



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:27 AM UTC

PDB ID : 1K25 / pdb_00001k25
Title : PBP2x from a Highly Penicillin-resistant *Streptococcus pneumoniae* Clinical Isolate
Authors : Dessen, A.; Mouz, N.; Hopkins, J.; Dideberg, O.
Deposited on : 2001-09-26
Resolution : 3.20 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

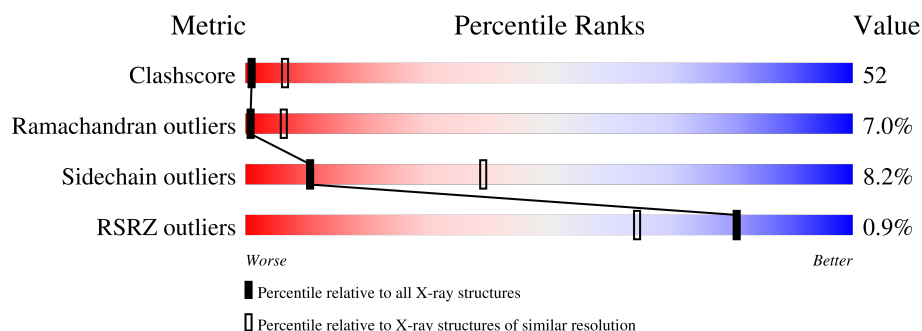
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	685	% 25% 45% 10% • 19%
1	B	685	% 25% 50% 9% 16%
1	C	685	28% 41% 11% • 20%
1	D	685	% 27% 42% 11% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16786 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 low-affinity PENICILLIN-BINDING PROTEIN 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4161	2606	691	849	15			
1	B	575	Total	C	N	O	S	0	0	0
			4311	2710	716	868	17			
1	C	550	Total	C	N	O	S	0	0	0
			4114	2580	685	834	15			
1	D	556	Total	C	N	O	S	0	0	0
			4179	2627	692	844	16			

There are 4 discrepancies between the modelled and reference sequences:

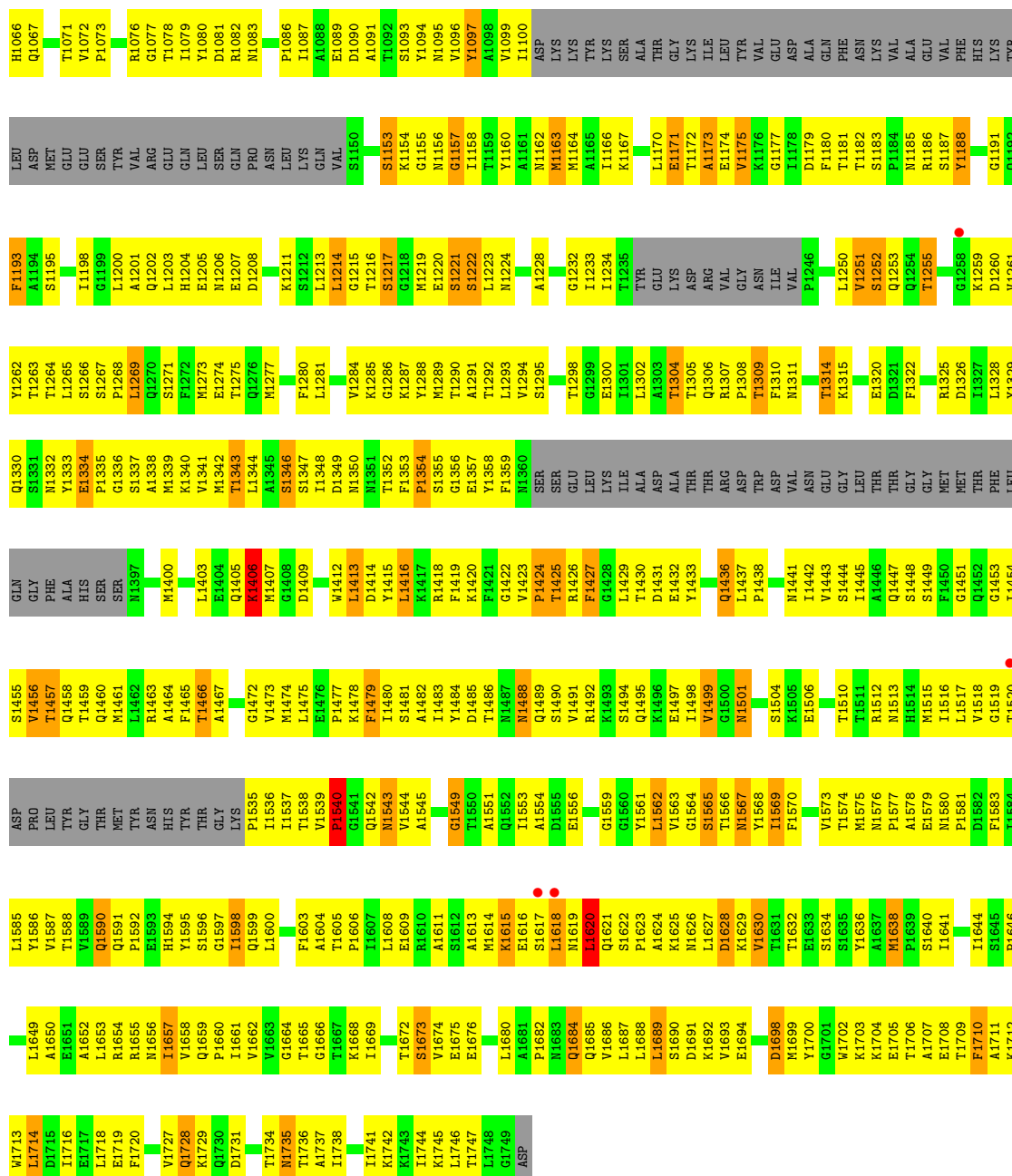
Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	PHE	engineered mutation	UNP O34006
B	1364	LEU	PHE	engineered mutation	UNP O34006
C	2364	LEU	PHE	engineered mutation	UNP O34006
D	3364	LEU	PHE	engineered mutation	UNP O34006

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	10	Total	O	0	0
			10	10		
2	C	2	Total	O	0	0
			2	2		
2	D	1	Total	O	0	0
			1	1		

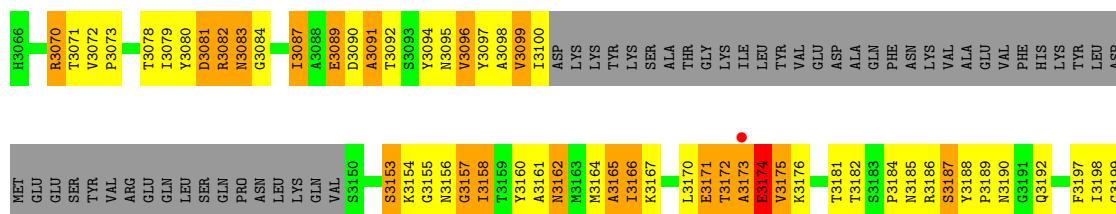
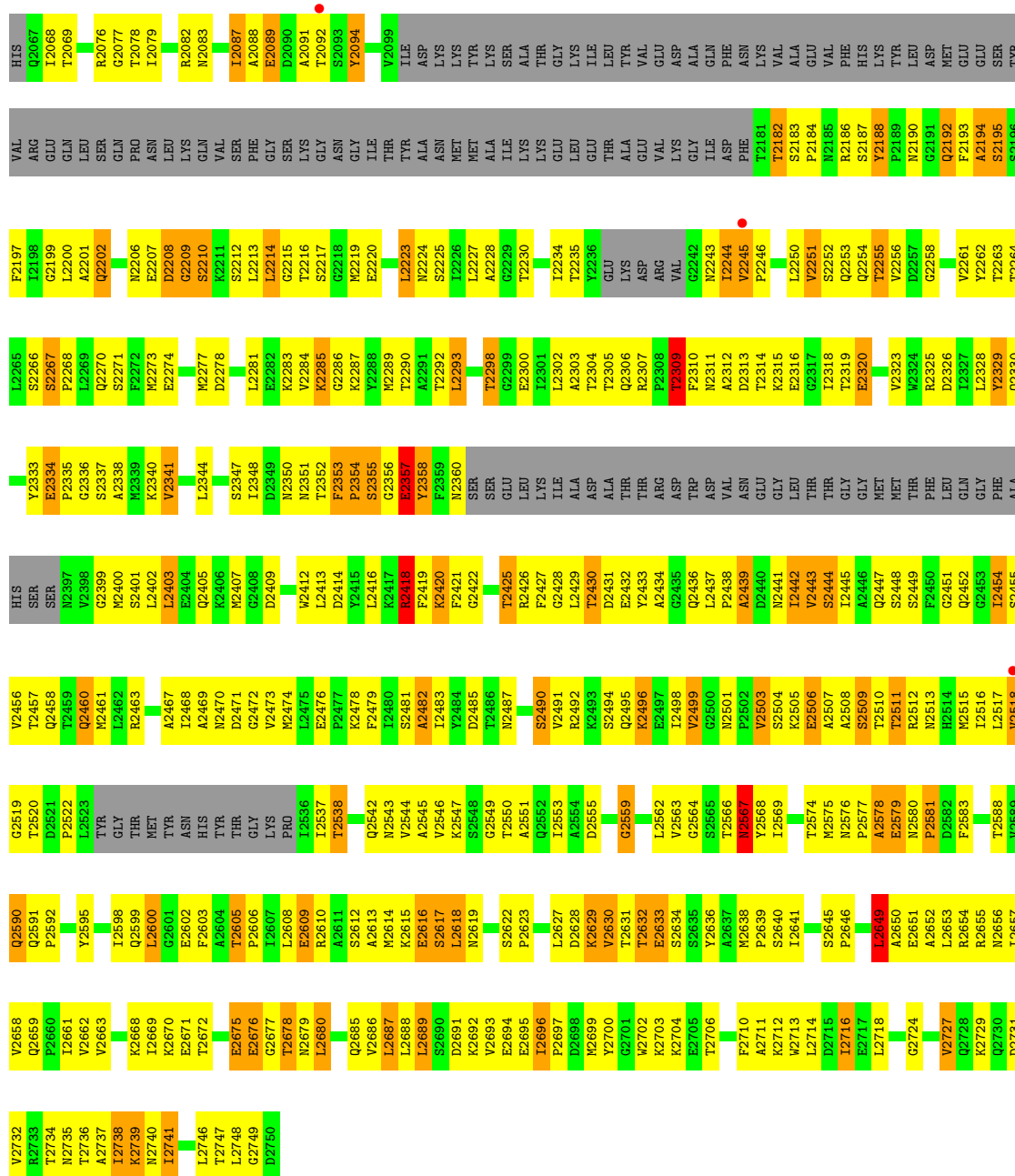


• Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X



• Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.56Å 146.56Å 132.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (19.90-3.20) 88.6 (19.90-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.23Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.312 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.148 for h,-h-k,-l 0.147 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	16786	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	0/4229	1.18	46/5747 (0.8%)
1	B	0.57	0/4383	1.12	29/5951 (0.5%)
1	C	0.61	0/4182	1.15	42/5684 (0.7%)
1	D	0.59	1/4248 (0.0%)	1.16	43/5766 (0.7%)
All	All	0.60	1/17042 (0.0%)	1.15	160/23148 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3219	MET	SD-CE	-5.74	1.65	1.79

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	VAL	N-CA-C	13.80	138.05	109.34
1	A	630	VAL	CB-CA-C	-10.76	93.64	111.29
1	D	3434	ALA	N-CA-C	10.64	122.57	110.97
1	B	1580	ASN	CA-C-N	10.47	132.93	119.84
1	B	1580	ASN	C-N-CA	10.47	132.93	119.84
1	C	2334	GLU	CA-C-N	10.36	132.79	119.84
1	C	2334	GLU	C-N-CA	10.36	132.79	119.84
1	A	309	THR	CB-CA-C	-9.71	102.27	114.40
1	C	2460	GLN	N-CA-C	-9.50	100.48	111.03
1	D	3280	PHE	N-CA-C	-9.24	101.78	113.23
1	D	3338	ALA	N-CA-C	-8.94	101.48	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	GLU	CA-C-N	8.46	130.41	119.84
1	A	334	GLU	C-N-CA	8.46	130.41	119.84
1	B	1673	SER	N-CA-C	-8.26	103.22	113.38
1	C	2357	GLU	N-CA-C	-8.20	102.84	112.92
1	C	2309	THR	CB-CA-C	-8.15	104.54	116.53
1	B	1334	GLU	CA-C-N	8.08	129.94	119.84
1	B	1334	GLU	C-N-CA	8.08	129.94	119.84
1	C	2228	ALA	N-CA-C	7.99	124.56	111.37
1	C	2358	TYR	N-CA-C	-7.95	103.18	113.12
1	D	3406	LYS	N-CA-C	-7.91	102.61	111.07
1	B	1188	TYR	CA-C-N	7.85	127.57	119.56
1	B	1188	TYR	C-N-CA	7.85	127.57	119.56
1	D	3081	ASP	N-CA-C	-7.83	98.93	110.52
1	C	2538	THR	N-CA-C	7.74	120.36	107.20
1	A	649	LEU	N-CA-C	-7.62	102.55	112.68
1	A	360	ASN	N-CA-C	-7.44	103.15	112.90
1	D	3604	ALA	N-CA-C	7.36	119.00	110.97
1	A	403	LEU	N-CA-C	-7.35	103.27	111.28
1	D	3096	VAL	N-CA-C	7.14	119.73	108.87
1	A	357	GLU	N-CA-C	-7.08	102.76	111.40
1	C	2425	THR	N-CA-C	-7.05	103.53	111.07
1	D	3504	SER	N-CA-C	7.04	120.43	110.50
1	A	87	ILE	N-CA-C	-7.03	106.07	111.62
1	A	580	ASN	CA-C-N	7.02	127.01	119.78
1	A	580	ASN	C-N-CA	7.02	127.01	119.78
1	D	3582	ASP	N-CA-C	-6.97	105.40	114.04
1	D	3166	ILE	N-CA-C	-6.93	101.92	111.89
1	D	3423	VAL	CA-C-N	6.86	128.41	119.84
1	D	3423	VAL	C-N-CA	6.86	128.41	119.84
1	A	451	GLY	N-CA-C	6.80	123.10	114.25
1	D	3197	PHE	N-CA-C	-6.73	103.87	111.07
1	A	356	GLY	N-CA-C	-6.71	106.90	115.42
1	C	2087	ILE	N-CA-C	-6.68	106.51	112.12
1	B	1549	GLY	N-CA-C	6.59	121.08	112.25
1	D	3698	ASP	N-CA-C	-6.48	98.62	108.67
1	D	3516	ILE	N-CA-C	-6.45	104.04	110.62
1	A	632	THR	N-CA-C	-6.41	97.16	110.80
1	D	3334	GLU	CA-C-N	6.32	127.74	119.84
1	D	3334	GLU	C-N-CA	6.32	127.74	119.84
1	A	597	GLY	N-CA-C	-6.31	105.16	112.73
1	A	581	PRO	N-CA-C	6.28	121.19	111.21
1	B	1261	VAL	CB-CA-C	-6.25	104.48	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ASN	N-CA-C	-6.25	104.70	113.20
1	C	2309	THR	CA-C-O	6.23	122.26	118.33
1	D	3451	GLY	N-CA-C	6.23	123.96	115.30
1	C	2418	ARG	N-CA-C	-6.21	103.23	111.24
1	C	2696	ILE	CA-C-N	-6.21	112.08	119.84
1	C	2696	ILE	C-N-CA	-6.21	112.08	119.84
1	C	2309	THR	N-CA-C	6.20	114.71	108.75
1	B	1543	ASN	N-CA-C	-6.16	99.61	109.96
1	C	2183	SER	CA-C-N	6.14	125.90	119.76
1	C	2183	SER	C-N-CA	6.14	125.90	119.76
1	B	1710	PHE	N-CA-C	-6.13	104.22	111.03
1	C	2420	LYS	N-CA-C	6.10	120.05	112.24
1	D	3580	ASN	CA-C-N	6.10	127.47	119.84
1	D	3580	ASN	C-N-CA	6.10	127.47	119.84
1	B	1698	ASP	N-CA-C	-6.09	101.27	110.28
1	B	1416	LEU	N-CA-C	-6.08	103.39	111.24
1	B	1544	VAL	N-CA-C	6.08	116.95	107.28
1	C	2738	ILE	N-CA-C	6.07	116.24	110.53
1	B	1457	THR	N-CA-C	-6.07	101.48	110.46
1	D	3435	GLY	N-CA-C	-6.07	103.83	112.81
1	A	435	GLY	N-CA-C	-6.05	101.68	112.58
1	B	1423	VAL	CA-C-N	6.04	127.39	119.84
1	B	1423	VAL	C-N-CA	6.04	127.39	119.84
1	A	416	LEU	N-CA-C	-6.03	104.39	110.97
1	B	1598	ILE	N-CA-C	-6.02	105.85	111.45
1	A	626	ASN	N-CA-C	-5.99	104.66	111.07
1	B	1423	VAL	N-CA-C	5.99	114.48	107.77
1	D	3089	GLU	N-CA-C	5.97	117.66	109.18
1	A	591	GLN	CA-C-N	5.96	126.46	120.14
1	A	591	GLN	C-N-CA	5.96	126.46	120.14
1	D	3296	ALA	N-CA-C	5.96	117.47	110.97
1	C	2089	GLU	N-CA-C	5.95	117.82	108.96
1	C	2261	VAL	N-CA-C	5.90	117.16	107.24
1	A	740	ASN	N-CA-C	5.90	119.74	111.30
1	C	2617	SER	N-CA-C	-5.89	98.25	110.80
1	C	2403	LEU	N-CA-C	-5.89	104.21	111.33
1	C	2083	ASN	N-CA-C	5.84	119.97	112.26
1	A	640	SER	N-CA-C	-5.83	102.02	110.24
1	A	590	GLN	N-CA-C	5.83	119.32	109.76
1	B	1171	GLU	N-CA-C	-5.80	104.32	111.75
1	B	1436	GLN	N-CA-C	5.80	118.67	108.75
1	D	3087	ILE	N-CA-C	-5.76	107.07	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3230	THR	N-CA-C	5.73	117.75	108.41
1	C	2341	VAL	N-CA-C	-5.68	104.82	110.62
1	C	2650	ALA	N-CA-C	-5.63	104.15	111.02
1	A	583	PHE	N-CA-C	5.59	118.74	109.46
1	D	3176	LYS	N-CA-C	5.58	117.50	108.34
1	A	401	SER	N-CA-C	-5.58	105.20	112.23
1	D	3557	LYS	N-CA-C	5.58	117.83	111.02
1	A	713	TRP	N-CA-C	5.55	118.85	111.75
1	A	699	MET	N-CA-C	5.52	120.70	113.30
1	A	89	GLU	N-CA-C	5.50	117.34	109.14
1	C	2094	TYR	N-CA-C	5.43	117.27	108.26
1	D	3463	ARG	N-CA-C	-5.43	105.26	111.07
1	C	2188	TYR	CA-C-N	5.43	126.62	119.84
1	C	2188	TYR	C-N-CA	5.43	126.62	119.84
1	B	1504	SER	N-CA-C	5.40	118.12	110.50
1	A	425	THR	N-CA-C	-5.38	105.49	111.36
1	A	630	VAL	CA-C-N	5.38	131.82	121.54
1	A	630	VAL	C-N-CA	5.38	131.82	121.54
1	B	1089	GLU	N-CA-C	5.38	118.04	109.81
1	A	414	ASP	N-CA-C	-5.38	105.11	110.97
1	C	2442	ILE	N-CA-C	5.38	115.52	110.30
1	A	227	LEU	N-CA-C	5.37	117.22	111.36
1	D	3419	PHE	N-CA-C	-5.37	106.71	113.20
1	A	423	VAL	CA-C-N	5.36	125.35	119.89
1	A	423	VAL	C-N-CA	5.36	125.35	119.89
1	B	1501	ASN	CA-C-N	5.31	124.76	119.24
1	B	1501	ASN	C-N-CA	5.31	124.76	119.24
1	C	2503	VAL	N-CA-C	5.30	116.29	108.45
1	D	3187	SER	N-CA-C	5.28	117.99	108.48
1	C	2187	SER	N-CA-C	5.28	117.50	108.90
1	C	2087	ILE	CB-CA-C	-5.27	105.74	110.91
1	D	3479	PHE	N-CA-C	-5.27	108.11	114.75
1	D	3598	ILE	N-CA-C	-5.27	105.57	110.53
1	D	3431	ASP	N-CA-C	5.27	118.71	111.54
1	C	2649	LEU	N-CA-C	-5.25	105.23	111.69
1	D	3189	PRO	N-CA-C	5.24	120.47	114.03
1	B	1499	VAL	N-CA-C	5.23	117.24	112.43
1	D	3673	SER	N-CA-C	-5.23	106.75	113.23
1	A	226	ILE	CB-CA-C	-5.22	105.29	111.97
1	A	83	ASN	N-CA-C	5.21	120.78	113.02
1	B	1590	GLN	N-CA-C	5.20	117.00	108.52
1	D	3165	ALA	N-CA-C	-5.19	106.64	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2274	GLU	N-CA-C	-5.16	105.54	111.07
1	B	1406	LYS	N-CA-C	-5.16	105.28	112.45
1	A	733	ARG	N-CA-C	5.16	117.77	110.50
1	C	2609	GLU	N-CA-C	-5.16	105.57	111.14
1	A	188	TYR	CA-C-N	5.16	126.29	119.84
1	A	188	TYR	C-N-CA	5.16	126.29	119.84
1	C	2590	GLN	N-CA-C	5.16	118.02	109.46
1	D	3458	GLN	N-CA-C	-5.16	107.16	113.50
1	B	1087	ILE	N-CA-C	-5.14	107.80	112.12
1	C	2605	THR	N-CA-C	5.12	121.14	109.81
1	A	442	ILE	N-CA-C	5.09	115.31	110.42
1	D	3513	ASN	N-CA-C	-5.08	105.64	111.07
1	C	2482	ALA	N-CA-C	5.07	115.03	107.88
1	D	3274	GLU	N-CA-C	-5.07	105.64	111.07
1	D	3469	ALA	N-CA-C	-5.06	105.95	112.68
1	C	2416	LEU	N-CA-C	-5.06	104.85	111.02
1	D	3445	ILE	N-CA-C	-5.05	104.67	111.44
1	C	2192	GLN	N-CA-C	-5.03	101.39	109.39
1	A	608	LEU	N-CA-C	-5.01	105.92	112.23
1	D	3174	GLU	N-CA-C	5.01	121.47	110.80
1	C	2414	ASP	N-CA-C	-5.00	105.47	111.03
1	D	3227	LEU	N-CA-C	5.00	119.66	113.50
1	A	598	ILE	CB-CA-C	-5.00	105.57	111.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2329	TYR	Sidechain

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	4161	0	4017	452	0
1	B	4311	0	4182	469	0
1	C	4114	0	3962	409	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4179	0	4052	396	0
2	A	8	0	0	1	0
2	B	10	0	0	5	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	16786	0	16213	1715	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 52.

All (1715) 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:A:629:LYS:O	1:A:630:VAL:HG13	1.43	1.18
1:A:618:LEU:HD23	1:A:618:LEU:H	1.04	1.11
1:D:3672:THR:HG22	1:D:3674:VAL:H	1.07	1.09
1:D:3590:GLN:HG2	1:D:3591:GLN:HG3	1.35	1.08
1:C:2714:LEU:HD13	1:C:2738:ILE:HD11	1.34	1.04
1:B:1515:MET:HE2	1:B:1545:ALA:HB1	1.43	1.01
1:C:2649:LEU:O	1:C:2653:LEU:HD12	1.61	0.99
1:A:276:GLN:HG3	1:A:607:ILE:HD11	1.41	0.99
1:D:3092:THR:HG22	1:D:3184:PRO:HA	1.45	0.99
1:A:551:ALA:HB3	1:A:569:ILE:HB	1.41	0.98
1:B:1232:GLY:HA3	1:B:1255:THR:HG22	1.44	0.98
1:A:402:LEU:HA	1:A:405:GLN:HB2	1.44	0.96
1:A:426:ARG:HB3	1:A:651:GLU:HG2	1.48	0.95
1:A:396:SER:HB3	1:A:400:MET:HG2	1.46	0.94
1:C:2629:LYS:HE3	1:C:2631:THR:N	1.82	0.94
1:D:3420:LYS:HD2	1:D:3474:MET:HE1	1.45	0.94
1:A:729:LYS:HB3	1:A:747:THR:HB	1.48	0.93
1:C:2069:THR:HG22	1:C:2235:THR:HG22	1.50	0.93
1:D:3684:GLN:HG2	1:D:3685:GLN:H	1.35	0.92
1:D:3693:VAL:HG11	1:D:3714:LEU:HD11	1.51	0.92
1:A:618:LEU:H	1:A:618:LEU:CD2	1.82	0.91
1:A:517:LEU:HA	1:A:520:THR:HB	1.50	0.91
1:D:3332:ASN:HD22	1:D:3332:ASN:N	1.69	0.91
1:A:501:ASN:C	1:A:501:ASN:HD22	1.79	0.90
1:A:629:LYS:O	1:A:630:VAL:CG1	2.19	0.90
1:A:633:GLU:HG2	1:A:682:PRO:HG2	1.54	0.90
1:B:1563:VAL:HG22	1:B:1564:GLY:H	1.36	0.90
1:A:618:LEU:HD23	1:A:618:LEU:N	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1284:VAL:CG1	1:B:1592:PRO:HB2	2.00	0.89
1:B:1618:LEU:H	1:B:1618:LEU:HD23	1.34	0.89
1:C:2714:LEU:HB2	1:C:2716:ILE:HD12	1.55	0.89
1:B:1264:THR:OG1	1:B:1479:PHE:HA	1.73	0.89
1:A:675:GLU:H	1:A:675:GLU:CD	1.81	0.88
1:C:2354:PRO:HB2	1:C:2358:TYR:CE2	2.07	0.88
1:B:1699:MET:HE3	1:B:1746:LEU:HD21	1.52	0.88
1:A:658:VAL:HG21	1:A:680:LEU:HD23	1.54	0.88
1:C:2251:VAL:O	1:C:2253:GLN:N	2.07	0.88
1:B:1619:ASN:O	1:B:1621:GLN:N	2.07	0.87
1:C:2492:ARG:HB3	1:C:2657:ILE:HD12	1.56	0.87
1:C:2661:ILE:HD13	1:C:2702:TRP:NE1	1.89	0.87
1:C:2491:VAL:HG12	1:C:2492:ARG:N	1.89	0.87
1:C:2283:LYS:HD3	1:C:2599:GLN:HG3	1.56	0.86
1:B:1698:ASP:HA	1:B:1734:THR:HG22	1.56	0.86
1:C:2290:THR:HG21	1:C:2458:GLN:OE1	1.75	0.86
1:B:1425:THR:HG23	1:B:1432:GLU:OE2	1.75	0.86
1:B:1337:SER:HB2	1:B:1549:GLY:HA2	1.56	0.86
1:C:2491:VAL:HG12	1:C:2492:ARG:H	1.39	0.86
1:D:3398:VAL:O	1:D:3402:LEU:HG	1.75	0.85
1:B:1332:ASN:HD21	1:B:1433:TYR:HD2	1.20	0.85
1:B:1344:LEU:HD12	1:B:1344:LEU:O	1.77	0.84
1:D:3672:THR:HG22	1:D:3674:VAL:N	1.91	0.84
1:B:1673:SER:HB3	1:B:1687:LEU:H	1.43	0.84
1:A:457:THR:OG1	1:A:460:GLN:HG3	1.78	0.84
1:B:1699:MET:CE	1:B:1746:LEU:HD21	2.07	0.84
1:B:1076:ARG:HD3	1:B:1186:ARG:CZ	2.06	0.84
1:A:422:GLY:HA3	1:A:437:LEU:CD2	2.08	0.83
1:B:1286:GLY:HA2	1:B:1592:PRO:HA	1.60	0.83
1:D:3462:LEU:O	1:D:3466:THR:HG23	1.77	0.83
1:C:2646:PRO:HG3	1:C:2669:ILE:HG12	1.58	0.83
1:A:245:VAL:HB	1:A:246:PRO:CD	2.09	0.82
1:B:1662:VAL:HG22	1:B:1688:LEU:HD12	1.59	0.82
1:D:3443:VAL:O	1:D:3447:GLN:HG3	1.79	0.82
1:C:2517:LEU:C	1:C:2519:GLY:H	1.84	0.82
1:C:2344:LEU:HG	1:C:2511:THR:HG23	1.60	0.82
1:B:1516:ILE:HG21	1:B:1543:ASN:HB3	1.60	0.82
1:B:1573:VAL:HG22	1:B:1586:TYR:HD1	1.43	0.82
1:A:696:ILE:HD11	1:A:744:ILE:HD13	1.62	0.81
1:C:2264:THR:OG1	1:C:2479:PHE:HA	1.80	0.81
1:D:3472:GLY:HA3	1:D:3503:VAL:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3340:LYS:HB3	1:D:3400:MET:HE2	1.62	0.81
1:A:517:LEU:C	1:A:519:GLY:H	1.86	0.81
1:B:1542:GLN:NE2	1:B:1577:PRO:HG3	1.95	0.81
1:C:2516:ILE:HD13	1:C:2543:ASN:HB3	1.62	0.81
1:A:491:VAL:HG12	1:A:492:ARG:N	1.94	0.81
1:B:1095:ASN:HD22	1:B:1156:ASN:HA	1.45	0.81
1:A:69:THR:HG22	1:A:235:THR:HB	1.63	0.81
1:D:3070:ARG:HB3	1:D:3070:ARG:HH11	1.45	0.81
1:C:2517:LEU:HA	1:C:2520:THR:HB	1.62	0.81
1:A:193:PHE:C	1:A:195:SER:H	1.89	0.80
1:B:1413:LEU:HA	1:B:1416:LEU:HD12	1.64	0.80
1:B:1661:ILE:HD11	1:B:1685:GLN:NE2	1.95	0.80
1:B:1618:LEU:H	1:B:1618:LEU:CD2	1.94	0.80
1:D:3095:ASN:HB2	1:D:3181:THR:OG1	1.82	0.80
1:B:1273:MET:SD	1:B:1305:THR:HG22	2.21	0.80
1:A:552:GLN:HB3	1:A:561:TYR:HD1	1.47	0.79
1:A:694:GLU:O	1:A:695:GLU:HG2	1.81	0.79
1:A:343:THR:HB	1:A:400:MET:CE	2.12	0.79
1:D:3644:ILE:HD11	1:D:3649:LEU:N	1.96	0.79
1:A:91:ALA:HB3	1:A:185:ASN:HB3	1.65	0.79
1:A:491:VAL:HG12	1:A:492:ARG:H	1.44	0.79
1:C:2201:ALA:HA	1:C:2214:LEU:O	1.81	0.79
1:B:1615:LYS:CA	1:B:1618:LEU:HD21	2.12	0.79
1:D:3166:ILE:O	1:D:3170:LEU:HB2	1.83	0.79
1:C:2227:LEU:O	1:C:2258:GLY:HA3	1.82	0.79
1:B:1710:PHE:CZ	1:B:1714:LEU:HD12	2.18	0.78
1:C:2687:LEU:HD12	1:C:2713:TRP:HZ3	1.47	0.78
1:D:3698:ASP:HA	1:D:3734:THR:HG22	1.65	0.78
1:A:737:ALA:O	1:A:741:ILE:HD11	1.83	0.78
1:B:1672:THR:HG22	1:B:1674:VAL:H	1.47	0.78
1:D:3343:THR:HG22	1:D:3412:TRP:CH2	2.19	0.78
1:B:1741:ILE:HG22	1:B:1741:ILE:O	1.83	0.78
1:B:1519:GLY:HA2	1:B:1535:PRO:HG2	1.66	0.78
1:B:1646:PRO:HG3	1:B:1669:ILE:HG12	1.66	0.78
1:D:3646:PRO:HG3	1:D:3669:ILE:HG12	1.64	0.77
1:A:337:SER:OG	1:A:549:GLY:HA3	1.84	0.77
1:B:1307:ARG:HD3	1:B:1309:THR:OG1	1.84	0.77
1:D:3070:ARG:HB3	1:D:3070:ARG:NH1	1.99	0.77
1:D:3638:MET:HG2	1:D:3674:VAL:HG12	1.66	0.77
1:B:1269:LEU:HD21	1:B:1611:ALA:HB2	1.66	0.77
1:B:1640:SER:HA	1:B:1676:GLU:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2714:LEU:HD13	1:C:2738:ILE:CD1	2.14	0.77
1:D:3281:LEU:HA	1:D:3289:MET:HE2	1.64	0.77
1:A:76:ARG:HE	1:A:186:ARG:NH2	1.83	0.77
1:A:193:PHE:O	1:A:195:SER:N	2.18	0.77
1:A:290:THR:HB	1:A:588:THR:OG1	1.85	0.76
1:B:1573:VAL:HG22	1:B:1586:TYR:CD1	2.20	0.76
1:B:1674:VAL:HG21	1:B:1686:VAL:HG22	1.67	0.76
1:C:2542:GLN:CD	1:C:2577:PRO:HB3	2.10	0.76
1:C:2069:THR:HG22	1:C:2235:THR:CG2	2.15	0.76
1:D:3511:THR:O	1:D:3515:MET:HG3	1.84	0.76
1:D:3563:VAL:HG22	1:D:3564:GLY:H	1.51	0.76
1:A:396:SER:OG	1:A:400:MET:N	2.16	0.76
1:A:649:LEU:HD13	1:A:688:LEU:HD11	1.66	0.76
1:C:2653:LEU:HB3	1:C:2658:VAL:HB	1.68	0.76
1:C:2629:LYS:HE3	1:C:2631:THR:H	1.47	0.76
1:D:3545:ALA:HB3	1:D:3575:MET:HB2	1.68	0.76
1:C:2590:GLN:HG2	1:C:2591:GLN:HG3	1.68	0.75
1:D:3551:ALA:HB3	1:D:3569:ILE:HB	1.69	0.75
1:A:344:LEU:HD11	1:A:348:ILE:HD11	1.68	0.75
1:C:2340:LYS:HG2	1:C:2400:MET:HG3	1.67	0.75
1:C:2576:ASN:OD1	1:C:2608:LEU:HD22	1.86	0.75
1:A:738:ILE:HA	1:A:741:ILE:HD13	1.69	0.75
1:C:2675:GLU:H	1:C:2675:GLU:CD	1.92	0.75
1:D:3516:ILE:HG21	1:D:3543:ASN:HB3	1.69	0.75
1:A:727:VAL:HG11	1:A:746:LEU:HD22	1.66	0.75
1:D:3343:THR:OG1	1:D:3400:MET:HE3	1.86	0.75
1:A:579:GLU:H	1:A:579:GLU:CD	1.95	0.75
1:B:1563:VAL:HG22	1:B:1564:GLY:N	2.01	0.74
1:B:1618:LEU:HD23	1:B:1618:LEU:N	2.02	0.74
1:B:1414:ASP:HB2	2:B:6:HOH:O	1.86	0.74
1:B:1340:LYS:HA	1:B:1343:THR:OG1	1.86	0.74
1:D:3684:GLN:HG2	1:D:3685:GLN:N	2.00	0.74
1:D:3741:ILE:CD1	1:D:3741:ILE:H	2.00	0.74
1:A:552:GLN:HB3	1:A:561:TYR:CD1	2.22	0.74
1:B:1465:PHE:CZ	1:B:1573:VAL:HG21	2.22	0.74
1:C:2716:ILE:HD13	1:C:2716:ILE:N	2.03	0.74
1:A:68:ILE:O	1:A:235:THR:HA	1.88	0.74
1:D:3284:VAL:HG13	1:D:3594:HIS:O	1.88	0.74
1:A:259:LYS:HB3	1:A:484:TYR:O	1.88	0.74
1:A:633:GLU:HG2	1:A:682:PRO:CG	2.18	0.74
1:C:2491:VAL:CG1	1:C:2492:ARG:H	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2737:ALA:O	1:C:2741:ILE:HD13	1.88	0.73
1:D:3413:LEU:HD23	1:D:3416:LEU:HD12	1.69	0.73
1:B:1638:MET:HB2	1:B:1680:LEU:HD13	1.71	0.73
1:B:1727:VAL:O	1:B:1728:GLN:HG2	1.88	0.73
1:A:223:LEU:HD21	1:A:480:ILE:HD11	1.70	0.73
1:C:2293:LEU:HD23	1:C:2302:LEU:HB2	1.71	0.73
1:A:625:LYS:O	1:A:628:ASP:HB2	1.87	0.73
1:C:2578:ALA:O	1:C:2581:PRO:HD3	1.89	0.73
1:C:2670:LYS:O	1:C:2671:GLU:HG3	1.89	0.73
1:D:3306:GLN:O	1:D:3307:ARG:HD3	1.88	0.72
1:D:3354:PRO:HB2	1:D:3359:PHE:CE1	2.25	0.72
1:C:2663:VAL:HG11	1:C:2710:PHE:HE1	1.53	0.72
1:A:79:ILE:O	1:A:87:ILE:HB	1.90	0.72
1:C:2201:ALA:HB2	1:C:2220:GLU:HG2	1.70	0.72
1:C:2649:LEU:HD13	1:C:2653:LEU:HD11	1.70	0.72
1:A:422:GLY:HA3	1:A:437:LEU:HD21	1.71	0.72
1:D:3488:ASN:HD22	1:D:3488:ASN:C	1.97	0.72
1:D:3339:MET:HE1	1:D:3421:PHE:CE2	2.25	0.72
1:D:3343:THR:HG22	1:D:3412:TRP:CZ2	2.24	0.72
1:B:1095:ASN:HB2	1:B:1181:THR:OG1	1.90	0.72
1:D:3222:SER:OG	1:D:3430:THR:HG23	1.90	0.72
1:C:2457:THR:OG1	1:C:2460:GLN:HG3	1.90	0.71
1:D:3680:LEU:HD21	1:D:3686:VAL:HG21	1.72	0.71
1:A:347:SER:HA	1:A:407:MET:HE2	1.72	0.71
1:A:396:SER:HG	1:A:400:MET:H	1.38	0.71
1:D:3250:LEU:HG	1:D:3251:VAL:H	1.54	0.71
1:A:615:LYS:O	1:A:618:LEU:HG	1.90	0.71
1:D:3078:THR:HG22	1:D:3089:GLU:HA	1.72	0.71
1:D:3603:PHE:O	1:D:3606:PRO:HD2	1.90	0.71
1:B:1222:SER:OG	1:B:1430:THR:HG23	1.91	0.71
1:D:3663:VAL:HB	1:D:3689:LEU:HA	1.73	0.71
1:A:716:ILE:HD13	1:A:716:ILE:H	1.56	0.71
1:B:1251:VAL:HG23	1:B:1252:SER:N	2.06	0.71
1:C:2273:MET:SD	1:C:2305:THR:HG22	2.31	0.71
1:C:2421:PHE:O	1:C:2437:LEU:HD21	1.90	0.71
1:C:2202:GLN:NE2	1:C:2216:THR:HG21	2.05	0.71
1:C:2555:ASP:HB3	1:C:2559:GLY:O	1.91	0.71
1:C:2649:LEU:CD1	1:C:2688:LEU:HD11	2.21	0.70
1:B:1095:ASN:ND2	1:B:1156:ASN:HA	2.05	0.70
1:D:3318:ILE:O	1:D:3318:ILE:HG22	1.89	0.70
1:C:2617:SER:O	1:C:2618:LEU:C	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG21	1:B:1204:HIS:NE2	2.06	0.70
1:A:728:GLN:OE1	1:A:749:GLY:HA3	1.92	0.70
1:A:251:VAL:CB	1:B:1214:LEU:HD21	2.21	0.70
1:A:576:ASN:OD1	1:A:608:LEU:HD22	1.91	0.70
1:B:1413:LEU:HD23	1:B:1416:LEU:HD12	1.74	0.70
1:B:1516:ILE:CG2	1:B:1543:ASN:HB3	2.22	0.70
1:C:2254:GLN:O	1:C:2256:VAL:HG23	1.92	0.70
1:C:2661:ILE:HD13	1:C:2702:TRP:HE1	1.56	0.70
1:C:2729:LYS:HB3	1:C:2747:THR:HB	1.73	0.70
1:D:3284:VAL:CG1	1:D:3592:PRO:HB2	2.22	0.70
1:C:2566:THR:O	1:C:2568:TYR:N	2.23	0.70
1:D:3710:PHE:CZ	1:D:3714:LEU:HD12	2.27	0.70
1:B:1545:ALA:HB3	1:B:1575:MET:HB2	1.74	0.70
1:C:2649:LEU:HD13	1:C:2653:LEU:CD1	2.22	0.70
1:C:2649:LEU:HD12	1:C:2688:LEU:HD11	1.74	0.70
1:D:3096:VAL:HG12	1:D:3155:GLY:HA2	1.74	0.70
1:A:251:VAL:O	1:A:253:GLN:N	2.24	0.69
1:B:1071:THR:O	1:B:1073:PRO:HD3	1.91	0.69
1:B:1334:GLU:HG2	1:B:1454:ILE:O	1.91	0.69
1:C:2448:SER:HA	1:C:2452:GLN:O	1.92	0.69
1:C:2580:ASN:C	1:C:2580:ASN:HD22	1.99	0.69
1:C:2640:SER:HA	1:C:2676:GLU:HG3	1.74	0.69
1:D:3232:GLY:HA3	1:D:3255:THR:HG22	1.73	0.69
1:D:3269:LEU:HD21	1:D:3611:ALA:HB2	1.74	0.69
1:D:3553:ILE:HD13	1:D:3591:GLN:HE21	1.57	0.69
1:A:396:SER:CB	1:A:400:MET:HG2	2.19	0.69
1:C:2328:LEU:O	1:C:2458:GLN:HB2	1.92	0.69
1:A:705:GLU:HG2	1:A:706:THR:N	2.07	0.69
1:B:1734:THR:O	1:B:1735:ASN:HB2	1.92	0.69
1:C:2649:LEU:CD1	1:C:2653:LEU:HD11	2.23	0.69
1:C:2471:ASP:O	1:C:2505:LYS:HA	1.92	0.69
1:A:193:PHE:C	1:A:195:SER:N	2.50	0.69
1:D:3516:ILE:CG2	1:D:3543:ASN:HB3	2.22	0.69
1:B:1233:ILE:N	1:B:1253:GLN:HB2	2.06	0.69
1:C:2517:LEU:C	1:C:2519:GLY:N	2.50	0.69
1:A:306:GLN:O	1:A:309:THR:HG23	1.93	0.68
1:A:343:THR:HB	1:A:400:MET:HE1	1.75	0.68
1:B:1718:LEU:HD23	1:B:1744:ILE:HB	1.74	0.68
1:D:3328:LEU:HD12	1:D:3458:GLN:HB2	1.75	0.68
1:C:2201:ALA:HB2	1:C:2220:GLU:CG	2.23	0.68
1:D:3399:GLY:O	1:D:3403:LEU:HG	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ILE:HD13	1:A:716:ILE:N	2.09	0.68
1:B:1072:VAL:HB	1:B:1255:THR:HG21	1.76	0.68
1:C:2428:GLY:O	1:C:2655:ARG:HD3	1.93	0.68
1:C:2727:VAL:HG11	1:C:2746:LEU:HD22	1.75	0.68
1:A:646:PRO:HG3	1:A:669:ILE:HG12	1.74	0.68
1:B:1214:LEU:HD13	1:B:1215:GLY:H	1.59	0.68
1:B:1595:TYR:OH	1:B:1600:LEU:HD22	1.93	0.68
1:A:74:ALA:HB2	1:A:255:THR:HG23	1.76	0.68
1:C:2352:THR:O	1:C:2353:PHE:HB3	1.94	0.68
1:B:1343:THR:HA	1:B:1412:TRP:CZ3	2.28	0.68
1:B:1618:LEU:HD12	1:B:1620:LEU:HD11	1.74	0.68
1:D:3070:ARG:NH1	1:D:3234:ILE:HB	2.09	0.68
1:A:245:VAL:HB	1:A:246:PRO:HD3	1.76	0.68
1:B:1492:ARG:HG3	1:B:1634:SER:HB2	1.74	0.68
1:B:1400:MET:HE1	1:B:1403:LEU:HD12	1.75	0.68
1:C:2629:LYS:C	1:C:2631:THR:H	2.00	0.68
1:D:3219:MET:HE1	1:D:3263:THR:HG21	1.75	0.68
1:D:3298:THR:OG1	1:D:3300:GLU:HG3	1.94	0.68
1:D:3412:TRP:O	1:D:3416:LEU:HG	1.94	0.68
1:A:479:PHE:CE1	1:A:480:ILE:HG13	2.28	0.67
1:C:2543:ASN:HB2	1:C:2579:GLU:OE2	1.94	0.67
1:B:1576:ASN:HA	1:B:1577:PRO:C	2.18	0.67
1:A:553:ILE:HB	1:A:562:LEU:HD12	1.75	0.67
1:A:485:ASP:OD1	1:A:487:ASN:HB2	1.95	0.67
1:C:2234:ILE:HG12	1:C:2250:LEU:CD1	2.24	0.67
1:D:3538:THR:O	1:D:3605:THR:HG23	1.93	0.67
1:D:3672:THR:HG22	1:D:3673:SER:N	2.09	0.67
1:A:673:SER:HB3	1:A:687:LEU:HB2	1.76	0.67
1:D:3198:ILE:HD13	1:D:3219:MET:HE2	1.76	0.67
1:C:2245:VAL:HB	1:C:2246:PRO:CD	2.25	0.67
1:C:2246:PRO:HD3	1:D:3330:GLN:HE22	1.58	0.67
1:C:2281:LEU:HA	1:C:2289:MET:HE2	1.76	0.67
1:B:1269:LEU:HD21	1:B:1611:ALA:CB	2.24	0.67
1:B:1714:LEU:HD13	1:B:1738:ILE:CD1	2.24	0.67
1:D:3741:ILE:N	1:D:3741:ILE:HD12	2.10	0.67
1:A:696:ILE:CD1	1:A:732:VAL:HB	2.24	0.67
1:B:1673:SER:HB2	1:B:1687:LEU:HB2	1.77	0.67
1:D:3278:ASP:OD1	1:D:3307:ARG:NH2	2.28	0.67
1:D:3689:LEU:HD23	1:D:3690:SER:O	1.94	0.67
1:A:281:LEU:HA	1:A:289:MET:HE2	1.76	0.66
1:A:563:VAL:HG22	1:A:564:GLY:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3200:LEU:C	1:D:3220:GLU:HG2	2.20	0.66
1:A:491:VAL:CG1	1:A:492:ARG:H	2.09	0.66
1:B:1620:LEU:HD13	1:B:1620:LEU:H	1.58	0.66
1:D:3413:LEU:O	1:D:3413:LEU:HD22	1.94	0.66
1:A:352:THR:HB	1:A:406:LYS:HZ3	1.59	0.66
1:A:409:ASP:HB3	1:A:445:ILE:HG21	1.76	0.66
1:B:1153:SER:C	1:B:1155:GLY:H	2.04	0.66
1:B:1673:SER:CB	1:B:1687:LEU:H	2.08	0.66
1:A:572:ALA:CB	1:A:600:LEU:HD21	2.26	0.66
1:A:650:ALA:HA	1:A:660:PRO:HG3	1.78	0.66
1:C:2330:GLN:HA	1:C:2433:TYR:CD1	2.31	0.66
1:D:3488:ASN:HD22	1:D:3489:GLN:N	1.93	0.66
1:A:310:PHE:CE2	1:A:312:ALA:HA	2.31	0.66
1:A:484:TYR:HD1	1:A:491:VAL:HG22	1.60	0.66
1:A:566:THR:HB	1:A:592:PRO:O	1.96	0.66
1:B:1202:GLN:HG3	1:B:1216:THR:HG21	1.78	0.66
1:B:1700:TYR:CE2	1:B:1728:GLN:HA	2.30	0.66
1:D:3293:LEU:CD2	1:D:3302:LEU:HB2	2.26	0.66
1:C:2699:MET:O	1:C:2702:TRP:HB2	1.96	0.66
1:D:3309:THR:HG22	1:D:3310:PHE:H	1.58	0.66
1:B:1467:ALA:O	1:B:1472:GLY:HA2	1.95	0.66
1:D:3277:MET:HG3	1:D:3307:ARG:NH2	2.11	0.66
1:A:335:PRO:HD3	1:A:456:VAL:HG22	1.78	0.66
1:C:2443:VAL:O	1:C:2447:GLN:HG3	1.96	0.66
1:A:354:PRO:HB3	1:A:357:GLU:HG2	1.78	0.66
1:C:2335:PRO:HD3	1:C:2456:VAL:HG22	1.78	0.66
1:C:2603:PHE:O	1:C:2606:PRO:HD2	1.95	0.66
1:D:3729:LYS:HB2	1:D:3747:THR:HB	1.78	0.65
1:A:501:ASN:HD22	1:A:502:PRO:N	1.94	0.65
1:B:1506:GLU:H	1:B:1506:GLU:CD	2.05	0.65
1:C:2347:SER:HA	1:C:2407:MET:HE2	1.76	0.65
1:C:2638:MET:HE1	1:C:2686:VAL:HG11	1.78	0.65
1:A:571:SER:HB3	1:A:588:THR:HG22	1.78	0.65
1:C:2629:LYS:CE	1:C:2631:THR:H	2.09	0.65
1:D:3267:SER:N	1:D:3268:PRO:HD2	2.11	0.65
1:D:3325:ARG:NH1	1:D:3325:ARG:HB2	2.11	0.65
1:B:1737:ALA:O	1:B:1741:ILE:HD13	1.96	0.65
1:D:3251:VAL:O	1:D:3252:SER:HB2	1.96	0.65
1:A:201:ALA:HA	1:A:214:LEU:O	1.97	0.65
1:A:714:LEU:HD13	1:A:738:ILE:HD11	1.78	0.65
1:B:1538:THR:O	1:B:1605:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASP:HB3	1:A:559:GLY:O	1.97	0.65
1:C:2092:THR:HA	1:C:2184:PRO:HA	1.77	0.65
1:D:3277:MET:HG3	1:D:3307:ARG:CZ	2.27	0.65
1:D:3350:ASN:ND2	1:D:3352:THR:OG1	2.30	0.65
1:B:1488:ASN:C	1:B:1488:ASN:HD22	2.05	0.65
1:C:2193:PHE:O	1:C:2195:SER:N	2.29	0.65
1:C:2292:THR:HG23	1:C:2304:THR:HB	1.78	0.65
1:D:3602:GLU:O	1:D:3606:PRO:HG2	1.97	0.65
1:D:3732:VAL:HG11	1:D:3741:ILE:CG1	2.27	0.65
1:A:566:THR:C	1:A:568:TYR:H	2.05	0.65
1:B:1729:LYS:HB3	1:B:1747:THR:HB	1.78	0.65
1:A:546:VAL:HG23	1:A:547:LYS:N	2.12	0.65
1:B:1251:VAL:HG23	1:B:1252:SER:H	1.60	0.65
1:B:1343:THR:HB	1:B:1400:MET:HE2	1.79	0.65
1:D:3333:TYR:O	1:D:3335:PRO:HD3	1.98	0.65
1:B:1203:LEU:HD23	1:B:1211:LYS:HB2	1.78	0.64
1:C:2202:GLN:HE21	1:C:2216:THR:HG21	1.60	0.64
1:C:2458:GLN:HE22	1:C:2588:THR:HG21	1.62	0.64
1:D:3350:ASN:ND2	1:D:3407:MET:HG2	2.11	0.64
1:D:3400:MET:HB3	1:D:3449:SER:O	1.97	0.64
1:D:3737:ALA:O	1:D:3741:ILE:HD13	1.98	0.64
1:D:3741:ILE:H	1:D:3741:ILE:HD12	1.61	0.64
1:C:2727:VAL:HG13	1:C:2746:LEU:HB3	1.77	0.64
1:D:3343:THR:HG21	1:D:3449:SER:O	1.97	0.64
1:D:3593:GLU:HB3	1:D:3594:HIS:CE1	2.32	0.64
1:D:3293:LEU:HD22	1:D:3302:LEU:HB2	1.79	0.64
1:B:1280:PHE:HB2	1:B:1603:PHE:HD1	1.62	0.64
1:C:2469:ALA:HB2	1:C:2575:MET:SD	2.38	0.64
1:C:2289:MET:O	1:C:2306:GLN:HA	1.98	0.64
1:C:2426:ARG:HB3	1:C:2651:GLU:HG2	1.80	0.64
1:D:3640:SER:HA	1:D:3676:GLU:HG3	1.78	0.64
1:C:2354:PRO:HD2	1:C:2358:TYR:OH	1.98	0.64
1:C:2517:LEU:HD23	1:C:2520:THR:HB	1.79	0.64
1:C:2649:LEU:O	1:C:2652:ALA:HB3	1.97	0.64
1:A:741:ILE:HD12	1:A:741:ILE:N	2.13	0.64
1:C:2329:TYR:HB2	1:C:2432:GLU:HG3	1.80	0.64
1:B:1628:ASP:O	1:B:1630:VAL:HG23	1.98	0.64
1:C:2354:PRO:HB3	1:C:2357:GLU:HG3	1.79	0.64
1:C:2649:LEU:HD12	1:C:2688:LEU:CD1	2.28	0.64
1:D:3563:VAL:HG22	1:D:3564:GLY:N	2.12	0.64
1:A:619:ASN:O	1:A:621:GLN:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1512:ARG:NH1	1:B:1579:GLU:O	2.31	0.64
1:D:3349:ASP:C	1:D:3351:ASN:H	2.06	0.64
1:B:1568:TYR:HB2	1:B:1570:PHE:CE1	2.33	0.63
1:B:1170:LEU:HD22	1:B:1175:VAL:HG11	1.80	0.63
1:B:1457:THR:OG1	1:B:1460:GLN:HG3	1.99	0.63
1:A:472:GLY:HA3	1:A:503:VAL:O	1.97	0.63
1:A:186:ARG:HG3	1:A:188:TYR:CE1	2.32	0.63
1:C:2245:VAL:HB	1:C:2246:PRO:HD3	1.80	0.63
1:D:3714:LEU:O	1:D:3716:ILE:HG13	1.98	0.63
1:A:629:LYS:O	1:A:630:VAL:CB	2.47	0.63
1:B:1216:THR:O	1:B:1217:SER:HB3	1.98	0.63
1:C:2334:GLU:O	1:C:2551:ALA:HB1	1.97	0.63
1:C:2672:THR:HG22	1:C:2688:LEU:HD23	1.81	0.63
1:C:2629:LYS:HE3	1:C:2631:THR:CA	2.28	0.63
1:C:2079:ILE:O	1:C:2079:ILE:HG22	1.98	0.63
1:D:3280:PHE:CE1	1:D:3600:LEU:HA	2.34	0.63
1:A:501:ASN:C	1:A:501:ASN:ND2	2.44	0.63
1:C:2716:ILE:HD13	1:C:2716:ILE:H	1.62	0.63
1:A:649:LEU:HD22	1:A:653:LEU:HG	1.81	0.62
1:C:2613:ALA:O	1:C:2614:MET:HB2	1.97	0.62
1:B:1284:VAL:HG13	1:B:1594:HIS:O	1.99	0.62
1:B:1512:ARG:NH1	1:B:1578:ALA:O	2.32	0.62
1:C:2076:ARG:HD3	1:C:2186:ARG:CZ	2.30	0.62
1:B:1741:ILE:O	1:B:1741:ILE:CG2	2.48	0.62
1:D:3174:GLU:O	1:D:3175:VAL:HG23	1.99	0.62
1:D:3542:GLN:NE2	1:D:3577:PRO:HG3	2.15	0.62
1:C:2201:ALA:HA	1:C:2215:GLY:HA2	1.82	0.62
1:C:2515:MET:HB2	1:C:2545:ALA:HB1	1.82	0.62
1:C:2515:MET:HE3	1:C:2547:LYS:HB2	1.81	0.62
1:D:3099:VAL:C	1:D:3100:ILE:HD12	2.25	0.62
1:D:3332:ASN:N	1:D:3332:ASN:ND2	2.40	0.62
1:D:3345:ALA:HB1	1:D:3468:ILE:HD11	1.81	0.62
1:D:3467:ALA:O	1:D:3472:GLY:N	2.33	0.62
1:B:1281:LEU:O	1:B:1285:LYS:N	2.31	0.62
1:D:3170:LEU:HD22	1:D:3175:VAL:HG11	1.81	0.62
1:D:3456:VAL:HG21	1:D:3461:MET:SD	2.38	0.62
1:B:1160:TYR:OH	1:B:1164:MET:HE2	2.00	0.62
1:C:2290:THR:HB	1:C:2588:THR:OG1	2.00	0.62
1:C:2512:ARG:HB2	1:C:2512:ARG:HH11	1.65	0.61
1:C:2727:VAL:HG11	1:C:2746:LEU:HD13	1.81	0.61
1:A:256:VAL:HG12	1:A:487:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HG2	1:A:400:MET:HG3	1.82	0.61
1:B:1309:THR:HG22	1:B:1310:PHE:H	1.66	0.61
1:B:1638:MET:HB2	1:B:1680:LEU:CD1	2.30	0.61
1:D:3478:LYS:HE3	1:D:3495:GLN:O	2.00	0.61
1:C:2069:THR:HG21	1:D:3204:HIS:NE2	2.16	0.61
1:C:2687:LEU:HD12	1:C:2713:TRP:CZ3	2.32	0.61
1:A:705:GLU:HG2	1:A:706:THR:H	1.65	0.61
1:B:1674:VAL:CG2	1:B:1686:VAL:HG22	2.29	0.61
1:D:3250:LEU:HG	1:D:3251:VAL:N	2.15	0.61
1:D:3729:LYS:HB2	1:D:3747:THR:CB	2.31	0.61
1:D:3732:VAL:HG21	1:D:3744:ILE:HG12	1.80	0.61
1:B:1081:ASP:HB2	1:B:1265:LEU:O	2.00	0.61
1:B:1284:VAL:HG13	1:B:1592:PRO:HB2	1.81	0.61
1:B:1615:LYS:C	1:B:1618:LEU:HD21	2.24	0.61
1:C:2629:LYS:HE2	1:C:2629:LYS:N	2.15	0.61
1:D:3273:MET:HE2	1:D:3291:ALA:HB1	1.80	0.61
1:A:468:ILE:O	1:A:508:ALA:HB1	2.01	0.61
1:B:1614:MET:O	1:B:1616:GLU:N	2.34	0.61
1:D:3098:ALA:O	1:D:3099:VAL:HB	2.00	0.61
1:A:343:THR:HB	1:A:400:MET:HE3	1.82	0.61
1:A:407:MET:HG2	1:A:411:THR:HB	1.82	0.61
1:B:1077:GLY:HA3	1:B:1259:LYS:O	2.00	0.61
1:B:1172:THR:O	1:B:1173:ALA:HB2	2.01	0.61
1:B:1615:LYS:HA	1:B:1618:LEU:HD21	1.82	0.61
1:B:1082:ARG:NH1	1:B:1620:LEU:HA	2.15	0.61
1:D:3201:ALA:HB2	1:D:3220:GLU:CG	2.30	0.61
1:A:287:LYS:HG3	1:A:591:GLN:HB2	1.82	0.61
1:A:550:THR:HG23	1:A:568:TYR:HB3	1.83	0.61
1:C:2658:VAL:HG21	1:C:2680:LEU:HD23	1.83	0.61
1:C:2702:TRP:O	1:C:2727:VAL:HG23	2.01	0.61
1:C:2727:VAL:CG1	1:C:2746:LEU:HB3	2.30	0.61
1:D:3350:ASN:O	1:D:3352:THR:N	2.25	0.61
1:D:3350:ASN:C	1:D:3352:THR:H	2.08	0.61
1:D:3562:LEU:HB3	1:D:3567:ASN:HD21	1.66	0.61
1:D:3649:LEU:HD22	1:D:3653:LEU:HD11	1.82	0.61
1:A:256:VAL:HG12	1:A:487:ASN:HD21	1.66	0.61
1:A:340:LYS:CB	1:A:400:MET:HE2	2.31	0.61
1:B:1336:GLY:HA3	1:B:1551:ALA:HB2	1.81	0.61
1:B:1457:THR:HA	2:B:5:HOH:O	2.00	0.61
1:C:2563:VAL:HG22	1:C:2564:GLY:N	2.16	0.61
1:C:2632:THR:O	1:C:2632:THR:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2731:ASP:OD1	1:C:2732:VAL:HG23	2.00	0.61
1:A:330:GLN:HA	1:A:433:TYR:CD1	2.35	0.60
1:A:632:THR:O	1:A:633:GLU:C	2.43	0.60
1:A:202:GLN:HE21	1:A:216:THR:HG21	1.67	0.60
1:A:355:SER:C	1:A:357:GLU:H	2.09	0.60
1:A:438:PRO:HB3	1:A:448:SER:HB3	1.82	0.60
1:A:632:THR:O	1:A:632:THR:HG22	2.01	0.60
1:B:1082:ARG:HH12	1:B:1620:LEU:HA	1.66	0.60
1:C:2352:THR:O	1:C:2353:PHE:CB	2.46	0.60
1:D:3092:THR:HG22	1:D:3184:PRO:CA	2.28	0.60
1:C:2729:LYS:HB3	1:C:2747:THR:CB	2.30	0.60
1:D:3641:ILE:CG1	1:D:3669:ILE:HB	2.30	0.60
1:A:619:ASN:HB3	1:A:622:SER:O	2.01	0.60
1:B:1414:ASP:O	1:B:1418:ARG:HG3	2.00	0.60
1:D:3094:TYR:O	1:D:3158:ILE:HG13	2.01	0.60
1:B:1427:PHE:HD1	1:B:1427:PHE:H	1.48	0.60
1:C:2328:LEU:HA	1:C:2458:GLN:HG3	1.83	0.60
1:C:2576:ASN:HA	1:C:2578:ALA:H	1.66	0.60
1:C:2714:LEU:CD1	1:C:2738:ILE:HD11	2.21	0.60
1:A:426:ARG:HA	1:A:651:GLU:OE2	2.02	0.60
1:A:576:ASN:ND2	1:A:612:SER:OG	2.34	0.60
1:A:631:THR:O	1:A:632:THR:OG1	2.18	0.60
1:B:1163:MET:C	1:B:1163:MET:HE2	2.26	0.60
1:A:670:LYS:O	1:A:671:GLU:HG3	2.01	0.60
1:B:1298:THR:C	1:B:1475:LEU:HD13	2.26	0.60
1:C:2197:PHE:CE1	1:C:2429:LEU:HD11	2.37	0.60
1:D:3262:TYR:O	1:D:3481:SER:HB3	2.02	0.60
1:A:281:LEU:HD12	1:A:285:LYS:HA	1.83	0.60
1:A:353:PHE:N	1:A:406:LYS:HZ1	2.00	0.60
1:D:3079:ILE:HG21	1:D:3219:MET:HE3	1.83	0.60
1:D:3080:TYR:HB2	1:D:3262:TYR:HA	1.84	0.60
1:D:3441:ASN:OD1	1:D:3443:VAL:N	2.35	0.60
1:B:1076:ARG:HD3	1:B:1186:ARG:NH2	2.16	0.60
1:B:1702:TRP:O	1:B:1727:VAL:HG23	2.02	0.60
1:D:3266:SER:C	1:D:3268:PRO:HD2	2.27	0.60
1:B:1264:THR:CG2	1:B:1300:GLU:HB3	2.32	0.59
1:B:1467:ALA:HB2	1:B:1474:MET:CG	2.31	0.59
1:C:2197:PHE:HE1	1:C:2429:LEU:HD11	1.67	0.59
1:C:2347:SER:HA	1:C:2407:MET:CE	2.32	0.59
1:D:3562:LEU:HB3	1:D:3567:ASN:ND2	2.17	0.59
1:A:195:SER:O	1:A:196:SER:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1290:THR:HG21	1:B:1458:GLN:OE1	2.01	0.59
1:B:1425:THR:HG21	1:B:1459:THR:CB	2.32	0.59
1:A:342:MET:HG3	1:A:419:PHE:CE1	2.37	0.59
1:C:2355:SER:C	1:C:2357:GLU:H	2.09	0.59
1:C:2617:SER:C	1:C:2618:LEU:HD23	2.27	0.59
1:D:3698:ASP:HA	1:D:3734:THR:CG2	2.32	0.59
1:B:1095:ASN:HA	1:B:1155:GLY:O	2.02	0.59
1:C:2298:THR:OG1	1:C:2300:GLU:HG3	2.03	0.59
1:D:3553:ILE:HG22	1:D:3554:ALA:N	2.17	0.59
1:B:1441:ASN:O	1:B:1443:VAL:N	2.35	0.59
1:A:657:ILE:HG22	1:A:657:ILE:O	2.02	0.59
1:B:1664:GLY:HA3	1:B:1690:SER:OG	2.02	0.59
1:B:1693:VAL:HG11	1:B:1714:LEU:HD11	1.83	0.59
1:B:1698:ASP:HA	1:B:1734:THR:CG2	2.30	0.59
1:C:2562:LEU:HD13	1:C:2567:ASN:ND2	2.17	0.59
1:D:3699:MET:CE	1:D:3746:LEU:HD21	2.33	0.59
1:D:3704:LYS:HG3	1:D:3720:PHE:CE1	2.37	0.59
1:A:556:GLU:HG2	1:A:556:GLU:O	2.02	0.59
1:D:3539:VAL:HB	1:D:3542:GLN:HB2	1.85	0.59
1:A:310:PHE:HE2	1:A:312:ALA:HA	1.67	0.59
1:B:1494:SER:O	1:B:1495:GLN:HG2	2.03	0.59
1:A:517:LEU:HD23	1:A:520:THR:HB	1.84	0.59
1:B:1288:TYR:HB2	1:B:1590:GLN:HB3	1.85	0.59
1:B:1562:LEU:CB	1:B:1567:ASN:HD21	2.16	0.59
1:B:1596:SER:HB3	1:B:1599:GLN:CD	2.28	0.59
1:C:2463:ARG:HG2	1:C:2474:MET:SD	2.43	0.59
1:D:3219:MET:HG3	1:D:3223:LEU:HD22	1.83	0.59
1:D:3425:THR:O	1:D:3426:ARG:C	2.46	0.59
1:D:3600:LEU:O	1:D:3603:PHE:HB3	2.02	0.59
1:A:480:ILE:HG21	1:A:657:ILE:HD11	1.86	0.58
1:A:694:GLU:C	1:A:695:GLU:HG2	2.27	0.58
1:B:1562:LEU:HB3	1:B:1567:ASN:HD21	1.66	0.58
1:D:3666:GLY:HA3	1:D:3690:SER:HB2	1.85	0.58
1:A:490:SER:HB3	1:A:632:THR:HG22	1.83	0.58
1:C:2201:ALA:CA	1:C:2214:LEU:O	2.51	0.58
1:C:2354:PRO:HB2	1:C:2358:TYR:CZ	2.38	0.58
1:A:69:THR:HG22	1:A:235:THR:CB	2.32	0.58
1:B:1627:LEU:O	1:B:1628:ASP:C	2.45	0.58
1:B:1658:VAL:HG11	1:B:1680:LEU:HD23	1.84	0.58
1:A:82:ARG:HD3	1:A:618:LEU:O	2.03	0.58
1:B:1461:MET:O	1:B:1464:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2244:ILE:HG22	1:C:2245:VAL:N	2.19	0.58
1:C:2617:SER:O	1:C:2618:LEU:O	2.22	0.58
1:C:2699:MET:HE3	1:C:2746:LEU:HD21	1.84	0.58
1:B:1162:ASN:O	1:B:1166:ILE:HG13	2.02	0.58
1:B:1265:LEU:HA	1:B:1302:LEU:O	2.01	0.58
1:B:1284:VAL:CG1	1:B:1592:PRO:CB	2.78	0.58
1:B:1293:LEU:HD23	1:B:1293:LEU:C	2.29	0.58
1:B:1400:MET:HA	1:B:1400:MET:HE3	1.84	0.58
1:D:3741:ILE:CD1	1:D:3741:ILE:N	2.64	0.58
1:A:282:GLU:O	1:A:285:LYS:HG2	2.03	0.58
1:A:563:VAL:HG22	1:A:564:GLY:H	1.68	0.58
1:B:1251:VAL:O	1:B:1252:SER:CB	2.51	0.58
1:B:1264:THR:HG21	1:B:1300:GLU:HB3	1.84	0.58
1:B:1307:ARG:HD3	1:B:1309:THR:HG1	1.66	0.58
1:B:1337:SER:HA	1:B:1340:LYS:HE3	1.85	0.58
1:C:2244:ILE:HG22	1:C:2245:VAL:H	1.68	0.58
1:C:2328:LEU:HA	1:C:2458:GLN:HB2	1.85	0.58
1:A:286:GLY:HA2	1:A:592:PRO:HA	1.84	0.58
1:A:357:GLU:O	1:A:360:ASN:OD1	2.22	0.58
1:A:439:ALA:HB3	1:A:444:SER:OG	2.04	0.58
1:A:605:THR:HB	1:A:606:PRO:HD3	1.86	0.58
1:A:614:MET:O	1:A:616:GLU:N	2.36	0.58
1:B:1561:TYR:O	1:B:1562:LEU:C	2.47	0.58
1:B:1727:VAL:HG12	1:B:1728:GLN:H	1.68	0.58
1:A:550:THR:HG21	1:A:568:TYR:CG	2.38	0.58
1:B:1185:ASN:CG	1:B:1186:ARG:H	2.12	0.58
1:B:1497:GLU:HG3	1:B:1659:GLN:CD	2.29	0.58
1:B:1641:ILE:HD11	1:B:1669:ILE:HG22	1.84	0.58
1:D:3100:ILE:HD12	1:D:3100:ILE:N	2.19	0.58
1:A:69:THR:HA	1:A:234:ILE:O	2.04	0.58
1:A:357:GLU:O	1:A:360:ASN:HB3	2.04	0.58
1:A:280:PHE:HE1	1:A:599:GLN:HB3	1.68	0.58
1:B:1096:VAL:HB	1:B:1180:PHE:CE2	2.38	0.58
1:B:1658:VAL:HG21	1:B:1680:LEU:HD23	1.85	0.58
1:C:2508:ALA:O	1:C:2511:THR:N	2.37	0.58
1:D:3289:MET:HB2	1:D:3307:ARG:HG2	1.86	0.58
1:D:3603:PHE:C	1:D:3606:PRO:HD2	2.27	0.58
1:B:1513:ASN:C	1:B:1515:MET:H	2.12	0.57
1:B:1596:SER:C	1:B:1598:ILE:H	2.11	0.57
1:D:3224:ASN:O	1:D:3227:LEU:N	2.31	0.57
1:D:3281:LEU:O	1:D:3285:LYS:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3506:GLU:CD	1:D:3506:GLU:H	2.11	0.57
1:A:699:MET:HG2	1:A:702:TRP:CE3	2.39	0.57
1:B:1700:TYR:HE2	1:B:1728:GLN:HA	1.69	0.57
1:C:2468:ILE:O	1:C:2508:ALA:HB1	2.04	0.57
1:C:2470:ASN:ND2	1:C:2473:VAL:HB	2.20	0.57
1:A:650:ALA:O	1:A:654:ARG:HG3	2.04	0.57
1:B:1233:ILE:HB	1:B:1253:GLN:HB2	1.85	0.57
1:D:3342:MET:O	1:D:3346:SER:N	2.37	0.57
1:D:3689:LEU:HD23	1:D:3689:LEU:C	2.30	0.57
1:C:2409:ASP:HB3	1:C:2445:ILE:HD13	1.86	0.57
1:C:2553:ILE:HD11	1:C:2569:ILE:HG13	1.86	0.57
1:D:3447:GLN:HA	1:D:3450:PHE:CE2	2.39	0.57
1:D:3732:VAL:HG11	1:D:3741:ILE:HG12	1.85	0.57
1:B:1311:ASN:CG	1:B:1314:THR:HG23	2.29	0.57
1:B:1325:ARG:NH2	1:B:1433:TYR:OH	2.38	0.57
1:C:2076:ARG:HD3	1:C:2186:ARG:NH1	2.19	0.57
1:B:1492:ARG:CG	1:B:1634:SER:HB2	2.34	0.57
1:B:1654:ARG:NH1	1:B:1660:PRO:HG2	2.19	0.57
1:C:2336:GLY:CA	1:C:2451:GLY:HA3	2.33	0.57
1:A:271:SER:O	1:A:274:GLU:HB2	2.04	0.57
1:A:361:SER:O	1:A:364:LEU:HG	2.04	0.57
1:A:416:LEU:O	1:A:419:PHE:N	2.36	0.57
1:B:1400:MET:CE	1:B:1403:LEU:HD12	2.34	0.57
1:B:1576:ASN:OD1	1:B:1583:PHE:HB2	2.04	0.57
1:B:1699:MET:HE3	1:B:1746:LEU:CD2	2.28	0.57
1:C:2344:LEU:HD11	1:C:2348:ILE:HD11	1.85	0.57
1:D:3436:GLN:N	1:D:3455:SER:O	2.33	0.57
1:B:1563:VAL:CG2	1:B:1564:GLY:H	2.14	0.57
1:C:2323:VAL:HG12	1:C:2325:ARG:HB3	1.86	0.57
1:A:729:LYS:CB	1:A:747:THR:HB	2.28	0.57
1:B:1277:MET:SD	1:B:1289:MET:HE3	2.45	0.57
1:B:1333:TYR:CE1	1:B:1458:GLN:HG2	2.40	0.57
1:C:2219:MET:HE1	1:C:2263:THR:HG22	1.86	0.57
1:C:2447:GLN:C	1:C:2449:SER:H	2.13	0.57
1:C:2598:ILE:O	1:C:2602:GLU:HG3	2.05	0.57
1:D:3693:VAL:HG11	1:D:3714:LEU:CD1	2.29	0.57
1:A:76:ARG:HE	1:A:186:ARG:HH21	1.53	0.57
1:A:357:GLU:O	1:A:360:ASN:N	2.37	0.57
1:B:1727:VAL:HG12	1:B:1728:GLN:N	2.20	0.57
1:D:3070:ARG:HH12	1:D:3234:ILE:HB	1.68	0.57
1:D:3329:TYR:HB2	1:D:3432:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HG2	1:A:274:GLU:OE1	2.05	0.56
1:A:653:LEU:HB3	1:A:658:VAL:CG1	2.34	0.56
1:B:1425:THR:HG21	1:B:1459:THR:OG1	2.05	0.56
1:B:1483:ILE:HG22	1:B:1483:ILE:O	2.05	0.56
1:D:3340:LYS:CB	1:D:3400:MET:HE2	2.33	0.56
1:B:1636:TYR:CE2	1:B:1656:ASN:HB2	2.40	0.56
1:C:2679:ASN:CG	1:C:2680:LEU:N	2.63	0.56
1:D:3321:ASP:N	1:D:3321:ASP:OD1	2.37	0.56
1:A:408:GLY:C	1:A:410:ALA:H	2.14	0.56
1:A:728:GLN:CD	1:A:749:GLY:HA3	2.29	0.56
1:B:1436:GLN:O	1:B:1454:ILE:HG13	2.05	0.56
1:B:1537:ILE:HD13	1:B:1574:THR:HG21	1.86	0.56
1:C:2566:THR:C	1:C:2568:TYR:H	2.12	0.56
1:D:3424:PRO:HG3	1:D:3434:ALA:HA	1.85	0.56
1:D:3467:ALA:HB2	1:D:3474:MET:HG2	1.88	0.56
1:B:1096:VAL:HG23	1:B:1179:ASP:O	2.05	0.56
1:D:3590:GLN:CG	1:D:3591:GLN:HG3	2.22	0.56
1:C:2506:GLU:O	1:C:2510:THR:HG23	2.06	0.56
1:D:3646:PRO:CG	1:D:3669:ILE:HG12	2.35	0.56
1:A:474:MET:HG3	1:A:502:PRO:HD3	1.87	0.56
1:B:1456:VAL:HG21	1:B:1461:MET:SD	2.45	0.56
1:C:2553:ILE:HD11	1:C:2568:TYR:C	2.31	0.56
1:D:3509:SER:HA	1:D:3512:ARG:NH2	2.20	0.56
1:A:81:ASP:O	1:A:83:ASN:N	2.38	0.56
1:A:469:ALA:HB2	1:A:575:MET:SD	2.46	0.56
1:B:1335:PRO:HG3	1:B:1456:VAL:HG22	1.88	0.56
1:A:336:GLY:O	1:A:451:GLY:HA3	2.06	0.56
1:A:424:PRO:HG3	1:A:434:ALA:HA	1.87	0.56
1:B:1156:ASN:O	1:B:1158:ILE:N	2.39	0.56
1:B:1251:VAL:O	1:B:1252:SER:HB2	2.06	0.56
1:B:1262:TYR:O	1:B:1481:SER:HB3	2.06	0.56
1:B:1644:ILE:HD13	1:B:1649:LEU:HB2	1.88	0.56
1:C:2438:PRO:HD3	1:C:2454:ILE:HB	1.88	0.56
1:A:69:THR:HG21	1:B:1204:HIS:CE1	2.41	0.56
1:A:209:GLY:O	1:A:210:SER:C	2.49	0.56
1:A:627:LEU:O	1:A:629:LYS:O	2.23	0.56
1:B:1641:ILE:O	1:B:1641:ILE:HG12	2.05	0.56
1:C:2507:ALA:O	1:C:2508:ALA:C	2.49	0.56
1:C:2629:LYS:C	1:C:2631:THR:N	2.63	0.56
1:D:3228:ALA:O	1:D:3229:GLY:C	2.48	0.56
1:A:328:LEU:HA	1:A:458:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:O	1:A:466:THR:HG23	2.05	0.56
1:D:3471:ASP:O	1:D:3473:VAL:HG23	2.05	0.56
1:B:1467:ALA:O	1:B:1472:GLY:CA	2.54	0.55
1:C:2199:GLY:HA3	1:C:2217:SER:O	2.07	0.55
1:D:3073:PRO:HB3	1:D:3184:PRO:HG2	1.88	0.55
1:D:3277:MET:C	1:D:3307:ARG:HH21	2.14	0.55
1:A:199:GLY:HA3	1:A:217:SER:O	2.05	0.55
1:D:3072:VAL:HB	1:D:3255:THR:CG2	2.36	0.55
1:D:3350:ASN:HD22	1:D:3407:MET:HG2	1.70	0.55
1:D:3718:LEU:HD23	1:D:3744:ILE:HB	1.87	0.55
1:C:2079:ILE:O	1:C:2087:ILE:HB	2.06	0.55
1:C:2350:ASN:O	1:C:2352:THR:HG23	2.06	0.55
1:C:2703:LYS:O	1:C:2706:THR:N	2.39	0.55
1:D:3339:MET:O	1:D:3339:MET:SD	2.64	0.55
1:D:3465:PHE:CZ	1:D:3573:VAL:HG21	2.41	0.55
1:A:447:GLN:HA	1:A:450:PHE:CE2	2.41	0.55
1:C:2219:MET:HE3	1:C:2223:LEU:CD2	2.37	0.55
1:C:2595:TYR:OH	1:C:2600:LEU:HD23	2.06	0.55
1:D:3332:ASN:HD22	1:D:3332:ASN:H	1.54	0.55
1:A:357:GLU:O	1:A:360:ASN:CB	2.54	0.55
1:B:1267:SER:N	1:B:1268:PRO:HD2	2.21	0.55
1:D:3447:GLN:HA	1:D:3450:PHE:CZ	2.41	0.55
1:A:272:PHE:O	1:A:275:THR:HB	2.07	0.55
1:D:3732:VAL:HG11	1:D:3741:ILE:HG13	1.88	0.55
1:B:1335:PRO:CB	1:B:1339:MET:HB2	2.37	0.55
1:B:1352:THR:C	1:B:1406:LYS:HZ1	2.14	0.55
1:B:1474:MET:HB3	1:B:1499:VAL:HG23	1.89	0.55
1:C:2663:VAL:HG11	1:C:2710:PHE:CE1	2.39	0.55
1:D:3284:VAL:HG13	1:D:3592:PRO:HB2	1.88	0.55
1:D:3673:SER:HB2	1:D:3687:LEU:HB2	1.87	0.55
1:D:3293:LEU:HD23	1:D:3293:LEU:C	2.32	0.55
1:A:426:ARG:HB3	1:A:651:GLU:CG	2.31	0.55
1:A:494:SER:HA	1:A:683:ASN:HD21	1.71	0.55
1:B:1348:ILE:HD13	1:B:1510:THR:CG2	2.36	0.55
1:B:1513:ASN:C	1:B:1515:MET:N	2.65	0.55
1:C:2082:ARG:HH22	1:C:2300:GLU:CD	2.14	0.55
1:C:2262:TYR:HB2	1:C:2482:ALA:HB3	1.89	0.55
1:C:2350:ASN:HD22	1:C:2352:THR:CG2	2.20	0.55
1:C:2580:ASN:C	1:C:2580:ASN:ND2	2.64	0.55
1:D:3492:ARG:HG3	1:D:3634:SER:HB2	1.89	0.55
1:D:3588:THR:O	1:D:3589:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:HG23	1:A:479:PHE:O	2.07	0.54
1:A:614:MET:O	1:A:615:LYS:C	2.48	0.54
1:B:1658:VAL:HG12	1:B:1659:GLN:N	2.22	0.54
1:D:3336:GLY:O	1:D:3451:GLY:HA3	2.07	0.54
1:D:3704:LYS:HD2	1:D:3748:LEU:HD11	1.89	0.54
1:D:3734:THR:O	1:D:3735:ASN:HB2	2.07	0.54
1:A:447:GLN:HG2	1:A:450:PHE:HE2	1.72	0.54
1:A:484:TYR:CG	1:A:485:ASP:N	2.76	0.54
1:A:491:VAL:O	1:A:633:GLU:HA	2.07	0.54
1:A:727:VAL:CG1	1:A:746:LEU:HD22	2.36	0.54
1:C:2619:ASN:HB3	1:C:2622:SER:O	2.08	0.54
1:C:2696:ILE:HG21	1:C:2732:VAL:HG12	1.89	0.54
1:A:506:GLU:O	1:A:509:SER:OG	2.25	0.54
1:D:3332:ASN:ND2	1:D:3433:TYR:HD2	2.05	0.54
1:D:3672:THR:CG2	1:D:3673:SER:N	2.70	0.54
1:A:282:GLU:HA	1:A:285:LYS:HD3	1.89	0.54
1:A:517:LEU:C	1:A:519:GLY:N	2.57	0.54
1:B:1290:THR:HB	1:B:1588:THR:OG1	2.07	0.54
1:B:1652:ALA:O	1:B:1655:ARG:HB2	2.07	0.54
1:D:3251:VAL:O	1:D:3252:SER:CB	2.56	0.54
1:B:1343:THR:HB	1:B:1400:MET:CE	2.37	0.54
1:B:1431:ASP:O	1:B:1432:GLU:C	2.48	0.54
1:C:2350:ASN:ND2	1:C:2352:THR:CG2	2.70	0.54
1:C:2495:GLN:O	1:C:2496:LYS:C	2.50	0.54
1:D:3337:SER:HB2	1:D:3549:GLY:CA	2.38	0.54
1:D:3542:GLN:CD	1:D:3577:PRO:HG3	2.33	0.54
1:B:1080:TYR:HE1	1:B:1086:PRO:HG3	1.73	0.54
1:B:1201:ALA:HA	1:B:1214:LEU:O	2.08	0.54
1:B:1488:ASN:HD22	1:B:1489:GLN:N	2.06	0.54
1:C:2360:ASN:CG	1:C:2360:ASN:O	2.51	0.54
1:D:3332:ASN:HD21	1:D:3433:TYR:HD2	1.56	0.54
1:D:3415:TYR:HA	1:D:3418:ARG:HD3	1.90	0.54
1:A:614:MET:C	1:A:618:LEU:HD21	2.33	0.54
1:A:682:PRO:O	1:A:683:ASN:HB2	2.06	0.54
1:D:3082:ARG:NH2	1:D:3300:GLU:OE1	2.28	0.54
1:D:3343:THR:HA	1:D:3412:TRP:CZ3	2.43	0.54
1:A:696:ILE:HG22	1:A:736:THR:H	1.73	0.54
1:A:714:LEU:HD13	1:A:738:ILE:CD1	2.38	0.54
1:C:2350:ASN:ND2	1:C:2352:THR:HG23	2.23	0.54
1:D:3162:ASN:O	1:D:3166:ILE:HG13	2.08	0.54
1:D:3400:MET:N	1:D:3400:MET:SD	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3638:MET:HE2	1:D:3672:THR:HG21	1.90	0.54
1:A:539:VAL:HG21	1:A:576:ASN:ND2	2.23	0.53
1:A:652:ALA:HB2	1:B:1250:LEU:HD22	1.91	0.53
1:B:1093:SER:HB2	1:B:1157:GLY:CA	2.38	0.53
1:B:1219:MET:HE1	1:B:1263:THR:HG21	1.88	0.53
1:D:3340:LYS:HG2	1:D:3400:MET:HG3	1.90	0.53
1:D:3513:ASN:HA	1:D:3516:ILE:CD1	2.38	0.53
1:D:3566:THR:O	1:D:3568:TYR:N	2.40	0.53
1:A:83:ASN:ND2	1:A:619:ASN:OD1	2.40	0.53
1:B:1731:ASP:OD1	1:B:1745:LYS:N	2.38	0.53
1:C:2193:PHE:C	1:C:2195:SER:N	2.65	0.53
1:C:2699:MET:CE	1:C:2746:LEU:HD21	2.38	0.53
1:D:3254:GLN:O	1:D:3256:VAL:HG23	2.08	0.53
1:B:1232:GLY:HA2	1:B:1253:GLN:O	2.09	0.53
1:C:2508:ALA:O	1:C:2509:SER:C	2.51	0.53
1:C:2741:ILE:N	1:C:2741:ILE:CD1	2.71	0.53
1:D:3228:ALA:O	1:D:3229:GLY:O	2.26	0.53
1:D:3488:ASN:ND2	1:D:3490:SER:H	2.06	0.53
1:A:290:THR:HG22	1:A:291:ALA:N	2.23	0.53
1:B:1405:GLN:OE1	1:B:1405:GLN:HA	2.08	0.53
1:B:1540:PRO:CD	1:B:1609:GLU:HG3	2.38	0.53
1:C:2661:ILE:HD13	1:C:2702:TRP:CD1	2.43	0.53
1:D:3354:PRO:HG2	1:D:3403:LEU:HD23	1.91	0.53
1:A:577:PRO:HG2	1:A:580:ASN:O	2.08	0.53
1:B:1314:THR:O	1:B:1315:LYS:HB2	2.08	0.53
1:D:3264:THR:OG1	1:D:3479:PHE:HA	2.07	0.53
1:A:206:ASN:C	1:A:208:ASP:H	2.16	0.53
1:B:1234:ILE:HG23	1:B:1250:LEU:O	2.08	0.53
1:B:1425:THR:HG21	1:B:1459:THR:HB	1.91	0.53
1:B:1608:LEU:O	1:B:1609:GLU:C	2.51	0.53
1:B:1706:THR:O	1:B:1707:ALA:C	2.52	0.53
1:B:1727:VAL:O	1:B:1728:GLN:CG	2.57	0.53
1:C:2341:VAL:HG12	1:C:2468:ILE:HG13	1.91	0.53
1:D:3201:ALA:HA	1:D:3214:LEU:O	2.09	0.53
1:A:243:ASN:C	1:A:243:ASN:OD1	2.52	0.53
1:B:1093:SER:HB2	1:B:1157:GLY:C	2.32	0.53
1:B:1355:SER:O	1:B:1356:GLY:C	2.51	0.53
1:B:1566:THR:O	1:B:1570:PHE:HE1	1.90	0.53
1:C:2283:LYS:HE2	1:C:2599:GLN:NE2	2.23	0.53
1:C:2501:ASN:HB2	1:C:2700:TYR:CG	2.44	0.53
1:C:2617:SER:OG	1:C:2618:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3640:SER:HA	1:D:3676:GLU:CG	2.39	0.53
1:A:76:ARG:HD3	1:A:186:ARG:CZ	2.39	0.53
1:A:264:THR:HG22	1:A:481:SER:HB2	1.91	0.53
1:A:354:PRO:HG3	1:A:406:LYS:HD3	1.89	0.53
1:A:474:MET:O	1:A:475:LEU:HD23	2.08	0.53
1:A:572:ALA:HB2	1:A:600:LEU:HD21	1.90	0.53
1:B:1078:THR:N	1:B:1260:ASP:OD1	2.37	0.53
1:B:1330:GLN:HA	1:B:1433:TYR:CD1	2.44	0.53
1:B:1624:ALA:C	1:B:1626:ASN:H	2.16	0.53
1:A:413:LEU:HD22	1:A:416:LEU:HD12	1.91	0.53
1:B:1100:ILE:HD12	1:B:1100:ILE:N	2.24	0.53
1:B:1205:GLU:HB2	1:B:1211:LYS:NZ	2.24	0.53
1:B:1467:ALA:HB2	1:B:1474:MET:HG2	1.90	0.53
1:B:1517:LEU:C	1:B:1519:GLY:N	2.63	0.53
1:D:3488:ASN:C	1:D:3488:ASN:ND2	2.61	0.53
1:A:293:LEU:HD22	1:A:302:LEU:HB2	1.91	0.52
1:B:1615:LYS:O	1:B:1615:LYS:HG2	2.09	0.52
1:A:347:SER:HA	1:A:407:MET:CE	2.40	0.52
1:A:696:ILE:HD11	1:A:744:ILE:CD1	2.37	0.52
1:B:1082:ARG:NH2	1:B:1300:GLU:OE1	2.42	0.52
1:B:1287:LYS:HD2	1:B:1591:GLN:OE1	2.10	0.52
1:D:3250:LEU:CG	1:D:3251:VAL:H	2.21	0.52
1:D:3325:ARG:HB2	1:D:3325:ARG:HH11	1.73	0.52
1:A:550:THR:CG2	1:A:568:TYR:CG	2.92	0.52
1:B:1335:PRO:HB2	1:B:1339:MET:HB2	1.91	0.52
1:B:1539:VAL:HG13	1:B:1540:PRO:HD2	1.91	0.52
1:C:2068:ILE:O	1:C:2235:THR:HA	2.09	0.52
1:C:2734:THR:O	1:C:2735:ASN:HB2	2.09	0.52
1:A:200:LEU:C	1:A:220:GLU:HG2	2.35	0.52
1:B:1438:PRO:HB3	1:B:1453:GLY:O	2.09	0.52
1:D:3090:ASP:OD1	1:D:3091:ALA:N	2.43	0.52
1:A:76:ARG:NE	1:A:186:ARG:NH2	2.57	0.52
1:A:711:ALA:HA	1:A:716:ILE:HD11	1.91	0.52
1:D:3291:ALA:O	1:D:3304:THR:HA	2.09	0.52
1:B:1277:MET:HB3	1:B:1307:ARG:NH2	2.25	0.52
1:B:1329:TYR:CE1	1:B:1429:LEU:HD12	2.44	0.52
1:B:1346:SER:OG	1:B:1415:TYR:HB3	2.10	0.52
1:B:1734:THR:HG23	2:B:14:HOH:O	2.09	0.52
1:C:2082:ARG:HH11	1:C:2082:ARG:HG3	1.74	0.52
1:C:2506:GLU:HA	1:C:2509:SER:OG	2.09	0.52
1:C:2741:ILE:N	1:C:2741:ILE:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:HB2	1:A:570:PHE:CE1	2.45	0.52
1:B:1566:THR:O	1:B:1568:TYR:N	2.43	0.52
1:C:2208:ASP:OD1	1:C:2210:SER:OG	2.27	0.52
1:D:3280:PHE:HE1	1:D:3600:LEU:HA	1.74	0.52
1:D:3640:SER:CA	1:D:3676:GLU:HG3	2.39	0.52
1:D:3663:VAL:HG21	1:D:3687:LEU:HD22	1.92	0.52
1:A:358:TYR:C	1:A:360:ASN:H	2.17	0.52
1:A:618:LEU:O	1:A:620:LEU:N	2.43	0.52
1:A:631:THR:O	1:A:632:THR:CB	2.56	0.52
1:C:2689:LEU:CD2	1:C:2693:VAL:HG21	2.40	0.52
1:A:340:LYS:HG2	1:A:400:MET:HE2	1.92	0.52
1:B:1202:GLN:HG3	1:B:1216:THR:CG2	2.38	0.52
1:C:2402:LEU:HA	1:C:2405:GLN:HB2	1.91	0.52
1:C:2537:ILE:HD13	1:C:2574:THR:HG21	1.91	0.52
1:C:2616:GLU:C	1:C:2617:SER:O	2.50	0.52
1:D:3273:MET:O	1:D:3277:MET:N	2.42	0.52
1:A:441:ASN:ND2	1:A:444:SER:OG	2.43	0.52
1:A:573:VAL:HA	1:A:585:LEU:O	2.10	0.52
1:A:574:THR:O	1:A:575:MET:HG3	2.11	0.52
1:A:696:ILE:HD13	1:A:732:VAL:O	2.10	0.52
1:B:1097:TYR:H	1:B:1097:TYR:HD2	1.57	0.52
1:B:1569:ILE:O	1:B:1569:ILE:HG22	2.10	0.52
1:B:1641:ILE:CG1	1:B:1669:ILE:HB	2.40	0.52
1:C:2219:MET:O	1:C:2220:GLU:C	2.53	0.52
1:D:3071:THR:HA	1:D:3232:GLY:O	2.08	0.52
1:A:208:ASP:HB3	1:B:1205:GLU:OE2	2.10	0.51
1:B:1202:GLN:HE21	1:B:1216:THR:HG21	1.74	0.51
1:B:1355:SER:C	1:B:1357:GLU:N	2.68	0.51
1:B:1615:LYS:N	1:B:1618:LEU:HD21	2.25	0.51
1:D:3553:ILE:HD11	1:D:3568:TYR:O	2.10	0.51
1:C:2254:GLN:O	1:C:2255:THR:C	2.53	0.51
1:D:3156:ASN:O	1:D:3157:GLY:C	2.52	0.51
1:D:3517:LEU:C	1:D:3519:GLY:N	2.68	0.51
1:D:3707:ALA:O	1:D:3718:LEU:HD11	2.09	0.51
1:A:447:GLN:C	1:A:449:SER:H	2.18	0.51
1:B:1614:MET:C	1:B:1616:GLU:H	2.17	0.51
1:C:2447:GLN:HB3	1:C:2452:GLN:HB2	1.92	0.51
1:D:3351:ASN:O	1:D:3353:PHE:N	2.43	0.51
1:B:1406:LYS:NZ	1:B:1406:LYS:HB3	2.26	0.51
1:B:1716:ILE:HG21	1:B:1744:ILE:CD1	2.40	0.51
1:C:2328:LEU:HA	1:C:2458:GLN:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2515:MET:HB3	1:C:2546:VAL:H	1.76	0.51
1:A:409:ASP:HB3	1:A:445:ILE:HD13	1.92	0.51
1:A:687:LEU:HG	1:A:706:THR:HG22	1.91	0.51
1:B:1200:LEU:C	1:B:1220:GLU:HG2	2.35	0.51
1:B:1335:PRO:HG3	1:B:1456:VAL:CG2	2.40	0.51
1:B:1492:ARG:NH1	1:B:1682:PRO:HG3	2.25	0.51
1:B:1693:VAL:HG21	1:B:1714:LEU:HD21	1.93	0.51
1:D:3666:GLY:CA	1:D:3690:SER:HB2	2.39	0.51
1:A:292:THR:HG23	1:A:304:THR:HB	1.91	0.51
1:D:3328:LEU:HD12	1:D:3458:GLN:CB	2.40	0.51
1:A:290:THR:HG21	1:A:458:GLN:OE1	2.10	0.51
1:A:491:VAL:HG21	1:A:630:VAL:HG11	1.92	0.51
1:B:1358:TYR:CD2	1:B:1406:LYS:HD3	2.45	0.51
1:B:1430:THR:O	1:B:1431:ASP:HB2	2.11	0.51
1:C:2470:ASN:HD22	1:C:2473:VAL:HB	1.75	0.51
1:D:3350:ASN:O	1:D:3352:THR:HG23	2.09	0.51
1:A:343:THR:HA	1:A:412:TRP:CH2	2.45	0.51
1:B:1347:SER:HA	1:B:1407:MET:HE2	1.92	0.51
1:B:1413:LEU:CD2	1:B:1437:LEU:HD12	2.41	0.51
1:B:1646:PRO:CG	1:B:1669:ILE:HG12	2.37	0.51
1:C:2224:ASN:O	1:C:2225:SER:C	2.52	0.51
1:C:2338:ALA:HB3	1:C:2461:MET:HE1	1.92	0.51
1:D:3224:ASN:O	1:D:3226:ILE:N	2.43	0.51
1:A:264:THR:HG23	1:A:479:PHE:C	2.36	0.51
1:B:1307:ARG:HA	1:B:1308:PRO:C	2.35	0.51
1:B:1536:ILE:HG23	1:B:1597:GLY:O	2.11	0.51
1:C:2209:GLY:O	1:C:2210:SER:C	2.54	0.51
1:C:2413:LEU:O	1:C:2413:LEU:HD23	2.11	0.51
1:A:286:GLY:O	1:A:287:LYS:C	2.54	0.51
1:A:563:VAL:CG2	1:A:564:GLY:N	2.75	0.51
1:A:732:VAL:HG21	1:A:744:ILE:HG12	1.91	0.51
1:B:1490:SER:HA	1:B:1632:THR:HG23	1.93	0.51
1:C:2283:LYS:HD3	1:C:2599:GLN:CG	2.36	0.51
1:D:3172:THR:O	1:D:3174:GLU:N	2.45	0.51
1:B:1675:GLU:O	1:B:1676:GLU:C	2.54	0.50
1:A:406:LYS:NZ	1:A:406:LYS:HB3	2.25	0.50
1:C:2687:LEU:HD23	1:C:2706:THR:HG23	1.93	0.50
1:C:2689:LEU:HD23	1:C:2693:VAL:HG21	1.92	0.50
1:C:2711:ALA:HA	1:C:2716:ILE:CG1	2.41	0.50
1:A:197:PHE:CE1	1:A:429:LEU:HD11	2.46	0.50
1:A:234:ILE:HG23	1:A:250:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1153:SER:C	1:B:1155:GLY:N	2.69	0.50
1:B:1506:GLU:CD	1:B:1506:GLU:N	2.69	0.50
1:B:1535:PRO:HD2	1:B:1538:THR:HG22	1.94	0.50
1:B:1627:LEU:HD23	1:B:1627:LEU:C	2.36	0.50
1:C:2482:ALA:O	1:C:2483:ILE:HG13	2.12	0.50
1:A:287:LYS:CG	1:A:591:GLN:HB2	2.40	0.50
1:A:287:LYS:HG2	1:A:591:GLN:O	2.10	0.50
1:A:565:SER:C	1:A:567:ASN:H	2.20	0.50
1:A:617:SER:C	1:A:619:ASN:H	2.20	0.50
1:A:736:THR:HG22	1:A:737:ALA:N	2.26	0.50
1:C:2267:SER:O	1:C:2268:PRO:C	2.53	0.50
1:C:2354:PRO:HB2	1:C:2358:TYR:CD2	2.47	0.50
1:C:2518:VAL:O	1:C:2518:VAL:HG12	2.11	0.50
1:D:3081:ASP:CB	1:D:3267:SER:OG	2.59	0.50
1:D:3663:VAL:CG2	1:D:3687:LEU:HD22	2.41	0.50
1:A:276:GLN:CG	1:A:607:ILE:HD11	2.27	0.50
1:B:1596:SER:C	1:B:1598:ILE:N	2.66	0.50
1:C:2309:THR:O	1:C:2310:PHE:HB3	2.12	0.50
1:D:3408:GLY:O	1:D:3411:THR:N	2.45	0.50
1:B:1153:SER:O	1:B:1155:GLY:N	2.44	0.50
1:C:2219:MET:HE1	1:C:2263:THR:CG2	2.42	0.50
1:A:337:SER:O	1:A:340:LYS:HB2	2.12	0.50
1:A:577:PRO:O	1:A:578:ALA:C	2.53	0.50
1:B:1100:ILE:O	1:B:1100:ILE:HG22	2.11	0.50
1:C:2566:THR:HB	1:C:2592:PRO:O	2.12	0.50
1:D:3463:ARG:HG2	1:D:3474:MET:SD	2.52	0.50
1:D:3699:MET:HE1	1:D:3746:LEU:HD21	1.93	0.50
1:B:1599:GLN:O	1:B:1600:LEU:C	2.54	0.50
1:C:2399:GLY:O	1:C:2402:LEU:N	2.36	0.50
1:D:3284:VAL:CG1	1:D:3592:PRO:CB	2.89	0.50
1:D:3555:ASP:HB2	1:D:3562:LEU:HG	1.93	0.50
1:A:296:ALA:O	1:A:297:LYS:C	2.53	0.50
1:B:1718:LEU:CD2	1:B:1744:ILE:HB	2.41	0.50
1:C:2193:PHE:C	1:C:2195:SER:H	2.20	0.50
1:C:2569:ILE:HG12	1:C:2590:GLN:HG3	1.93	0.50
1:D:3714:LEU:HD13	1:D:3738:ILE:CD1	2.41	0.50
1:A:82:ARG:HH22	1:A:300:GLU:CD	2.20	0.49
1:A:328:LEU:O	1:A:459:THR:HG23	2.12	0.49
1:B:1337:SER:CB	1:B:1549:GLY:HA2	2.36	0.49
1:B:1438:PRO:HD3	1:B:1454:ILE:HD12	1.94	0.49
1:C:2439:ALA:HB3	1:C:2441:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3420:LYS:HD2	1:D:3474:MET:CE	2.31	0.49
1:D:3467:ALA:HB2	1:D:3474:MET:CG	2.41	0.49
1:A:286:GLY:O	1:A:288:TYR:N	2.45	0.49
1:A:467:ALA:O	1:A:472:GLY:N	2.43	0.49
1:A:498:ILE:HG22	1:A:500:GLY:H	1.76	0.49
1:A:550:THR:HG22	1:A:551:ALA:N	2.26	0.49
1:A:679:ASN:CG	1:A:680:LEU:N	2.70	0.49
1:B:1203:LEU:HD23	1:B:1211:LYS:CB	2.41	0.49
1:B:1718:LEU:HD23	1:B:1744:ILE:O	2.12	0.49
1:C:2649:LEU:O	1:C:2649:LEU:HD22	2.12	0.49
1:C:2739:LYS:CG	1:C:2740:ASN:N	2.74	0.49
1:D:3173:ALA:O	1:D:3174:GLU:C	2.54	0.49
1:A:344:LEU:HD11	1:A:348:ILE:CD1	2.40	0.49
1:B:1306:GLN:O	1:B:1307:ARG:NH1	2.30	0.49
1:C:2646:PRO:HB3	1:C:2662:VAL:HG13	1.94	0.49
1:A:219:MET:HE3	1:A:223:LEU:HD22	1.94	0.49
1:A:310:PHE:HB2	1:A:318:ILE:HG13	1.94	0.49
1:A:342:MET:HG3	1:A:419:PHE:CZ	2.47	0.49
1:B:1221:SER:O	1:B:1222:SER:C	2.56	0.49
1:B:1271:SER:O	1:B:1274:GLU:HB2	2.13	0.49
1:B:1463:ARG:HA	1:B:1466:THR:OG1	2.13	0.49
1:C:2314:THR:O	1:C:2316:GLU:N	2.46	0.49
1:C:2578:ALA:O	1:C:2580:ASN:N	2.44	0.49
1:C:2699:MET:O	1:C:2700:TYR:C	2.55	0.49
1:A:711:ALA:HB2	1:A:718:LEU:HG	1.94	0.49
1:B:1457:THR:CA	2:B:5:HOH:O	2.58	0.49
1:C:2566:THR:C	1:C:2568:TYR:N	2.67	0.49
1:D:3717:GLU:HG3	1:D:3742:LYS:O	2.12	0.49
1:A:352:THR:HB	1:A:406:LYS:NZ	2.27	0.49
1:A:422:GLY:HA3	1:A:437:LEU:HD22	1.94	0.49
1:A:737:ALA:O	1:A:741:ILE:CD1	2.57	0.49
1:B:1223:LEU:HD21	1:B:1480:ILE:HD11	1.95	0.49
1:B:1332:ASN:ND2	1:B:1433:TYR:CD2	2.78	0.49
1:B:1707:ALA:O	1:B:1710:PHE:HB3	2.12	0.49
1:C:2354:PRO:HB3	1:C:2357:GLU:CG	2.43	0.49
1:C:2653:LEU:HD12	1:C:2653:LEU:H	1.76	0.49
1:C:2653:LEU:HD23	1:C:2658:VAL:HG11	1.93	0.49
1:D:3202:GLN:NE2	1:D:3216:THR:HG21	2.27	0.49
1:D:3282:GLU:HA	1:D:3285:LYS:HD3	1.95	0.49
1:D:3289:MET:O	1:D:3306:GLN:HA	2.13	0.49
1:D:3354:PRO:HG2	1:D:3403:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3427:PHE:HB2	1:D:3477:PRO:O	2.13	0.49
1:D:3517:LEU:C	1:D:3519:GLY:H	2.18	0.49
1:D:3701:GLY:O	1:D:3702:TRP:O	2.30	0.49
1:A:542:GLN:CD	1:A:577:PRO:HB3	2.38	0.49
1:C:2515:MET:HB3	1:C:2546:VAL:N	2.27	0.49
1:C:2711:ALA:HA	1:C:2716:ILE:HG12	1.94	0.49
1:C:2741:ILE:CD1	1:C:2741:ILE:H	2.25	0.49
1:D:3185:ASN:CG	1:D:3186:ARG:H	2.21	0.49
1:A:294:VAL:HG12	1:A:295:SER:N	2.28	0.49
1:A:516:ILE:HG23	2:A:4:HOH:O	2.13	0.49
1:D:3070:ARG:HH12	1:D:3234:ILE:CB	2.26	0.49
1:D:3335:PRO:CG	1:D:3456:VAL:HG22	2.43	0.49
1:A:254:GLN:O	1:A:256:VAL:HG22	2.13	0.49
1:A:515:MET:HE3	1:A:547:LYS:HB2	1.95	0.49
1:B:1290:THR:HG22	1:B:1291:ALA:N	2.27	0.49
1:B:1347:SER:CA	1:B:1407:MET:HE2	2.43	0.49
1:B:1716:ILE:HG21	1:B:1744:ILE:HG13	1.95	0.49
1:C:2425:THR:O	1:C:2426:ARG:HB2	2.12	0.49
1:C:2711:ALA:O	1:C:2716:ILE:HD13	2.13	0.49
1:D:3335:PRO:HG3	1:D:3456:VAL:HG22	1.93	0.49
1:A:447:GLN:HA	1:A:450:PHE:HE2	1.78	0.49
1:B:1422:GLY:HA3	1:B:1437:LEU:CD2	2.43	0.49
1:B:1719:GLU:OE2	1:B:1745:LYS:NZ	2.46	0.49
1:C:2188:TYR:N	1:C:2188:TYR:CD1	2.81	0.49
1:C:2358:TYR:C	1:C:2360:ASN:H	2.20	0.49
1:C:2646:PRO:CG	1:C:2669:ILE:HG12	2.36	0.49
1:D:3729:LYS:HB2	1:D:3747:THR:OG1	2.13	0.49
1:A:354:PRO:HD3	1:A:406:LYS:NZ	2.27	0.48
1:A:467:ALA:HB2	1:A:474:MET:HG2	1.94	0.48
1:A:545:ALA:HB3	1:A:575:MET:HB2	1.95	0.48
1:A:676:GLU:C	1:A:678:THR:H	2.21	0.48
1:B:1604:ALA:O	1:B:1605:THR:C	2.55	0.48
1:B:1661:ILE:O	1:B:1662:VAL:C	2.55	0.48
1:C:2277:MET:HE2	1:C:2603:PHE:CE1	2.48	0.48
1:C:2311:ASN:O	1:C:2313:ASP:N	2.46	0.48
1:C:2420:LYS:HD2	1:C:2474:MET:HE1	1.95	0.48
1:C:2436:GLN:N	1:C:2455:SER:OG	2.46	0.48
1:A:263:THR:O	1:A:481:SER:HB3	2.14	0.48
1:A:647:GLY:C	1:A:649:LEU:H	2.21	0.48
1:B:1350:ASN:HB2	1:B:1415:TYR:CE2	2.49	0.48
1:C:2333:TYR:O	1:C:2455:SER:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3293:LEU:HD23	1:D:3293:LEU:O	2.13	0.48
1:D:3323:VAL:HG12	1:D:3325:ARG:HB3	1.94	0.48
1:B:1467:ALA:HB2	1:B:1474:MET:HG3	1.94	0.48
1:D:3188:TYR:O	1:D:3313:ASP:HB2	2.14	0.48
1:D:3516:ILE:HG12	1:D:3578:ALA:CB	2.43	0.48
1:D:3576:ASN:OD1	1:D:3608:LEU:HD22	2.13	0.48
1:A:517:LEU:HD23	1:A:520:THR:CG2	2.43	0.48
1:B:1298:THR:CA	1:B:1475:LEU:HD13	2.43	0.48
1:C:2287:LYS:HG3	1:C:2591:GLN:HB2	1.94	0.48
1:C:2355:SER:O	1:C:2357:GLU:N	2.47	0.48
1:C:2520:THR:O	1:C:2522:PRO:HD3	2.14	0.48
1:C:2599:GLN:HA	1:C:2602:GLU:OE1	2.13	0.48
1:D:3078:THR:CG2	1:D:3089:GLU:HA	2.42	0.48
1:D:3341:VAL:O	1:D:3341:VAL:HG12	2.13	0.48
1:A:194:ALA:O	1:A:195:SER:C	2.56	0.48
1:A:219:MET:O	1:A:220:GLU:C	2.56	0.48
1:A:647:GLY:C	1:A:649:LEU:N	2.71	0.48
1:B:1202:GLN:CG	1:B:1216:THR:HG21	2.42	0.48
1:C:2711:ALA:O	1:C:2716:ILE:CD1	2.62	0.48
1:D:3198:ILE:O	1:D:3219:MET:HB3	2.13	0.48
1:D:3277:MET:HG3	1:D:3307:ARG:NE	2.29	0.48
1:D:3566:THR:O	1:D:3570:PHE:HE1	1.95	0.48
1:B:1348:ILE:HD13	1:B:1510:THR:HG21	1.96	0.48
1:C:2082:ARG:HD3	1:C:2619:ASN:O	2.12	0.48
1:C:2553:ILE:CG1	1:C:2569:ILE:HG13	2.44	0.48
1:C:2613:ALA:O	1:C:2614:MET:CB	2.62	0.48
1:C:2695:GLU:HB3	1:C:2735:ASN:O	2.13	0.48
1:D:3081:ASP:O	1:D:3083:ASN:N	2.46	0.48
1:D:3267:SER:N	1:D:3268:PRO:CD	2.77	0.48
1:D:3425:THR:N	1:D:3432:GLU:OE2	2.46	0.48
1:D:3644:ILE:HD11	1:D:3649:LEU:CA	2.43	0.48
1:C:2251:VAL:C	1:C:2253:GLN:N	2.71	0.48
1:C:2724:GLY:N	1:C:2748:LEU:HB3	2.28	0.48
1:A:286:GLY:C	1:A:288:TYR:N	2.71	0.48
1:B:1343:THR:HA	1:B:1412:TRP:CH2	2.48	0.48
1:B:1478:LYS:HE3	1:B:1495:GLN:O	2.14	0.48
1:D:3072:VAL:HB	1:D:3255:THR:HG21	1.93	0.48
1:D:3420:LYS:CD	1:D:3474:MET:HE1	2.32	0.48
1:D:3456:VAL:HG23	1:D:3457:THR:O	2.13	0.48
1:A:208:ASP:O	1:A:209:GLY:C	2.56	0.48
1:B:1170:LEU:HD22	1:B:1175:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1465:PHE:HB3	1:B:1575:MET:HE2	1.95	0.48
1:C:2418:ARG:C	1:C:2420:LYS:H	2.22	0.48
1:D:3512:ARG:O	1:D:3515:MET:HB2	2.13	0.48
1:D:3553:ILE:CG2	1:D:3554:ALA:N	2.76	0.48
1:D:3704:LYS:O	1:D:3705:GLU:C	2.57	0.48
1:A:427:PHE:HB2	1:A:477:PRO:O	2.14	0.47
1:A:580:ASN:ND2	1:A:580:ASN:C	2.69	0.47
1:B:1326:ASP:OD1	1:B:1328:LEU:HB3	2.14	0.47
1:B:1628:ASP:HB3	1:B:1630:VAL:CG2	2.43	0.47
1:C:2441:ASN:ND2	1:C:2444:SER:OG	2.45	0.47
1:C:2629:LYS:HE2	1:C:2630:VAL:N	2.29	0.47
1:C:2629:LYS:HG2	1:C:2631:THR:H	1.79	0.47
1:D:3638:MET:O	1:D:3677:GLY:N	2.47	0.47
1:A:512:ARG:O	1:A:515:MET:N	2.38	0.47
1:A:563:VAL:CG2	1:A:564:GLY:H	2.28	0.47
1:B:1163:MET:HE3	1:B:1167:LYS:HE3	1.96	0.47
1:C:2426:ARG:HB3	1:C:2651:GLU:CG	2.42	0.47
1:D:3198:ILE:HG22	1:D:3199:GLY:O	2.14	0.47
1:D:3286:GLY:HA2	1:D:3592:PRO:HA	1.97	0.47
1:D:3716:ILE:HD11	1:D:3738:ILE:HD11	1.95	0.47
1:A:96:VAL:HG22	1:A:97:TYR:N	2.28	0.47
1:A:310:PHE:CB	1:A:318:ILE:HG13	2.44	0.47
1:A:729:LYS:HB3	1:A:747:THR:CB	2.34	0.47
1:C:2328:LEU:HA	1:C:2458:GLN:CG	2.45	0.47
1:C:2338:ALA:HB3	1:C:2461:MET:CE	2.44	0.47
1:D:3165:ALA:C	1:D:3167:LYS:N	2.71	0.47
1:D:3537:ILE:HD13	1:D:3574:THR:HG21	1.96	0.47
1:A:457:THR:O	1:A:458:GLN:C	2.57	0.47
1:B:1329:TYR:OH	1:B:1429:LEU:HB3	2.15	0.47
1:B:1329:TYR:HB2	1:B:1432:GLU:HG3	1.96	0.47
1:B:1413:LEU:HD23	1:B:1416:LEU:CD1	2.43	0.47
1:C:2430:THR:O	1:C:2431:ASP:HB2	2.15	0.47
1:C:2433:TYR:CD1	1:C:2433:TYR:N	2.83	0.47
1:D:3426:ARG:O	1:D:3654:ARG:HD2	2.14	0.47
1:A:296:ALA:O	1:A:298:THR:N	2.47	0.47
1:A:599:GLN:HA	1:A:599:GLN:HE21	1.79	0.47
1:B:1400:MET:HA	1:B:1400:MET:CE	2.43	0.47
1:C:2264:THR:HG22	1:C:2481:SER:HB2	1.96	0.47
1:C:2473:VAL:HG12	1:C:2498:ILE:HG23	1.96	0.47
1:D:3414:ASP:O	1:D:3418:ARG:HG3	2.14	0.47
1:A:293:LEU:CD2	1:A:302:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:HA	1:A:335:PRO:HD2	1.60	0.47
1:A:646:PRO:HA	1:A:669:ILE:HD11	1.96	0.47
1:A:663:VAL:HG11	1:A:710:PHE:CE1	2.50	0.47
1:A:696:ILE:HD12	1:A:732:VAL:CG1	2.44	0.47
1:A:696:ILE:HD12	1:A:732:VAL:HB	1.96	0.47
1:B:1082:ARG:NH2	1:B:1300:GLU:CD	2.73	0.47
1:B:1082:ARG:O	1:B:1083:ASN:ND2	2.48	0.47
1:B:1233:ILE:O	1:B:1233:ILE:HG22	2.15	0.47
1:B:1280:PHE:CB	1:B:1603:PHE:HD1	2.28	0.47
1:B:1689:LEU:HD12	1:B:1713:TRP:CD2	2.50	0.47
1:B:1734:THR:O	1:B:1735:ASN:CB	2.62	0.47
1:D:3167:LYS:HB3	1:D:3171:GLU:OE1	2.15	0.47
1:D:3335:PRO:HB3	1:D:3461:MET:HE2	1.96	0.47
1:A:340:LYS:CA	1:A:400:MET:HE2	2.44	0.47
1:B:1188:TYR:OH	1:B:1200:LEU:HA	2.14	0.47
1:B:1699:MET:HE1	1:B:1746:LEU:HD21	1.92	0.47
1:D:3230:THR:HG22	1:D:3231:ASP:O	2.14	0.47
1:D:3605:THR:N	1:D:3606:PRO:CD	2.78	0.47
1:B:1221:SER:O	1:B:1224:ASN:N	2.48	0.47
1:B:1223:LEU:HD12	1:B:1655:ARG:HD2	1.97	0.47
1:B:1224:ASN:O	1:B:1228:ALA:N	2.42	0.47
1:B:1354:PRO:HB3	1:B:1358:TYR:HD2	1.80	0.47
1:B:1545:ALA:N	1:B:1578:ALA:HB2	2.30	0.47
1:B:1600:LEU:O	1:B:1603:PHE:HB3	2.14	0.47
1:C:2478:LYS:HE3	1:C:2494:SER:OG	2.15	0.47
1:C:2695:GLU:HB3	1:C:2735:ASN:HA	1.96	0.47
1:A:649:LEU:HD13	1:A:688:LEU:CD1	2.41	0.47
1:B:1457:THR:HB	2:B:5:HOH:O	2.15	0.47
1:C:2714:LEU:HB2	1:C:2716:ILE:CD1	2.36	0.47
1:D:3233:ILE:N	1:D:3253:GLN:HB2	2.30	0.47
1:D:3461:MET:O	1:D:3465:PHE:N	2.44	0.47
1:A:361:SER:O	1:A:362:SER:C	2.58	0.46
1:B:1488:ASN:ND2	1:B:1490:SER:H	2.13	0.46
1:C:2704:LYS:HG3	1:C:2748:LEU:HD11	1.97	0.46
1:D:3420:LYS:HE3	1:D:3499:VAL:O	2.14	0.46
1:A:276:GLN:HB3	1:A:603:PHE:HD1	1.79	0.46
1:A:474:MET:CB	1:A:499:VAL:HG23	2.45	0.46
1:A:566:THR:C	1:A:568:TYR:N	2.68	0.46
1:B:1640:SER:CA	1:B:1676:GLU:HG3	2.41	0.46
1:C:2266:SER:O	1:C:2267:SER:C	2.58	0.46
1:C:2422:GLY:HA3	1:C:2437:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2491:VAL:CG1	1:C:2492:ARG:N	2.57	0.46
1:C:2724:GLY:H	1:C:2748:LEU:HB3	1.81	0.46
1:A:69:THR:HA	1:A:235:THR:HA	1.97	0.46
1:B:1628:ASP:O	1:B:1630:VAL:N	2.44	0.46
1:C:2340:LYS:HG2	1:C:2400:MET:CG	2.43	0.46
1:C:2452:GLN:HA	1:C:2452:GLN:HE21	1.81	0.46
1:C:2499:VAL:O	1:C:2499:VAL:HG23	2.15	0.46
1:D:3337:SER:HB2	1:D:3549:GLY:HA3	1.97	0.46
1:D:3513:ASN:O	1:D:3517:LEU:HG	2.15	0.46
1:A:624:ALA:O	1:A:627:LEU:HB2	2.15	0.46
1:A:700:TYR:C	1:A:700:TYR:CD1	2.93	0.46
1:B:1293:LEU:HD22	1:B:1302:LEU:HB2	1.97	0.46
1:B:1353:PHE:O	1:B:1354:PRO:C	2.58	0.46
1:C:2350:ASN:HD22	1:C:2352:THR:HG21	1.79	0.46
1:C:2355:SER:C	1:C:2357:GLU:N	2.70	0.46
1:C:2618:LEU:O	1:C:2618:LEU:HG	2.15	0.46
1:D:3095:ASN:ND2	1:D:3157:GLY:N	2.64	0.46
1:D:3263:THR:O	1:D:3481:SER:HB3	2.16	0.46
1:D:3458:GLN:O	1:D:3462:LEU:HG	2.16	0.46
1:D:3472:GLY:O	1:D:3501:ASN:HA	2.15	0.46
1:D:3641:ILE:HD11	1:D:3669:ILE:HG22	1.97	0.46
1:A:272:PHE:CE2	1:A:607:ILE:HD13	2.51	0.46
1:A:352:THR:O	1:A:353:PHE:O	2.32	0.46
1:B:1343:THR:CB	1:B:1400:MET:HE2	2.44	0.46
1:B:1355:SER:O	1:B:1357:GLU:N	2.48	0.46
1:C:2262:TYR:CD1	1:C:2627:LEU:HD11	2.51	0.46
1:C:2314:THR:C	1:C:2316:GLU:H	2.23	0.46
1:D:3512:ARG:O	1:D:3516:ILE:HG13	2.15	0.46
1:A:629:LYS:O	1:A:630:VAL:HG22	2.15	0.46
1:B:1352:THR:C	1:B:1406:LYS:NZ	2.74	0.46
1:B:1443:VAL:O	1:B:1444:SER:C	2.59	0.46
1:B:1641:ILE:HG13	1:B:1669:ILE:HB	1.96	0.46
1:B:1644:ILE:HD11	1:B:1649:LEU:N	2.30	0.46
1:B:1710:PHE:CZ	1:B:1714:LEU:CD1	2.95	0.46
1:C:2082:ARG:NH2	1:C:2300:GLU:CD	2.74	0.46
1:C:2245:VAL:HG12	1:D:3431:ASP:HB3	1.97	0.46
1:C:2344:LEU:O	1:C:2348:ILE:HG13	2.16	0.46
1:C:2562:LEU:HB3	1:C:2567:ASN:HD22	1.80	0.46
1:D:3607:ILE:O	1:D:3610:ARG:HB3	2.15	0.46
1:D:3637:ALA:O	1:D:3639:PRO:HD3	2.16	0.46
1:A:92:THR:HA	1:A:184:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:SER:OG	1:A:399:GLY:N	2.49	0.46
1:A:484:TYR:CD1	1:A:490:SER:O	2.69	0.46
1:A:659:GLN:O	1:A:685:GLN:HA	2.15	0.46
1:B:1097:TYR:CD2	1:B:1097:TYR:N	2.84	0.46
1:B:1280:PHE:CD2	1:B:1289:MET:HE1	2.51	0.46
1:B:1338:ALA:O	1:B:1341:VAL:HG23	2.15	0.46
1:B:1342:MET:HG3	1:B:1419:PHE:CZ	2.50	0.46
1:B:1574:THR:OG1	1:B:1585:LEU:HB3	2.15	0.46
1:C:2344:LEU:CG	1:C:2511:THR:HG23	2.38	0.46
1:C:2677:GLY:O	1:C:2678:THR:C	2.59	0.46
1:D:3079:ILE:CG2	1:D:3219:MET:HE3	2.45	0.46
1:D:3081:ASP:HB3	1:D:3267:SER:OG	2.16	0.46
1:D:3641:ILE:HG13	1:D:3669:ILE:HB	1.98	0.46
1:A:223:LEU:HD21	1:A:480:ILE:CD1	2.44	0.46
1:B:1292:THR:HG23	1:B:1304:THR:OG1	2.16	0.46
1:B:1590:GLN:HG2	1:B:1591:GLN:OE1	2.16	0.46
1:B:1646:PRO:O	1:B:1650:ALA:HB2	2.16	0.46
1:C:2442:ILE:HG13	1:C:2443:VAL:H	1.80	0.46
1:D:3160:TYR:OH	1:D:3164:MET:HE2	2.16	0.46
1:D:3281:LEU:O	1:D:3285:LYS:N	2.49	0.46
1:A:294:VAL:HG21	1:A:462:LEU:HD13	1.97	0.46
1:A:462:LEU:HA	1:A:465:PHE:HB2	1.98	0.46
1:A:653:LEU:O	1:A:658:VAL:HB	2.16	0.46
1:A:690:SER:C	1:A:692:LYS:H	2.24	0.46
1:B:1666:GLY:HA3	1:B:1691:ASP:OD1	2.15	0.46
1:C:2447:GLN:C	1:C:2449:SER:N	2.74	0.46
1:C:2583:PHE:HE2	1:C:2612:SER:HA	1.81	0.46
1:C:2645:SER:O	1:C:2646:PRO:C	2.59	0.46
1:C:2672:THR:HG22	1:C:2688:LEU:CD2	2.46	0.46
1:D:3192:GLN:O	1:D:3274:GLU:HG3	2.16	0.46
1:D:3701:GLY:O	1:D:3702:TRP:C	2.58	0.46
1:A:344:LEU:O	1:A:344:LEU:HD12	2.16	0.46
1:A:350:ASN:O	1:A:352:THR:HG23	2.16	0.46
1:A:668:LYS:O	1:A:690:SER:HA	2.16	0.46
1:B:1553:ILE:HG22	1:B:1554:ALA:N	2.30	0.46
1:B:1603:PHE:CD2	1:B:1603:PHE:C	2.94	0.46
1:B:1689:LEU:HD12	1:B:1713:TRP:CE3	2.51	0.46
1:B:1708:GLU:O	1:B:1711:ALA:N	2.49	0.46
1:C:2472:GLY:HA3	1:C:2503:VAL:O	2.16	0.46
1:A:81:ASP:C	1:A:83:ASN:N	2.73	0.45
1:A:469:ALA:HA	1:A:512:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:SER:HB2	1:B:1157:GLY:HA2	1.99	0.45
1:B:1314:THR:O	1:B:1315:LYS:CB	2.64	0.45
1:C:2610:ARG:O	1:C:2613:ALA:O	2.34	0.45
1:D:3153:SER:C	1:D:3155:GLY:N	2.73	0.45
1:D:3488:ASN:ND2	1:D:3490:SER:N	2.64	0.45
1:B:1479:PHE:CD2	1:B:1479:PHE:N	2.85	0.45
1:B:1516:ILE:C	1:B:1518:VAL:N	2.73	0.45
1:C:2329:TYR:CE2	1:C:2330:GLN:HG3	2.51	0.45
1:C:2336:GLY:HA2	1:C:2451:GLY:HA3	1.97	0.45
1:C:2463:ARG:HD2	1:C:2499:VAL:HG21	1.98	0.45
1:C:2512:ARG:HB2	1:C:2512:ARG:NH1	2.31	0.45
1:D:3412:TRP:CZ2	1:D:3416:LEU:HD21	2.51	0.45
1:D:3553:ILE:HD11	1:D:3568:TYR:C	2.41	0.45
1:C:2254:GLN:O	1:C:2256:VAL:CG2	2.61	0.45
1:C:2736:THR:O	1:C:2737:ALA:C	2.59	0.45
1:D:3354:PRO:HB2	1:D:3359:PHE:HE1	1.77	0.45
1:A:277:MET:HE1	1:A:291:ALA:HB2	1.98	0.45
1:A:290:THR:CG2	1:A:291:ALA:N	2.79	0.45
1:A:710:PHE:CZ	1:A:714:LEU:HD12	2.51	0.45
1:B:1097:TYR:HD2	1:B:1097:TYR:N	2.14	0.45
1:B:1347:SER:N	1:B:1407:MET:HE2	2.32	0.45
1:C:2629:LYS:O	1:C:2631:THR:N	2.48	0.45
1:C:2711:ALA:HA	1:C:2716:ILE:HD11	1.99	0.45
1:D:3544:VAL:HG22	1:D:3576:ASN:HB3	1.98	0.45
1:B:1072:VAL:HB	1:B:1255:THR:CG2	2.44	0.45
1:B:1191:GLY:HA2	1:B:1311:ASN:OD1	2.17	0.45
1:B:1517:LEU:O	1:B:1518:VAL:C	2.60	0.45
1:B:1640:SER:HA	1:B:1676:GLU:CG	2.43	0.45
1:C:2287:LYS:HG2	1:C:2591:GLN:O	2.17	0.45
1:C:2448:SER:CA	1:C:2452:GLN:O	2.64	0.45
1:C:2485:ASP:OD1	1:C:2487:ASN:HB2	2.17	0.45
1:A:409:ASP:HB3	1:A:445:ILE:CD1	2.47	0.45
1:A:442:ILE:HG13	1:A:443:VAL:N	2.31	0.45
1:B:1066:HIS:N	1:B:1066:HIS:HD1	2.15	0.45
1:B:1491:VAL:CB	1:B:1630:VAL:HG11	2.47	0.45
1:C:2314:THR:C	1:C:2316:GLU:N	2.74	0.45
1:C:2662:VAL:HA	1:C:2688:LEU:HB2	1.99	0.45
1:D:3413:LEU:O	1:D:3416:LEU:HB2	2.17	0.45
1:D:3645:SER:O	1:D:3646:PRO:C	2.59	0.45
1:D:3711:ALA:HB2	1:D:3718:LEU:CD1	2.47	0.45
1:A:413:LEU:O	1:A:413:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LEU:HB2	1:A:716:ILE:HD12	1.99	0.45
1:B:1259:LYS:HE2	1:B:1485:ASP:OD2	2.17	0.45
1:B:1736:THR:O	1:B:1737:ALA:C	2.59	0.45
1:C:2402:LEU:O	1:C:2403:LEU:C	2.59	0.45
1:C:2439:ALA:HB3	1:C:2444:SER:OG	2.16	0.45
1:D:3599:GLN:O	1:D:3600:LEU:C	2.59	0.45
1:A:439:ALA:H	1:A:444:SER:HB3	1.82	0.45
1:A:566:THR:O	1:A:591:GLN:HA	2.17	0.45
1:A:629:LYS:C	1:A:630:VAL:HG13	2.30	0.45
1:A:727:VAL:HG21	1:A:746:LEU:HD13	1.98	0.45
1:B:1185:ASN:CG	1:B:1186:ARG:N	2.73	0.45
1:C:2208:ASP:O	1:C:2210:SER:N	2.49	0.45
1:D:3251:VAL:HG23	1:D:3252:SER:N	2.32	0.45
1:D:3359:PHE:O	1:D:3360:ASN:C	2.60	0.45
1:A:508:ALA:O	1:A:511:THR:N	2.48	0.45
1:B:1406:LYS:HB3	1:B:1406:LYS:HZ3	1.81	0.45
1:B:1484:TYR:CE2	1:B:1486:THR:HG22	2.51	0.45
1:B:1488:ASN:C	1:B:1488:ASN:ND2	2.71	0.45
1:B:1641:ILE:HD11	1:B:1669:ILE:O	2.17	0.45
1:A:653:LEU:HD22	1:A:658:VAL:HG11	1.99	0.45
1:B:1200:LEU:O	1:B:1220:GLU:HG2	2.17	0.45
1:B:1447:GLN:C	1:B:1449:SER:H	2.25	0.45
1:B:1619:ASN:C	1:B:1621:GLN:N	2.75	0.45
1:C:2289:MET:HB2	1:C:2307:ARG:HB2	1.97	0.45
1:D:3345:ALA:CB	1:D:3468:ILE:HD11	2.46	0.45
1:B:1700:TYR:CD2	1:B:1728:GLN:HA	2.52	0.44
1:D:3264:THR:HG23	1:D:3479:PHE:C	2.42	0.44
1:D:3644:ILE:CD1	1:D:3649:LEU:HB2	2.47	0.44
1:A:315:LYS:N	1:A:315:LYS:HD3	2.31	0.44
1:A:474:MET:HG3	1:A:502:PRO:CD	2.47	0.44
1:B:1193:PHE:CD1	1:B:1193:PHE:C	2.94	0.44
1:D:3224:ASN:O	1:D:3225:SER:C	2.60	0.44
1:D:3274:GLU:OE1	1:D:3274:GLU:HA	2.17	0.44
1:D:3436:GLN:N	1:D:3455:SER:OG	2.50	0.44
1:D:3699:MET:HE3	1:D:3746:LEU:HD21	1.99	0.44
1:A:251:VAL:O	1:A:252:SER:C	2.60	0.44
1:A:254:GLN:O	1:A:255:THR:C	2.59	0.44
1:A:490:SER:HB3	1:A:632:THR:CG2	2.45	0.44
1:B:1198:ILE:HD11	1:B:1265:LEU:CD1	2.48	0.44
1:B:1266:SER:O	1:B:1267:SER:C	2.59	0.44
1:B:1294:VAL:HG12	1:B:1295:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:TYR:CZ	1:B:1429:LEU:HB3	2.52	0.44
1:C:2457:THR:O	1:C:2460:GLN:N	2.47	0.44
1:C:2563:VAL:CG2	1:C:2564:GLY:N	2.80	0.44
1:C:2636:TYR:CZ	1:C:2656:ASN:ND2	2.86	0.44
1:C:2649:LEU:HD13	1:C:2688:LEU:HD11	1.95	0.44
1:D:3596:SER:C	1:D:3598:ILE:N	2.75	0.44
1:A:416:LEU:O	1:A:417:LYS:C	2.59	0.44
1:A:467:ALA:HB2	1:A:474:MET:CG	2.47	0.44
1:B:1172:THR:O	1:B:1173:ALA:CB	2.65	0.44
1:B:1714:LEU:HD13	1:B:1738:ILE:HD11	1.99	0.44
1:C:2426:ARG:O	1:C:2654:ARG:NH1	2.51	0.44
1:C:2433:TYR:N	1:C:2433:TYR:HD1	2.16	0.44
1:C:2629:LYS:HE3	1:C:2631:THR:HA	1.99	0.44
1:C:2656:ASN:C	1:C:2657:ILE:HG13	2.43	0.44
1:D:3221:SER:O	1:D:3224:ASN:HB2	2.16	0.44
1:D:3590:GLN:O	1:D:3591:GLN:C	2.60	0.44
1:D:3717:GLU:O	1:D:3743:LYS:HA	2.18	0.44
1:A:338:ALA:HB3	1:A:461:MET:HE1	1.98	0.44
1:A:452:GLN:HA	1:A:452:GLN:HE21	1.81	0.44
1:A:630:VAL:O	1:A:631:THR:OG1	2.29	0.44
1:B:1640:SER:HB2	1:B:1676:GLU:CD	2.42	0.44
1:B:1658:VAL:CG1	1:B:1680:LEU:HD23	2.47	0.44
1:C:2293:LEU:HD23	1:C:2302:LEU:CB	2.44	0.44
1:C:2304:THR:O	1:C:2305:THR:HB	2.18	0.44
1:C:2490:SER:C	1:C:2491:VAL:HG23	2.42	0.44
1:C:2605:THR:HG22	1:C:2609:GLU:OE1	2.18	0.44
1:D:3348:ILE:CD1	1:D:3510:THR:CG2	2.95	0.44
1:D:3702:TRP:O	1:D:3727:VAL:HG23	2.18	0.44
1:A:296:ALA:N	1:A:582:ASP:O	2.45	0.44
1:A:461:MET:O	1:A:462:LEU:C	2.60	0.44
1:A:470:ASN:O	1:A:470:ASN:CG	2.59	0.44
1:A:470:ASN:O	1:A:472:GLY:N	2.50	0.44
1:B:1516:ILE:O	1:B:1517:LEU:C	2.61	0.44
1:B:1596:SER:HB3	1:B:1599:GLN:NE2	2.33	0.44
1:B:1702:TRP:HE3	1:B:1707:ALA:HA	1.82	0.44
1:C:2694:GLU:C	1:C:2738:ILE:HG22	2.43	0.44
1:D:3413:LEU:HA	1:D:3416:LEU:HD12	2.00	0.44
1:D:3441:ASN:OD1	1:D:3441:ASN:C	2.59	0.44
1:D:3512:ARG:NH1	1:D:3578:ALA:O	2.51	0.44
1:D:3564:GLY:O	1:D:3565:SER:C	2.60	0.44
1:D:3649:LEU:HD22	1:D:3653:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:O	1:A:285:LYS:HA	2.18	0.44
1:A:281:LEU:O	1:A:285:LYS:N	2.47	0.44
1:A:399:GLY:O	1:A:402:LEU:HB2	2.17	0.44
1:A:517:LEU:HA	1:A:520:THR:CB	2.36	0.44
1:A:739:LYS:CE	1:A:740:ASN:HD21	2.31	0.44
1:B:1193:PHE:C	1:B:1195:SER:N	2.74	0.44
1:B:1474:MET:HB3	1:B:1499:VAL:CG2	2.47	0.44
1:B:1519:GLY:O	1:B:1520:THR:C	2.60	0.44
1:C:2281:LEU:HD13	1:C:2289:MET:HG3	1.99	0.44
1:D:3334:GLU:O	1:D:3551:ALA:HB1	2.17	0.44
1:D:3515:MET:HE1	1:D:3575:MET:HE3	1.99	0.44
1:D:3687:LEU:HG	1:D:3706:THR:HG23	1.99	0.44
1:A:81:ASP:C	1:A:83:ASN:H	2.26	0.44
1:A:676:GLU:HG2	1:A:677:GLY:N	2.33	0.44
1:B:1545:ALA:H	1:B:1578:ALA:HB2	1.83	0.44
1:B:1652:ALA:HA	1:B:1655:ARG:CZ	2.47	0.44
1:B:1672:THR:HG22	1:B:1673:SER:N	2.33	0.44
1:B:1704:LYS:O	1:B:1705:GLU:C	2.61	0.44
1:C:2267:SER:O	1:C:2271:SER:HB2	2.17	0.44
1:D:3282:GLU:HA	1:D:3285:LYS:CD	2.48	0.44
1:A:699:MET:HG2	1:A:702:TRP:CD2	2.52	0.44
1:B:1447:GLN:C	1:B:1449:SER:N	2.75	0.44
1:A:232:GLY:HA3	1:A:255:THR:OG1	2.18	0.43
1:A:430:THR:HG21	1:B:1067:GLN:OE1	2.17	0.43
1:A:504:SER:O	1:A:507:ALA:HB3	2.17	0.43
1:B:1413:LEU:O	1:B:1416:LEU:HB2	2.18	0.43
1:C:2206:ASN:C	1:C:2208:ASP:H	2.26	0.43
1:C:2429:LEU:HD21	1:C:2479:PHE:CZ	2.53	0.43
1:C:2504:SER:O	1:C:2507:ALA:HB3	2.17	0.43
1:A:234:ILE:HG23	1:A:250:LEU:CD1	2.48	0.43
1:A:459:THR:O	1:A:460:GLN:C	2.61	0.43
1:B:1170:LEU:C	1:B:1172:THR:N	2.69	0.43
1:B:1553:ILE:CG2	1:B:1554:ALA:N	2.82	0.43
1:B:1702:TRP:H	1:B:1702:TRP:CD1	2.34	0.43
1:C:2501:ASN:C	1:C:2501:ASN:HD22	2.25	0.43
1:D:3415:TYR:O	1:D:3419:PHE:HD2	2.00	0.43
1:D:3425:THR:HG21	1:D:3459:THR:C	2.43	0.43
1:D:3476:GLU:OE1	1:D:3476:GLU:HA	2.18	0.43
1:D:3740:ASN:O	1:D:3741:ILE:C	2.61	0.43
1:A:96:VAL:CG2	1:A:97:TYR:N	2.81	0.43
1:A:629:LYS:O	1:A:630:VAL:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:SER:O	1:A:646:PRO:C	2.60	0.43
1:B:1353:PHE:C	1:B:1353:PHE:CD2	2.96	0.43
1:B:1426:ARG:N	1:B:1432:GLU:OE1	2.50	0.43
1:B:1473:VAL:CG1	1:B:1498:ILE:HG23	2.48	0.43
1:B:1497:GLU:HG3	1:B:1659:GLN:NE2	2.32	0.43
1:B:1564:GLY:C	1:B:1565:SER:O	2.61	0.43
1:C:2199:GLY:O	1:C:2200:LEU:HG	2.18	0.43
1:C:2309:THR:HB	1:C:2310:PHE:H	1.20	0.43
1:C:2420:LYS:HB3	1:C:2463:ARG:NH2	2.33	0.43
1:C:2632:THR:O	1:C:2633:GLU:C	2.61	0.43
1:C:2689:LEU:HD12	1:C:2713:TRP:CD2	2.54	0.43
1:A:94:TYR:N	1:A:94:TYR:CD1	2.86	0.43
1:A:645:SER:O	1:A:647:GLY:N	2.50	0.43
1:C:2270:GLN:OE1	1:C:2304:THR:N	2.48	0.43
1:C:2409:ASP:HB3	1:C:2445:ILE:HG21	2.00	0.43
1:D:3601:GLY:C	1:D:3603:PHE:N	2.76	0.43
1:A:652:ALA:HA	1:A:655:ARG:NH2	2.33	0.43
1:A:681:ALA:HB1	1:A:682:PRO:HD2	2.00	0.43
1:A:711:ALA:HA	1:A:716:ILE:CD1	2.49	0.43
1:A:714:LEU:HB2	1:A:716:ILE:CD1	2.49	0.43
1:B:1644:ILE:CD1	1:B:1649:LEU:HB2	2.49	0.43
1:B:1668:LYS:HB2	1:B:1691:ASP:CG	2.44	0.43
1:C:2491:VAL:O	1:C:2492:ARG:HG3	2.18	0.43
1:C:2547:LYS:HA	1:C:2547:LYS:HD2	1.83	0.43
1:C:2615:LYS:O	1:C:2617:SER:O	2.37	0.43
1:D:3094:TYR:C	1:D:3095:ASN:HD22	2.26	0.43
1:D:3355:SER:O	1:D:3356:GLY:C	2.61	0.43
1:D:3501:ASN:HB2	1:D:3700:TYR:CG	2.53	0.43
1:D:3537:ILE:CD1	1:D:3574:THR:HG21	2.48	0.43
1:A:689:LEU:CD2	1:A:693:VAL:HG21	2.48	0.43
1:B:1293:LEU:CD2	1:B:1302:LEU:HB2	2.49	0.43
1:B:1483:ILE:HG13	1:B:1657:ILE:HD11	2.01	0.43
1:C:2082:ARG:HG3	1:C:2082:ARG:NH1	2.33	0.43
1:D:3254:GLN:O	1:D:3255:THR:C	2.62	0.43
1:A:90:ASP:OD2	1:A:92:THR:HG22	2.18	0.43
1:A:480:ILE:CG2	1:A:657:ILE:HD11	2.48	0.43
1:B:1704:LYS:HE2	1:B:1720:PHE:CD2	2.53	0.43
1:C:2550:THR:HG23	1:C:2568:TYR:HB3	1.99	0.43
1:D:3292:THR:HG23	1:D:3304:THR:OG1	2.19	0.43
1:D:3404:GLU:OE2	1:D:3409:ASP:OD1	2.35	0.43
1:A:81:ASP:OD1	1:A:85:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:O	1:A:329:TYR:N	2.52	0.43
1:A:339:MET:HE3	1:A:454:ILE:HD13	1.99	0.43
1:A:647:GLY:O	1:A:649:LEU:N	2.51	0.43
1:B:1193:PHE:HD1	1:B:1193:PHE:O	2.02	0.43
1:B:1605:THR:O	1:B:1609:GLU:HB2	2.18	0.43
1:B:1684:GLN:HG2	1:B:1685:GLN:N	2.33	0.43
1:C:2483:ILE:O	1:C:2483:ILE:HG22	2.18	0.43
1:C:2668:LYS:HB2	1:C:2691:ASP:CG	2.44	0.43
1:D:3167:LYS:HB3	1:D:3171:GLU:CD	2.44	0.43
1:A:427:PHE:N	1:A:427:PHE:CD1	2.87	0.43
1:A:508:ALA:O	1:A:511:THR:HB	2.18	0.43
1:B:1214:LEU:CD1	1:B:1215:GLY:H	2.31	0.43
1:B:1262:TYR:HB2	1:B:1482:ALA:HB3	2.00	0.43
1:B:1516:ILE:O	1:B:1518:VAL:N	2.52	0.43
1:B:1719:GLU:HB3	1:B:1745:LYS:HG3	2.01	0.43
1:C:2194:ALA:O	1:C:2195:SER:C	2.62	0.43
1:C:2509:SER:O	1:C:2513:ASN:OD1	2.37	0.43
1:D:3643:ASP:C	1:D:3644:ILE:HG22	2.43	0.43
1:B:1090:ASP:OD1	1:B:1091:ALA:N	2.51	0.43
1:B:1234:ILE:HA	1:B:1251:VAL:HA	2.00	0.43
1:B:1266:SER:C	1:B:1268:PRO:HD2	2.43	0.43
1:B:1436:GLN:N	1:B:1455:SER:OG	2.52	0.43
1:C:2490:SER:HB3	1:C:2632:THR:O	2.18	0.43
1:C:2512:ARG:HH11	1:C:2512:ARG:CB	2.30	0.43
1:D:3277:MET:HE2	1:D:3603:PHE:CE1	2.54	0.43
1:A:302:LEU:O	1:A:303:ALA:HB2	2.18	0.42
1:A:340:LYS:CG	1:A:400:MET:HE2	2.48	0.42
1:A:470:ASN:C	1:A:472:GLY:N	2.75	0.42
1:A:571:SER:HA	1:A:587:VAL:O	2.19	0.42
1:B:1079:ILE:HG21	1:B:1219:MET:HE3	2.01	0.42
1:B:1290:THR:O	1:B:1587:VAL:HG13	2.18	0.42
1:B:1441:ASN:C	1:B:1443:VAL:N	2.76	0.42
1:B:1445:ILE:O	1:B:1448:SER:OG	2.35	0.42
1:C:2078:THR:HG22	1:C:2089:GLU:HA	2.01	0.42
1:D:3072:VAL:HB	1:D:3255:THR:HG22	1.99	0.42
1:D:3327:ILE:H	1:D:3327:ILE:HG13	1.59	0.42
1:D:3680:LEU:HD12	1:D:3684:GLN:OE1	2.19	0.42
1:A:329:TYR:CE1	1:A:429:LEU:HD12	2.53	0.42
1:B:1079:ILE:HG21	1:B:1219:MET:CE	2.49	0.42
1:B:1354:PRO:HB2	1:B:1359:PHE:CE2	2.54	0.42
1:B:1618:LEU:O	1:B:1619:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2542:GLN:NE2	1:C:2577:PRO:HB3	2.35	0.42
1:C:2553:ILE:HD11	1:C:2568:TYR:O	2.19	0.42
1:C:2578:ALA:C	1:C:2580:ASN:N	2.76	0.42
1:C:2638:MET:SD	1:C:2639:PRO:HD2	2.59	0.42
1:C:2711:ALA:HB2	1:C:2718:LEU:HD12	2.01	0.42
1:D:3081:ASP:C	1:D:3083:ASN:H	2.26	0.42
1:D:3403:LEU:O	1:D:3407:MET:HE3	2.18	0.42
1:A:652:ALA:CB	1:B:1250:LEU:HD22	2.49	0.42
1:B:1081:ASP:OD1	1:B:1081:ASP:C	2.62	0.42
1:B:1222:SER:CB	1:B:1430:THR:HG23	2.49	0.42
1:B:1517:LEU:C	1:B:1519:GLY:H	2.28	0.42
1:B:1619:ASN:O	1:B:1620:LEU:C	2.60	0.42
1:D:3687:LEU:O	1:D:3688:LEU:HD23	2.18	0.42
1:A:354:PRO:HB2	1:A:358:TYR:CE2	2.53	0.42
1:A:650:ALA:CA	1:A:660:PRO:HG3	2.47	0.42
1:A:666:GLY:CA	1:A:690:SER:HB2	2.49	0.42
1:B:1492:ARG:HD2	1:B:1634:SER:HB2	2.02	0.42
1:B:1689:LEU:HB2	1:B:1713:TRP:CZ3	2.54	0.42
1:B:1708:GLU:O	1:B:1709:THR:C	2.62	0.42
1:C:2318:ILE:HG22	1:C:2318:ILE:O	2.17	0.42
1:C:2490:SER:HB2	1:C:2634:SER:OG	2.19	0.42
1:C:2729:LYS:HB3	1:C:2747:THR:OG1	2.20	0.42
1:D:3461:MET:O	1:D:3464:ALA:HB3	2.20	0.42
1:A:354:PRO:HB2	1:A:358:TYR:CZ	2.54	0.42
1:A:399:GLY:O	1:A:402:LEU:N	2.52	0.42
1:A:425:THR:HG21	1:A:459:THR:HB	2.02	0.42
1:A:636:TYR:CZ	1:A:656:ASN:ND2	2.87	0.42
1:B:1083:ASN:HD22	1:B:1083:ASN:HA	1.72	0.42
1:B:1298:THR:HA	1:B:1475:LEU:HD13	2.02	0.42
1:B:1513:ASN:HA	1:B:1516:ILE:HG13	2.02	0.42
1:B:1605:THR:N	1:B:1606:PRO:CD	2.82	0.42
1:B:1672:THR:HG22	1:B:1673:SER:H	1.84	0.42
1:C:2335:PRO:HB3	1:C:2456:VAL:HG21	2.01	0.42
1:C:2711:ALA:HB2	1:C:2718:LEU:CD1	2.49	0.42
1:D:3553:ILE:HG13	1:D:3568:TYR:HA	2.01	0.42
1:A:447:GLN:C	1:A:449:SER:N	2.77	0.42
1:A:476:GLU:HB2	1:A:499:VAL:HG13	2.00	0.42
1:B:1406:LYS:NZ	1:B:1406:LYS:CB	2.83	0.42
1:B:1570:PHE:N	1:B:1570:PHE:CD1	2.87	0.42
1:C:2273:MET:HE3	1:C:2303:ALA:CB	2.50	0.42
1:C:2505:LYS:O	1:C:2507:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2659:GLN:O	1:C:2685:GLN:HA	2.18	0.42
1:D:3080:TYR:CD1	1:D:3084:GLY:O	2.72	0.42
1:A:251:VAL:C	1:A:253:GLN:N	2.78	0.42
1:A:472:GLY:O	1:A:501:ASN:ND2	2.53	0.42
1:B:1700:TYR:OH	1:B:1728:GLN:NE2	2.53	0.42
1:D:3153:SER:O	1:D:3155:GLY:N	2.52	0.42
1:D:3232:GLY:HA2	1:D:3253:GLN:O	2.19	0.42
1:A:434:ALA:O	1:A:460:GLN:NE2	2.52	0.42
1:A:470:ASN:C	1:A:472:GLY:H	2.27	0.42
1:A:573:VAL:HG22	1:A:574:THR:N	2.34	0.42
1:B:1624:ALA:O	1:B:1626:ASN:N	2.52	0.42
1:B:1658:VAL:CG2	1:B:1680:LEU:HD23	2.48	0.42
1:C:2079:ILE:HB	1:C:2088:ALA:HB3	2.01	0.42
1:C:2474:MET:HB3	1:C:2499:VAL:HG22	2.02	0.42
1:C:2476:GLU:OE2	1:C:2654:ARG:CZ	2.67	0.42
1:D:3338:ALA:O	1:D:3340:LYS:N	2.52	0.42
1:D:3469:ALA:HB2	1:D:3584:ILE:HD11	2.02	0.42
1:A:192:GLN:NE2	1:A:278:ASP:OD2	2.53	0.42
1:A:219:MET:HE2	1:A:219:MET:HB3	1.80	0.42
1:A:681:ALA:HB1	1:A:682:PRO:CD	2.49	0.42
1:B:1427:PHE:CE1	1:B:1459:THR:HG21	2.55	0.42
1:B:1517:LEU:O	1:B:1519:GLY:N	2.53	0.42
1:B:1540:PRO:HD2	1:B:1609:GLU:HG3	2.00	0.42
1:D:3097:TYR:CD2	1:D:3181:THR:HG23	2.54	0.42
1:D:3259:LYS:HB3	1:D:3484:TYR:O	2.20	0.42
1:D:3563:VAL:CG2	1:D:3564:GLY:H	2.28	0.42
1:D:3731:ASP:CG	1:D:3745:LYS:H	2.26	0.42
1:A:68:ILE:O	1:A:235:THR:CA	2.62	0.42
1:A:336:GLY:O	1:A:451:GLY:CA	2.68	0.42
1:A:340:LYS:HA	1:A:400:MET:HE2	2.02	0.42
1:A:411:THR:HG22	1:A:415:TYR:CE2	2.55	0.42
1:B:1076:ARG:HD3	1:B:1186:ARG:NH1	2.34	0.42
1:B:1320:GLU:C	1:B:1322:PHE:H	2.28	0.42
1:B:1658:VAL:HG11	1:B:1680:LEU:CD2	2.50	0.42
1:C:2082:ARG:NH2	1:C:2300:GLU:OE1	2.53	0.42
1:C:2082:ARG:HA	1:C:2263:THR:O	2.19	0.42
1:C:2246:PRO:HD3	1:D:3330:GLN:NE2	2.30	0.42
1:C:2326:ASP:O	1:C:2330:GLN:N	2.53	0.42
1:C:2336:GLY:HA3	1:C:2551:ALA:HA	2.02	0.42
1:C:2703:LYS:O	1:C:2704:LYS:C	2.62	0.42
1:D:3343:THR:HG21	1:D:3449:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3738:ILE:O	1:D:3740:ASN:N	2.53	0.42
1:A:327:ILE:C	1:A:329:TYR:N	2.78	0.41
1:A:357:GLU:O	1:A:358:TYR:C	2.63	0.41
1:A:408:GLY:C	1:A:410:ALA:N	2.75	0.41
1:B:1426:ARG:O	1:B:1654:ARG:HD2	2.19	0.41
1:B:1465:PHE:O	1:B:1466:THR:C	2.63	0.41
1:B:1562:LEU:CB	1:B:1567:ASN:ND2	2.82	0.41
1:C:2576:ASN:HA	1:C:2578:ALA:N	2.34	0.41
1:D:3201:ALA:HB2	1:D:3220:GLU:CD	2.45	0.41
1:A:428:GLY:O	1:A:429:LEU:C	2.62	0.41
1:B:1441:ASN:C	1:B:1443:VAL:H	2.28	0.41
1:B:1653:LEU:C	1:B:1655:ARG:N	2.78	0.41
1:C:2094:TYR:CE2	1:C:2182:THR:HB	2.55	0.41
1:C:2193:PHE:O	1:C:2194:ALA:C	2.63	0.41
1:C:2319:THR:O	1:C:2320:GLU:C	2.63	0.41
1:C:2399:GLY:C	1:C:2401:SER:N	2.78	0.41
1:C:2412:TRP:CE3	1:C:2412:TRP:HA	2.55	0.41
1:C:2543:ASN:O	1:C:2578:ALA:CB	2.68	0.41
1:D:3492:ARG:HD2	1:D:3634:SER:HB2	2.02	0.41
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.91	0.41
1:A:328:LEU:O	1:A:329:TYR:HB3	2.20	0.41
1:A:637:ALA:O	1:A:639:PRO:HD3	2.20	0.41
1:A:687:LEU:HD11	1:A:706:THR:O	2.20	0.41
1:A:738:ILE:HA	1:A:741:ILE:CD1	2.46	0.41
1:B:1692:LYS:NZ	1:B:1694:GLU:OE1	2.47	0.41
1:B:1711:ALA:O	1:B:1712:LYS:C	2.62	0.41
1:C:2284:VAL:O	1:C:2285:LYS:C	2.63	0.41
1:C:2357:GLU:O	1:C:2360:ASN:OD1	2.39	0.41
1:C:2661:ILE:CD1	1:C:2702:TRP:CD1	3.03	0.41
1:D:3350:ASN:C	1:D:3352:THR:N	2.72	0.41
1:D:3672:THR:CG2	1:D:3673:SER:H	2.33	0.41
1:A:327:ILE:C	1:A:329:TYR:H	2.28	0.41
1:A:425:THR:OG1	1:A:426:ARG:N	2.54	0.41
1:A:447:GLN:HG2	1:A:450:PHE:CE2	2.53	0.41
1:A:539:VAL:CG2	1:A:608:LEU:HB3	2.50	0.41
1:B:1170:LEU:O	1:B:1171:GLU:C	2.64	0.41
1:B:1206:ASN:O	1:B:1207:GLU:C	2.63	0.41
1:D:3654:ARG:CZ	1:D:3660:PRO:HG2	2.50	0.41
1:D:3699:MET:HE1	1:D:3746:LEU:HD11	2.03	0.41
1:A:343:THR:HA	1:A:412:TRP:CZ3	2.55	0.41
1:A:517:LEU:HD23	1:A:520:THR:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:THR:O	1:A:606:PRO:C	2.63	0.41
1:C:2537:ILE:HD13	1:C:2574:THR:CG2	2.51	0.41
1:C:2605:THR:HB	1:C:2606:PRO:HD3	2.03	0.41
1:D:3353:PHE:O	1:D:3354:PRO:C	2.63	0.41
1:D:3665:THR:O	1:D:3666:GLY:C	2.61	0.41
1:D:3718:LEU:CD2	1:D:3744:ILE:HB	2.49	0.41
1:D:3737:ALA:O	1:D:3741:ILE:CD1	2.68	0.41
1:A:284:VAL:O	1:A:285:LYS:C	2.63	0.41
1:A:358:TYR:C	1:A:360:ASN:N	2.79	0.41
1:C:2076:ARG:HH21	1:C:2220:GLU:HG3	1.86	0.41
1:A:281:LEU:O	1:A:285:LYS:CA	2.69	0.41
1:A:471:ASP:O	1:A:505:LYS:HA	2.21	0.41
1:A:600:LEU:C	1:A:600:LEU:HD12	2.46	0.41
1:A:645:SER:HA	1:A:667:THR:O	2.21	0.41
1:A:647:GLY:O	1:A:650:ALA:N	2.54	0.41
1:B:1170:LEU:HB3	1:B:1175:VAL:HB	2.01	0.41
1:B:1646:PRO:HA	1:B:1669:ILE:HD11	2.02	0.41
1:B:1702:TRP:C	1:B:1703:LYS:O	2.61	0.41
1:B:1718:LEU:HD22	1:B:1746:LEU:HG	2.01	0.41
1:C:2347:SER:CA	1:C:2407:MET:CE	2.99	0.41
1:C:2537:ILE:H	1:C:2537:ILE:HG13	1.67	0.41
1:C:2694:GLU:O	1:C:2695:GLU:HG2	2.20	0.41
1:D:3081:ASP:C	1:D:3081:ASP:OD1	2.63	0.41
1:D:3639:PRO:C	1:D:3676:GLU:HG3	2.45	0.41
1:A:437:LEU:O	1:A:438:PRO:C	2.61	0.41
1:A:474:MET:HB3	1:A:499:VAL:HG23	2.02	0.41
1:A:645:SER:C	1:A:647:GLY:N	2.78	0.41
1:A:703:LYS:O	1:A:704:LYS:C	2.63	0.41
1:B:1183:SER:O	1:B:1183:SER:OG	2.32	0.41
1:B:1277:MET:HA	1:B:1603:PHE:HE1	1.86	0.41
1:B:1349:ASP:OD2	1:B:1415:TYR:OH	2.27	0.41
1:B:1427:PHE:HB2	1:B:1477:PRO:O	2.21	0.41
1:C:2278:ASP:CG	1:C:2307:ARG:HH21	2.29	0.41
1:C:2437:LEU:O	1:C:2438:PRO:C	2.62	0.41
1:D:3224:ASN:C	1:D:3226:ILE:N	2.78	0.41
1:D:3402:LEU:C	1:D:3404:GLU:N	2.77	0.41
1:D:3497:GLU:OE2	1:D:3654:ARG:NH2	2.46	0.41
1:D:3498:ILE:HG21	1:D:3700:TYR:CD1	2.55	0.41
1:A:264:THR:OG1	1:A:479:PHE:HA	2.20	0.41
1:A:339:MET:CE	1:A:454:ILE:HD13	2.51	0.41
1:A:419:PHE:HB3	1:A:421:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LYS:HB2	1:A:691:ASP:CG	2.46	0.41
1:B:1156:ASN:O	1:B:1157:GLY:C	2.63	0.41
1:B:1336:GLY:O	1:B:1451:GLY:HA3	2.21	0.41
1:B:1512:ARG:O	1:B:1515:MET:HB2	2.20	0.41
1:B:1562:LEU:HB3	1:B:1567:ASN:ND2	2.34	0.41
1:B:1675:GLU:N	1:B:1675:GLU:CD	2.79	0.41
1:C:2286:GLY:O	1:C:2287:LYS:C	2.64	0.41
1:C:2328:LEU:HD12	1:C:2458:GLN:HB2	2.03	0.41
1:C:2335:PRO:CB	1:C:2461:MET:HE2	2.51	0.41
1:C:2503:VAL:O	1:C:2503:VAL:HG23	2.20	0.41
1:C:2517:LEU:O	1:C:2519:GLY:N	2.54	0.41
1:C:2724:GLY:HA3	1:C:2749:GLY:C	2.46	0.41
1:D:3096:VAL:HG12	1:D:3155:GLY:CA	2.48	0.41
1:D:3156:ASN:O	1:D:3158:ILE:N	2.54	0.41
1:D:3198:ILE:HD13	1:D:3198:ILE:HA	1.83	0.41
1:D:3566:THR:HA	1:D:3570:PHE:HZ	1.86	0.41
1:A:76:ARG:NH2	1:A:220:GLU:HG3	2.36	0.41
1:A:234:ILE:HG12	1:A:250:LEU:CD1	2.51	0.41
1:A:427:PHE:N	1:A:427:PHE:HD1	2.19	0.41
1:A:515:MET:HB2	1:A:545:ALA:HB1	2.03	0.41
1:A:553:ILE:H	1:A:553:ILE:HG13	1.66	0.41
1:A:639:PRO:O	1:A:640:SER:C	2.64	0.41
1:A:652:ALA:HA	1:A:655:ARG:CZ	2.51	0.41
1:A:711:ALA:CB	1:A:718:LEU:HG	2.51	0.41
1:A:732:VAL:HG21	1:A:741:ILE:HG21	2.02	0.41
1:B:1420:LYS:NZ	1:B:1499:VAL:O	2.44	0.41
1:B:1501:ASN:HB2	1:B:1700:TYR:HB2	2.02	0.41
1:B:1619:ASN:O	1:B:1622:SER:N	2.54	0.41
1:C:2334:GLU:HA	1:C:2335:PRO:HD2	1.66	0.41
1:C:2337:SER:CB	1:C:2549:GLY:HA3	2.51	0.41
1:C:2457:THR:O	1:C:2458:GLN:C	2.63	0.41
1:C:2729:LYS:HE3	1:C:2729:LYS:HB2	1.74	0.41
1:D:3509:SER:HA	1:D:3512:ARG:HH21	1.86	0.41
1:A:234:ILE:HG12	1:A:250:LEU:HD11	2.02	0.40
1:A:276:GLN:O	1:A:279:ALA:N	2.54	0.40
1:A:481:SER:O	1:A:482:ALA:HB2	2.19	0.40
1:A:537:ILE:HA	1:A:605:THR:OG1	2.21	0.40
1:A:657:ILE:HD12	1:A:657:ILE:N	2.35	0.40
1:C:2354:PRO:O	1:C:2355:SER:HB3	2.21	0.40
1:C:2638:MET:HA	1:C:2639:PRO:HD3	1.97	0.40
1:C:2640:SER:CA	1:C:2676:GLU:HG3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2646:PRO:HG3	1:C:2669:ILE:CG1	2.39	0.40
1:D:3427:PHE:CE1	1:D:3429:LEU:HB2	2.56	0.40
1:D:3593:GLU:HB3	1:D:3594:HIS:ND1	2.37	0.40
1:A:301:ILE:HG13	1:A:478:LYS:O	2.21	0.40
1:A:487:ASN:C	1:A:489:GLN:H	2.29	0.40
1:A:677:GLY:O	1:A:678:THR:C	2.63	0.40
1:B:1346:SER:OG	1:B:1415:TYR:CG	2.74	0.40
1:B:1609:GLU:O	1:B:1613:ALA:HB2	2.21	0.40
1:C:2695:GLU:HB3	1:C:2735:ASN:C	2.46	0.40
1:D:3275:THR:HG22	1:D:3276:GLN:N	2.36	0.40
1:D:3348:ILE:HD13	1:D:3510:THR:HG21	2.02	0.40
1:A:244:ILE:HG22	1:A:245:VAL:N	2.36	0.40
1:A:282:GLU:OE2	1:A:285:LYS:HD3	2.21	0.40
1:A:596:SER:HB3	1:A:599:GLN:CD	2.46	0.40
1:B:1334:GLU:HA	1:B:1335:PRO:HD3	1.82	0.40
1:B:1400:MET:O	1:B:1403:LEU:N	2.54	0.40
1:C:2434:ALA:O	1:C:2460:GLN:NE2	2.54	0.40
1:C:2469:ALA:HA	1:C:2512:ARG:HD3	2.04	0.40
1:C:2473:VAL:CG1	1:C:2498:ILE:HG23	2.51	0.40
1:C:2646:PRO:O	1:C:2649:LEU:HB3	2.21	0.40
1:D:3082:ARG:HB3	1:D:3264:THR:HA	2.04	0.40
1:D:3087:ILE:HA	1:D:3190:ASN:HD21	1.86	0.40
1:D:3357:GLU:O	1:D:3360:ASN:N	2.54	0.40
1:D:3514:HIS:HA	1:D:3517:LEU:HD12	2.04	0.40
1:D:3593:GLU:C	1:D:3594:HIS:ND1	2.80	0.40
1:A:340:LYS:HB3	1:A:400:MET:HE2	2.04	0.40
1:A:550:THR:HG21	1:A:568:TYR:CD2	2.57	0.40
1:B:1579:GLU:C	1:B:1581:PRO:HD3	2.46	0.40
1:B:1596:SER:O	1:B:1598:ILE:N	2.54	0.40
1:B:1653:LEU:C	1:B:1655:ARG:H	2.29	0.40
1:C:2538:THR:O	1:C:2538:THR:HG23	2.21	0.40
1:C:2579:GLU:H	1:C:2579:GLU:CD	2.29	0.40
1:D:3234:ILE:CG2	1:D:3235:THR:N	2.84	0.40
1:D:3610:ARG:C	1:D:3612:SER:H	2.28	0.40
1:D:3672:THR:HG21	1:D:3674:VAL:O	2.21	0.40
1:D:3699:MET:HE1	1:D:3744:ILE:HG21	2.03	0.40
1:A:208:ASP:O	1:A:210:SER:N	2.54	0.40
1:A:412:TRP:CZ2	1:A:449:SER:HA	2.57	0.40
1:A:413:LEU:HD13	1:A:413:LEU:C	2.46	0.40
1:B:1094:TYR:CD1	1:B:1094:TYR:N	2.88	0.40
1:B:1264:THR:HG21	1:B:1300:GLU:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1614:MET:C	1:B:1616:GLU:N	2.77	0.40
1:C:2467:ALA:HB2	1:C:2474:MET:HG3	2.04	0.40
1:C:2544:VAL:HG12	1:C:2546:VAL:CG1	2.51	0.40
1:C:2600:LEU:HD13	1:C:2600:LEU:C	2.46	0.40
1:D:3357:GLU:O	1:D:3360:ASN:ND2	2.54	0.40
1:D:3571:SER:O	1:D:3572:ALA:HB2	2.21	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	546/685 (80%)	401 (73%)	105 (19%)	40 (7%)	1	6
1	B	565/685 (82%)	431 (76%)	99 (18%)	35 (6%)	1	9
1	C	540/685 (79%)	390 (72%)	106 (20%)	44 (8%)	1	4
1	D	544/685 (79%)	430 (79%)	80 (15%)	34 (6%)	1	8
All	All	2195/2740 (80%)	1652 (75%)	390 (18%)	153 (7%)	1	6

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	194	ALA
1	A	209	GLY
1	A	251	VAL
1	A	252	SER
1	A	615	LYS
1	A	630	VAL
1	A	632	THR
1	B	1153	SER

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Mol	Chain	Res	Type
1	B	1157	GLY
1	B	1173	ALA
1	B	1208	ASP
1	B	1221	SER
1	B	1222	SER
1	B	1442	ILE
1	B	1567	ASN
1	B	1615	LYS
1	B	1620	LEU
1	C	2194	ALA
1	C	2252	SER
1	C	2354	PRO
1	C	2581	PRO
1	C	2623	PRO
1	D	3091	ALA
1	D	3153	SER
1	D	3157	GLY
1	D	3173	ALA
1	D	3352	THR
1	D	3567	ASN
1	D	3702	TRP
1	A	195	SER
1	A	208	ASP
1	A	210	SER
1	A	255	THR
1	A	329	TYR
1	A	355	SER
1	A	471	ASP
1	A	487	ASN
1	A	578	ALA
1	B	1154	LYS
1	B	1251	VAL
1	B	1252	SER
1	B	1409	ASP
1	B	1562	LEU
1	B	1628	ASP
1	B	1684	GLN
1	B	1728	GLN
1	C	2207	GLU
1	C	2208	ASP
1	C	2209	GLY
1	C	2243	ASN

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Mol	Chain	Res	Type
1	C	2312	ALA
1	C	2315	LYS
1	C	2351	ASN
1	C	2355	SER
1	C	2506	GLU
1	C	2559	GLY
1	C	2578	ALA
1	C	2579	GLU
1	C	2630	VAL
1	C	2632	THR
1	C	2633	GLU
1	C	2676	GLU
1	D	3082	ARG
1	D	3174	GLU
1	D	3225	SER
1	D	3229	GLY
1	D	3252	SER
1	D	3263	THR
1	D	3312	ALA
1	D	3339	MET
1	D	3407	MET
1	D	3589	VAL
1	D	3739	LYS
1	A	328	LEU
1	A	353	PHE
1	A	496	LYS
1	A	518	VAL
1	A	623	PRO
1	A	631	THR
1	A	633	GLU
1	B	1174	GLU
1	B	1217	SER
1	B	1625	LYS
1	C	2195	SER
1	C	2210	SER
1	C	2244	ILE
1	C	2255	THR
1	C	2356	GLY
1	C	2419	PHE
1	C	2439	ALA
1	C	2496	LYS
1	C	2567	ASN

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Mol	Chain	Res	Type
1	C	2692	LYS
1	D	3099	VAL
1	D	3171	GLU
1	D	3175	VAL
1	D	3354	PRO
1	D	3358	TYR
1	D	3644	ILE
1	D	3741	ILE
1	A	287	LYS
1	A	297	LYS
1	A	504	SER
1	A	618	LEU
1	A	648	GLU
1	A	691	ASP
1	B	1354	PRO
1	B	1424	PRO
1	B	1540	PRO
1	B	1565	SER
1	B	1629	LYS
1	B	1714	LEU
1	B	1735	ASN
1	C	2077	GLY
1	C	2267	SER
1	C	2285	LYS
1	C	2353	PHE
1	C	2618	LEU
1	D	3161	ALA
1	D	3351	ASN
1	D	3409	ASP
1	A	351	ASN
1	A	354	PRO
1	A	519	GLY
1	A	619	ASN
1	B	1099	VAL
1	B	1623	PRO
1	B	1742	LYS
1	C	2444	SER
1	D	3154	LYS
1	D	3285	LYS
1	A	212	SER
1	A	291	ALA
1	A	303	ALA

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Mol	Chain	Res	Type
1	A	620	LEU
1	C	2091	ALA
1	C	2245	VAL
1	C	2678	THR
1	D	3251	VAL
1	D	3540	PRO
1	B	1175	VAL
1	B	1657	ILE
1	C	2641	ILE
1	C	2697	PRO
1	D	3606	PRO
1	B	1177	GLY
1	C	2251	VAL
1	A	245	VAL
1	A	502	PRO
1	B	1559	GLY
1	D	3472	GLY
1	C	2518	VAL

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	449/583 (77%)	409 (91%)	40 (9%)	9	34
1	B	461/583 (79%)	427 (93%)	34 (7%)	13	43
1	C	439/583 (75%)	401 (91%)	38 (9%)	9	36
1	D	448/583 (77%)	412 (92%)	36 (8%)	11	40
All	All	1797/2332 (77%)	1649 (92%)	148 (8%)	10	39

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	182	THR
1	A	230	THR

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Mol	Chain	Res	Type
1	A	235	THR
1	A	243	ASN
1	A	256	VAL
1	A	275	THR
1	A	282	GLU
1	A	298	THR
1	A	304	THR
1	A	320	GLU
1	A	357	GLU
1	A	364	LEU
1	A	396	SER
1	A	405	GLN
1	A	406	LYS
1	A	427	PHE
1	A	443	VAL
1	A	465	PHE
1	A	501	ASN
1	A	504	SER
1	A	538	THR
1	A	546	VAL
1	A	548	SER
1	A	556	GLU
1	A	558	ASN
1	A	567	ASN
1	A	588	THR
1	A	599	GLN
1	A	600	LEU
1	A	615	LYS
1	A	618	LEU
1	A	627	LEU
1	A	640	SER
1	A	649	LEU
1	A	658	VAL
1	A	675	GLU
1	A	706	THR
1	A	712	LYS
1	A	716	ILE
1	B	1097	TYR
1	B	1163	MET
1	B	1182	THR
1	B	1187	SER
1	B	1193	PHE

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Mol	Chain	Res	Type
1	B	1213	LEU
1	B	1214	LEU
1	B	1255	THR
1	B	1269	LEU
1	B	1275	THR
1	B	1304	THR
1	B	1309	THR
1	B	1314	THR
1	B	1343	THR
1	B	1346	SER
1	B	1406	LYS
1	B	1413	LEU
1	B	1424	PRO
1	B	1425	THR
1	B	1427	PHE
1	B	1456	VAL
1	B	1466	THR
1	B	1479	PHE
1	B	1488	ASN
1	B	1540	PRO
1	B	1556	GLU
1	B	1569	ILE
1	B	1617	SER
1	B	1618	LEU
1	B	1620	LEU
1	B	1630	VAL
1	B	1638	MET
1	B	1665	THR
1	B	1689	LEU
1	C	2182	THR
1	C	2190	ASN
1	C	2192	GLN
1	C	2202	GLN
1	C	2212	SER
1	C	2213	LEU
1	C	2214	LEU
1	C	2223	LEU
1	C	2230	THR
1	C	2293	LEU
1	C	2298	THR
1	C	2309	THR
1	C	2320	GLU

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Mol	Chain	Res	Type
1	C	2357	GLU
1	C	2418	ARG
1	C	2427	PHE
1	C	2430	THR
1	C	2443	VAL
1	C	2454	ILE
1	C	2490	SER
1	C	2499	VAL
1	C	2509	SER
1	C	2511	THR
1	C	2567	ASN
1	C	2600	LEU
1	C	2616	GLU
1	C	2628	ASP
1	C	2629	LYS
1	C	2649	LEU
1	C	2675	GLU
1	C	2680	LEU
1	C	2687	LEU
1	C	2689	LEU
1	C	2712	LYS
1	C	2716	ILE
1	C	2727	VAL
1	C	2739	LYS
1	C	2741	ILE
1	D	3070	ARG
1	D	3083	ASN
1	D	3158	ILE
1	D	3162	ASN
1	D	3172	THR
1	D	3182	THR
1	D	3187	SER
1	D	3205	GLU
1	D	3214	LEU
1	D	3223	LEU
1	D	3235	THR
1	D	3275	THR
1	D	3304	THR
1	D	3309	THR
1	D	3321	ASP
1	D	3332	ASN
1	D	3354	PRO

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Mol	Chain	Res	Type
1	D	3413	LEU
1	D	3427	PHE
1	D	3456	VAL
1	D	3457	THR
1	D	3471	ASP
1	D	3477	PRO
1	D	3488	ASN
1	D	3499	VAL
1	D	3540	PRO
1	D	3550	THR
1	D	3556	GLU
1	D	3587	VAL
1	D	3594	HIS
1	D	3644	ILE
1	D	3649	LEU
1	D	3712	LYS
1	D	3715	ASP
1	D	3732	VAL
1	D	3741	ILE

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

Mol	Chain	Res	Type
1	A	202	GLN
1	A	350	ASN
1	A	360	ASN
1	A	405	GLN
1	A	441	ASN
1	A	452	GLN
1	A	487	ASN
1	A	501	ASN
1	A	567	ASN
1	A	580	ASN
1	A	599	GLN
1	A	656	ASN
1	A	740	ASN
1	B	1083	ASN
1	B	1095	ASN
1	B	1202	GLN
1	B	1488	ASN
1	B	1501	ASN
1	B	1567	ASN

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Mol	Chain	Res	Type
1	B	1580	ASN
1	B	1619	ASN
1	B	1659	GLN
1	B	1679	ASN
1	B	1728	GLN
1	C	2083	ASN
1	C	2202	GLN
1	C	2206	ASN
1	C	2276	GLN
1	C	2350	ASN
1	C	2470	ASN
1	C	2495	GLN
1	C	2501	ASN
1	C	2542	GLN
1	C	2567	ASN
1	C	2580	ASN
1	C	2599	GLN
1	C	2619	ASN
1	C	2656	ASN
1	C	2684	GLN
1	D	3083	ASN
1	D	3095	ASN
1	D	3156	ASN
1	D	3190	ASN
1	D	3202	GLN
1	D	3332	ASN
1	D	3350	ASN
1	D	3452	GLN
1	D	3488	ASN
1	D	3501	ASN
1	D	3567	ASN
1	D	3580	ASN
1	D	3679	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	556/685 (81%)	0.01	9 (1%) 70 51	3, 26, 59, 100	0
1	B	575/685 (83%)	0.01	4 (0%) 84 69	7, 29, 62, 81	0
1	C	550/685 (80%)	-0.03	3 (0%) 87 76	4, 27, 58, 99	0
1	D	556/685 (81%)	-0.02	4 (0%) 84 69	7, 30, 56, 88	0
All	All	2237/2740 (81%)	-0.01	20 (0%) 81 64	3, 28, 59, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1617	SER	3.6
1	A	520	THR	3.4
1	D	3520	THR	3.1
1	A	518	VAL	3.0
1	D	3675	GLU	3.0
1	B	1258	GLY	2.9
1	D	3173	ALA	2.9
1	C	2245	VAL	2.8
1	B	1618	LEU	2.8
1	A	395	SER	2.7
1	D	3518	VAL	2.6
1	B	1520	THR	2.5
1	C	2092	THR	2.5
1	C	2518	VAL	2.5
1	A	363	GLU	2.5
1	A	631	THR	2.5
1	A	628	ASP	2.4
1	A	92	THR	2.2
1	A	354	PRO	2.2
1	A	617	SER	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.