP:O	2.72	0.42
1:C:603:VAL:CB	1:C:626:ASN:HD22	2.32	0.42
1:A:392:GLU:OE2	1:B:122:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:O	1:A:442:ASP:CG	2.63	0.42
1:B:631:LYS:HB2	1:B:668:VAL:HG13	2.02	0.42
1:B:634:LEU:HD11	1:B:663:ASN:HB3	2.01	0.42
1:C:484:LYS:O	1:C:487:VAL:HG12	2.19	0.42
1:C:525:LYS:HG2	1:C:526:PRO:HD2	2.02	0.42
1:D:207:ASP:C	1:D:208:ILE:HD13	2.44	0.42
1:D:662:LYS:HG3	1:D:663:ASN:N	2.34	0.42
1:A:133:GLY:C	1:A:135:ALA:H	2.27	0.42
1:A:377:TRP:CH2	1:A:448:VAL:HG11	2.55	0.42
1:A:633:TYR:HD2	1:A:638:GLU:N	2.18	0.42
1:B:205:SER:HB2	1:B:261:LEU:O	2.20	0.42
1:B:387:THR:N	1:B:390:GLU:OE2	2.40	0.42
1:B:574:ARG:HG3	1:B:576:MET:HG3	2.01	0.42
1:C:202:SER:O	1:C:203:LYS:C	2.63	0.42
1:D:299:ARG:C	1:D:299:ARG:CD	2.92	0.42
1:D:471:ARG:HA	1:D:471:ARG:NE	2.34	0.42
1:D:555:LEU:C	1:D:555:LEU:HD12	2.45	0.42
1:B:60:ILE:N	1:B:60:ILE:HD13	2.33	0.42
1:B:152:ALA:HB1	1:B:159:VAL:O	2.20	0.42
1:B:671:THR:C	1:B:673:GLY:N	2.75	0.42
1:C:370:ASP:CG	1:C:409:PRO:HD2	2.45	0.42
1:D:216:ASN:HB3	1:D:248:SER:O	2.20	0.42
1:A:40:PHE:HA	1:A:50:GLN:HE22	1.84	0.42
1:A:509:ASN:O	1:A:511:ALA:N	2.52	0.42
1:B:40:PHE:O	1:B:41:ALA:C	2.63	0.42
1:B:388:GLY:HA2	1:B:426:TYR:CZ	2.54	0.42
1:B:557:ASN:O	1:B:578:GLY:HA2	2.19	0.42
1:B:658:LEU:CA	1:B:663:ASN:HD21	2.33	0.42
1:D:612:ALA:O	1:D:683:ASN:HB2	2.20	0.42
1:B:61:PRO:HD2	1:B:335:LYS:HZ3	1.83	0.42
1:B:125:TYR:CG	1:B:359:TYR:HB2	2.55	0.42
1:B:151:LYS:HZ2	1:B:151:LYS:HG3	1.70	0.42
1:B:203:LYS:O	1:B:264:PRO:HD2	2.19	0.42
1:C:299:ARG:HH21	1:C:409:PRO:CA	2.32	0.42
1:D:325:GLN:HB2	3:D:714:HOH:O	2.18	0.42
1:A:654:ASP:HA	1:A:655:ASN:HA	1.81	0.42
1:B:157:ILE:HG13	1:B:397:GLN:NE2	2.35	0.42
1:B:182:ASN:HA	1:B:215:ASP:O	2.19	0.42
1:D:684:TYR:HD2	1:D:685:SER:CA	2.32	0.42
1:A:280:CYS:O	1:A:291:GLU:HA	2.20	0.41
1:A:353:THR:HG23	1:A:554:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:O	1:B:71:VAL:HG12	2.20	0.41
1:D:357:ALA:HB1	1:D:358:HIS:CG	2.55	0.41
1:B:116:LYS:HE3	1:B:116:LYS:HB2	1.61	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.83	0.41
1:B:229:THR:CG2	1:B:230:ILE:N	2.83	0.41
1:C:47:ALA:O	1:C:48:ALA:C	2.63	0.41
1:C:447:THR:O	1:C:465:ASP:HB2	2.20	0.41
1:D:63:THR:O	1:D:63:THR:HG23	2.19	0.41
1:D:311:LEU:O	1:D:312:ASN:C	2.63	0.41
1:D:565:MET:C	1:D:566:TRP:CG	2.97	0.41
1:A:403:ARG:NE	1:A:441:GLU:OE2	2.48	0.41
1:B:205:SER:HG	1:B:260:LYS:HE3	1.81	0.41
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.82	0.41
1:B:592:PHE:O	1:B:593:TRP:C	2.61	0.41
1:C:525:LYS:HD2	1:C:694:SER:CB	2.50	0.41
1:C:642:ILE:CD1	1:C:653:PHE:CZ	2.84	0.41
1:D:261:LEU:HD12	1:D:261:LEU:HA	1.78	0.41
1:D:538:GLU:OE2	1:D:624:TYR:OH	2.33	0.41
1:A:357:ALA:HA	1:A:358:HIS:HA	1.86	0.41
1:B:82:TYR:CZ	1:B:147:LYS:HG2	2.55	0.41
1:B:626:ASN:C	1:B:627:ILE:HG23	2.45	0.41
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.90	0.41
1:C:618:THR:HA	1:C:656:VAL:O	2.20	0.41
1:D:617:ARG:HA	1:D:684:TYR:CE1	2.56	0.41
1:A:113:VAL:O	1:A:114:ASN:C	2.64	0.41
1:A:583:ASP:O	1:A:584:ARG:HB2	2.20	0.41
1:A:606:LEU:HD12	1:A:678:ASP:O	2.20	0.41
1:B:633:TYR:CD1	1:B:638:GLU:N	2.88	0.41
1:B:658:LEU:HD22	1:B:663:ASN:CG	2.46	0.41
1:D:460:VAL:O	1:D:460:VAL:HG13	2.21	0.41
1:A:47:ALA:HA	1:A:50:GLN:HE21	1.85	0.41
1:A:481:GLN:N	1:A:481:GLN:CD	2.79	0.41
1:A:484:LYS:CB	1:A:485:PRO:CD	2.93	0.41
1:B:635:ASN:OD1	1:B:663:ASN:HA	2.20	0.41
1:C:447:THR:H	1:C:465:ASP:HB2	1.86	0.41
1:C:475:TRP:CZ2	1:C:507:ASP:HB2	2.55	0.41
1:A:179:THR:HG22	1:A:180:GLU:CA	2.51	0.41
1:A:668:VAL:CG1	1:A:675:GLU:OE2	2.68	0.41
1:B:533:GLN:O	1:B:536:THR:HB	2.20	0.41
1:C:232:THR:O	1:C:235:GLY:N	2.49	0.41
1:C:377:TRP:HD1	1:C:377:TRP:O	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ASN:ND2	1:D:558:MET:N	2.52	0.41
1:A:320:GLY:HA2	1:A:353:THR:HG23	2.02	0.41
1:B:243:ARG:HG2	1:B:244:SER:N	2.35	0.41
1:B:415:GLY:HA2	1:B:448:VAL:HG13	2.03	0.41
1:B:538:GLU:HA	1:B:593:TRP:CZ2	2.56	0.41
1:B:579:LEU:HD12	1:B:579:LEU:HA	1.76	0.41
1:B:634:LEU:HD22	1:B:656:VAL:HG11	1.99	0.41
1:C:181:GLN:HE21	1:C:181:GLN:HA	1.85	0.41
1:C:475:TRP:CZ3	1:C:521:LEU:HD22	2.55	0.41
1:C:516:TYR:CZ	1:C:616:LYS:CE	3.02	0.41
1:D:355:ARG:HG3	1:D:377:TRP:CD2	2.55	0.41
1:A:346:ILE:HG23	1:A:351:ALA:HB3	2.02	0.41
1:A:513:GLN:O	1:A:514:THR:HB	2.20	0.41
1:A:514:THR:O	1:A:531:THR:HG21	2.20	0.41
1:A:594:TYR:O	1:A:595:LYS:C	2.60	0.41
1:B:37:LYS:CD	1:B:77:TYR:CE2	3.02	0.41
1:B:357:ALA:HB1	1:B:358:HIS:CE1	2.56	0.41
1:B:357:ALA:HA	1:B:358:HIS:HA	1.82	0.41
1:B:508:ALA:HB1	1:B:530:GLU:HA	2.03	0.41
1:B:575:ASN:OD1	1:B:577:LYS:HG3	2.21	0.41
1:B:658:LEU:HA	1:B:663:ASN:HD21	1.85	0.41
1:C:481:GLN:HA	1:C:539:TYR:CE1	2.56	0.41
1:D:59:GLU:O	1:D:62:HIS:HB2	2.21	0.41
1:D:122:LYS:HE3	1:D:122:LYS:HB2	1.84	0.41
1:D:132:ILE:O	1:D:133:GLY:C	2.63	0.41
1:D:619:THR:HG23	1:D:620:ALA:O	2.21	0.41
1:D:630:PRO:HA	1:D:669:VAL:HG13	1.89	0.41
1:C:668:VAL:HA	1:C:676:TYR:O	2.21	0.41
1:D:413:VAL:HG22	1:D:414:TRP:N	2.36	0.41
1:D:574:ARG:HG2	1:D:576:MET:CG	2.51	0.41
1:A:65:ASN:HA	1:A:68:ASP:OD1	2.21	0.40
1:A:521:LEU:HG	1:A:522:ASN:O	2.21	0.40
1:A:634:LEU:CD2	1:A:656:VAL:CG1	2.94	0.40
1:C:247:LEU:HD12	1:C:248:SER:N	2.36	0.40
1:C:306:GLY:HA2	1:C:549:TYR:HA	2.03	0.40
1:C:583:ASP:O	1:C:584:ARG:CB	2.49	0.40
1:D:184:ILE:O	1:D:185:THR:C	2.63	0.40
1:D:307:LYS:HE3	1:D:307:LYS:HB3	1.81	0.40
1:D:325:GLN:HG2	1:D:359:TYR:HE1	1.84	0.40
1:D:356:PHE:HB3	1:D:361:GLN:NE2	2.35	0.40
1:D:479:LYS:O	1:D:480:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLN:HA	1:A:539:TYR:CE1	2.56	0.40
1:A:665:LEU:O	1:A:679:GLU:HA	2.22	0.40
1:B:219:LEU:N	1:B:219:LEU:CD1	2.83	0.40
1:B:417:HIS:CD2	1:B:417:HIS:O	2.74	0.40
1:C:125:TYR:O	1:C:360:GLN:HB3	2.21	0.40
1:C:284:ALA:O	1:C:285:ASP:HB2	2.21	0.40
1:C:497:GLN:H	1:C:497:GLN:HG2	1.75	0.40
1:D:353:THR:HG23	1:D:554:TYR:CE1	2.56	0.40
1:D:458:HIS:CG	1:D:459:PRO:HD2	2.57	0.40
1:A:37:LYS:HG2	1:A:38:GLY:O	2.21	0.40
1:A:100:LEU:O	1:A:129:ALA:HA	2.21	0.40
1:B:327:TRP:CZ3	1:B:338:HIS:HD2	2.40	0.40
1:B:408:HIS:HB2	1:B:411:ILE:HD12	2.02	0.40
1:C:189:CYS:O	1:C:190:ALA:C	2.63	0.40
1:C:490:LEU:HD12	1:C:490:LEU:HA	1.90	0.40
1:C:549:TYR:O	1:C:551:ILE:HD12	2.22	0.40
1:D:76:PHE:CE2	1:D:564:PRO:HB2	2.57	0.40
1:D:408:HIS:HA	1:D:409:PRO:HD2	1.93	0.40
1:D:411:ILE:HG21	1:D:414:TRP:CH2	2.57	0.40
1:A:448:VAL:CG2	1:A:449:SER:N	2.83	0.40
1:A:614:ARG:NH2	1:A:682:TRP:CE2	2.89	0.40
1:A:629:THR:HA	1:A:630:PRO:HD3	1.95	0.40
1:B:283:MET:HG2	1:B:288:VAL:HA	2.04	0.40
1:C:166:VAL:O	1:C:167:TYR:C	2.64	0.40
1:C:377:TRP:CH2	1:C:448:VAL:HG11	2.56	0.40
1:D:302:GLU:HG2	1:D:303:ILE:N	2.37	0.40
1:D:518:GLY:O	1:D:535:LYS:NZ	2.54	0.40
1:D:538:GLU:HA	1:D:593:TRP:CZ2	2.57	0.40
1:A:303:ILE:CG2	1:A:498:LYS:HD3	2.52	0.40
1:A:604:LEU:HA	1:A:624:TYR:O	2.22	0.40
1:C:84:ARG:CD	1:C:143:GLU:OE2	2.66	0.40
1:C:555:LEU:HD12	1:C:555:LEU:O	2.21	0.40
1:C:607:THR:O	1:C:608:GLN:HB2	2.22	0.40
1:D:82:TYR:CZ	1:D:147:LYS:HG2	2.57	0.40
1:D:357:ALA:HA	1:D:358:HIS:HA	1.85	0.40
1:D:666:LYS:HA	1:D:678:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	670/692 (97%)	617 (92%)	50 (8%)	3 (0%)	30	54
1	B	670/692 (97%)	613 (92%)	51 (8%)	6 (1%)	14	35
1	C	671/692 (97%)	626 (93%)	44 (7%)	1 (0%)	48	73
1	D	664/692 (96%)	620 (93%)	40 (6%)	4 (1%)	21	44
All	All	2675/2768 (97%)	2476 (93%)	185 (7%)	14 (0%)	24	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	C	238	VAL
1	A	692	ILE
1	B	627	ILE
1	B	638	GLU
1	B	672	LYS
1	B	685	SER
1	D	648	ASP
1	D	673	GLY
1	B	636	GLY
1	B	689	ASN
1	D	133	GLY
1	A	528	TYR
1	D	642	ILE

5.3.2 Protein sidechains [i](#)

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	570/591 (96%)	513 (90%)	57 (10%)	7	19
1	B	564/591 (95%)	489 (87%)	75 (13%)	4	10
1	C	571/591 (97%)	522 (91%)	49 (9%)	10	25
1	D	564/591 (95%)	512 (91%)	52 (9%)	8	22
All	All	2269/2364 (96%)	2036 (90%)	233 (10%)	7	18

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	58	VAL
1	A	78	GLU
1	A	86	THR
1	A	96	LYS
1	A	111	VAL
1	A	120	THR
1	A	130	CYS
1	A	138	LEU
1	A	147	LYS
1	A	163	LEU
1	A	179	THR
1	A	181	GLN
1	A	187	THR
1	A	194	VAL
1	A	197	THR
1	A	199	LYS
1	A	243	ARG
1	A	258	THR
1	A	260	LYS
1	A	261	LEU
1	A	271	LYS
1	A	277	LYS
1	A	285	ASP
1	A	291	GLU
1	A	300	LYS
1	A	314	GLU
1	A	330	LEU
1	A	337	GLU
1	A	374	LEU
1	A	377	TRP
1	A	399	ARG
1	A	416	LEU

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Mol	Chain	Res	Type
1	A	417	HIS
1	A	451	ASN
1	A	460	VAL
1	A	471	ARG
1	A	481	GLN
1	A	492	LYS
1	A	497	GLN
1	A	499	LEU
1	A	521	LEU
1	A	543	ILE
1	A	600	GLU
1	A	609	ARG
1	A	616	LYS
1	A	617	ARG
1	A	619	THR
1	A	643	ARG
1	A	652	VAL
1	A	658	LEU
1	A	663	ASN
1	A	664	ILE
1	A	666	LYS
1	A	674	LYS
1	A	677	THR
1	A	692	ILE
1	B	22	LEU
1	B	31	THR
1	B	42	THR
1	B	43	ASP
1	B	49	SER
1	B	52	ASP
1	B	60	ILE
1	B	67	MET
1	B	86	THR
1	B	93	LEU
1	B	94	GLU
1	B	98	VAL
1	B	111	VAL
1	B	113	VAL
1	B	116	LYS
1	B	130	CYS
1	B	147	LYS
1	B	151	LYS

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Mol	Chain	Res	Type
1	B	153	ARG
1	B	163	LEU
1	B	176	LEU
1	B	181	GLN
1	B	182	ASN
1	B	186	VAL
1	B	187	THR
1	B	194	VAL
1	B	199	LYS
1	B	204	LYS
1	B	207	ASP
1	B	208	ILE
1	B	219	LEU
1	B	241	HIS
1	B	242	SER
1	B	252	THR
1	B	257	SER
1	B	261	LEU
1	B	289	ILE
1	B	292	VAL
1	B	293	VAL
1	B	298	VAL
1	B	307	LYS
1	B	330	LEU
1	B	335	LYS
1	B	337	GLU
1	B	362	SER
1	B	374	LEU
1	B	377	TRP
1	B	416	LEU
1	B	417	HIS
1	B	419	GLU
1	B	436	ASP
1	B	456	MET
1	B	481	GLN
1	B	484	LYS
1	B	499	LEU
1	B	567	THR
1	B	571	VAL
1	B	577	LYS
1	B	579	LEU
1	B	586	THR

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Mol	Chain	Res	Type
1	B	601	GLU
1	B	609	ARG
1	B	617	ARG
1	B	621	VAL
1	B	622	THR
1	B	629	THR
1	B	637	GLN
1	B	654	ASP
1	B	655	ASN
1	B	657	SER
1	B	662	LYS
1	B	664	ILE
1	B	669	VAL
1	B	677	THR
1	B	685	SER
1	C	31	THR
1	C	42	THR
1	C	56	GLU
1	C	57	THR
1	C	58	VAL
1	C	63	THR
1	C	71	VAL
1	C	72	GLN
1	C	86	THR
1	C	120	THR
1	C	163	LEU
1	C	182	ASN
1	C	186	VAL
1	C	187	THR
1	C	208	ILE
1	C	211	LYS
1	C	234	GLU
1	C	238	VAL
1	C	252	THR
1	C	259	PHE
1	C	261	LEU
1	C	277	LYS
1	C	292	VAL
1	C	293	VAL
1	C	298	VAL
1	C	299	ARG
1	C	314	GLU

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Mol	Chain	Res	Type
1	C	337	GLU
1	C	374	LEU
1	C	377	TRP
1	C	390	GLU
1	C	417	HIS
1	C	483	ILE
1	C	490	LEU
1	C	492	LYS
1	C	500	MET
1	C	525	LYS
1	C	565	MET
1	C	571	VAL
1	C	601	GLU
1	C	629	THR
1	C	649	VAL
1	C	664	ILE
1	C	670	SER
1	C	671	THR
1	C	677	THR
1	C	688	LYS
1	C	691	GLU
1	C	694	SER
1	D	22	LEU
1	D	31	THR
1	D	57	THR
1	D	58	VAL
1	D	86	THR
1	D	94	GLU
1	D	113	VAL
1	D	130	CYS
1	D	137	LYS
1	D	147	LYS
1	D	153	ARG
1	D	163	LEU
1	D	181	GLN
1	D	186	VAL
1	D	204	LYS
1	D	211	LYS
1	D	260	LYS
1	D	261	LEU
1	D	293	VAL
1	D	299	ARG

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Mol	Chain	Res	Type
1	D	314	GLU
1	D	330	LEU
1	D	337	GLU
1	D	349	VAL
1	D	374	LEU
1	D	377	TRP
1	D	390	GLU
1	D	399	ARG
1	D	416	LEU
1	D	460	VAL
1	D	471	ARG
1	D	481	GLN
1	D	490	LEU
1	D	514	THR
1	D	557	ASN
1	D	565	MET
1	D	571	VAL
1	D	579	LEU
1	D	590	SER
1	D	601	GLU
1	D	606	LEU
1	D	619	THR
1	D	621	VAL
1	D	625	SER
1	D	632	VAL
1	D	634	LEU
1	D	649	VAL
1	D	662	LYS
1	D	663	ASN
1	D	666	LYS
1	D	677	THR
1	D	684	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	91	HIS
1	A	114	ASN
1	A	121	HIS
1	A	162	ASN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	228	ASN
1	A	253	GLN
1	A	263	ASN
1	A	336	ASN
1	A	451	ASN
1	A	481	GLN
1	A	489	GLN
1	A	512	HIS
1	A	547	HIS
1	A	557	ASN
1	A	597	ASN
1	A	637	GLN
1	A	644	ASN
1	A	655	ASN
1	B	34	GLN
1	B	50	GLN
1	B	114	ASN
1	B	121	HIS
1	B	162	ASN
1	B	181	GLN
1	B	182	ASN
1	B	183	ASN
1	B	250	GLN
1	B	253	GLN
1	B	336	ASN
1	B	455	HIS
1	B	467	GLN
1	B	481	GLN
1	B	489	GLN
1	B	637	GLN
1	B	644	ASN
1	B	663	ASN
1	C	91	HIS
1	C	121	HIS
1	C	162	ASN
1	C	181	GLN
1	C	182	ASN
1	C	228	ASN
1	C	336	ASN
1	C	455	HIS
1	C	463	ASN

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Mol	Chain	Res	Type
1	C	481	GLN
1	C	522	ASN
1	C	597	ASN
1	C	626	ASN
1	C	663	ASN
1	D	91	HIS
1	D	162	ASN
1	D	182	ASN
1	D	233	GLN
1	D	236	GLN
1	D	253	GLN
1	D	263	ASN
1	D	336	ASN
1	D	455	HIS
1	D	481	GLN
1	D	513	GLN
1	D	533	GLN
1	D	557	ASN
1	D	635	ASN
1	D	655	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 ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	672/692 (97%)	-0.12	5 (0%) 84 83	23, 36, 61, 81	0
1	B	672/692 (97%)	0.03	4 (0%) 85 85	22, 40, 62, 87	0
1	C	673/692 (97%)	-0.24	5 (0%) 84 83	22, 36, 53, 72	0
1	D	666/692 (96%)	-0.19	2 (0%) 90 89	21, 36, 61, 77	0
All	All	2683/2768 (96%)	-0.13	16 (0%) 85 85	21, 37, 60, 87	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	694	SER	3.0
1	C	524	GLY	2.8
1	B	693	ASP	2.8
1	C	523	TRP	2.6
1	B	690	ARG	2.4
1	D	686	GLY	2.4
1	A	568	ARG	2.4
1	A	683	ASN	2.3
1	A	693	ASP	2.3
1	B	67	MET	2.3
1	C	59	GLU	2.2
1	A	67	MET	2.2
1	A	692	ILE	2.2
1	C	671	THR	2.1
1	B	42	THR	2.0
1	D	566	TRP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	807	1/1	0.82	0.29	78,78,78,78	0
2	CL	D	804	1/1	0.87	0.29	74,74,74,74	0
2	CL	A	802	1/1	0.95	0.26	50,50,50,50	0
2	CL	D	803	1/1	0.96	0.26	56,56,56,56	0
2	CL	C	805	1/1	0.96	0.29	59,59,59,59	0
2	CL	D	806	1/1	0.97	0.19	48,48,48,48	0
2	CL	A	801	1/1	0.98	0.23	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.