



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:55 AM UTC

PDB ID : 3FHN / pdb_00003fhn
Title : Structure of Tip20p
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Deposited on : 2008-12-09
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

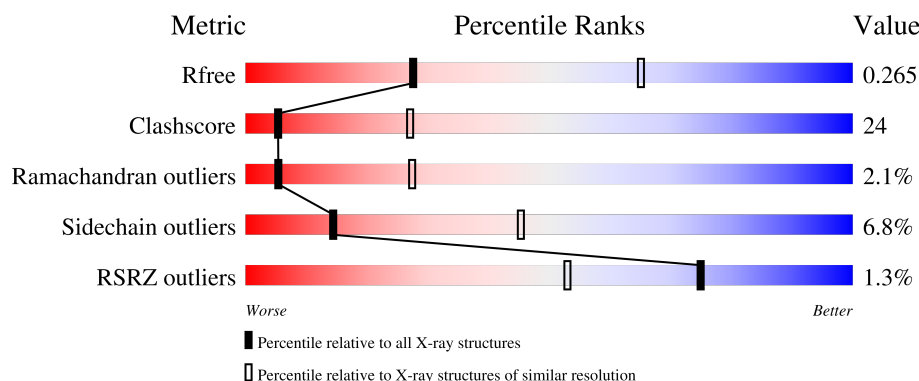
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	706	2% 48% 41% 6% 5%
1	B	706	% 55% 35% 5% 5%
1	C	706	% 56% 36% • 5%
1	D	706	2% 50% 38% 7% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22040 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 Protein transport protein TIP20.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	Se	0	0	0
			5510	3532	910	1053	5	10			
1	B	673	Total	C	N	O	S	Se	0	0	0
			5510	3532	910	1053	5	10			
1	C	673	Total	C	N	O	S	Se	0	0	0
			5510	3532	910	1053	5	10			
1	D	673	Total	C	N	O	S	Se	0	0	0
			5510	3532	910	1053	5	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P33891
A	-3	ALA	-	expression tag	UNP P33891
A	-2	MSE	-	expression tag	UNP P33891
A	-1	GLY	-	expression tag	UNP P33891
A	0	SER	-	expression tag	UNP P33891
A	1	MSE	-	expression tag	UNP P33891
B	-4	GLY	-	expression tag	UNP P33891
B	-3	ALA	-	expression tag	UNP P33891
B	-2	MSE	-	expression tag	UNP P33891
B	-1	GLY	-	expression tag	UNP P33891
B	0	SER	-	expression tag	UNP P33891
B	1	MSE	-	expression tag	UNP P33891
C	-4	GLY	-	expression tag	UNP P33891
C	-3	ALA	-	expression tag	UNP P33891
C	-2	MSE	-	expression tag	UNP P33891
C	-1	GLY	-	expression tag	UNP P33891
C	0	SER	-	expression tag	UNP P33891
C	1	MSE	-	expression tag	UNP P33891
D	-4	GLY	-	expression tag	UNP P33891
D	-3	ALA	-	expression tag	UNP P33891
D	-2	MSE	-	expression tag	UNP P33891

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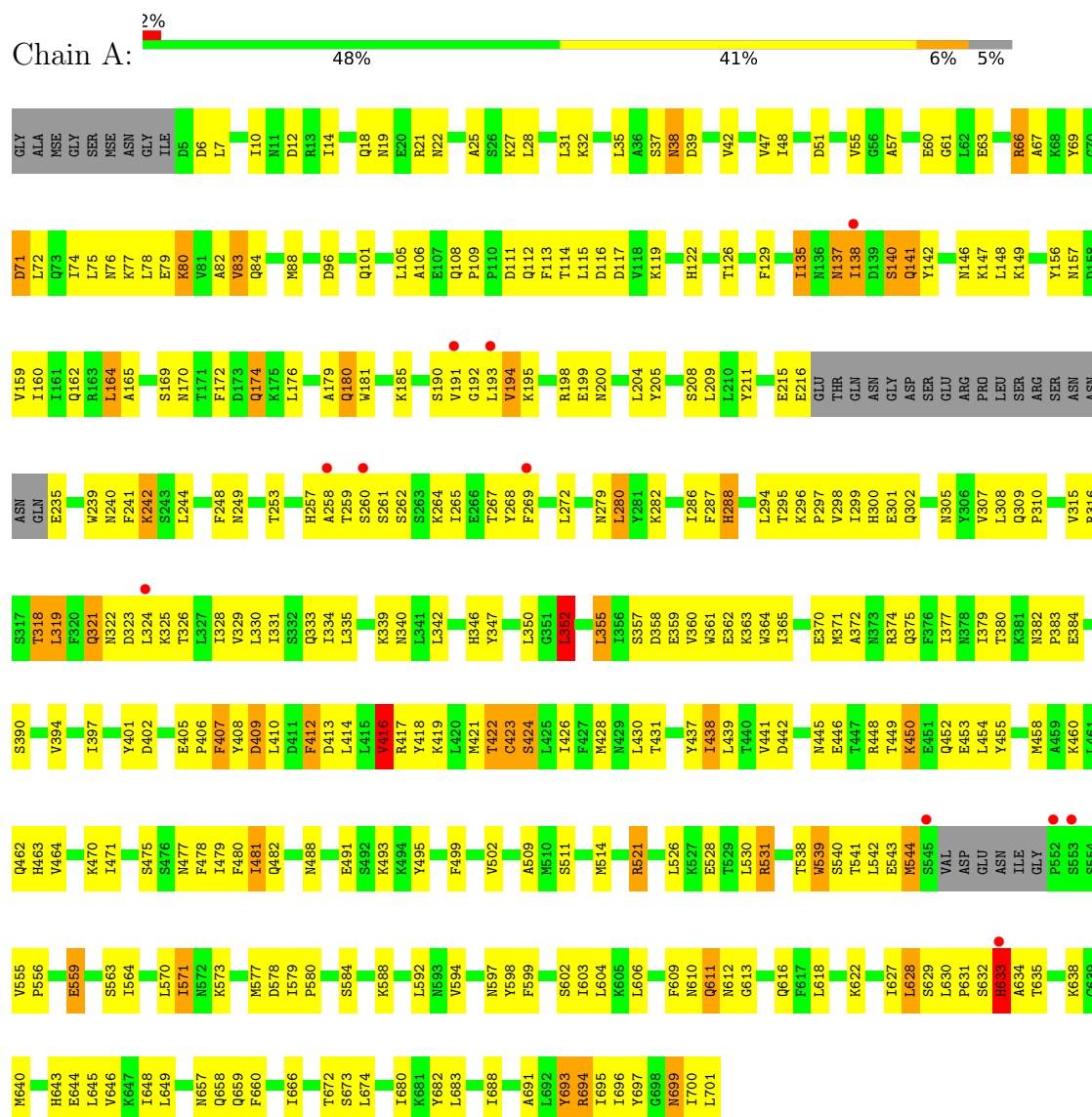
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P33891
D	0	SER	-	expression tag	UNP P33891
D	1	MSE	-	expression tag	UNP P33891

3 Residue-property plots

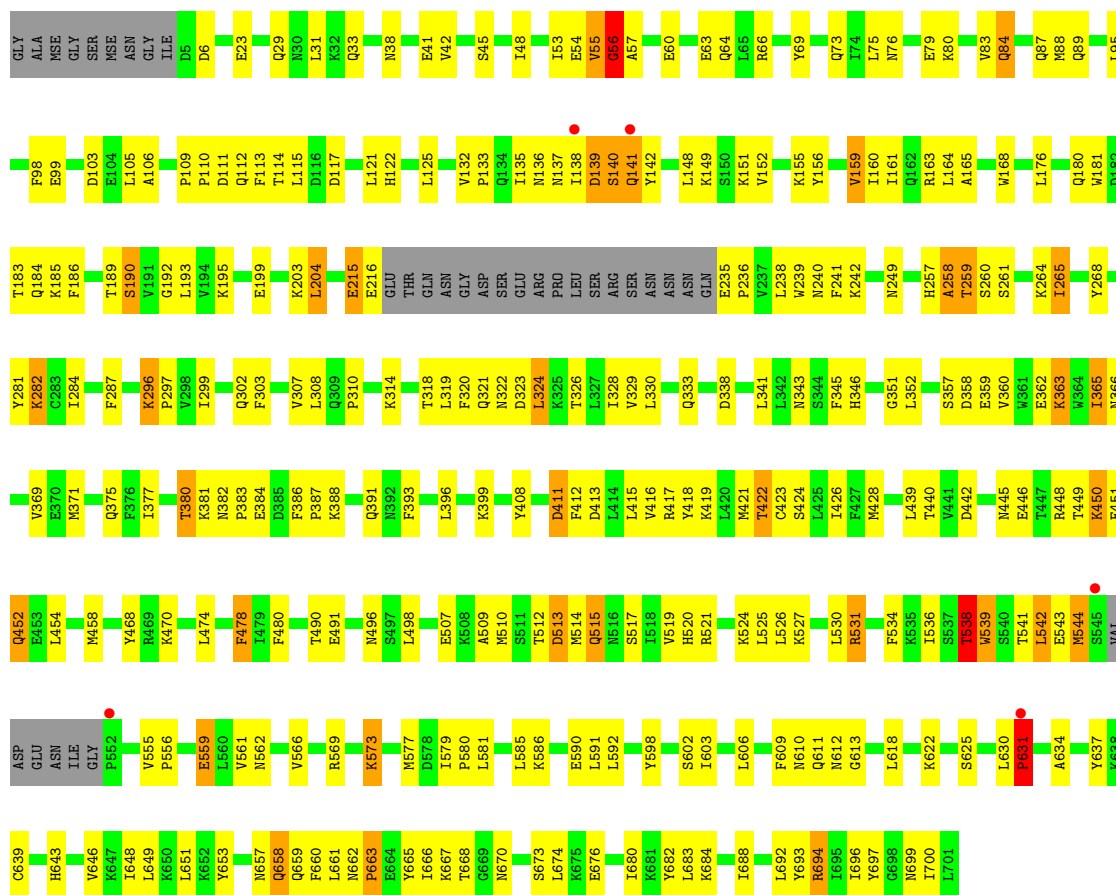
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein transport protein TIP20

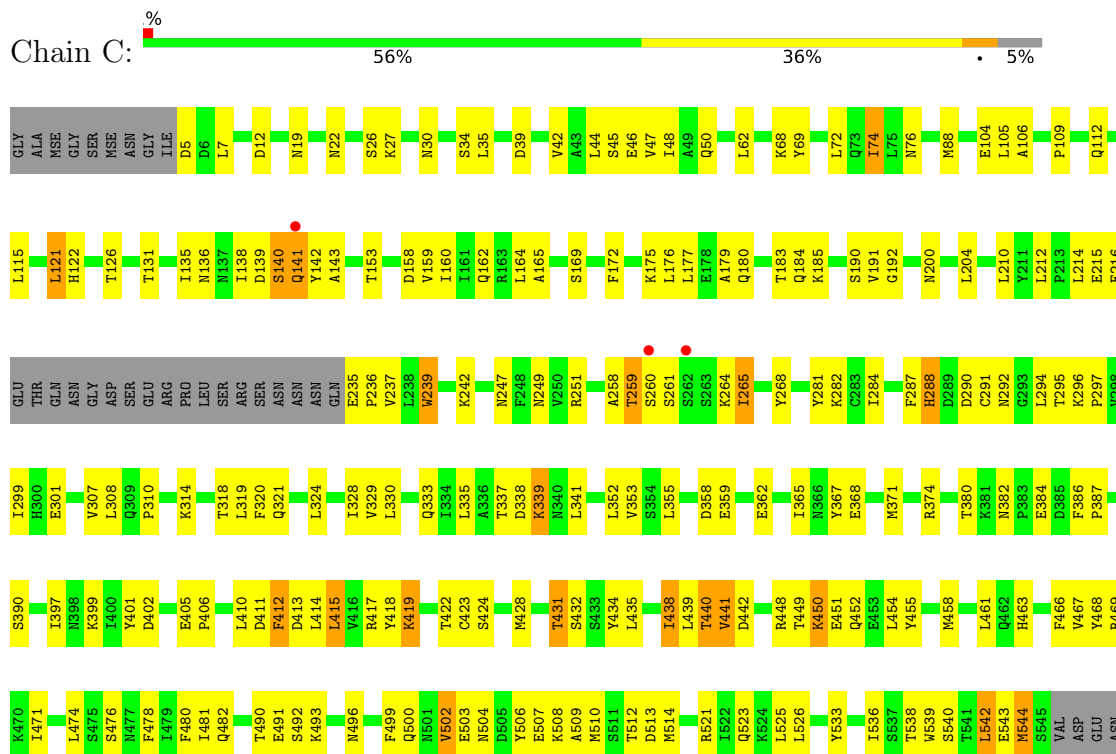


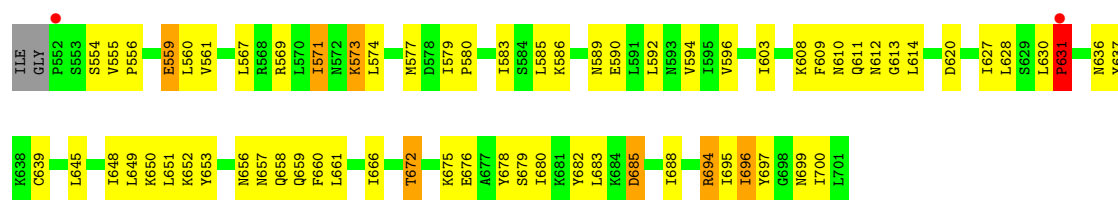
• Molecule 1: Protein transport protein TIP20



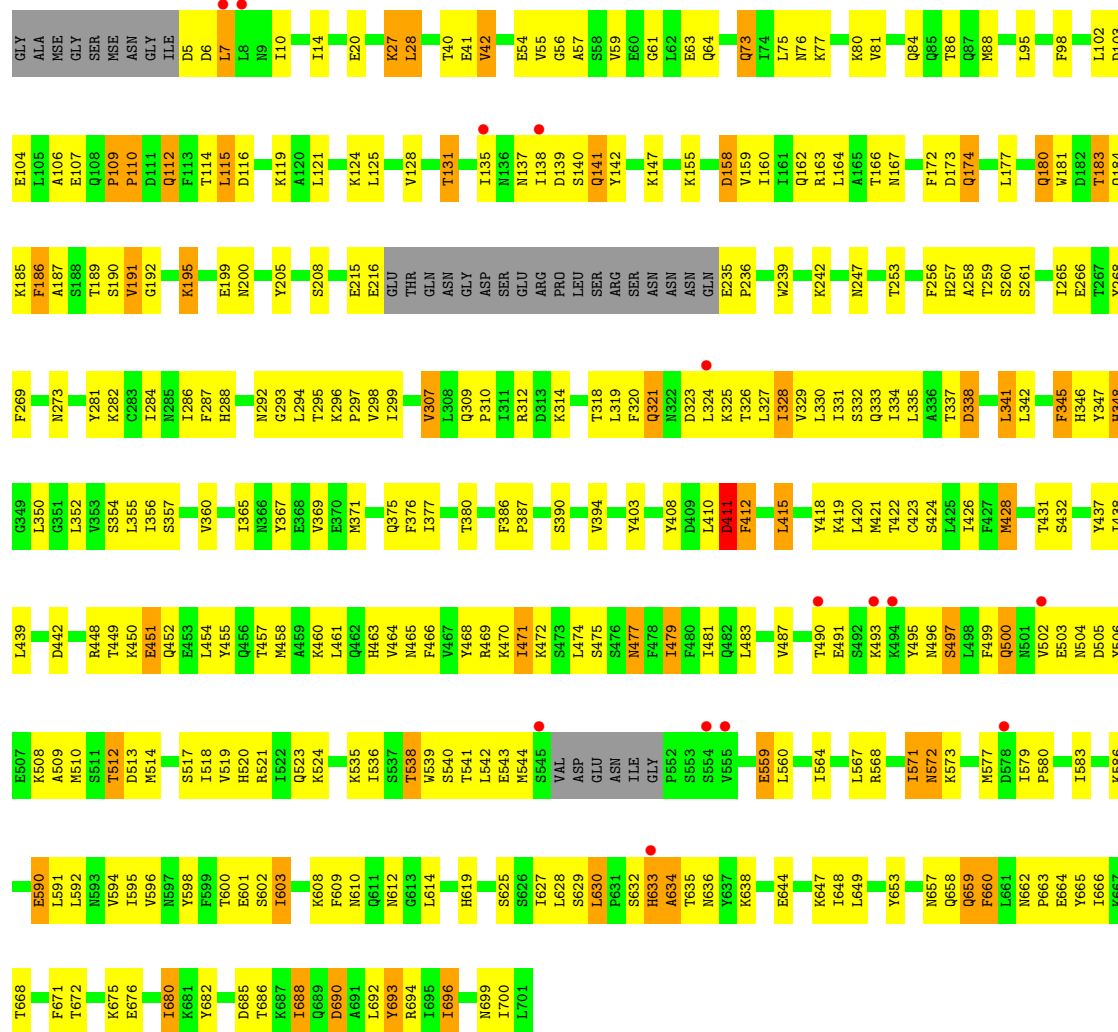


• Molecule 1: Protein transport protein TIP20





● Molecule 1: Protein transport protein TIP20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.48Å 111.62Å 149.84Å 77.09° 88.12° 70.35°	Depositor
Resolution (Å)	29.90 – 3.00 29.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.90-3.00) 98.2 (29.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.265 0.220 , 0.265	Depositor DCC
R_{free} test set	5006 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22040	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% 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	0.51	0/5601	1.00	25/7561 (0.3%)
1	B	0.56	0/5601	1.01	26/7561 (0.3%)
1	C	0.55	0/5601	0.96	14/7561 (0.2%)
1	D	0.49	0/5601	0.96	21/7561 (0.3%)
All	All	0.53	0/22404	0.98	86/30244 (0.3%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	PHE	N-CA-C	-12.35	94.87	110.19
1	C	141	GLN	N-CA-C	-10.02	99.54	113.37
1	B	141	GLN	N-CA-C	-9.79	101.50	113.15
1	A	141	GLN	N-CA-C	-9.75	101.59	113.19
1	B	190	SER	N-CA-C	-9.08	102.34	113.50
1	B	80	LYS	N-CA-C	-8.09	102.15	110.97
1	D	109	PRO	CA-C-N	8.04	129.89	119.84
1	D	109	PRO	C-N-CA	8.04	129.89	119.84
1	A	80	LYS	N-CA-C	-7.91	102.34	110.97
1	B	381	LYS	N-CA-C	7.83	120.91	111.82
1	B	573	LYS	N-CA-C	-7.78	102.80	111.28
1	B	282	LYS	N-CA-C	-7.65	102.94	111.28
1	B	287	PHE	N-CA-C	7.50	122.62	113.17
1	B	6	ASP	N-CA-C	-7.09	103.89	112.54
1	D	287	PHE	N-CA-C	6.99	121.98	113.17
1	C	74	ILE	N-CA-C	-6.98	102.51	112.35
1	A	66	ARG	N-CA-C	-6.92	105.37	113.88
1	C	72	LEU	N-CA-C	6.85	121.47	113.18
1	B	139	ASP	N-CA-C	6.78	118.84	110.91
1	C	282	LYS	N-CA-C	-6.65	104.11	111.36
1	C	672	THR	N-CA-C	-6.56	104.45	113.18
1	D	286	ILE	N-CA-C	6.53	117.28	110.62
1	C	287	PHE	N-CA-C	6.44	121.15	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	LEU	N-CA-C	-6.44	105.39	113.18
1	D	174	GLN	N-CA-C	-6.30	103.94	111.69
1	A	109	PRO	CA-C-N	6.28	127.69	119.84
1	A	109	PRO	C-N-CA	6.28	127.69	119.84
1	B	324	LEU	N-CA-C	6.24	118.89	111.33
1	A	321	GLN	N-CA-C	-6.23	106.37	112.97
1	D	242	LYS	N-CA-C	-6.21	104.51	111.28
1	D	539	TRP	N-CA-C	6.19	120.39	112.34
1	D	292	ASN	N-CA-C	6.15	119.73	112.72
1	B	268	TYR	N-CA-C	-6.13	104.52	111.14
1	C	419	LYS	N-CA-C	-6.10	104.71	111.36
1	B	159	VAL	N-CA-C	6.06	118.63	111.05
1	D	660	PHE	N-CA-C	-6.04	106.07	113.50
1	A	424	SER	N-CA-C	5.99	118.29	111.11
1	D	80	LYS	N-CA-C	-5.97	104.40	111.03
1	D	603	ILE	N-CA-C	5.97	116.34	111.62
1	C	268	TYR	N-CA-C	-5.96	104.69	111.07
1	B	117	ASP	N-CA-C	-5.94	104.88	111.71
1	B	625	SER	N-CA-C	5.84	117.64	111.28
1	A	174	GLN	N-CA-C	-5.82	104.30	111.40
1	A	628	LEU	N-CA-C	-5.81	105.03	111.71
1	B	365	ILE	CB-CA-C	-5.80	104.55	111.97
1	B	561	VAL	N-CA-C	5.79	116.52	110.62
1	A	511	SER	N-CA-C	5.77	118.51	111.82
1	B	132	VAL	CA-C-N	5.74	127.02	119.84
1	B	132	VAL	C-N-CA	5.74	127.02	119.84
1	D	688	ILE	N-CA-C	-5.70	104.31	112.35
1	A	6	ASP	N-CA-C	-5.64	106.23	113.23
1	C	561	VAL	N-CA-C	5.55	116.29	110.62
1	B	363	LYS	N-CA-C	-5.50	105.83	112.54
1	B	136	ASN	N-CA-C	5.49	116.91	109.11
1	A	67	ALA	N-CA-C	-5.49	105.68	112.38
1	A	339	LYS	N-CA-C	-5.47	105.48	111.82
1	D	115	LEU	N-CA-C	-5.45	105.73	112.38
1	A	162	GLN	N-CA-C	5.42	116.99	111.14
1	B	496	ASN	N-CA-C	-5.41	105.03	111.69
1	D	324	LEU	N-CA-C	-5.39	106.78	113.19
1	A	242	LYS	N-CA-C	-5.38	105.31	111.07
1	A	402	ASP	N-CA-C	-5.37	105.43	111.28
1	A	287	PHE	N-CA-C	5.36	120.48	113.30
1	A	635	THR	N-CA-C	5.34	118.24	109.76
1	B	161	ILE	N-CA-C	5.33	115.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	TRP	N-CA-C	5.30	117.06	111.28
1	A	416	VAL	N-CA-C	-5.29	105.61	113.39
1	A	616	GLN	N-CA-C	-5.26	105.55	111.28
1	A	672	THR	N-CA-C	-5.25	107.54	114.31
1	C	242	LYS	N-CA-C	-5.24	105.57	111.28
1	D	505	ASP	N-CA-C	-5.24	105.68	111.71
1	C	175	LYS	N-CA-C	-5.23	106.74	113.23
1	B	470	LYS	N-CA-C	-5.22	105.76	111.82
1	B	498	LEU	N-CA-C	-5.21	106.18	112.54
1	A	481	ILE	N-CA-C	-5.20	105.32	110.62
1	C	68	LYS	N-CA-C	5.17	118.05	111.69
1	D	479	ILE	N-CA-C	5.13	115.86	110.62
1	A	57	ALA	N-CA-C	-5.10	107.45	113.97
1	D	619	HIS	N-CA-C	-5.09	105.64	111.14
1	D	432	SER	N-CA-C	-5.07	105.84	111.36
1	D	471	ILE	N-CA-C	-5.07	105.56	110.42
1	D	634	ALA	N-CA-C	5.06	116.79	111.28
1	B	538	THR	N-CA-C	5.05	118.54	112.38
1	C	299	ILE	CB-CA-C	-5.03	105.53	111.97
1	D	500	GLN	N-CA-C	5.03	117.16	111.02
1	B	56	GLY	N-CA-C	5.02	125.07	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5510	0	5545	331	0
1	B	5510	0	5545	253	0
1	C	5510	0	5545	226	0
1	D	5510	0	5545	292	0
All	All	22040	0	22180	1067	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 24.

All (1067) 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:531:ARG:HH21	1:B:383:PRO:HD3	1.13	1.14
1:C:183:THR:HG22	1:C:185:LYS:H	1.10	1.14
1:B:365:ILE:HD11	1:B:418:TYR:HD2	1.19	1.05
1:A:295:THR:CG2	1:A:297:PRO:HD2	1.88	1.04
1:B:183:THR:HG22	1:B:185:LYS:H	1.22	1.03
1:A:531:ARG:HH11	1:A:531:ARG:HB2	1.18	1.03
1:A:295:THR:HG22	1:A:297:PRO:CD	1.89	1.01
1:A:564:ILE:HG23	1:A:627:ILE:HD11	1.44	0.99
1:C:424:SER:HA	1:C:428:MSE:HG3	1.45	0.99
1:C:538:THR:HG22	1:C:542:LEU:HB3	1.42	0.99
1:D:583:ILE:HA	1:D:586:LYS:HD2	1.45	0.98
1:A:521:ARG:HG3	1:A:521:ARG:HH11	1.29	0.96
1:D:183:THR:HG23	1:D:185:LYS:H	1.30	0.96
1:D:544:MSE:H	1:D:612:ASN:ND2	1.64	0.95
1:C:419:LYS:O	1:C:422:THR:HG22	1.64	0.95
1:A:295:THR:HG22	1:A:297:PRO:HD2	0.96	0.95
1:B:538:THR:HG22	1:B:542:LEU:HB3	1.48	0.95
1:A:335:LEU:HD21	1:A:410:LEU:HD11	1.49	0.94
1:A:531:ARG:NH2	1:B:383:PRO:HD3	1.83	0.93
1:D:235:GLU:N	1:D:236:PRO:HA	1.85	0.92
1:A:419:LYS:O	1:A:422:THR:HG22	1.68	0.92
1:D:439:LEU:HD21	1:D:514:MSE:HE2	1.50	0.92
1:C:649:LEU:HD22	1:C:700:ILE:HD11	1.49	0.91
1:C:695:ILE:HG12	1:C:700:ILE:HD12	1.49	0.91
1:C:338:ASP:OD1	1:C:353:VAL:HG23	1.71	0.91
1:D:592:LEU:HD23	1:D:636:ASN:HD22	1.34	0.90
1:C:365:ILE:HD11	1:C:418:TYR:HB3	1.53	0.89
1:B:265:ILE:HD12	1:B:330:LEU:HD22	1.53	0.88
1:B:658:GLN:HG3	1:B:661:LEU:HD12	1.55	0.88
1:D:449:THR:HG22	1:D:451:GLU:H	1.38	0.88
1:B:419:LYS:O	1:B:422:THR:HG22	1.73	0.88
1:C:88:MSE:HE1	1:C:141:GLN:HB2	1.57	0.86
1:D:449:THR:HB	1:D:452:GLN:HG3	1.57	0.86
1:D:394:VAL:HG13	1:D:470:LYS:HG2	1.55	0.85
1:C:140:SER:C	1:C:142:TYR:H	1.85	0.85
1:A:377:ILE:HD13	1:B:534:PHE:HZ	1.41	0.85
1:B:259:THR:HG22	1:B:260:SER:H	1.41	0.84
1:B:666:ILE:HD12	1:B:696:ILE:HD12	1.60	0.84
1:C:586:LYS:O	1:C:590:GLU:HG2	1.78	0.84
1:C:450:LYS:HD2	1:C:525:LEU:HD23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:MSE:HE1	1:C:374:ARG:HH21	1.43	0.83
1:D:140:SER:C	1:D:142:TYR:H	1.82	0.83
1:B:630:LEU:HB3	1:B:631:PRO:HD2	1.61	0.82
1:C:412:PHE:O	1:C:415:LEU:HD22	1.78	0.82
1:B:555:VAL:HG12	1:B:556:PRO:HD2	1.62	0.82
1:C:458:MSE:HE2	1:C:574:LEU:HD13	1.60	0.82
1:B:531:ARG:HH11	1:B:531:ARG:HB2	1.44	0.81
1:A:137:ASN:HB2	1:A:140:SER:OG	1.81	0.81
1:A:666:ILE:HD12	1:A:696:ILE:HD12	1.62	0.81
1:D:544:MSE:H	1:D:612:ASN:HD22	1.27	0.81
1:C:648:ILE:HD11	1:C:680:ILE:HD13	1.61	0.81
1:A:599:PHE:HA	1:A:603:ILE:HD13	1.63	0.80
1:C:666:ILE:HD12	1:C:696:ILE:HD12	1.63	0.80
1:B:235:GLU:HB3	1:B:236:PRO:HD3	1.62	0.80
1:B:365:ILE:HD11	1:B:418:TYR:CD2	2.11	0.79
1:A:215:GLU:HG2	1:A:216:GLU:HG3	1.64	0.79
1:C:358:ASP:O	1:C:362:GLU:HG2	1.83	0.79
1:D:455:TYR:HD1	1:D:458:MSE:HE2	1.48	0.79
1:B:630:LEU:HB2	1:B:634:ALA:HB3	1.64	0.79
1:D:672:THR:O	1:D:676:GLU:HG2	1.83	0.78
1:D:424:SER:HA	1:D:428:MSE:HB2	1.64	0.78
1:A:428:MSE:HE2	1:A:499:PHE:HA	1.64	0.78
1:D:455:TYR:CD1	1:D:458:MSE:HE2	2.19	0.78
1:D:487:VAL:HA	1:D:490:THR:HG22	1.65	0.77
1:B:329:VAL:O	1:B:333:GLN:HG3	1.84	0.77
1:C:672:THR:O	1:C:676:GLU:HG2	1.84	0.77
1:D:542:LEU:HD12	1:D:612:ASN:HB3	1.66	0.77
1:B:649:LEU:HD22	1:B:700:ILE:HD11	1.67	0.77
1:A:316:ARG:HH12	1:A:357:SER:HB2	1.50	0.76
1:A:261:SER:HB3	1:A:264:LYS:HG3	1.67	0.76
1:D:458:MSE:HE1	1:D:573:LYS:HB3	1.67	0.76
1:A:531:ARG:HB2	1:A:531:ARG:NH1	1.96	0.76
1:D:499:PHE:O	1:D:503:GLU:HB2	1.85	0.76
1:B:648:ILE:HD11	1:B:680:ILE:HD13	1.67	0.76
1:B:84:GLN:HG2	1:B:135:ILE:HD13	1.67	0.76
1:A:618:LEU:HD11	1:A:646:VAL:HG21	1.67	0.76
1:A:88:MSE:HE3	1:A:141:GLN:HB2	1.67	0.75
1:C:666:ILE:HD12	1:C:696:ILE:CD1	2.17	0.75
1:D:560:LEU:O	1:D:564:ILE:HG13	1.85	0.75
1:A:448:ARG:HH22	1:B:450:LYS:HE3	1.51	0.75
1:B:140:SER:C	1:B:142:TYR:H	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:LEU:HB3	1:C:631:PRO:HD2	1.67	0.74
1:A:371:MSE:O	1:A:375:GLN:HG3	1.87	0.74
1:D:564:ILE:HG22	1:D:627:ILE:HD11	1.68	0.74
1:C:432:SER:HB3	1:C:502:VAL:HG12	1.69	0.74
1:A:140:SER:C	1:A:142:TYR:H	1.94	0.73
1:A:521:ARG:HG3	1:A:521:ARG:NH1	1.96	0.73
1:C:7:LEU:O	1:C:7:LEU:HD23	1.89	0.73
1:A:316:ARG:NH1	1:A:357:SER:HB2	2.03	0.73
1:D:325:LYS:HG2	1:D:367:TYR:OH	1.88	0.73
1:B:450:LYS:HB2	1:B:450:LYS:NZ	2.02	0.73
1:C:503:GLU:O	1:C:507:GLU:HG3	1.88	0.73
1:C:510:MSE:HE2	1:C:583:ILE:HD12	1.71	0.73
1:A:598:TYR:CE2	1:A:603:ILE:HD11	2.24	0.72
1:A:405:GLU:HB3	1:A:406:PRO:HD3	1.71	0.72
1:C:449:THR:HB	1:C:452:GLN:HG3	1.72	0.72
1:A:454:LEU:HG	1:A:458:MSE:HE2	1.71	0.72
1:D:648:ILE:HD13	1:D:688:ILE:HG23	1.71	0.72
1:A:649:LEU:HG	1:A:700:ILE:HD11	1.71	0.72
1:A:322:ASN:ND2	1:A:323:ASP:H	1.87	0.72
1:B:362:GLU:HG2	1:B:418:TYR:HE2	1.54	0.72
1:C:555:VAL:CG1	1:C:556:PRO:HD2	2.19	0.71
1:D:474:LEU:O	1:D:477:ASN:HB2	1.89	0.71
1:A:455:TYR:CE1	1:A:573:LYS:HG3	2.26	0.71
1:D:371:MSE:O	1:D:375:GLN:HG3	1.89	0.71
1:B:651:LEU:HB3	1:B:661:LEU:HD21	1.72	0.71
1:A:571:ILE:HD12	1:A:628:LEU:HA	1.72	0.70
1:C:139:ASP:OD1	1:C:143:ALA:HB2	1.90	0.70
1:B:449:THR:HG22	1:B:452:GLN:CD	2.16	0.70
1:C:308:LEU:HD22	1:C:352:LEU:HD21	1.72	0.70
1:D:376:PHE:O	1:D:380:THR:HG22	1.91	0.70
1:C:696:ILE:HG22	1:C:697:TYR:CD2	2.26	0.70
1:A:325:LYS:O	1:A:328:ILE:HG22	1.91	0.70
1:B:113:PHE:HB2	1:B:164:LEU:HD11	1.73	0.70
1:B:660:PHE:HD2	1:B:665:TYR:CE2	2.10	0.70
1:B:449:THR:HG23	1:B:452:GLN:H	1.57	0.69
1:C:449:THR:HG22	1:C:451:GLU:H	1.57	0.69
1:B:365:ILE:O	1:B:369:VAL:HG23	1.91	0.69
1:B:555:VAL:CG1	1:B:556:PRO:HD2	2.22	0.69
1:C:259:THR:HG22	1:C:260:SER:H	1.56	0.69
1:A:449:THR:HG23	1:A:452:GLN:H	1.55	0.69
1:C:685:ASP:HA	1:C:688:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ASN:C	1:B:659:GLN:H	2.00	0.69
1:D:350:LEU:HD11	1:D:354:SER:HB3	1.72	0.69
1:D:438:ILE:HD11	1:D:463:HIS:HB3	1.75	0.69
1:C:509:ALA:HB1	1:C:514:MSE:HE2	1.75	0.68
1:C:324:LEU:HD13	1:C:367:TYR:HB2	1.75	0.68
1:A:439:LEU:HD21	1:A:514:MSE:HE2	1.75	0.68
1:A:357:SER:HB3	1:A:360:VAL:HG23	1.75	0.68
1:C:183:THR:HG22	1:C:185:LYS:N	1.96	0.68
1:A:428:MSE:CE	1:A:499:PHE:HA	2.24	0.68
1:C:371:MSE:CE	1:C:374:ARG:HH21	2.06	0.68
1:A:31:LEU:O	1:A:35:LEU:HD12	1.94	0.68
1:D:592:LEU:HD23	1:D:636:ASN:ND2	2.07	0.68
1:A:648:ILE:HD11	1:A:680:ILE:HD13	1.76	0.68
1:D:183:THR:HG23	1:D:185:LYS:N	2.07	0.68
1:D:88:MSE:HE1	1:D:141:GLN:HB2	1.75	0.67
1:D:439:LEU:CD2	1:D:514:MSE:HE2	2.23	0.67
1:D:504:ASN:HB3	1:D:508:LYS:HE3	1.76	0.67
1:B:618:LEU:O	1:B:622:LYS:HG3	1.94	0.67
1:D:7:LEU:HD23	1:D:7:LEU:H	1.58	0.67
1:A:55:VAL:HG12	1:A:61:GLY:HA3	1.76	0.67
1:C:424:SER:O	1:C:428:MSE:HB2	1.94	0.67
1:A:428:MSE:HE1	1:A:502:VAL:HB	1.76	0.67
1:D:543:GLU:HA	1:D:612:ASN:ND2	2.10	0.67
1:D:259:THR:HG22	1:D:260:SER:H	1.59	0.67
1:A:478:PHE:O	1:A:481:ILE:HG12	1.94	0.67
1:C:259:THR:HG22	1:C:260:SER:N	2.10	0.67
1:D:185:LYS:HE2	1:D:185:LYS:HA	1.75	0.67
1:D:408:TYR:HA	1:D:419:LYS:HE2	1.77	0.66
1:A:322:ASN:OD1	1:A:326:THR:HG21	1.95	0.66
1:D:449:THR:HG22	1:D:451:GLU:N	2.09	0.66
1:A:282:LYS:O	1:A:286:ILE:HG13	1.95	0.66
1:B:450:LYS:HB2	1:B:450:LYS:HZ2	1.60	0.66
1:C:567:LEU:HD23	1:C:627:ILE:HD12	1.77	0.66
1:D:390:SER:O	1:D:394:VAL:HG23	1.96	0.66
1:D:55:VAL:CG1	1:D:61:GLY:HA3	2.26	0.66
1:D:648:ILE:HD11	1:D:680:ILE:HG12	1.76	0.66
1:D:259:THR:HG22	1:D:260:SER:N	2.10	0.66
1:A:544:MSE:H	1:A:612:ASN:HB3	1.60	0.65
1:C:585:LEU:HD21	1:C:631:PRO:HD3	1.76	0.65
1:A:7:LEU:CD1	1:D:77:LYS:HB3	2.27	0.65
1:D:465:ASN:OD1	1:D:580:PRO:HD3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:THR:HG22	1:B:260:SER:N	2.11	0.65
1:A:269:PHE:CE1	1:A:352:LEU:HD11	2.32	0.65
1:D:542:LEU:CD1	1:D:612:ASN:HB3	2.26	0.65
1:B:666:ILE:HD12	1:B:696:ILE:CD1	2.25	0.65
1:B:424:SER:HA	1:B:428:MSE:HE3	1.78	0.65
1:D:140:SER:C	1:D:142:TYR:N	2.47	0.65
1:A:564:ILE:HG23	1:A:627:ILE:CD1	2.25	0.65
1:D:55:VAL:O	1:D:57:ALA:N	2.30	0.65
1:D:487:VAL:HA	1:D:490:THR:CG2	2.26	0.65
1:A:555:VAL:HG22	1:A:556:PRO:HD2	1.79	0.65
1:B:618:LEU:HD22	1:B:646:VAL:HG11	1.79	0.65
1:C:523:GLN:HG3	1:C:594:VAL:HG11	1.78	0.64
1:C:630:LEU:HD12	1:C:630:LEU:H	1.62	0.64
1:D:579:ILE:HG23	1:D:580:PRO:HD2	1.78	0.64
1:D:662:ASN:HD21	1:D:665:TYR:HB2	1.61	0.64
1:D:140:SER:O	1:D:142:TYR:N	2.30	0.64
1:D:509:ALA:HB1	1:D:514:MSE:HE3	1.79	0.64
1:A:657:ASN:C	1:A:659:GLN:H	2.04	0.64
1:C:172:PHE:CE1	1:C:200:ASN:HB3	2.32	0.64
1:C:544:MSE:CE	1:C:554:SER:HB3	2.28	0.64
1:A:7:LEU:HD13	1:D:77:LYS:HB3	1.79	0.64
1:A:413:ASP:HA	1:A:416:VAL:HG23	1.78	0.64
1:A:540:SER:C	1:A:610:ASN:HD22	2.06	0.64
1:B:630:LEU:H	1:B:630:LEU:HD12	1.62	0.64
1:D:665:TYR:O	1:D:668:THR:HB	1.98	0.64
1:A:288:HIS:CD2	1:A:296:LYS:HE3	2.32	0.64
1:B:159:VAL:HG12	1:B:160:ILE:HD12	1.80	0.64
1:A:113:PHE:HB2	1:A:164:LEU:HD11	1.80	0.63
1:A:394:VAL:HG13	1:A:470:LYS:HG2	1.80	0.63
1:B:451:GLU:CD	1:B:569:ARG:HH12	2.06	0.63
1:C:592:LEU:HD22	1:C:639:CYS:SG	2.38	0.63
1:D:564:ILE:CG2	1:D:627:ILE:HD11	2.28	0.63
1:B:454:LEU:HG	1:B:458:MSE:HE2	1.79	0.63
1:C:265:ILE:HG21	1:C:330:LEU:HD22	1.79	0.63
1:D:428:MSE:HE3	1:D:428:MSE:HA	1.79	0.63
1:B:55:VAL:CG2	1:B:56:GLY:N	2.62	0.63
1:C:48:ILE:HG12	1:C:69:TYR:CE2	2.33	0.63
1:B:536:ILE:HD11	1:B:559:GLU:HG2	1.80	0.63
1:C:424:SER:HA	1:C:428:MSE:CG	2.26	0.63
1:C:510:MSE:HA	1:C:514:MSE:HE3	1.80	0.63
1:D:491:GLU:HB3	1:D:493:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:C	1:A:142:TYR:N	2.57	0.63
1:A:454:LEU:HG	1:A:458:MSE:CE	2.28	0.63
1:C:538:THR:CG2	1:C:542:LEU:HB3	2.23	0.63
1:A:295:THR:O	1:A:298:VAL:HB	1.99	0.62
1:A:407:PHE:O	1:A:408:TYR:HB2	1.98	0.62
1:A:618:LEU:HD13	1:A:646:VAL:HG11	1.80	0.62
1:C:7:LEU:HD23	1:C:7:LEU:C	2.24	0.62
1:B:343:ASN:ND2	1:C:339:LYS:HD2	2.13	0.62
1:B:517:SER:O	1:B:521:ARG:HG3	1.99	0.62
1:C:109:PRO:HG2	1:C:112:GLN:HG3	1.82	0.62
1:C:512:THR:HG22	1:C:513:ASP:N	2.14	0.62
1:C:215:GLU:O	1:C:216:GLU:HB2	1.97	0.62
1:C:657:ASN:C	1:C:659:GLN:H	2.07	0.62
1:A:370:GLU:O	1:A:374:ARG:HG2	2.00	0.62
1:C:544:MSE:HE1	1:C:554:SER:HB3	1.81	0.62
1:C:555:VAL:HG12	1:C:556:PRO:HD2	1.82	0.62
1:B:630:LEU:HB3	1:B:631:PRO:CD	2.29	0.62
1:D:454:LEU:O	1:D:458:MSE:HG3	1.98	0.62
1:B:66:ARG:NH2	1:B:76:ASN:OD1	2.33	0.62
1:D:215:GLU:O	1:D:216:GLU:HB2	2.00	0.62
1:A:573:LYS:O	1:A:577:MSE:HG2	2.00	0.61
1:B:648:ILE:HD13	1:B:688:ILE:HG23	1.82	0.61
1:D:269:PHE:CE2	1:D:352:LEU:HD11	2.35	0.61
1:A:14:ILE:O	1:A:18:GLN:HG3	2.00	0.61
1:C:308:LEU:HD22	1:C:352:LEU:CD2	2.30	0.61
1:C:542:LEU:HD11	1:C:613:GLY:N	2.15	0.61
1:A:401:TYR:OH	1:A:479:ILE:HD12	2.00	0.61
1:A:185:LYS:O	1:A:185:LYS:HD3	2.00	0.61
1:A:363:LYS:HA	1:B:697:TYR:HE2	1.64	0.61
1:C:542:LEU:HD11	1:C:613:GLY:CA	2.30	0.61
1:C:636:ASN:HD22	1:C:639:CYS:H	1.48	0.61
1:D:121:LEU:HD13	1:D:160:ILE:HD13	1.82	0.61
1:C:658:GLN:HG3	1:C:661:LEU:HD12	1.82	0.61
1:A:431:THR:CG2	1:A:471:ILE:HD11	2.31	0.61
1:A:431:THR:HG23	1:A:471:ILE:HD11	1.82	0.61
1:A:509:ALA:HB1	1:A:514:MSE:HE1	1.83	0.61
1:C:261:SER:HB3	1:C:264:LYS:HD2	1.83	0.61
1:A:531:ARG:HH11	1:A:531:ARG:CB	2.05	0.61
1:B:660:PHE:HD2	1:B:665:TYR:HE2	1.49	0.61
1:A:335:LEU:HD22	1:A:410:LEU:HD21	1.83	0.60
1:C:318:THR:O	1:C:321:GLN:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:GLU:N	1:D:236:PRO:CA	2.61	0.60
1:A:38:ASN:HD21	1:D:6:ASP:HB2	1.66	0.60
1:A:335:LEU:CD2	1:A:410:LEU:HD11	2.29	0.60
1:A:372:ALA:HB1	1:A:430:LEU:HD11	1.83	0.60
1:B:190:SER:HB3	1:B:193:LEU:HB3	1.82	0.60
1:D:337:THR:O	1:D:341:LEU:HB2	2.00	0.60
1:A:588:LYS:HD3	1:A:628:LEU:O	2.01	0.60
1:B:358:ASP:O	1:B:362:GLU:HG3	2.02	0.60
1:C:183:THR:HG22	1:C:184:GLN:N	2.14	0.60
1:D:158:ASP:O	1:D:162:GLN:HB3	2.01	0.60
1:B:573:LYS:O	1:B:577:MSE:HG2	2.00	0.60
1:C:630:LEU:HD12	1:C:630:LEU:N	2.15	0.60
1:A:135:ILE:HG22	1:A:137:ASN:ND2	2.17	0.60
1:A:401:TYR:HH	1:A:479:ILE:HD12	1.67	0.60
1:C:320:PHE:CE1	1:C:321:GLN:HB3	2.36	0.60
1:C:442:ASP:CG	1:C:448:ARG:HH12	2.09	0.60
1:A:48:ILE:HG12	1:A:69:TYR:CE2	2.36	0.60
1:A:108:GLN:HG3	1:A:112:GLN:NE2	2.17	0.60
1:D:633:HIS:CD2	1:D:634:ALA:H	2.19	0.60
1:A:72:LEU:HB2	1:A:75:LEU:HD13	1.84	0.60
1:B:180:GLN:OE1	1:B:185:LYS:HD3	2.02	0.60
1:D:420:LEU:HD23	1:D:483:LEU:HD22	1.82	0.60
1:B:382:ASN:HB3	1:B:384:GLU:CD	2.27	0.60
1:C:183:THR:CG2	1:C:185:LYS:HG2	2.31	0.60
1:C:455:TYR:CE1	1:C:573:LYS:HG3	2.37	0.60
1:D:307:VAL:O	1:D:310:PRO:HD2	2.01	0.60
1:A:406:PRO:C	1:A:407:PHE:O	2.38	0.59
1:A:405:GLU:O	1:A:407:PHE:O	2.20	0.59
1:C:695:ILE:CG1	1:C:700:ILE:HD12	2.29	0.59
1:B:371:MSE:O	1:B:375:GLN:HG3	2.02	0.59
1:B:450:LYS:HD2	1:B:525:LEU:HD23	1.84	0.59
1:D:309:GLN:OE1	1:D:312:ARG:HD2	2.03	0.59
1:A:21:ARG:NH2	1:D:28:LEU:HD21	2.17	0.59
1:A:603:ILE:N	1:A:603:ILE:HD12	2.17	0.59
1:D:390:SER:HB3	1:D:466:PHE:HD2	1.67	0.59
1:A:645:LEU:HD12	1:A:683:LEU:HD21	1.83	0.59
1:D:183:THR:CG2	1:D:185:LYS:HB2	2.32	0.59
1:D:479:ILE:HG13	1:D:483:LEU:HD12	1.83	0.59
1:D:544:MSE:N	1:D:612:ASN:ND2	2.46	0.59
1:D:520:HIS:HB3	1:D:524:LYS:NZ	2.17	0.59
1:B:140:SER:C	1:B:142:TYR:N	2.58	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:SER:O	1:B:192:GLY:N	2.35	0.59
1:A:449:THR:HG22	1:A:452:GLN:HG3	1.83	0.59
1:C:478:PHE:O	1:C:482:GLN:HG2	2.03	0.59
1:A:455:TYR:HD1	1:A:458:MSE:HE3	1.67	0.59
1:C:88:MSE:CE	1:C:141:GLN:HB2	2.31	0.59
1:D:320:PHE:HD1	1:D:320:PHE:O	1.86	0.59
1:B:539:TRP:O	1:B:609:PHE:HA	2.03	0.58
1:D:590:GLU:O	1:D:594:VAL:HG23	2.02	0.58
1:D:649:LEU:HD22	1:D:700:ILE:HD12	1.84	0.58
1:A:428:MSE:CE	1:A:502:VAL:HB	2.33	0.58
1:A:530:LEU:HD13	1:A:598:TYR:CE2	2.38	0.58
1:C:579:ILE:HG23	1:C:580:PRO:HD2	1.84	0.58
1:A:666:ILE:CD1	1:A:696:ILE:HD12	2.33	0.58
1:D:538:THR:O	1:D:542:LEU:HD23	2.03	0.58
1:A:406:PRO:O	1:A:409:ASP:HB2	2.02	0.58
1:A:408:TYR:HA	1:A:419:LYS:HE2	1.84	0.58
1:B:543:GLU:O	1:B:543:GLU:HG2	2.03	0.58
1:D:190:SER:O	1:D:192:GLY:N	2.28	0.58
1:A:195:LYS:NZ	1:A:198:ARG:HH21	2.02	0.58
1:A:584:SER:O	1:A:588:LYS:HG3	2.03	0.58
1:C:105:LEU:HD13	1:C:121:LEU:HD11	1.86	0.58
1:D:394:VAL:CG1	1:D:470:LYS:HG2	2.31	0.58
1:D:491:GLU:HB3	1:D:493:LYS:HZ3	1.67	0.58
1:A:179:ALA:O	1:A:180:GLN:C	2.45	0.58
1:A:449:THR:HG22	1:A:452:GLN:OE1	2.04	0.58
1:C:249:ASN:OD1	1:C:310:PRO:HB3	2.03	0.58
1:D:332:SER:O	1:D:335:LEU:HB3	2.04	0.58
1:D:657:ASN:C	1:D:659:GLN:H	2.11	0.58
1:A:571:ILE:CD1	1:A:628:LEU:HA	2.34	0.58
1:A:543:GLU:O	1:A:543:GLU:HG2	2.03	0.58
1:B:359:GLU:O	1:B:363:LYS:HG2	2.04	0.58
1:A:618:LEU:CD1	1:A:646:VAL:HG21	2.34	0.58
1:A:377:ILE:HD13	1:B:534:PHE:CZ	2.32	0.57
1:A:449:THR:HG22	1:A:452:GLN:CG	2.34	0.57
1:A:96:ASP:OD1	1:A:148:LEU:HD21	2.04	0.57
1:C:439:LEU:O	1:C:440:THR:HG23	2.04	0.57
1:D:124:LYS:O	1:D:128:VAL:HG23	2.04	0.57
1:A:176:LEU:HD22	1:A:181:TRP:CD1	2.39	0.57
1:B:29:GLN:O	1:B:33:GLN:HG3	2.04	0.57
1:C:542:LEU:HD12	1:C:542:LEU:C	2.28	0.57
1:D:512:THR:HG22	1:D:513:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ALA:HB1	1:A:514:MSE:CE	2.35	0.57
1:C:106:ALA:HB2	1:C:159:VAL:HG11	1.86	0.57
1:D:660:PHE:HD2	1:D:665:TYR:CE2	2.23	0.57
1:A:542:LEU:HD11	1:A:613:GLY:N	2.20	0.57
1:B:559:GLU:H	1:B:559:GLU:CD	2.11	0.57
1:C:46:GLU:O	1:C:50:GLN:HG2	2.03	0.57
1:A:449:THR:CG2	1:A:452:GLN:HG3	2.35	0.57
1:D:602:SER:C	1:D:603:ILE:HD12	2.29	0.57
1:D:649:LEU:HD13	1:D:700:ILE:HD11	1.85	0.57
1:D:160:ILE:O	1:D:164:LEU:HG	2.05	0.57
1:D:536:ILE:HD11	1:D:559:GLU:HG3	1.87	0.57
1:C:509:ALA:CB	1:C:514:MSE:HE2	2.35	0.57
1:A:84:GLN:NE2	1:A:135:ILE:HG21	2.19	0.57
1:A:542:LEU:HD11	1:A:613:GLY:CA	2.34	0.57
1:A:606:LEU:HD13	1:B:377:ILE:HD11	1.86	0.57
1:A:538:THR:HG22	1:A:542:LEU:HD23	1.87	0.56
1:D:609:PHE:HB2	1:D:614:LEU:HD13	1.86	0.56
1:B:555:VAL:HG12	1:B:556:PRO:CD	2.33	0.56
1:B:602:SER:C	1:B:603:ILE:HD12	2.30	0.56
1:D:509:ALA:HB1	1:D:514:MSE:CE	2.35	0.56
1:A:77:LYS:HE3	1:D:7:LEU:HB3	1.86	0.56
1:C:140:SER:C	1:C:142:TYR:N	2.50	0.56
1:C:183:THR:CG2	1:C:184:GLN:N	2.68	0.56
1:A:362:GLU:HG3	1:B:667:LYS:NZ	2.21	0.56
1:B:530:LEU:HD13	1:B:598:TYR:CE2	2.40	0.56
1:A:190:SER:C	1:A:192:GLY:H	2.13	0.56
1:A:260:SER:HB2	1:A:318:THR:HB	1.87	0.56
1:D:496:ASN:HB2	1:D:500:GLN:NE2	2.20	0.56
1:A:648:ILE:HD12	1:A:683:LEU:HD23	1.88	0.56
1:B:585:LEU:HD22	1:B:631:PRO:HD3	1.87	0.56
1:D:183:THR:CG2	1:D:185:LYS:H	2.13	0.56
1:B:103:ASP:OD1	1:B:155:LYS:HE2	2.06	0.56
1:B:541:THR:HG22	1:B:541:THR:O	2.05	0.56
1:C:533:TYR:HE2	1:C:603:ILE:HD13	1.70	0.56
1:D:591:LEU:O	1:D:595:ILE:HG13	2.06	0.56
1:A:269:PHE:CZ	1:A:352:LEU:HD11	2.40	0.55
1:D:411:ASP:O	1:D:412:PHE:O	2.24	0.55
1:D:483:LEU:O	1:D:487:VAL:HG23	2.06	0.55
1:A:412:PHE:CE1	1:A:414:LEU:HD12	2.41	0.55
1:C:367:TYR:CE1	1:C:371:MSE:HE3	2.41	0.55
1:B:357:SER:OG	1:B:360:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD21	1:C:660:PHE:HB2	1.86	0.55
1:D:662:ASN:OD1	1:D:665:TYR:N	2.35	0.55
1:B:55:VAL:O	1:B:57:ALA:N	2.39	0.55
1:B:88:MSE:HE1	1:B:141:GLN:C	2.31	0.55
1:C:42:VAL:HG12	1:C:42:VAL:O	2.07	0.55
1:D:573:LYS:O	1:D:577:MSE:HG2	2.06	0.55
1:D:491:GLU:O	1:D:493:LYS:HD2	2.06	0.55
1:B:113:PHE:CB	1:B:164:LEU:HD11	2.37	0.55
1:D:538:THR:HG22	1:D:542:LEU:HB3	1.87	0.55
1:B:261:SER:HB3	1:B:264:LYS:HG3	1.89	0.55
1:C:555:VAL:HG13	1:C:556:PRO:HD2	1.87	0.55
1:D:55:VAL:HG11	1:D:61:GLY:HA3	1.89	0.55
1:C:542:LEU:HD12	1:C:542:LEU:O	2.07	0.55
1:B:160:ILE:O	1:B:164:LEU:HD23	2.07	0.55
1:B:649:LEU:HD22	1:B:700:ILE:CD1	2.36	0.55
1:C:165:ALA:HB1	1:C:239:TRP:CG	2.42	0.55
1:D:510:MSE:HB3	1:D:583:ILE:CD1	2.36	0.55
1:C:140:SER:HB2	1:C:142:TYR:HB2	1.89	0.54
1:D:59:VAL:O	1:D:63:GLU:HG2	2.07	0.54
1:D:487:VAL:CA	1:D:490:THR:HG22	2.37	0.54
1:A:648:ILE:HD11	1:A:680:ILE:CD1	2.37	0.54
1:B:168:TRP:CE3	1:B:203:LYS:HE3	2.42	0.54
1:B:538:THR:CG2	1:B:542:LEU:HB3	2.30	0.54
1:C:434:TYR:CE2	1:C:467:VAL:HG21	2.42	0.54
1:D:544:MSE:N	1:D:612:ASN:HD22	2.01	0.54
1:A:408:TYR:CE2	1:A:422:THR:HG21	2.42	0.54
1:D:422:THR:O	1:D:426:ILE:HB	2.07	0.54
1:B:338:ASP:OD1	1:B:351:GLY:HA3	2.07	0.54
1:B:658:GLN:HG3	1:B:661:LEU:CD1	2.35	0.54
1:D:666:ILE:HD12	1:D:696:ILE:HD12	1.88	0.54
1:B:490:THR:O	1:B:490:THR:HG22	2.07	0.54
1:C:435:LEU:HB2	1:C:506:TYR:CE1	2.42	0.54
1:D:139:ASP:C	1:D:140:SER:O	2.49	0.54
1:D:411:ASP:O	1:D:412:PHE:C	2.50	0.54
1:D:490:THR:HG23	1:D:491:GLU:CD	2.33	0.54
1:B:83:VAL:O	1:B:87:GLN:HG3	2.07	0.54
1:D:345:PHE:O	1:D:347:TYR:N	2.40	0.54
1:A:316:ARG:HH12	1:A:357:SER:CB	2.20	0.54
1:C:5:ASP:C	1:C:7:LEU:H	2.15	0.54
1:D:84:GLN:HG3	1:D:135:ILE:HD12	1.90	0.54
1:C:160:ILE:O	1:C:164:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:GLU:O	1:C:493:LYS:HG3	2.07	0.54
1:C:510:MSE:HB3	1:C:583:ILE:CD1	2.37	0.54
1:A:330:LEU:O	1:A:334:ILE:HG13	2.08	0.53
1:A:359:GLU:HG3	1:B:667:LYS:HE3	1.89	0.53
1:A:659:GLN:HG3	1:A:660:PHE:N	2.23	0.53
1:B:189:THR:O	1:B:189:THR:HG22	2.08	0.53
1:B:611:GLN:HB2	1:B:653:TYR:CE2	2.44	0.53
1:C:382:ASN:HB3	1:C:384:GLU:OE2	2.08	0.53
1:B:520:HIS:O	1:B:524:LYS:HG3	2.09	0.53
1:B:630:LEU:O	1:B:631:PRO:C	2.51	0.53
1:C:261:SER:HB3	1:C:264:LYS:CD	2.38	0.53
1:D:536:ILE:CD1	1:D:559:GLU:HG3	2.39	0.53
1:D:540:SER:C	1:D:610:ASN:ND2	2.66	0.53
1:A:538:THR:CG2	1:A:542:LEU:HD23	2.38	0.53
1:B:66:ARG:HH21	1:B:76:ASN:HA	1.73	0.53
1:A:140:SER:HB2	1:A:142:TYR:HB2	1.89	0.53
1:A:610:ASN:O	1:A:613:GLY:N	2.40	0.53
1:A:438:ILE:HD13	1:A:464:VAL:HG23	1.91	0.53
1:B:422:THR:CG2	1:B:423:CYS:N	2.71	0.53
1:B:666:ILE:HD13	1:B:692:LEU:HB3	1.91	0.53
1:D:660:PHE:HD2	1:D:665:TYR:HE2	1.55	0.53
1:A:137:ASN:N	1:A:137:ASN:HD22	2.06	0.53
1:A:383:PRO:HG2	1:A:384:GLU:OE1	2.09	0.53
1:A:441:VAL:HG22	1:A:442:ASP:N	2.22	0.53
1:A:475:SER:HB3	1:A:499:PHE:HD2	1.74	0.53
1:A:695:ILE:HG12	1:A:700:ILE:HD12	1.91	0.53
1:B:84:GLN:HG2	1:B:135:ILE:CD1	2.37	0.53
1:C:694:ARG:O	1:C:699:ASN:HB2	2.09	0.53
1:D:540:SER:HA	1:D:610:ASN:ND2	2.23	0.53
1:A:315:VAL:HG11	1:A:355:LEU:HD21	1.90	0.53
1:A:359:GLU:HG3	1:B:667:LYS:CE	2.39	0.53
1:A:697:TYR:CE2	1:B:363:LYS:HD3	2.44	0.53
1:C:431:THR:HG23	1:C:471:ILE:HD11	1.90	0.53
1:D:121:LEU:HD13	1:D:160:ILE:CD1	2.39	0.53
1:B:55:VAL:HG23	1:B:56:GLY:N	2.24	0.53
1:D:183:THR:HG23	1:D:184:GLN:N	2.24	0.53
1:D:496:ASN:HB2	1:D:500:GLN:CD	2.35	0.52
1:A:66:ARG:HD3	1:A:71:ASP:OD1	2.08	0.52
1:A:542:LEU:HD11	1:A:613:GLY:HA2	1.92	0.52
1:A:455:TYR:CD1	1:A:458:MSE:HE3	2.44	0.52
1:D:106:ALA:HA	1:D:163:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:O	1:D:199:GLU:HG3	2.09	0.52
1:D:694:ARG:O	1:D:699:ASN:HB2	2.10	0.52
1:A:63:GLU:HG2	1:A:79:GLU:OE2	2.09	0.52
1:A:509:ALA:O	1:A:514:MSE:HE3	2.09	0.52
1:A:610:ASN:O	1:A:611:GLN:C	2.53	0.52
1:B:657:ASN:C	1:B:659:GLN:N	2.68	0.52
1:B:326:THR:O	1:B:330:LEU:HG	2.10	0.52
1:B:388:LYS:HD3	1:B:391:GLN:NE2	2.25	0.52
1:B:509:ALA:O	1:B:514:MSE:HE3	2.10	0.52
1:D:330:LEU:O	1:D:334:ILE:HG13	2.10	0.52
1:D:442:ASP:CG	1:D:448:ARG:HH12	2.16	0.52
1:B:510:MSE:HE1	1:B:580:PRO:CD	2.39	0.52
1:A:261:SER:HB3	1:A:264:LYS:CG	2.38	0.52
1:A:382:ASN:HA	1:B:531:ARG:HH21	1.75	0.52
1:D:461:LEU:HD23	1:D:579:ILE:HD13	1.92	0.52
1:D:490:THR:HG23	1:D:491:GLU:N	2.25	0.52
1:A:261:SER:H	1:A:264:LYS:HB2	1.74	0.52
1:A:342:LEU:O	1:A:346:HIS:HA	2.09	0.52
1:D:103:ASP:OD1	1:D:155:LYS:HE2	2.10	0.52
1:A:538:THR:CG2	1:A:542:LEU:HB3	2.40	0.52
1:C:411:ASP:O	1:C:413:ASP:N	2.43	0.52
1:A:530:LEU:HD23	1:A:563:SER:OG	2.10	0.52
1:B:509:ALA:HB1	1:B:514:MSE:CE	2.40	0.52
1:C:510:MSE:HE1	1:C:580:PRO:CD	2.40	0.52
1:D:568:ARG:O	1:D:572:ASN:HB2	2.09	0.52
1:C:329:VAL:O	1:C:333:GLN:HG3	2.10	0.51
1:A:101:GLN:O	1:A:105:LEU:HG	2.10	0.51
1:A:559:GLU:CD	1:A:559:GLU:H	2.17	0.51
1:B:148:LEU:O	1:B:152:VAL:HG23	2.10	0.51
1:D:464:VAL:HG21	1:D:514:MSE:SE	2.61	0.51
1:A:335:LEU:CD2	1:A:410:LEU:HD21	2.40	0.51
1:C:165:ALA:HB1	1:C:239:TRP:CD1	2.46	0.51
1:D:177:LEU:HD23	1:D:247:ASN:OD1	2.10	0.51
1:B:531:ARG:HB2	1:B:531:ARG:NH1	2.19	0.51
1:C:45:SER:OG	1:C:48:ILE:HG13	2.10	0.51
1:C:592:LEU:O	1:C:596:VAL:HG23	2.11	0.51
1:D:284:ILE:CG2	1:D:296:LYS:HG2	2.41	0.51
1:A:477:ASN:HB3	1:A:480:PHE:HD1	1.76	0.51
1:A:555:VAL:CG2	1:A:556:PRO:HD2	2.40	0.51
1:B:637:TYR:CE2	1:B:682:TYR:HB3	2.45	0.51
1:C:290:ASP:C	1:C:292:ASN:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:ILE:HG22	1:C:697:TYR:HD2	1.73	0.51
1:A:66:ARG:NH2	1:A:76:ASN:OD1	2.43	0.51
1:B:559:GLU:CD	1:B:559:GLU:N	2.69	0.51
1:C:454:LEU:HA	1:C:521:ARG:HD3	1.93	0.51
1:D:27:LYS:HB2	1:D:27:LYS:NZ	2.26	0.51
1:A:165:ALA:HB1	1:A:239:TRP:CG	2.45	0.51
1:B:657:ASN:HB3	1:B:660:PHE:CE1	2.45	0.51
1:C:536:ILE:HD11	1:C:559:GLU:CG	2.41	0.51
1:A:355:LEU:C	1:A:355:LEU:HD12	2.36	0.51
1:B:106:ALA:HB2	1:B:159:VAL:HG11	1.92	0.51
1:C:190:SER:O	1:C:192:GLY:N	2.37	0.51
1:C:414:LEU:O	1:C:414:LEU:HD23	2.11	0.51
1:C:510:MSE:HB3	1:C:583:ILE:HD11	1.92	0.51
1:D:649:LEU:HB3	1:D:700:ILE:CD1	2.40	0.51
1:A:543:GLU:OE2	1:A:543:GLU:N	2.44	0.51
1:B:48:ILE:HG12	1:B:69:TYR:CD2	2.46	0.51
1:A:77:LYS:CE	1:D:7:LEU:HB3	2.41	0.50
1:A:352:LEU:HB3	1:A:355:LEU:HD23	1.94	0.50
1:C:261:SER:HB3	1:C:264:LYS:CG	2.40	0.50
1:D:428:MSE:HE2	1:D:502:VAL:HB	1.92	0.50
1:C:284:ILE:O	1:C:288:HIS:HB3	2.11	0.50
1:C:653:TYR:CD1	1:C:653:TYR:N	2.79	0.50
1:D:592:LEU:CD1	1:D:625:SER:HB2	2.41	0.50
1:A:113:PHE:CB	1:A:164:LEU:HD11	2.41	0.50
1:A:371:MSE:HA	1:A:371:MSE:HE2	1.92	0.50
1:B:536:ILE:HD11	1:B:559:GLU:CG	2.42	0.50
1:C:386:PHE:N	1:C:387:PRO:HD2	2.27	0.50
1:C:450:LYS:HD2	1:C:525:LEU:CD2	2.39	0.50
1:C:649:LEU:CD2	1:C:700:ILE:HD11	2.33	0.50
1:D:102:LEU:C	1:D:104:GLU:H	2.20	0.50
1:D:657:ASN:O	1:D:659:GLN:N	2.44	0.50
1:A:248:PHE:CD2	1:A:307:VAL:HG13	2.47	0.50
1:B:622:LYS:HE2	1:B:643:HIS:HE1	1.76	0.50
1:C:590:GLU:O	1:C:594:VAL:HG23	2.12	0.50
1:D:690:ASP:O	1:D:694:ARG:HG3	2.12	0.50
1:A:618:LEU:HD23	1:A:622:LYS:NZ	2.27	0.50
1:A:694:ARG:HG3	1:A:699:ASN:HB2	1.94	0.50
1:B:442:ASP:OD2	1:B:448:ARG:NH1	2.39	0.50
1:D:181:TRP:HA	1:D:186:PHE:HB2	1.92	0.50
1:D:471:ILE:HG23	1:D:499:PHE:HD2	1.76	0.50
1:A:296:LYS:HB2	1:A:297:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TRP:O	1:A:609:PHE:HA	2.12	0.50
1:D:172:PHE:CE1	1:D:200:ASN:HB3	2.46	0.50
1:D:183:THR:HG21	1:D:185:LYS:HB2	1.94	0.50
1:D:256:PHE:CD2	1:D:268:TYR:HE2	2.30	0.50
1:D:475:SER:HB2	1:D:497:SER:OG	2.12	0.50
1:D:682:TYR:CD1	1:D:682:TYR:N	2.80	0.50
1:B:586:LYS:O	1:B:590:GLU:HG2	2.11	0.49
1:B:611:GLN:N	1:B:653:TYR:OH	2.45	0.49
1:C:510:MSE:HE1	1:C:580:PRO:HD3	1.94	0.49
1:D:295:THR:CG2	1:D:297:PRO:HD2	2.42	0.49
1:A:408:TYR:OH	1:A:422:THR:HG21	2.12	0.49
1:C:451:GLU:CD	1:C:569:ARG:HH12	2.19	0.49
1:C:685:ASP:HA	1:C:688:ILE:CD1	2.42	0.49
1:A:170:ASN:O	1:A:174:GLN:HG3	2.12	0.49
1:A:262:SER:O	1:A:333:GLN:OE1	2.30	0.49
1:A:324:LEU:CD2	1:A:363:LYS:HE2	2.42	0.49
1:B:215:GLU:O	1:B:216:GLU:HB2	2.12	0.49
1:C:571:ILE:HG12	1:C:628:LEU:HD23	1.93	0.49
1:D:331:ILE:HG23	1:D:410:LEU:HD11	1.94	0.49
1:A:579:ILE:HG23	1:A:580:PRO:HD2	1.95	0.49
1:B:422:THR:O	1:B:426:ILE:HB	2.13	0.49
1:D:41:GLU:O	1:D:42:VAL:C	2.54	0.49
1:D:98:PHE:CE2	1:D:125:LEU:HD22	2.48	0.49
1:A:657:ASN:O	1:A:659:GLN:N	2.46	0.49
1:B:181:TRP:O	1:B:282:LYS:HE2	2.12	0.49
1:B:439:LEU:HD21	1:B:514:MSE:HE2	1.94	0.49
1:C:177:LEU:HD23	1:C:247:ASN:OD1	2.12	0.49
1:D:106:ALA:HB2	1:D:159:VAL:HG11	1.94	0.49
1:A:205:TYR:CG	1:A:294:LEU:HD21	2.48	0.49
1:A:380:THR:HB	1:A:437:TYR:CE2	2.47	0.49
1:D:320:PHE:O	1:D:320:PHE:CD1	2.66	0.49
1:D:469:ARG:HG2	1:D:469:ARG:HH11	1.78	0.49
1:D:666:ILE:HG12	1:D:692:LEU:HD13	1.94	0.49
1:A:359:GLU:OE2	1:B:667:LYS:HE3	2.12	0.49
1:B:694:ARG:O	1:B:699:ASN:HB2	2.12	0.49
1:C:109:PRO:HG2	1:C:112:GLN:CG	2.42	0.49
1:A:352:LEU:N	1:A:352:LEU:HD23	2.27	0.49
1:B:45:SER:OG	1:B:48:ILE:HG13	2.13	0.49
1:B:105:LEU:HD13	1:B:121:LEU:HD11	1.93	0.49
1:C:543:GLU:HA	1:C:612:ASN:ND2	2.28	0.49
1:C:648:ILE:HD12	1:C:683:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:SER:HA	1:A:428:MSE:HB2	1.94	0.49
1:B:122:HIS:HB2	1:B:156:TYR:OH	2.12	0.49
1:B:413:ASP:O	1:B:416:VAL:HG12	2.13	0.49
1:C:26:SER:O	1:C:30:ASN:ND2	2.45	0.49
1:C:630:LEU:HB3	1:C:631:PRO:CD	2.38	0.49
1:D:580:PRO:CG	1:D:583:ILE:HD12	2.43	0.49
1:A:37:SER:C	1:A:39:ASP:H	2.21	0.49
1:A:116:ASP:O	1:A:117:ASP:C	2.56	0.49
1:A:491:GLU:O	1:A:493:LYS:HG3	2.13	0.49
1:D:109:PRO:HA	1:D:110:PRO:HD3	1.72	0.49
1:D:471:ILE:HG23	1:D:499:PHE:CD2	2.47	0.49
1:D:506:TYR:O	1:D:510:MSE:HG3	2.13	0.49
1:D:579:ILE:CG2	1:D:580:PRO:HD2	2.42	0.49
1:C:555:VAL:HG12	1:C:556:PRO:CD	2.43	0.48
1:C:573:LYS:O	1:C:577:MSE:HG2	2.13	0.48
1:D:84:GLN:HE21	1:D:135:ILE:HD13	1.78	0.48
1:A:269:PHE:HE1	1:A:352:LEU:HD11	1.78	0.48
1:A:610:ASN:O	1:A:612:ASN:N	2.46	0.48
1:A:632:SER:O	1:A:633:HIS:C	2.55	0.48
1:D:128:VAL:O	1:D:131:THR:HB	2.13	0.48
1:A:260:SER:HB2	1:A:318:THR:CB	2.43	0.48
1:C:458:MSE:HE2	1:C:574:LEU:CD1	2.40	0.48
1:D:115:LEU:O	1:D:119:LYS:HG3	2.12	0.48
1:B:195:LYS:O	1:B:199:GLU:HG3	2.13	0.48
1:B:408:TYR:OH	1:B:422:THR:CG2	2.61	0.48
1:C:183:THR:HG21	1:C:185:LYS:HG2	1.96	0.48
1:D:635:THR:HG22	1:D:635:THR:O	2.11	0.48
1:A:441:VAL:CG1	1:A:460:LYS:HE2	2.43	0.48
1:A:450:LYS:HE3	1:B:448:ARG:HH22	1.78	0.48
1:A:540:SER:C	1:A:610:ASN:ND2	2.72	0.48
1:C:109:PRO:HG2	1:C:112:GLN:CD	2.38	0.48
1:C:158:ASP:HA	1:C:162:GLN:HB2	1.95	0.48
1:C:235:GLU:HB2	1:C:236:PRO:HD3	1.94	0.48
1:D:166:THR:HG22	1:D:167:ASN:N	2.29	0.48
1:D:644:GLU:OE2	1:D:682:TYR:CD1	2.66	0.48
1:A:205:TYR:CE2	1:A:209:LEU:HD11	2.49	0.48
1:C:338:ASP:CG	1:C:352:LEU:H	2.20	0.48
1:C:648:ILE:HD11	1:C:680:ILE:CD1	2.37	0.48
1:D:288:HIS:HA	1:D:299:ILE:HD12	1.95	0.48
1:A:129:PHE:CD2	1:A:149:LYS:HE3	2.49	0.48
1:A:438:ILE:HD11	1:A:463:HIS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ILE:CG2	1:C:296:LYS:HG2	2.43	0.48
1:C:496:ASN:N	1:C:500:GLN:OE1	2.35	0.48
1:A:383:PRO:HD3	1:B:531:ARG:NH2	2.29	0.48
1:B:137:ASN:O	1:B:139:ASP:N	2.47	0.48
1:B:261:SER:H	1:B:264:LYS:HD2	1.78	0.48
1:B:542:LEU:C	1:B:542:LEU:HD12	2.38	0.48
1:D:187:ALA:C	1:D:189:THR:H	2.20	0.48
1:A:88:MSE:SE	1:A:142:TYR:HD1	2.47	0.48
1:A:649:LEU:CG	1:A:700:ILE:HD11	2.41	0.48
1:D:690:ASP:HA	1:D:693:TYR:HB2	1.95	0.48
1:A:407:PHE:O	1:A:409:ASP:N	2.37	0.48
1:A:454:LEU:HD23	1:A:570:LEU:HD22	1.96	0.48
1:A:538:THR:HG22	1:A:542:LEU:HB3	1.95	0.48
1:A:645:LEU:O	1:A:649:LEU:HD13	2.14	0.48
1:B:468:TYR:CE1	1:B:507:GLU:HG3	2.49	0.48
1:A:42:VAL:HG12	1:A:42:VAL:O	2.13	0.47
1:A:47:VAL:HG13	1:A:48:ILE:N	2.29	0.47
1:A:106:ALA:HB2	1:A:159:VAL:HG11	1.96	0.47
1:A:417:ARG:O	1:A:421:MSE:HG3	2.14	0.47
1:A:441:VAL:HG12	1:A:460:LYS:HE2	1.95	0.47
1:A:604:LEU:HG	1:A:694:ARG:HH22	1.79	0.47
1:B:88:MSE:HE1	1:B:141:GLN:CB	2.44	0.47
1:B:109:PRO:C	1:B:111:ASP:H	2.21	0.47
1:D:328:ILE:HG13	1:D:403:TYR:CZ	2.49	0.47
1:D:536:ILE:HG12	1:D:559:GLU:HG3	1.96	0.47
1:A:39:ASP:HB2	1:A:74:ILE:HD12	1.95	0.47
1:B:450:LYS:NZ	1:B:450:LYS:CB	2.74	0.47
1:B:651:LEU:O	1:B:661:LEU:HD11	2.14	0.47
1:C:476:SER:HA	1:C:481:ILE:HD11	1.96	0.47
1:C:542:LEU:HD11	1:C:613:GLY:HA2	1.95	0.47
1:A:542:LEU:HD12	1:A:542:LEU:C	2.39	0.47
1:B:109:PRO:O	1:B:111:ASP:N	2.48	0.47
1:B:544:MSE:H	1:B:612:ASN:HB3	1.79	0.47
1:C:540:SER:HB3	1:C:608:LYS:O	2.14	0.47
1:D:686:THR:O	1:D:690:ASP:OD1	2.32	0.47
1:B:303:PHE:O	1:B:307:VAL:HG23	2.14	0.47
1:D:239:TRP:H	1:D:239:TRP:CD1	2.31	0.47
1:D:259:THR:CG2	1:D:260:SER:H	2.26	0.47
1:A:48:ILE:HG12	1:A:69:TYR:CD2	2.50	0.47
1:A:422:THR:CG2	1:A:423:CYS:N	2.77	0.47
1:C:384:GLU:O	1:C:387:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:PRO:HG2	1:D:664:GLU:OE1	2.15	0.47
1:A:137:ASN:HB2	1:A:140:SER:HG	1.78	0.47
1:A:347:TYR:HE2	1:A:350:LEU:O	1.98	0.47
1:A:688:ILE:O	1:A:691:ALA:HB3	2.15	0.47
1:B:386:PHE:N	1:B:387:PRO:HD2	2.30	0.47
1:B:515:GLN:O	1:B:519:VAL:HG23	2.15	0.47
1:B:539:TRP:HB3	1:B:609:PHE:CD2	2.50	0.47
1:C:362:GLU:OE2	1:C:417:ARG:NH1	2.47	0.47
1:A:122:HIS:O	1:A:126:THR:HG23	2.14	0.47
1:A:308:LEU:HD22	1:A:352:LEU:HD21	1.97	0.47
1:A:422:THR:O	1:A:426:ILE:HB	2.14	0.47
1:A:694:ARG:HD2	1:A:699:ASN:OD1	2.15	0.47
1:C:122:HIS:NE2	1:C:212:LEU:HD21	2.29	0.47
1:C:153:THR:HB	1:C:214:LEU:CD2	2.45	0.47
1:C:335:LEU:HD22	1:C:410:LEU:HD11	1.96	0.47
1:C:365:ILE:HD11	1:C:418:TYR:CB	2.33	0.47
1:D:102:LEU:C	1:D:104:GLU:N	2.73	0.47
1:D:109:PRO:HG2	1:D:112:GLN:CD	2.39	0.47
1:D:295:THR:HB	1:D:298:VAL:HG23	1.95	0.47
1:D:657:ASN:HB3	1:D:660:PHE:CE1	2.50	0.47
1:A:195:LYS:HZ3	1:A:198:ARG:HH21	1.63	0.47
1:B:204:LEU:HD12	1:B:239:TRP:HB2	1.96	0.47
1:B:527:LYS:NZ	1:B:598:TYR:HB2	2.30	0.47
1:A:190:SER:O	1:A:192:GLY:N	2.44	0.47
1:A:660:PHE:CD1	1:A:674:LEU:HD13	2.50	0.47
1:D:662:ASN:ND2	1:D:665:TYR:HB2	2.30	0.47
1:B:84:GLN:HE21	1:B:135:ILE:HD13	1.80	0.46
1:D:158:ASP:C	1:D:158:ASP:OD1	2.58	0.46
1:A:157:ASN:ND2	1:A:211:TYR:CE1	2.83	0.46
1:A:319:LEU:HD21	1:A:360:VAL:HG11	1.98	0.46
1:A:462:GLN:HG3	1:A:578:ASP:H	1.79	0.46
1:B:478:PHE:H	1:B:478:PHE:HD2	1.60	0.46
1:C:390:SER:HB2	1:C:466:PHE:HD2	1.79	0.46
1:D:420:LEU:CD2	1:D:483:LEU:HD22	2.44	0.46
1:A:408:TYR:OH	1:A:422:THR:CG2	2.63	0.46
1:D:431:THR:HB	1:D:502:VAL:HG11	1.97	0.46
1:A:108:GLN:HG3	1:A:112:GLN:HE21	1.78	0.46
1:B:180:GLN:O	1:B:183:THR:HB	2.15	0.46
1:C:281:TYR:HA	1:C:284:ILE:HD12	1.98	0.46
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.72	0.46
1:D:261:SER:O	1:D:265:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:MSE:HB3	1:D:583:ILE:HD11	1.98	0.46
1:D:657:ASN:C	1:D:659:GLN:N	2.73	0.46
1:A:240:ASN:OD1	1:A:241:PHE:CD1	2.68	0.46
1:A:592:LEU:HD13	1:A:628:LEU:HD12	1.98	0.46
1:C:648:ILE:HD12	1:C:683:LEU:CD2	2.45	0.46
1:D:671:PHE:HE2	1:D:692:LEU:CD1	2.29	0.46
1:D:700:ILE:O	1:D:700:ILE:HG22	2.15	0.46
1:A:390:SER:OG	1:A:463:HIS:CG	2.68	0.46
1:B:140:SER:HB2	1:B:142:TYR:HB2	1.98	0.46
1:B:164:LEU:O	1:B:165:ALA:C	2.57	0.46
1:B:168:TRP:CZ3	1:B:203:LYS:HE3	2.50	0.46
1:B:284:ILE:HA	1:B:299:ILE:HG21	1.96	0.46
1:B:296:LYS:CB	1:B:297:PRO:HD3	2.45	0.46
1:C:499:PHE:O	1:C:502:VAL:HG23	2.16	0.46
1:D:61:GLY:O	1:D:64:GLN:HB2	2.15	0.46
1:B:258:ALA:HB1	1:B:264:LYS:HZ3	1.81	0.46
1:B:259:THR:CG2	1:B:260:SER:H	2.20	0.46
1:C:165:ALA:HB1	1:C:239:TRP:CD2	2.51	0.46
1:C:650:LYS:C	1:C:652:LYS:H	2.23	0.46
1:D:205:TYR:CG	1:D:294:LEU:HD21	2.51	0.46
1:A:137:ASN:ND2	1:A:137:ASN:N	2.64	0.46
1:A:438:ILE:HG22	1:A:439:LEU:HD23	1.97	0.46
1:B:451:GLU:OE2	1:B:569:ARG:NH1	2.49	0.46
1:B:693:TYR:HD2	1:B:697:TYR:CE1	2.34	0.46
1:C:371:MSE:HE1	1:C:374:ARG:NH2	2.23	0.46
1:C:658:GLN:HG3	1:C:661:LEU:CD1	2.46	0.46
1:D:512:THR:O	1:D:513:ASP:C	2.59	0.46
1:B:543:GLU:N	1:B:543:GLU:OE2	2.48	0.45
1:B:684:LYS:O	1:B:688:ILE:HG13	2.15	0.45
1:C:610:ASN:O	1:C:611:GLN:C	2.59	0.45
1:D:259:THR:CG2	1:D:260:SER:N	2.78	0.45
1:A:308:LEU:HD22	1:A:352:LEU:CD2	2.46	0.45
1:A:331:ILE:HD12	1:A:364:TRP:CD1	2.52	0.45
1:A:604:LEU:HD12	1:A:609:PHE:CE1	2.50	0.45
1:B:55:VAL:HG22	1:B:56:GLY:H	1.81	0.45
1:B:109:PRO:HD2	1:B:112:GLN:OE1	2.16	0.45
1:B:490:THR:O	1:B:491:GLU:HG3	2.17	0.45
1:B:622:LYS:HE2	1:B:643:HIS:CE1	2.51	0.45
1:C:307:VAL:O	1:C:307:VAL:HG12	2.16	0.45
1:A:205:TYR:O	1:A:208:SER:HB2	2.16	0.45
1:A:592:LEU:HD22	1:A:630:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:MSE:HE2	1:A:640:MSE:HA	1.98	0.45
1:C:490:THR:HG22	1:C:490:THR:O	2.16	0.45
1:D:41:GLU:HG2	1:D:73:GLN:NE2	2.32	0.45
1:A:454:LEU:CG	1:A:458:MSE:HE2	2.43	0.45
1:A:531:ARG:HH21	1:B:383:PRO:CD	2.04	0.45
1:A:602:SER:C	1:A:603:ILE:HD12	2.41	0.45
1:A:666:ILE:HG21	1:A:693:TYR:CE2	2.51	0.45
1:B:512:THR:OG1	1:B:513:ASP:N	2.49	0.45
1:C:585:LEU:CD2	1:C:631:PRO:HD3	2.45	0.45
1:D:106:ALA:HA	1:D:163:ARG:HH12	1.81	0.45
1:A:38:ASN:HD21	1:D:6:ASP:CB	2.29	0.45
1:B:95:LEU:HD13	1:B:149:LYS:HA	1.99	0.45
1:C:658:GLN:CG	1:C:661:LEU:HD12	2.45	0.45
1:D:431:THR:CG2	1:D:471:ILE:HD11	2.46	0.45
1:A:299:ILE:O	1:A:300:HIS:C	2.58	0.45
1:A:448:ARG:HH12	1:B:450:LYS:HG3	1.81	0.45
1:A:481:ILE:HG13	1:A:482:GLN:N	2.30	0.45
1:A:694:ARG:O	1:A:699:ASN:HB2	2.16	0.45
1:C:359:GLU:H	1:C:359:GLU:CD	2.24	0.45
1:D:42:VAL:HG12	1:D:42:VAL:O	2.17	0.45
1:A:116:ASP:O	1:A:119:LYS:N	2.50	0.45
1:A:407:PHE:C	1:A:409:ASP:H	2.23	0.45
1:C:543:GLU:HA	1:C:612:ASN:HD22	1.81	0.45
1:D:461:LEU:HD21	1:D:583:ILE:HG21	1.99	0.45
1:A:644:GLU:O	1:A:648:ILE:HG13	2.16	0.45
1:B:258:ALA:CB	1:B:264:LYS:HZ3	2.29	0.45
1:C:44:LEU:HD11	1:C:74:ILE:HD13	1.98	0.45
1:C:259:THR:CG2	1:C:260:SER:H	2.26	0.45
1:D:365:ILE:HD12	1:D:418:TYR:HD2	1.81	0.45
1:D:415:LEU:HD13	1:D:419:LYS:HE3	1.99	0.45
1:D:468:TYR:CZ	1:D:472:LYS:HE3	2.52	0.45
1:D:644:GLU:OE2	1:D:682:TYR:HD1	1.99	0.45
1:C:438:ILE:HD11	1:C:463:HIS:HB2	1.99	0.45
1:D:5:ASP:N	1:D:7:LEU:HD21	2.31	0.45
1:D:377:ILE:HA	1:D:380:THR:CG2	2.47	0.45
1:D:428:MSE:HA	1:D:428:MSE:CE	2.47	0.45
1:D:438:ILE:CD1	1:D:463:HIS:HB3	2.46	0.45
1:D:600:THR:HG22	1:D:601:GLU:OE2	2.16	0.45
1:A:445:ASN:O	1:A:446:GLU:C	2.59	0.45
1:A:622:LYS:HE2	1:A:643:HIS:NE2	2.32	0.45
1:B:159:VAL:O	1:B:163:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ILE:HD11	1:C:559:GLU:HG2	1.98	0.45
1:D:493:LYS:HG2	1:D:495:TYR:HE1	1.81	0.45
1:D:567:LEU:O	1:D:571:ILE:HB	2.15	0.45
1:B:666:ILE:HG22	1:B:693:TYR:CE1	2.52	0.44
1:C:135:ILE:HG22	1:C:136:ASN:N	2.32	0.44
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.78	0.44
1:B:512:THR:O	1:B:513:ASP:C	2.60	0.44
1:C:5:ASP:C	1:C:7:LEU:N	2.75	0.44
1:C:637:TYR:CD1	1:C:682:TYR:HD2	2.35	0.44
1:A:76:ASN:C	1:A:78:LEU:H	2.25	0.44
1:A:488:ASN:HD21	1:A:495:TYR:H	1.64	0.44
1:D:580:PRO:HG2	1:D:583:ILE:HD12	2.00	0.44
1:D:647:LYS:HB2	1:D:647:LYS:HE3	1.83	0.44
1:C:320:PHE:CD1	1:C:321:GLN:N	2.85	0.44
1:A:321:GLN:O	1:A:321:GLN:HG3	2.18	0.44
1:A:597:ASN:HD21	1:A:638:LYS:HE2	1.83	0.44
1:D:5:ASP:N	1:D:7:LEU:CD2	2.80	0.44
1:D:365:ILE:O	1:D:369:VAL:HG23	2.18	0.44
1:D:536:ILE:CG1	1:D:559:GLU:HG3	2.48	0.44
1:D:628:LEU:C	1:D:630:LEU:N	2.75	0.44
1:A:10:ILE:O	1:A:14:ILE:HG13	2.17	0.44
1:A:538:THR:O	1:A:540:SER:N	2.50	0.44
1:B:249:ASN:ND2	1:B:310:PRO:HB3	2.32	0.44
1:C:468:TYR:CE1	1:C:507:GLU:HG2	2.53	0.44
1:C:539:TRP:O	1:C:609:PHE:HA	2.17	0.44
1:C:678:TYR:O	1:C:679:SER:C	2.60	0.44
1:D:592:LEU:HD13	1:D:628:LEU:HD12	1.97	0.44
1:A:265:ILE:HA	1:A:268:TYR:CD1	2.53	0.44
1:A:328:ILE:HG23	1:A:329:VAL:N	2.33	0.44
1:A:363:LYS:HA	1:B:697:TYR:CE2	2.50	0.44
1:A:377:ILE:CD1	1:B:534:PHE:HZ	2.20	0.44
1:B:338:ASP:OD2	1:B:352:LEU:N	2.51	0.44
1:B:637:TYR:HE2	1:B:682:TYR:HB3	1.80	0.44
1:B:665:TYR:O	1:B:668:THR:HB	2.18	0.44
1:D:181:TRP:HA	1:D:186:PHE:CG	2.52	0.44
1:D:318:THR:O	1:D:319:LEU:C	2.59	0.44
1:D:523:GLN:NE2	1:D:594:VAL:HG13	2.32	0.44
1:A:521:ARG:HH11	1:A:521:ARG:CG	2.07	0.44
1:D:293:GLY:O	1:D:298:VAL:HG21	2.17	0.44
1:D:365:ILE:HG21	1:D:421:MSE:HE2	1.98	0.44
1:A:542:LEU:HD12	1:A:542:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:GLN:HG3	1:A:660:PHE:H	1.81	0.44
1:C:318:THR:O	1:C:319:LEU:C	2.60	0.44
1:D:338:ASP:O	1:D:342:LEU:HB2	2.18	0.44
1:D:350:LEU:HD21	1:D:354:SER:CB	2.47	0.44
1:D:355:LEU:HD12	1:D:355:LEU:C	2.43	0.44
1:D:386:PHE:N	1:D:387:PRO:HD2	2.33	0.44
1:D:465:ASN:CG	1:D:580:PRO:HD3	2.43	0.44
1:D:540:SER:C	1:D:610:ASN:HD22	2.24	0.44
1:D:634:ALA:C	1:D:636:ASN:H	2.26	0.44
1:A:179:ALA:O	1:A:181:TRP:N	2.51	0.43
1:B:55:VAL:CG2	1:B:56:GLY:H	2.31	0.43
1:B:240:ASN:OD1	1:B:241:PHE:N	2.51	0.43
1:B:284:ILE:HG21	1:B:296:LYS:HG3	2.00	0.43
1:B:657:ASN:HB3	1:B:660:PHE:HE1	1.83	0.43
1:C:355:LEU:C	1:C:355:LEU:HD12	2.43	0.43
1:A:362:GLU:HG3	1:B:667:LYS:HZ1	1.82	0.43
1:A:597:ASN:ND2	1:A:638:LYS:HE2	2.33	0.43
1:B:422:THR:HG22	1:B:423:CYS:N	2.33	0.43
1:D:323:ASP:C	1:D:325:LYS:H	2.24	0.43
1:D:535:LYS:O	1:D:535:LYS:HG2	2.19	0.43
1:A:114:THR:HG22	1:A:115:LEU:N	2.33	0.43
1:C:533:TYR:CD1	1:C:560:LEU:HB2	2.53	0.43
1:D:257:HIS:ND1	1:D:258:ALA:N	2.66	0.43
1:D:577:MSE:HB3	1:D:579:ILE:HG13	1.99	0.43
1:A:7:LEU:HD11	1:D:77:LYS:HB3	1.99	0.43
1:A:27:LYS:HD2	1:D:20:GLU:OE2	2.19	0.43
1:A:648:ILE:HG12	1:A:680:ILE:HD11	2.01	0.43
1:B:657:ASN:O	1:B:659:GLN:N	2.50	0.43
1:C:259:THR:CG2	1:C:260:SER:N	2.79	0.43
1:C:630:LEU:O	1:C:631:PRO:C	2.60	0.43
1:D:321:GLN:HG2	1:D:321:GLN:O	2.18	0.43
1:D:662:ASN:HD21	1:D:665:TYR:CB	2.30	0.43
1:B:362:GLU:HG2	1:B:418:TYR:CE2	2.44	0.43
1:B:408:TYR:OH	1:B:422:THR:HG21	2.17	0.43
1:C:169:SER:HA	1:C:204:LEU:HD21	2.01	0.43
1:C:461:LEU:HD23	1:C:579:ILE:HD13	2.01	0.43
1:B:382:ASN:HB3	1:B:384:GLU:OE1	2.19	0.43
1:B:478:PHE:N	1:B:478:PHE:CD2	2.86	0.43
1:C:295:THR:OG1	1:C:297:PRO:HD2	2.18	0.43
1:D:510:MSE:HE2	1:D:583:ILE:HD12	2.01	0.43
1:A:156:TYR:O	1:A:160:ILE:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:NH1	1:B:450:LYS:HG3	2.33	0.43
1:B:41:GLU:OE1	1:B:73:GLN:HB3	2.18	0.43
1:B:88:MSE:HE1	1:B:141:GLN:HB2	2.01	0.43
1:B:424:SER:CA	1:B:428:MSE:HE3	2.46	0.43
1:B:660:PHE:HE2	1:B:673:SER:HB2	1.83	0.43
1:C:320:PHE:CZ	1:C:321:GLN:NE2	2.87	0.43
1:C:405:GLU:HB3	1:C:406:PRO:CD	2.48	0.43
1:D:114:THR:C	1:D:116:ASP:N	2.76	0.43
1:D:377:ILE:HA	1:D:380:THR:HG22	2.01	0.43
1:A:365:ILE:HD11	1:A:418:TYR:HB3	1.99	0.43
1:B:66:ARG:NH2	1:B:76:ASN:HA	2.33	0.43
1:C:319:LEU:HA	1:C:319:LEU:HD12	1.77	0.43
1:D:568:ARG:HA	1:D:627:ILE:HG21	2.00	0.43
1:D:598:TYR:O	1:D:602:SER:HB2	2.18	0.43
1:D:603:ILE:HD12	1:D:603:ILE:N	2.34	0.43
1:D:627:ILE:C	1:D:629:SER:N	2.76	0.43
1:D:630:LEU:HD22	1:D:632:SER:H	1.84	0.43
1:A:80:LYS:O	1:A:83:VAL:HG12	2.19	0.43
1:A:632:SER:O	1:A:634:ALA:N	2.52	0.43
1:B:31:LEU:HD23	1:B:53:ILE:HG12	2.01	0.43
1:B:183:THR:HG22	1:B:185:LYS:N	2.07	0.43
1:B:449:THR:HG22	1:B:452:GLN:NE2	2.34	0.43
1:C:34:SER:O	1:C:35:LEU:C	2.61	0.43
1:A:249:ASN:OD1	1:A:310:PRO:HB3	2.19	0.43
1:A:297:PRO:O	1:A:301:GLU:HB2	2.19	0.43
1:A:644:GLU:OE2	1:A:682:TYR:HD1	2.01	0.43
1:B:176:LEU:HD22	1:B:181:TRP:CD1	2.53	0.43
1:B:260:SER:HB2	1:B:318:THR:OG1	2.19	0.43
1:B:324:LEU:O	1:B:328:ILE:HG12	2.19	0.43
1:C:7:LEU:C	1:C:7:LEU:CD2	2.91	0.43
1:D:295:THR:HG22	1:D:297:PRO:HD2	2.00	0.43
1:D:355:LEU:HD12	1:D:356:ILE:N	2.34	0.43
1:D:627:ILE:C	1:D:629:SER:H	2.27	0.43
1:A:431:THR:CG2	1:A:502:VAL:HG11	2.49	0.42
1:C:474:LEU:HD22	1:C:480:PHE:HE1	1.84	0.42
1:C:560:LEU:CD2	1:C:620:ASP:HB3	2.49	0.42
1:D:571:ILE:HD12	1:D:571:ILE:HA	1.79	0.42
1:B:440:THR:O	1:B:440:THR:OG1	2.37	0.42
1:B:445:ASN:O	1:B:446:GLU:C	2.62	0.42
1:B:610:ASN:O	1:B:611:GLN:C	2.62	0.42
1:C:510:MSE:CA	1:C:514:MSE:HE3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:THR:HG22	1:C:538:THR:O	2.18	0.42
1:D:348:HIS:O	1:D:348:HIS:ND1	2.52	0.42
1:A:315:VAL:O	1:A:318:THR:HG22	2.19	0.42
1:B:319:LEU:O	1:B:322:ASN:HB2	2.19	0.42
1:B:365:ILE:CD1	1:B:421:MSE:SE	3.17	0.42
1:B:591:LEU:HD23	1:B:591:LEU:HA	1.79	0.42
1:C:27:LYS:HD2	1:C:27:LYS:HA	1.79	0.42
1:C:265:ILE:HG21	1:C:330:LEU:CD2	2.48	0.42
1:C:411:ASP:O	1:C:412:PHE:C	2.63	0.42
1:D:323:ASP:C	1:D:325:LYS:N	2.77	0.42
1:A:28:LEU:HG	1:A:32:LYS:NZ	2.34	0.42
1:A:240:ASN:OD1	1:A:241:PHE:HD1	2.03	0.42
1:A:269:PHE:HA	1:A:272:LEU:HB3	2.00	0.42
1:B:60:GLU:O	1:B:64:GLN:HG3	2.20	0.42
1:B:183:THR:CG2	1:B:184:GLN:N	2.82	0.42
1:B:320:PHE:CG	1:B:321:GLN:N	2.87	0.42
1:B:592:LEU:HD11	1:B:639:CYS:SG	2.59	0.42
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.88	0.42
1:C:533:TYR:CE2	1:C:603:ILE:HD13	2.52	0.42
1:D:84:GLN:HG3	1:D:135:ILE:CD1	2.49	0.42
1:D:415:LEU:C	1:D:415:LEU:HD12	2.44	0.42
1:D:519:VAL:HG21	1:D:590:GLU:HB3	2.02	0.42
1:D:632:SER:O	1:D:633:HIS:C	2.61	0.42
1:A:19:ASN:O	1:A:22:ASN:N	2.52	0.42
1:A:259:THR:HG22	1:A:260:SER:N	2.35	0.42
1:A:309:GLN:HB3	1:A:310:PRO:CD	2.50	0.42
1:A:377:ILE:HD11	1:B:606:LEU:CD1	2.49	0.42
1:A:488:ASN:ND2	1:A:495:TYR:H	2.18	0.42
1:A:521:ARG:NH1	1:A:521:ARG:CG	2.67	0.42
1:B:99:GLU:OE2	1:B:151:LYS:HE3	2.20	0.42
1:B:362:GLU:O	1:B:366:ASN:HB2	2.20	0.42
1:C:39:ASP:HB2	1:C:74:ILE:HD12	2.01	0.42
1:C:115:LEU:HD12	1:C:115:LEU:O	2.19	0.42
1:D:180:GLN:O	1:D:183:THR:HG22	2.19	0.42
1:D:380:THR:OG1	1:D:437:TYR:CE2	2.72	0.42
1:A:74:ILE:HG23	1:A:75:LEU:HD12	2.01	0.42
1:B:284:ILE:CG2	1:B:296:LYS:HG3	2.49	0.42
1:D:137:ASN:CB	1:D:140:SER:HB2	2.50	0.42
1:D:295:THR:HG22	1:D:297:PRO:CD	2.49	0.42
1:D:590:GLU:OE1	1:D:590:GLU:HA	2.18	0.42
1:A:137:ASN:O	1:A:138:ILE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MSE:HE3	1:A:502:VAL:CG2	2.49	0.42
1:B:41:GLU:O	1:B:42:VAL:C	2.62	0.42
1:D:357:SER:HB3	1:D:360:VAL:HG23	2.02	0.42
1:B:98:PHE:CD2	1:B:125:LEU:HD13	2.55	0.42
1:B:651:LEU:HD11	1:B:674:LEU:HD11	2.01	0.42
1:D:295:THR:HB	1:D:297:PRO:HD2	2.00	0.42
1:B:417:ARG:HG3	1:B:418:TYR:N	2.34	0.42
1:B:581:LEU:O	1:B:585:LEU:HG	2.20	0.42
1:D:95:LEU:O	1:D:98:PHE:N	2.51	0.42
1:D:460:LYS:O	1:D:464:VAL:HG23	2.19	0.42
1:B:88:MSE:HE1	1:B:141:GLN:O	2.20	0.42
1:B:204:LEU:HB3	1:B:240:ASN:HB3	2.01	0.42
1:B:302:GLN:OE1	1:B:302:GLN:HA	2.19	0.42
1:B:659:GLN:HG3	1:B:660:PHE:N	2.34	0.42
1:C:62:LEU:HA	1:C:62:LEU:HD23	1.85	0.42
1:D:10:ILE:O	1:D:14:ILE:HG13	2.19	0.42
1:D:195:LYS:HB2	1:D:195:LYS:NZ	2.35	0.42
1:A:631:PRO:HG2	1:A:634:ALA:CB	2.49	0.41
1:B:63:GLU:HG2	1:B:79:GLU:OE1	2.19	0.41
1:C:614:LEU:HD12	1:C:614:LEU:HA	1.92	0.41
1:A:195:LYS:O	1:A:199:GLU:HG3	2.19	0.41
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.91	0.41
1:B:258:ALA:CB	1:B:264:LYS:NZ	2.83	0.41
1:B:542:LEU:HD11	1:B:613:GLY:N	2.34	0.41
1:B:683:LEU:HD12	1:B:683:LEU:HA	1.88	0.41
1:C:338:ASP:HA	1:C:341:LEU:HD12	2.02	0.41
1:C:431:THR:HG22	1:C:432:SER:N	2.34	0.41
1:A:302:GLN:O	1:A:305:ASN:HB3	2.21	0.41
1:A:660:PHE:CZ	1:A:673:SER:HB3	2.55	0.41
1:B:257:HIS:O	1:B:258:ALA:C	2.62	0.41
1:D:592:LEU:HD11	1:D:625:SER:HB2	2.01	0.41
1:A:205:TYR:CD1	1:A:294:LEU:HD21	2.55	0.41
1:A:318:THR:O	1:A:322:ASN:HB2	2.20	0.41
1:A:450:LYS:HE3	1:B:448:ARG:NH2	2.35	0.41
1:A:462:GLN:HG3	1:A:578:ASP:N	2.35	0.41
1:A:627:ILE:C	1:A:629:SER:N	2.77	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.82	0.41
1:B:474:LEU:HD22	1:B:480:PHE:CE1	2.56	0.41
1:C:508:LYS:O	1:C:509:ALA:C	2.63	0.41
1:D:657:ASN:HB3	1:D:660:PHE:HE1	1.85	0.41
1:D:671:PHE:O	1:D:675:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:CD	1:A:453:GLU:OE1	2.68	0.41
1:A:683:LEU:HD12	1:A:683:LEU:HA	1.90	0.41
1:B:490:THR:C	1:B:491:GLU:HG3	2.46	0.41
1:C:645:LEU:O	1:C:649:LEU:HG	2.21	0.41
1:D:390:SER:HB3	1:D:466:PHE:CD2	2.52	0.41
1:A:31:LEU:HG	1:A:35:LEU:HD11	2.01	0.41
1:A:358:ASP:OD1	1:A:418:TYR:OH	2.38	0.41
1:A:431:THR:HG21	1:A:471:ILE:CD1	2.51	0.41
1:A:431:THR:HG21	1:A:471:ILE:HD11	2.03	0.41
1:A:648:ILE:HD13	1:A:688:ILE:HG23	2.02	0.41
1:A:649:LEU:HG	1:A:700:ILE:CD1	2.47	0.41
1:B:377:ILE:HA	1:B:380:THR:HG22	2.02	0.41
1:D:256:PHE:CD2	1:D:268:TYR:CE2	3.08	0.41
1:D:330:LEU:HG	1:D:334:ILE:HD11	2.03	0.41
1:A:76:ASN:C	1:A:78:LEU:N	2.78	0.41
1:A:79:GLU:HA	1:A:82:ALA:HB3	2.03	0.41
1:A:172:PHE:CE1	1:A:200:ASN:HB3	2.56	0.41
1:A:542:LEU:HD12	1:A:612:ASN:HB2	2.02	0.41
1:A:693:TYR:O	1:A:697:TYR:HD1	2.04	0.41
1:B:114:THR:HG22	1:B:115:LEU:N	2.36	0.41
1:B:165:ALA:HB1	1:B:239:TRP:CG	2.56	0.41
1:C:172:PHE:CE2	1:C:176:LEU:HD11	2.55	0.41
1:C:401:TYR:CD1	1:C:401:TYR:C	2.99	0.41
1:A:571:ILE:HD11	1:A:628:LEU:HD23	2.03	0.41
1:A:638:LYS:HE3	1:A:638:LYS:HB3	1.81	0.41
1:B:308:LEU:HD22	1:B:352:LEU:HD21	2.03	0.41
1:D:541:THR:O	1:D:541:THR:HG22	2.21	0.41
1:A:22:ASN:O	1:A:25:ALA:HB3	2.21	0.41
1:A:279:ASN:O	1:A:280:LEU:C	2.63	0.41
1:A:371:MSE:HA	1:A:371:MSE:CE	2.49	0.41
1:A:478:PHE:CD1	1:A:481:ILE:HD11	2.55	0.41
1:A:509:ALA:C	1:A:514:MSE:HE3	2.46	0.41
1:A:630:LEU:HB3	1:A:631:PRO:HD2	2.02	0.41
1:A:660:PHE:HD1	1:A:674:LEU:HD13	1.85	0.41
1:B:181:TRP:HA	1:B:186:PHE:CD1	2.56	0.41
1:B:562:ASN:O	1:B:566:VAL:HG23	2.21	0.41
1:B:668:THR:HG22	1:B:670:ASN:H	1.84	0.41
1:C:179:ALA:O	1:C:180:GLN:C	2.64	0.41
1:C:320:PHE:CG	1:C:321:GLN:N	2.89	0.41
1:C:422:THR:CG2	1:C:423:CYS:N	2.84	0.41
1:C:675:LYS:HE3	1:C:675:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:O	1:D:164:LEU:C	2.64	0.41
1:D:281:TYR:CD1	1:D:282:LYS:N	2.89	0.41
1:D:431:THR:HG23	1:D:471:ILE:HD11	2.02	0.41
1:D:490:THR:HG23	1:D:491:GLU:H	1.86	0.41
1:D:543:GLU:HG2	1:D:543:GLU:O	2.20	0.41
1:D:608:LYS:HA	1:D:699:ASN:O	2.20	0.41
1:D:634:ALA:C	1:D:636:ASN:N	2.79	0.41
1:A:165:ALA:HB1	1:A:239:TRP:CD2	2.56	0.41
1:A:699:ASN:HD22	1:A:699:ASN:HA	1.55	0.41
1:C:204:LEU:HD12	1:C:204:LEU:HA	1.87	0.41
1:D:114:THR:HG22	1:D:115:LEU:N	2.36	0.41
1:D:477:ASN:O	1:D:481:ILE:HG13	2.21	0.41
1:B:345:PHE:O	1:B:346:HIS:HB2	2.21	0.40
1:B:393:PHE:O	1:B:396:LEU:HB3	2.21	0.40
1:B:416:VAL:O	1:B:416:VAL:HG22	2.21	0.40
1:B:602:SER:O	1:B:603:ILE:HD12	2.21	0.40
1:C:415:LEU:HD23	1:C:415:LEU:C	2.46	0.40
1:C:432:SER:HB3	1:C:502:VAL:CG1	2.46	0.40
1:D:208:SER:OG	1:D:239:TRP:HD1	2.04	0.40
1:D:281:TYR:CD1	1:D:281:TYR:C	2.98	0.40
1:D:329:VAL:O	1:D:333:GLN:HG3	2.20	0.40
1:D:439:LEU:HD21	1:D:514:MSE:CE	2.35	0.40
1:D:638:LYS:HE3	1:D:638:LYS:HB3	1.88	0.40
1:A:169:SER:HA	1:A:204:LEU:HD21	2.02	0.40
1:B:84:GLN:CG	1:B:135:ILE:HD13	2.45	0.40
1:A:379:ILE:HG13	1:A:380:THR:HG23	2.02	0.40
1:A:588:LYS:CB	1:A:630:LEU:HD21	2.51	0.40
1:B:281:TYR:HB2	1:C:481:ILE:HD12	2.03	0.40
1:B:649:LEU:HB3	1:B:700:ILE:HD13	2.03	0.40
1:D:671:PHE:HE2	1:D:692:LEU:HD12	1.86	0.40
1:A:7:LEU:HB2	1:D:81:VAL:HG21	2.04	0.40
1:A:540:SER:HB2	1:A:701:LEU:HD12	2.03	0.40
1:B:658:GLN:HG2	1:B:658:GLN:O	2.21	0.40
1:C:542:LEU:C	1:C:542:LEU:CD1	2.94	0.40
1:C:657:ASN:C	1:C:659:GLN:N	2.74	0.40
1:C:666:ILE:HD12	1:C:696:ILE:HD11	1.99	0.40
1:D:106:ALA:HB2	1:D:159:VAL:CG1	2.51	0.40
1:A:193:LEU:O	1:A:194:VAL:C	2.65	0.40
1:A:361:TRP:O	1:A:364:TRP:HB3	2.22	0.40
1:B:411:ASP:O	1:B:412:PHE:C	2.64	0.40
1:C:19:ASN:O	1:C:22:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:PHE:CD1	1:C:200:ASN:HB3	2.56	0.40
1:C:294:LEU:HD23	1:C:294:LEU:HA	1.90	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	667/706 (94%)	589 (88%)	64 (10%)	14 (2%)	5	27
1	B	667/706 (94%)	610 (92%)	43 (6%)	14 (2%)	5	27
1	C	667/706 (94%)	606 (91%)	49 (7%)	12 (2%)	6	31
1	D	667/706 (94%)	592 (89%)	59 (9%)	16 (2%)	4	24
All	All	2668/2824 (94%)	2397 (90%)	215 (8%)	56 (2%)	5	27

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	TRP
1	A	611	GLN
1	A	633	HIS
1	B	56	GLY
1	B	138	ILE
1	B	631	PRO
1	C	138	ILE
1	C	412	PHE
1	C	631	PRO
1	D	56	GLY
1	D	412	PHE
1	D	512	THR
1	D	633	HIS

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Mol	Chain	Res	Type
1	A	138	ILE
1	A	140	SER
1	A	180	GLN
1	A	191	VAL
1	A	544	MSE
1	B	544	MSE
1	C	492	SER
1	D	138	ILE
1	D	141	GLN
1	D	658	GLN
1	A	258	ALA
1	A	658	GLN
1	B	110	PRO
1	C	259	THR
1	C	685	ASP
1	D	158	ASP
1	D	321	GLN
1	D	411	ASP
1	B	258	ALA
1	B	259	THR
1	B	513	ASP
1	B	539	TRP
1	C	140	SER
1	D	685	ASP
1	A	38	ASN
1	A	319	LEU
1	A	423	CYS
1	B	140	SER
1	B	265	ILE
1	B	658	GLN
1	C	291	CYS
1	C	544	MSE
1	D	110	PRO
1	D	186	PHE
1	D	497	SER
1	B	663	PRO
1	C	191	VAL
1	C	258	ALA
1	D	191	VAL
1	C	441	VAL
1	D	42	VAL
1	B	133	PRO

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Mol	Chain	Res	Type
1	A	194	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	633/648 (98%)	591 (93%)	42 (7%)	15	46
1	B	633/648 (98%)	599 (95%)	34 (5%)	20	53
1	C	633/648 (98%)	593 (94%)	40 (6%)	16	48
1	D	633/648 (98%)	577 (91%)	56 (9%)	9	35
All	All	2532/2592 (98%)	2360 (93%)	172 (7%)	14	45

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	51	ASP
1	A	60	GLU
1	A	71	ASP
1	A	83	VAL
1	A	111	ASP
1	A	135	ILE
1	A	137	ASN
1	A	146	ASN
1	A	147	LYS
1	A	164	LEU
1	A	235	GLU
1	A	242	LYS
1	A	244	LEU
1	A	253	THR
1	A	257	HIS
1	A	267	THR
1	A	280	LEU
1	A	288	HIS
1	A	318	THR

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	352	LEU
1	A	355	LEU
1	A	397	ILE
1	A	409	ASP
1	A	412	PHE
1	A	416	VAL
1	A	422	THR
1	A	438	ILE
1	A	450	LYS
1	A	521	ARG
1	A	526	LEU
1	A	528	GLU
1	A	531	ARG
1	A	541	THR
1	A	559	GLU
1	A	571	ILE
1	A	594	VAL
1	A	633	HIS
1	A	693	TYR
1	A	694	ARG
1	A	699	ASN
1	B	23	GLU
1	B	38	ASN
1	B	54	GLU
1	B	55	VAL
1	B	75	LEU
1	B	84	GLN
1	B	89	GLN
1	B	204	LEU
1	B	215	GLU
1	B	242	LYS
1	B	296	LYS
1	B	314	LYS
1	B	323	ASP
1	B	341	LEU
1	B	380	THR
1	B	399	LYS
1	B	411	ASP
1	B	415	LEU
1	B	422	THR
1	B	450	LYS

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Mol	Chain	Res	Type
1	B	452	GLN
1	B	478	PHE
1	B	515	GLN
1	B	526	LEU
1	B	531	ARG
1	B	538	THR
1	B	542	LEU
1	B	559	GLU
1	B	579	ILE
1	B	631	PRO
1	B	662	ASN
1	B	663	PRO
1	B	676	GLU
1	B	694	ARG
1	C	12	ASP
1	C	47	VAL
1	C	76	ASN
1	C	104	GLU
1	C	121	LEU
1	C	126	THR
1	C	131	THR
1	C	237	VAL
1	C	251	ARG
1	C	265	ILE
1	C	288	HIS
1	C	301	GLU
1	C	314	LYS
1	C	328	ILE
1	C	337	THR
1	C	339	LYS
1	C	368	GLU
1	C	380	THR
1	C	397	ILE
1	C	399	LYS
1	C	402	ASP
1	C	415	LEU
1	C	431	THR
1	C	438	ILE
1	C	440	THR
1	C	441	VAL
1	C	450	LYS
1	C	469	ARG

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Mol	Chain	Res	Type
1	C	502	VAL
1	C	504	ASN
1	C	526	LEU
1	C	542	LEU
1	C	559	GLU
1	C	571	ILE
1	C	573	LYS
1	C	589	ASN
1	C	631	PRO
1	C	656	ASN
1	C	694	ARG
1	C	696	ILE
1	D	7	LEU
1	D	27	LYS
1	D	28	LEU
1	D	40	THR
1	D	54	GLU
1	D	73	GLN
1	D	75	LEU
1	D	76	ASN
1	D	86	THR
1	D	107	GLU
1	D	112	GLN
1	D	131	THR
1	D	147	LYS
1	D	173	ASP
1	D	174	GLN
1	D	180	GLN
1	D	183	THR
1	D	191	VAL
1	D	195	LYS
1	D	253	THR
1	D	266	GLU
1	D	273	ASN
1	D	307	VAL
1	D	314	LYS
1	D	326	THR
1	D	327	LEU
1	D	328	ILE
1	D	338	ASP
1	D	341	LEU
1	D	345	PHE

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Mol	Chain	Res	Type
1	D	346	HIS
1	D	348	HIS
1	D	411	ASP
1	D	415	LEU
1	D	423	CYS
1	D	428	MSE
1	D	450	LYS
1	D	451	GLU
1	D	457	THR
1	D	477	ASN
1	D	517	SER
1	D	518	ILE
1	D	521	ARG
1	D	538	THR
1	D	559	GLU
1	D	571	ILE
1	D	572	ASN
1	D	590	GLU
1	D	596	VAL
1	D	630	LEU
1	D	653	TYR
1	D	659	GLN
1	D	680	ILE
1	D	690	ASP
1	D	693	TYR
1	D	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	84	GLN
1	A	85	GLN
1	A	87	GLN
1	A	108	GLN
1	A	112	GLN
1	A	137	ASN
1	A	174	GLN
1	A	180	GLN
1	A	206	GLN
1	A	300	HIS
1	A	322	ASN

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	343	ASN
1	A	346	HIS
1	A	378	ASN
1	A	392	ASN
1	A	398	ASN
1	A	465	ASN
1	A	488	ASN
1	A	572	ASN
1	A	610	ASN
1	A	616	GLN
1	A	633	HIS
1	A	689	GLN
1	B	22	ASN
1	B	29	GLN
1	B	84	GLN
1	B	134	GLN
1	B	206	GLN
1	B	279	ASN
1	B	288	HIS
1	B	321	GLN
1	B	348	HIS
1	B	373	ASN
1	B	382	ASN
1	B	391	GLN
1	B	429	ASN
1	B	456	GLN
1	B	482	GLN
1	B	496	ASN
1	B	500	GLN
1	B	562	ASN
1	B	589	ASN
1	B	612	ASN
1	B	615	ASN
1	B	619	HIS
1	B	633	HIS
1	B	656	ASN
1	C	22	ASN
1	C	33	GLN
1	C	50	GLN
1	C	85	GLN
1	C	87	GLN

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Mol	Chain	Res	Type
1	C	112	GLN
1	C	134	GLN
1	C	137	ASN
1	C	206	GLN
1	C	246	ASN
1	C	255	HIS
1	C	273	ASN
1	C	302	GLN
1	C	321	GLN
1	C	322	ASN
1	C	343	ASN
1	C	373	ASN
1	C	429	ASN
1	C	465	ASN
1	C	496	ASN
1	C	589	ASN
1	C	612	ASN
1	C	636	ASN
1	D	38	ASN
1	D	50	GLN
1	D	84	GLN
1	D	108	GLN
1	D	137	ASN
1	D	141	GLN
1	D	146	ASN
1	D	174	GLN
1	D	200	ASN
1	D	375	GLN
1	D	391	GLN
1	D	392	ASN
1	D	500	GLN
1	D	504	ASN
1	D	523	GLN
1	D	593	ASN
1	D	611	GLN
1	D	612	ASN
1	D	633	HIS
1	D	636	ASN
1	D	659	GLN
1	D	670	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	663/706 (93%)	-0.02	11 (1%) 69 45	47, 83, 125, 155	0
1	B	663/706 (93%)	-0.27	5 (0%) 82 64	44, 70, 121, 160	0
1	C	663/706 (93%)	-0.21	5 (0%) 82 64	42, 71, 127, 161	0
1	D	663/706 (93%)	0.00	14 (2%) 63 40	52, 86, 128, 162	0
All	All	2652/2824 (93%)	-0.13	35 (1%) 75 53	42, 77, 125, 162	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	SER	4.2
1	D	7	LEU	4.2
1	A	324	LEU	3.4
1	C	260	SER	3.4
1	A	138	ILE	3.4
1	A	552	PRO	3.2
1	D	8	LEU	3.2
1	D	138	ILE	3.2
1	D	502	VAL	3.1
1	D	490	THR	3.0
1	B	631	PRO	3.0
1	A	633	HIS	3.0
1	A	260	SER	2.9
1	D	135	ILE	2.9
1	B	552	PRO	2.8
1	D	578	ASP	2.7
1	B	138	ILE	2.6
1	C	552	PRO	2.6
1	B	141	GLN	2.5
1	D	554	SER	2.5
1	A	269	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	493	LYS	2.5
1	D	555	VAL	2.4
1	A	258	ALA	2.3
1	A	545	SER	2.3
1	D	324	LEU	2.3
1	D	494	LYS	2.3
1	D	633	HIS	2.2
1	A	191	VAL	2.1
1	B	545	SER	2.1
1	D	545	SER	2.1
1	C	141	GLN	2.1
1	A	193	LEU	2.1
1	A	553	SER	2.1
1	C	631	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.