



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:58 PM UTC

PDB ID : 3F7F / pdb_00003f7f
Title : Structure of Nup120
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Deposited on : 2008-11-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

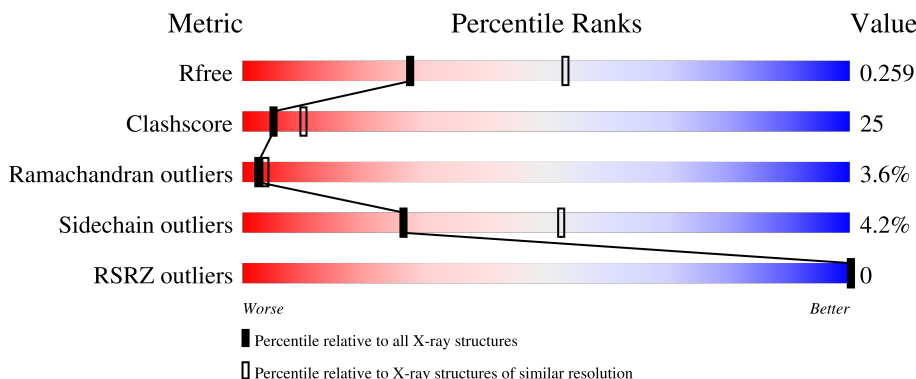
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	729	
1	B	729	
1	C	729	
1	D	729	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22876 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 Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5716	3700	908	1089	19			
1	B	701	Total	C	N	O	S	0	0	0
			5716	3700	908	1089	19			
1	C	701	Total	C	N	O	S	0	0	0
			5716	3700	908	1089	19			
1	D	701	Total	C	N	O	S	0	0	0
			5716	3700	908	1089	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	SER	engineered mutation	UNP P35729
B	207	CYS	SER	engineered mutation	UNP P35729
C	207	CYS	SER	engineered mutation	UNP P35729
D	207	CYS	SER	engineered mutation	UNP P35729

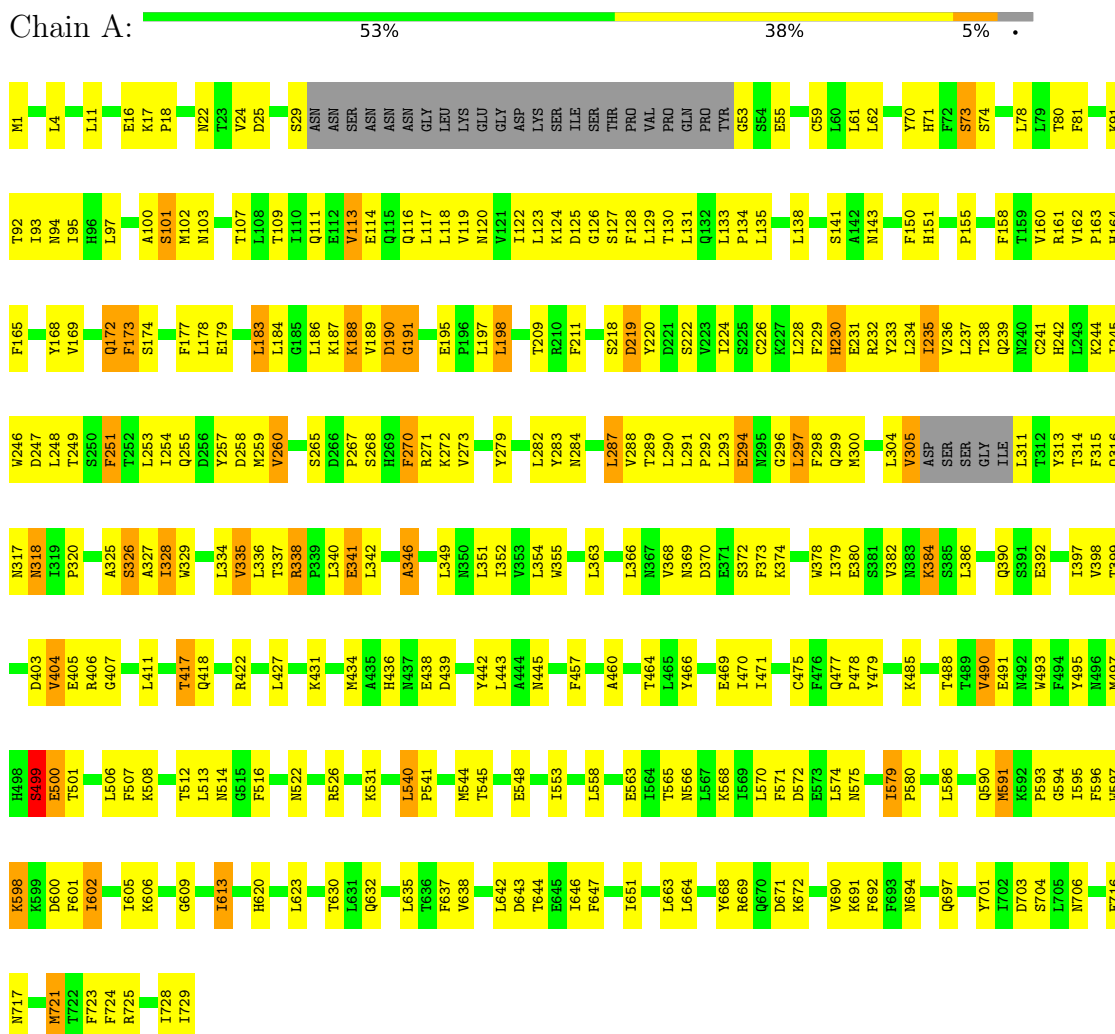
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Hg	0	0
			3	3		
2	B	3	Total	Hg	0	0
			3	3		
2	C	3	Total	Hg	0	0
			3	3		
2	D	3	Total	Hg	0	0
			3	3		

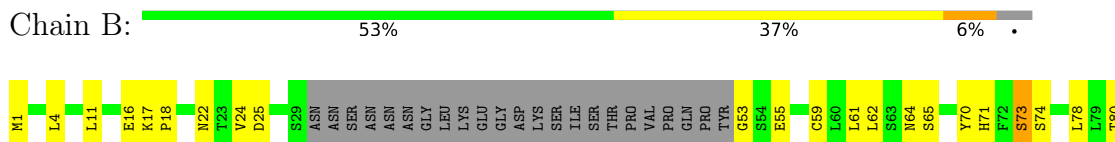
3 Residue-property plots

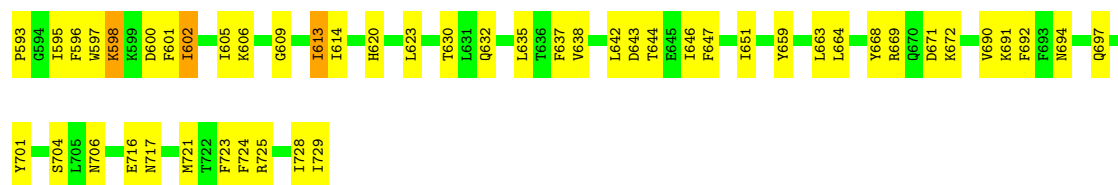
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoporin NUP120



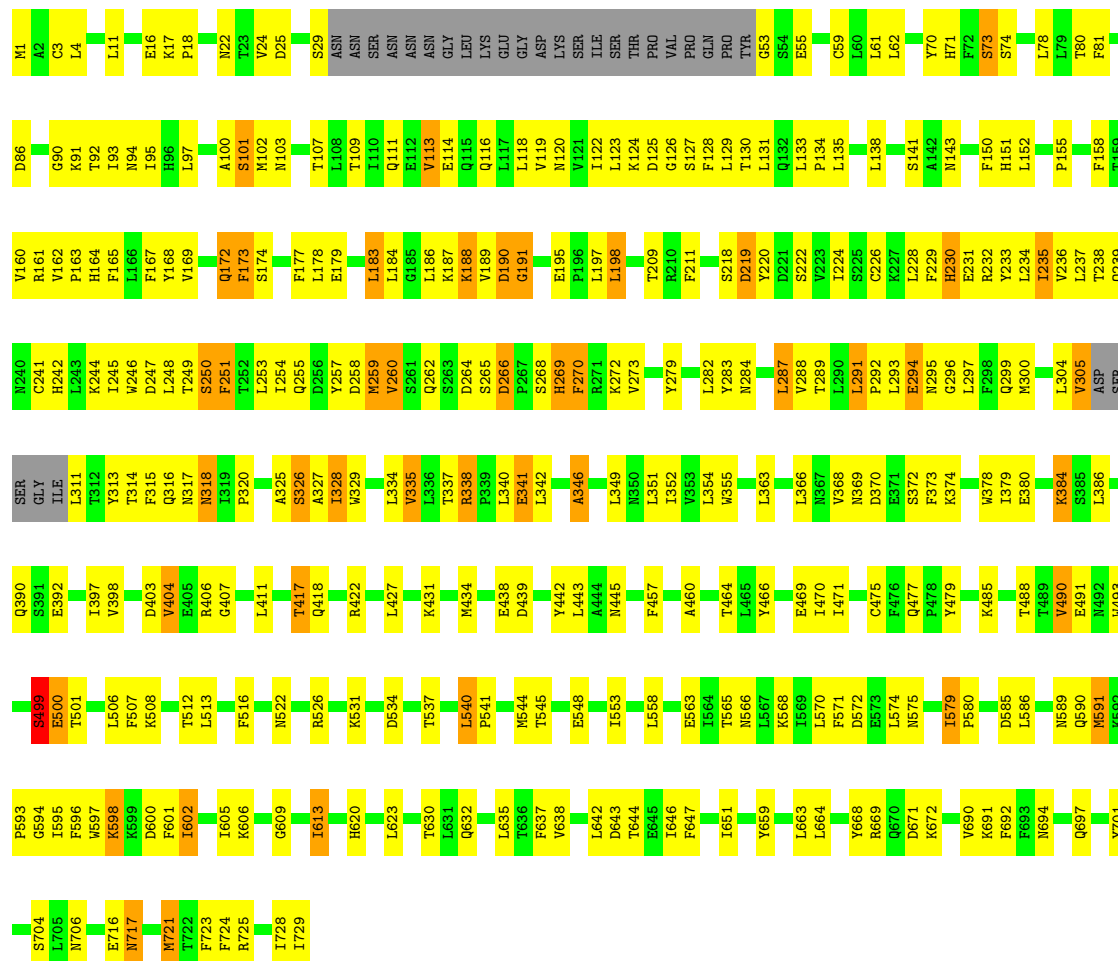
• Molecule 1: Nucleoporin NUP120





• Molecule 1: Nucleoporin NUP120

Chain D: 53% 37% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.68Å 117.48Å 146.29Å 89.94° 89.77° 89.89°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 88.7 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.254 0.237 , 0.259	Depositor DCC
R_{free} test set	19985 reflections (9.60%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l 0.468 for -h,k,-l 0.440 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22876	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.50	0/5845	0.98	25/7935 (0.3%)
1	B	0.50	0/5845	0.98	26/7935 (0.3%)
1	C	0.50	0/5845	0.98	26/7935 (0.3%)
1	D	0.50	0/5845	0.98	28/7935 (0.4%)
All	All	0.50	0/23380	0.98	105/31740 (0.3%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	VAL	N-CA-C	8.71	119.51	110.72
1	A	597	TRP	N-CA-C	-8.02	100.56	111.55
1	C	597	TRP	N-CA-C	-7.92	100.70	111.55
1	B	597	TRP	N-CA-C	-7.90	100.72	111.55
1	D	597	TRP	N-CA-C	-7.89	100.74	111.55
1	C	260	VAL	N-CA-C	7.68	120.69	111.09
1	D	728	ILE	N-CA-C	7.65	118.57	111.45
1	A	294	GLU	N-CA-C	-7.59	102.24	113.40
1	A	728	ILE	N-CA-C	7.58	118.50	111.45
1	C	728	ILE	N-CA-C	7.57	118.49	111.45
1	B	728	ILE	N-CA-C	7.55	118.47	111.45
1	C	294	GLU	N-CA-C	-7.54	102.31	113.40
1	D	294	GLU	N-CA-C	-7.54	102.31	113.40
1	B	294	GLU	N-CA-C	-7.48	102.40	113.40
1	D	251	PHE	N-CA-C	-7.48	103.45	112.58
1	C	398	VAL	N-CA-C	6.69	117.31	110.82
1	B	398	VAL	N-CA-C	6.50	117.13	110.82
1	D	398	VAL	N-CA-C	6.50	117.12	110.82
1	A	406	ARG	N-CA-C	-6.49	104.28	111.36
1	B	260	VAL	N-CA-C	6.44	119.15	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	SER	N-CA-C	-6.40	102.27	110.53
1	A	398	VAL	N-CA-C	6.35	116.98	110.82
1	B	406	ARG	N-CA-C	-6.35	104.44	111.36
1	C	406	ARG	N-CA-C	-6.35	104.44	111.36
1	C	417	THR	N-CA-C	6.33	118.18	111.28
1	D	101	SER	N-CA-C	-6.30	102.40	110.53
1	B	101	SER	N-CA-C	-6.29	102.41	110.53
1	C	101	SER	N-CA-C	-6.24	102.48	110.53
1	A	417	THR	N-CA-C	6.22	118.06	111.28
1	D	406	ARG	N-CA-C	-6.22	104.58	111.36
1	B	591	MET	N-CA-C	6.18	117.81	111.14
1	D	260	VAL	N-CA-C	6.17	119.70	111.44
1	A	591	MET	N-CA-C	6.16	117.80	111.14
1	C	249	THR	N-CA-C	-6.16	103.88	111.40
1	C	141	SER	N-CA-C	-6.12	105.61	114.12
1	C	251	PHE	N-CA-C	-6.06	103.56	111.74
1	A	198	LEU	N-CA-C	6.05	119.01	110.23
1	C	198	LEU	N-CA-C	6.03	118.98	110.23
1	B	198	LEU	N-CA-C	5.98	118.90	110.23
1	D	249	THR	N-CA-C	-5.98	102.41	111.56
1	B	262	GLN	N-CA-C	5.98	118.28	111.11
1	B	141	SER	N-CA-C	-5.97	105.82	114.12
1	D	198	LEU	N-CA-C	5.97	118.89	110.23
1	A	141	SER	N-CA-C	-5.96	105.83	114.12
1	D	141	SER	N-CA-C	-5.95	105.85	114.12
1	D	591	MET	N-CA-C	5.93	117.55	111.14
1	C	591	MET	N-CA-C	5.85	117.46	111.14
1	B	417	THR	N-CA-C	5.85	117.66	111.28
1	C	540	LEU	N-CA-C	-5.76	97.10	109.01
1	D	97	LEU	CA-C-N	5.66	125.12	119.24
1	D	97	LEU	C-N-CA	5.66	125.12	119.24
1	B	475	CYS	N-CA-C	5.65	118.79	110.59
1	D	417	THR	N-CA-C	5.64	117.43	111.28
1	D	475	CYS	N-CA-C	5.62	118.74	110.59
1	A	249	THR	N-CA-C	-5.61	106.27	113.23
1	A	540	LEU	N-CA-C	-5.61	97.40	109.01
1	B	540	LEU	N-CA-C	-5.59	97.43	109.01
1	D	540	LEU	CA-C-N	5.57	126.81	119.84
1	D	540	LEU	C-N-CA	5.57	126.81	119.84
1	A	475	CYS	N-CA-C	5.57	118.66	110.59
1	D	540	LEU	N-CA-C	-5.55	97.51	109.01
1	C	475	CYS	N-CA-C	5.55	118.64	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	LEU	CA-C-N	5.53	126.76	119.84
1	A	540	LEU	C-N-CA	5.53	126.76	119.84
1	B	540	LEU	CA-C-N	5.53	126.75	119.84
1	B	540	LEU	C-N-CA	5.53	126.75	119.84
1	B	97	LEU	CA-C-N	5.49	124.95	119.24
1	B	97	LEU	C-N-CA	5.49	124.95	119.24
1	A	251	PHE	N-CA-C	-5.48	104.35	111.74
1	D	384	LYS	N-CA-C	-5.47	100.75	109.23
1	C	540	LEU	CA-C-N	5.46	126.67	119.84
1	C	540	LEU	C-N-CA	5.46	126.67	119.84
1	C	97	LEU	CA-C-N	5.43	124.89	119.24
1	C	97	LEU	C-N-CA	5.43	124.89	119.24
1	B	249	THR	N-CA-C	-5.42	104.78	111.40
1	B	384	LYS	N-CA-C	-5.38	100.90	109.23
1	C	485	LYS	N-CA-C	5.37	118.00	109.24
1	C	384	LYS	N-CA-C	-5.35	100.93	109.23
1	D	485	LYS	N-CA-C	5.34	117.94	109.24
1	A	485	LYS	N-CA-C	5.31	117.90	109.24
1	A	97	LEU	CA-C-N	5.29	124.74	119.24
1	A	97	LEU	C-N-CA	5.29	124.74	119.24
1	B	558	LEU	N-CA-C	5.26	119.79	112.90
1	A	384	LYS	N-CA-C	-5.24	101.11	109.23
1	D	173	PHE	N-CA-C	5.23	117.42	108.90
1	C	269	HIS	N-CA-C	5.22	116.70	107.61
1	C	262	GLN	N-CA-C	5.18	117.66	111.71
1	D	269	HIS	N-CA-C	5.17	117.79	108.48
1	A	173	PHE	N-CA-C	5.17	117.33	108.90
1	D	717	ASN	N-CA-C	5.16	119.29	113.15
1	D	558	LEU	N-CA-C	5.16	119.65	112.90
1	C	173	PHE	N-CA-C	5.15	117.30	108.90
1	B	485	LYS	N-CA-C	5.15	117.63	109.24
1	A	558	LEU	N-CA-C	5.14	119.64	112.90
1	B	173	PHE	N-CA-C	5.13	117.26	108.90
1	B	291	LEU	CA-C-N	5.11	126.22	119.84
1	B	291	LEU	C-N-CA	5.11	126.22	119.84
1	C	297	LEU	N-CA-C	5.07	116.65	108.34
1	B	162	VAL	N-CA-C	5.06	114.47	108.96
1	C	162	VAL	N-CA-C	5.05	114.47	108.96
1	A	297	LEU	N-CA-C	5.04	116.61	108.34
1	A	594	GLY	N-CA-C	5.04	118.50	111.14
1	D	594	GLY	N-CA-C	5.01	118.46	111.14
1	D	291	LEU	CA-C-N	5.01	126.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	LEU	C-N-CA	5.01	126.10	119.84

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	5716	0	5626	282	0
1	B	5716	0	5626	286	0
1	C	5716	0	5626	288	0
1	D	5716	0	5626	282	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
All	All	22876	0	22504	1127	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 25.

All (1127) 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:113:VAL:HG23	1:A:114:GLU:H	1.07	1.18
1:B:113:VAL:HG23	1:B:114:GLU:H	1.08	1.16
1:C:113:VAL:HG23	1:C:114:GLU:H	1.08	1.14
1:D:113:VAL:HG23	1:D:114:GLU:H	1.09	1.12
1:A:160:VAL:HG23	1:A:161:ARG:H	1.23	1.03
1:B:160:VAL:HG23	1:B:161:ARG:H	1.23	1.03
1:B:342:LEU:HD13	1:B:379:ILE:HD12	1.39	1.02
1:C:342:LEU:HD13	1:C:379:ILE:HD12	1.39	1.01
1:A:342:LEU:HD13	1:A:379:ILE:HD12	1.40	1.01
1:D:342:LEU:HD13	1:D:379:ILE:HD12	1.39	1.01
1:C:160:VAL:HG23	1:C:161:ARG:H	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:VAL:HG23	1:D:161:ARG:H	1.23	0.99
1:D:288:VAL:HG12	1:D:300:MET:HB3	1.45	0.99
1:C:288:VAL:HG12	1:C:300:MET:HB3	1.45	0.99
1:A:288:VAL:HG12	1:A:300:MET:HB3	1.46	0.95
1:A:119:VAL:HB	1:A:131:LEU:HB2	1.48	0.95
1:B:18:PRO:HB3	1:B:417:THR:HG22	1.47	0.95
1:B:119:VAL:HB	1:B:131:LEU:HB2	1.49	0.94
1:B:288:VAL:HG12	1:B:300:MET:HB3	1.47	0.94
1:A:18:PRO:HB3	1:A:417:THR:HG22	1.48	0.94
1:D:119:VAL:HB	1:D:131:LEU:HB2	1.48	0.93
1:C:119:VAL:HB	1:C:131:LEU:HB2	1.48	0.93
1:D:18:PRO:HB3	1:D:417:THR:HG22	1.48	0.92
1:C:235:ILE:HD12	1:C:235:ILE:H	1.32	0.92
1:B:235:ILE:HD12	1:B:235:ILE:H	1.33	0.92
1:D:235:ILE:H	1:D:235:ILE:HD12	1.34	0.92
1:C:18:PRO:HB3	1:C:417:THR:HG22	1.49	0.91
1:A:235:ILE:HD12	1:A:235:ILE:H	1.33	0.91
1:D:541:PRO:HD2	1:D:544:MET:HE2	1.52	0.91
1:C:541:PRO:HD2	1:C:544:MET:HE2	1.53	0.89
1:A:541:PRO:HD2	1:A:544:MET:HE2	1.53	0.88
1:A:545:THR:HG23	1:A:548:GLU:OE1	1.72	0.88
1:C:109:THR:CG2	1:C:120:ASN:HB2	2.03	0.87
1:C:623:LEU:HD12	1:C:664:LEU:CD2	2.04	0.87
1:B:541:PRO:HD2	1:B:544:MET:HE2	1.54	0.87
1:D:109:THR:CG2	1:D:120:ASN:HB2	2.04	0.87
1:B:623:LEU:HD12	1:B:664:LEU:CD2	2.04	0.87
1:A:109:THR:CG2	1:A:120:ASN:HB2	2.03	0.87
1:D:545:THR:HG23	1:D:548:GLU:OE1	1.74	0.87
1:D:623:LEU:HD12	1:D:664:LEU:CD2	2.05	0.87
1:D:643:ASP:OD1	1:D:646:ILE:HG13	1.75	0.86
1:C:62:LEU:HD13	1:C:135:LEU:HD11	1.58	0.86
1:D:62:LEU:HD13	1:D:135:LEU:HD11	1.57	0.86
1:C:545:THR:HG23	1:C:548:GLU:OE1	1.75	0.86
1:B:109:THR:CG2	1:B:120:ASN:HB2	2.05	0.86
1:A:623:LEU:HD12	1:A:664:LEU:CD2	2.04	0.85
1:C:643:ASP:OD1	1:C:646:ILE:HG13	1.76	0.85
1:D:297:LEU:HD13	1:D:318:ASN:ND2	1.91	0.85
1:C:113:VAL:HG23	1:C:114:GLU:N	1.90	0.85
1:A:62:LEU:HD13	1:A:135:LEU:HD11	1.58	0.85
1:B:62:LEU:HD13	1:B:135:LEU:HD11	1.57	0.85
1:B:545:THR:HG23	1:B:548:GLU:OE1	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HE2	1:B:191:GLY:HA2	1.59	0.85
1:D:53:GLY:HA2	1:D:73:SER:HA	1.59	0.85
1:D:262:GLN:HG3	1:D:299:GLN:HE22	1.42	0.85
1:B:53:GLY:HA2	1:B:73:SER:HA	1.59	0.85
1:B:643:ASP:OD1	1:B:646:ILE:HG13	1.76	0.85
1:A:188:LYS:HE2	1:A:191:GLY:HA2	1.59	0.85
1:C:297:LEU:HD13	1:C:318:ASN:ND2	1.92	0.85
1:D:113:VAL:HG23	1:D:114:GLU:N	1.91	0.85
1:A:53:GLY:HA2	1:A:73:SER:HA	1.59	0.84
1:C:53:GLY:HA2	1:C:73:SER:HA	1.59	0.84
1:C:623:LEU:HD12	1:C:664:LEU:HD22	1.59	0.84
1:B:297:LEU:HD13	1:B:318:ASN:ND2	1.91	0.84
1:A:297:LEU:HD13	1:A:318:ASN:ND2	1.92	0.83
1:A:113:VAL:HG23	1:A:114:GLU:N	1.89	0.83
1:A:623:LEU:HD12	1:A:664:LEU:HD22	1.60	0.83
1:D:188:LYS:HE2	1:D:191:GLY:HA2	1.59	0.83
1:A:643:ASP:OD1	1:A:646:ILE:HG13	1.78	0.83
1:C:188:LYS:HE2	1:C:191:GLY:HA2	1.60	0.83
1:C:17:LYS:HE2	1:C:17:LYS:HA	1.61	0.82
1:B:113:VAL:HG23	1:B:114:GLU:N	1.90	0.82
1:D:623:LEU:HD12	1:D:664:LEU:HD22	1.61	0.82
1:C:113:VAL:CG2	1:C:114:GLU:H	1.92	0.81
1:D:17:LYS:HA	1:D:17:LYS:HE2	1.61	0.81
1:D:113:VAL:CG2	1:D:114:GLU:H	1.93	0.81
1:C:245:ILE:HG21	1:C:311:LEU:HD23	1.62	0.81
1:B:623:LEU:HD12	1:B:664:LEU:HD22	1.62	0.81
1:A:245:ILE:HG21	1:A:311:LEU:HD23	1.63	0.80
1:A:17:LYS:HE2	1:A:17:LYS:HA	1.61	0.80
1:B:17:LYS:HA	1:B:17:LYS:HE2	1.61	0.80
1:A:55:GLU:HB2	1:A:74:SER:HA	1.64	0.79
1:C:247:ASP:HB2	1:C:254:ILE:HG13	1.63	0.79
1:D:247:ASP:HB2	1:D:254:ILE:HG13	1.63	0.79
1:B:55:GLU:HB2	1:B:74:SER:HA	1.65	0.78
1:D:352:ILE:HD13	1:D:471:ILE:HG12	1.66	0.78
1:C:293:LEU:HD13	1:C:297:LEU:HD12	1.66	0.78
1:A:297:LEU:HD13	1:A:318:ASN:HD22	1.49	0.78
1:A:352:ILE:HD13	1:A:471:ILE:HG12	1.65	0.78
1:A:293:LEU:HD13	1:A:297:LEU:HD12	1.66	0.78
1:B:297:LEU:HD13	1:B:318:ASN:HD22	1.49	0.78
1:B:335:VAL:HG13	1:B:352:ILE:HB	1.66	0.77
1:C:352:ILE:HD13	1:C:471:ILE:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LEU:HD13	1:D:297:LEU:HD12	1.66	0.77
1:D:335:VAL:HG13	1:D:352:ILE:HB	1.66	0.77
1:A:335:VAL:HG13	1:A:352:ILE:HB	1.66	0.77
1:B:293:LEU:HD13	1:B:297:LEU:HD12	1.67	0.77
1:C:335:VAL:HG13	1:C:352:ILE:HB	1.66	0.77
1:D:404:VAL:HG11	1:D:438:GLU:HA	1.67	0.77
1:C:55:GLU:HB2	1:C:74:SER:HA	1.65	0.76
1:B:404:VAL:HG11	1:B:438:GLU:HA	1.67	0.76
1:D:297:LEU:HD13	1:D:318:ASN:HD22	1.49	0.76
1:D:102:MET:HB3	1:D:107:THR:HG21	1.67	0.76
1:D:55:GLU:HB2	1:D:74:SER:HA	1.66	0.76
1:A:102:MET:HB3	1:A:107:THR:HG21	1.66	0.75
1:C:160:VAL:HG23	1:C:161:ARG:N	2.01	0.75
1:C:591:MET:HE1	1:C:630:THR:OG1	1.87	0.75
1:C:102:MET:HB3	1:C:107:THR:HG21	1.67	0.75
1:D:602:ILE:HB	1:D:691:LYS:HB2	1.68	0.75
1:A:233:TYR:CG	1:A:311:LEU:HD22	2.22	0.75
1:B:102:MET:HB3	1:B:107:THR:HG21	1.67	0.75
1:B:245:ILE:HG21	1:B:311:LEU:HD23	1.68	0.75
1:B:602:ILE:HB	1:B:691:LYS:HB2	1.69	0.75
1:C:297:LEU:HD13	1:C:318:ASN:HD22	1.49	0.75
1:D:160:VAL:HG23	1:D:161:ARG:N	2.01	0.75
1:A:22:ASN:ND2	1:A:91:LYS:HB2	2.02	0.74
1:C:235:ILE:HD12	1:C:235:ILE:N	2.01	0.74
1:B:235:ILE:HD12	1:B:235:ILE:N	2.00	0.74
1:B:397:ILE:HG23	1:B:526:ARG:HG2	1.69	0.74
1:A:602:ILE:HB	1:A:691:LYS:HB2	1.69	0.74
1:C:602:ILE:HB	1:C:691:LYS:HB2	1.69	0.74
1:B:22:ASN:ND2	1:B:91:LYS:HB2	2.03	0.74
1:A:235:ILE:HD12	1:A:235:ILE:N	2.01	0.74
1:D:235:ILE:HD12	1:D:235:ILE:N	2.02	0.74
1:D:236:VAL:HG22	1:D:244:LYS:O	1.88	0.74
1:C:259:MET:HE1	1:C:313:TYR:HE2	1.53	0.74
1:D:92:THR:HG21	1:D:479:TYR:OH	1.88	0.74
1:C:236:VAL:HG22	1:C:244:LYS:O	1.88	0.74
1:D:591:MET:HE1	1:D:630:THR:OG1	1.88	0.74
1:A:724:PHE:HB3	1:B:724:PHE:HB3	1.69	0.73
1:B:92:THR:HG21	1:B:479:TYR:OH	1.87	0.73
1:A:259:MET:HE1	1:A:313:TYR:HE2	1.53	0.73
1:B:233:TYR:CG	1:B:311:LEU:HD22	2.23	0.73
1:A:16:GLU:O	1:A:417:THR:HG21	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG22	1:A:244:LYS:O	1.88	0.73
1:B:236:VAL:HG22	1:B:244:LYS:O	1.88	0.73
1:C:22:ASN:ND2	1:C:91:LYS:HB2	2.02	0.73
1:C:92:THR:HG21	1:C:479:TYR:OH	1.88	0.73
1:A:160:VAL:HG23	1:A:161:ARG:N	2.02	0.73
1:D:22:ASN:ND2	1:D:91:LYS:HB2	2.03	0.73
1:B:160:VAL:HG23	1:B:161:ARG:N	2.02	0.73
1:B:352:ILE:HD13	1:B:471:ILE:HG12	1.70	0.73
1:D:245:ILE:HG21	1:D:311:LEU:HD23	1.70	0.73
1:A:694:ASN:ND2	1:A:697:GLN:HE21	1.88	0.72
1:D:397:ILE:HG23	1:D:526:ARG:HG2	1.71	0.72
1:A:92:THR:HG21	1:A:479:TYR:OH	1.88	0.72
1:D:434:MET:HE3	1:D:442:TYR:HD1	1.55	0.72
1:B:591:MET:HE1	1:B:630:THR:OG1	1.90	0.72
1:D:169:VAL:HG13	1:D:228:LEU:HD22	1.72	0.72
1:C:169:VAL:HG13	1:C:228:LEU:HD22	1.71	0.72
1:A:130:THR:O	1:A:150:PHE:HA	1.90	0.71
1:A:397:ILE:HG23	1:A:526:ARG:HG2	1.72	0.71
1:A:169:VAL:HG13	1:A:228:LEU:HD22	1.70	0.71
1:A:591:MET:HE1	1:A:630:THR:OG1	1.90	0.71
1:A:113:VAL:CG2	1:A:114:GLU:H	1.91	0.71
1:D:130:THR:O	1:D:150:PHE:HA	1.91	0.71
1:A:717:ASN:OD1	1:A:721:MET:HG3	1.90	0.71
1:C:404:VAL:HG11	1:C:438:GLU:HA	1.73	0.71
1:C:259:MET:HE1	1:C:313:TYR:CE2	2.26	0.71
1:C:130:THR:O	1:C:150:PHE:HA	1.91	0.71
1:C:717:ASN:OD1	1:C:721:MET:HG3	1.90	0.71
1:B:717:ASN:OD1	1:B:721:MET:HG3	1.91	0.71
1:D:717:ASN:OD1	1:D:721:MET:HG3	1.90	0.71
1:B:113:VAL:CG2	1:B:114:GLU:H	1.92	0.70
1:B:130:THR:O	1:B:150:PHE:HA	1.91	0.70
1:B:434:MET:HE3	1:B:442:TYR:HD1	1.56	0.70
1:C:16:GLU:O	1:C:417:THR:HG21	1.91	0.70
1:D:694:ASN:ND2	1:D:697:GLN:HE21	1.88	0.70
1:A:247:ASP:HB2	1:A:254:ILE:HG13	1.72	0.70
1:B:694:ASN:ND2	1:B:697:GLN:HE21	1.90	0.70
1:C:694:ASN:ND2	1:C:697:GLN:HE21	1.88	0.70
1:B:293:LEU:HD22	1:B:297:LEU:HD11	1.73	0.70
1:D:233:TYR:CG	1:D:311:LEU:HD22	2.26	0.70
1:A:259:MET:HE1	1:A:313:TYR:CE2	2.26	0.70
1:B:169:VAL:HG13	1:B:228:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ILE:HG23	1:C:526:ARG:HG2	1.74	0.70
1:A:293:LEU:HD22	1:A:297:LEU:HD11	1.73	0.70
1:C:233:TYR:CG	1:C:311:LEU:HD22	2.26	0.70
1:D:16:GLU:O	1:D:417:THR:HG21	1.92	0.70
1:C:427:LEU:HD13	1:C:442:TYR:CE2	2.27	0.70
1:D:596:PHE:CZ	1:D:704:SER:HA	2.27	0.70
1:C:24:VAL:HG11	1:C:143:ASN:HA	1.74	0.69
1:C:434:MET:HE3	1:C:442:TYR:HD1	1.57	0.69
1:C:270:PHE:C	1:C:270:PHE:CD2	2.71	0.69
1:D:102:MET:HE3	1:D:163:PRO:HD2	1.73	0.69
1:A:102:MET:HE3	1:A:163:PRO:HD2	1.73	0.69
1:D:24:VAL:HG11	1:D:143:ASN:HA	1.74	0.69
1:B:16:GLU:O	1:B:417:THR:HG21	1.93	0.69
1:A:258:ASP:OD2	1:A:260:VAL:HG22	1.93	0.69
1:B:102:MET:HE3	1:B:163:PRO:HD2	1.74	0.69
1:B:235:ILE:H	1:B:235:ILE:CD1	2.06	0.69
1:B:596:PHE:CZ	1:B:704:SER:HA	2.28	0.69
1:C:292:PRO:C	1:C:293:LEU:HD12	2.17	0.69
1:D:293:LEU:HD22	1:D:297:LEU:HD11	1.74	0.69
1:B:292:PRO:C	1:B:293:LEU:HD12	2.17	0.69
1:A:292:PRO:C	1:A:293:LEU:HD12	2.17	0.69
1:A:235:ILE:H	1:A:235:ILE:CD1	2.06	0.68
1:A:427:LEU:HD13	1:A:442:TYR:CE2	2.28	0.68
1:A:434:MET:HE3	1:A:442:TYR:HD1	1.58	0.68
1:A:24:VAL:HG11	1:A:143:ASN:HA	1.74	0.68
1:C:427:LEU:HD13	1:C:442:TYR:HE2	1.58	0.68
1:C:102:MET:HE3	1:C:163:PRO:HD2	1.74	0.68
1:B:427:LEU:HD13	1:B:442:TYR:CE2	2.29	0.68
1:C:293:LEU:HD22	1:C:297:LEU:HD11	1.74	0.68
1:D:292:PRO:C	1:D:293:LEU:HD12	2.18	0.68
1:C:235:ILE:H	1:C:235:ILE:CD1	2.05	0.68
1:B:24:VAL:HG11	1:B:143:ASN:HA	1.74	0.68
1:B:247:ASP:HB2	1:B:254:ILE:HG13	1.75	0.68
1:D:95:ILE:HD11	1:D:133:LEU:HD11	1.76	0.68
1:A:596:PHE:CZ	1:A:704:SER:HA	2.29	0.67
1:C:596:PHE:CZ	1:C:704:SER:HA	2.30	0.67
1:C:95:ILE:HD11	1:C:133:LEU:HD11	1.76	0.67
1:A:95:ILE:HD11	1:A:133:LEU:HD11	1.77	0.67
1:B:95:ILE:HD11	1:B:133:LEU:HD11	1.77	0.67
1:D:235:ILE:H	1:D:235:ILE:CD1	2.06	0.67
1:A:270:PHE:CD2	1:A:270:PHE:C	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:MET:HE1	1:D:313:TYR:CE2	2.30	0.67
1:C:172:GLN:HB3	1:C:188:LYS:HZ2	1.61	0.66
1:A:404:VAL:HG11	1:A:438:GLU:HA	1.76	0.66
1:C:434:MET:HB2	1:C:442:TYR:CE1	2.30	0.66
1:B:270:PHE:C	1:B:270:PHE:CD2	2.73	0.66
1:D:259:MET:HE1	1:D:313:TYR:HE2	1.61	0.66
1:D:305:VAL:HG21	1:D:311:LEU:N	2.11	0.66
1:A:623:LEU:CD1	1:A:664:LEU:HD22	2.24	0.66
1:A:721:MET:HE2	1:B:721:MET:HE2	1.78	0.66
1:A:24:VAL:HG23	1:A:93:ILE:HG23	1.78	0.66
1:C:160:VAL:CG2	1:C:161:ARG:H	2.05	0.66
1:D:172:GLN:HB3	1:D:188:LYS:HZ2	1.61	0.66
1:A:160:VAL:CG2	1:A:161:ARG:H	2.06	0.66
1:D:160:VAL:CG2	1:D:161:ARG:H	2.05	0.65
1:A:109:THR:HG22	1:A:120:ASN:HB2	1.79	0.65
1:D:434:MET:HB2	1:D:442:TYR:CE1	2.31	0.65
1:B:109:THR:HG22	1:B:120:ASN:HB2	1.79	0.65
1:B:427:LEU:HD13	1:B:442:TYR:HE2	1.59	0.65
1:A:427:LEU:HD13	1:A:442:TYR:HE2	1.59	0.65
1:C:296:GLY:O	1:C:320:PRO:HA	1.97	0.65
1:D:427:LEU:HD13	1:D:442:TYR:CE2	2.31	0.65
1:A:434:MET:HB2	1:A:442:TYR:CE1	2.30	0.65
1:C:300:MET:O	1:C:316:GLN:HB2	1.97	0.65
1:D:296:GLY:O	1:D:320:PRO:HA	1.97	0.65
1:D:623:LEU:CD1	1:D:664:LEU:HD22	2.26	0.65
1:B:293:LEU:HD22	1:B:297:LEU:CD1	2.27	0.65
1:D:325:ALA:O	1:D:326:SER:HB3	1.97	0.65
1:A:325:ALA:O	1:A:326:SER:HB3	1.97	0.65
1:B:258:ASP:OD2	1:B:260:VAL:HG22	1.97	0.65
1:C:623:LEU:CD1	1:C:664:LEU:HD22	2.25	0.65
1:B:116:GLN:HG2	1:B:134:PRO:HA	1.78	0.65
1:C:305:VAL:HG21	1:C:311:LEU:N	2.13	0.65
1:C:325:ALA:O	1:C:326:SER:HB3	1.97	0.65
1:A:293:LEU:HD22	1:A:297:LEU:CD1	2.27	0.64
1:A:29:SER:HB2	1:C:501:THR:HG23	1.78	0.64
1:B:325:ALA:O	1:B:326:SER:HB3	1.97	0.64
1:B:434:MET:HB2	1:B:442:TYR:CE1	2.31	0.64
1:B:259:MET:HE1	1:B:313:TYR:HE2	1.62	0.64
1:D:427:LEU:HD13	1:D:442:TYR:HE2	1.62	0.64
1:A:116:GLN:HG2	1:A:134:PRO:HA	1.79	0.64
1:B:172:GLN:HB3	1:B:188:LYS:HZ2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:O	1:A:316:GLN:HB2	1.98	0.64
1:B:305:VAL:HG21	1:B:311:LEU:N	2.12	0.64
1:D:300:MET:O	1:D:316:GLN:HB2	1.98	0.64
1:A:172:GLN:HB3	1:A:188:LYS:HZ2	1.62	0.64
1:B:300:MET:O	1:B:316:GLN:HB2	1.98	0.64
1:B:623:LEU:CD1	1:B:664:LEU:HD22	2.27	0.64
1:D:116:GLN:HG2	1:D:134:PRO:HA	1.78	0.64
1:B:232:ARG:HD3	1:B:233:TYR:CE1	2.33	0.64
1:D:260:VAL:HG11	1:D:270:PHE:CE1	2.33	0.64
1:A:296:GLY:O	1:A:320:PRO:HA	1.97	0.64
1:B:296:GLY:O	1:B:320:PRO:HA	1.97	0.63
1:C:293:LEU:HD22	1:C:297:LEU:CD1	2.28	0.63
1:A:305:VAL:HG21	1:A:311:LEU:N	2.12	0.63
1:B:24:VAL:HG23	1:B:93:ILE:HG23	1.81	0.63
1:C:109:THR:HG22	1:C:120:ASN:HB2	1.78	0.63
1:D:531:LYS:HB3	1:D:553:ILE:HG12	1.79	0.63
1:A:232:ARG:HD3	1:A:233:TYR:CE1	2.34	0.63
1:D:293:LEU:HD22	1:D:297:LEU:CD1	2.28	0.63
1:C:232:ARG:HD3	1:C:233:TYR:CE1	2.34	0.63
1:D:690:VAL:HG12	1:D:691:LYS:N	2.13	0.63
1:B:187:LYS:HD3	1:B:197:LEU:HD11	1.81	0.63
1:C:24:VAL:HG23	1:C:93:ILE:HG23	1.79	0.63
1:C:116:GLN:HG2	1:C:134:PRO:HA	1.79	0.63
1:D:24:VAL:HG23	1:D:93:ILE:HG23	1.79	0.63
1:D:232:ARG:HD3	1:D:233:TYR:CE1	2.34	0.63
1:B:690:VAL:HG12	1:B:691:LYS:N	2.13	0.63
1:C:690:VAL:HG12	1:C:691:LYS:N	2.13	0.63
1:B:541:PRO:CD	1:B:544:MET:HE2	2.28	0.63
1:C:442:TYR:O	1:C:445:ASN:N	2.29	0.63
1:A:541:PRO:CD	1:A:544:MET:HE2	2.28	0.62
1:A:690:VAL:HG12	1:A:691:LYS:N	2.13	0.62
1:C:531:LYS:HB3	1:C:553:ILE:HG12	1.80	0.62
1:D:109:THR:HG22	1:D:120:ASN:HB2	1.78	0.62
1:D:442:TYR:O	1:D:445:ASN:N	2.30	0.62
1:A:70:TYR:HA	1:A:80:THR:O	1.99	0.62
1:A:522:ASN:O	1:A:526:ARG:HG3	1.99	0.62
1:B:690:VAL:CG1	1:B:691:LYS:N	2.63	0.62
1:A:187:LYS:HD3	1:A:197:LEU:HD11	1.82	0.62
1:A:690:VAL:CG1	1:A:691:LYS:N	2.63	0.62
1:B:434:MET:HE3	1:B:442:TYR:CD1	2.35	0.62
1:C:247:ASP:HB2	1:C:254:ILE:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:HA	1:B:80:THR:O	2.00	0.62
1:B:500:GLU:HB2	1:B:507:PHE:CZ	2.35	0.62
1:B:531:LYS:HB3	1:B:553:ILE:HG12	1.80	0.62
1:A:531:LYS:HB3	1:A:553:ILE:HG12	1.80	0.62
1:B:160:VAL:CG2	1:B:161:ARG:H	2.05	0.62
1:C:70:TYR:HA	1:C:80:THR:O	1.99	0.62
1:D:541:PRO:CD	1:D:544:MET:HE2	2.26	0.62
1:B:172:GLN:CB	1:B:188:LYS:HZ2	2.13	0.61
1:B:551:THR:HA	1:C:211:PHE:CE1	2.34	0.61
1:B:522:ASN:O	1:B:526:ARG:HG3	2.00	0.61
1:D:187:LYS:HD3	1:D:197:LEU:HD11	1.81	0.61
1:A:172:GLN:CB	1:A:188:LYS:HZ2	2.13	0.61
1:A:282:LEU:HB3	1:A:287:LEU:HD12	1.81	0.61
1:C:541:PRO:CD	1:C:544:MET:HE2	2.27	0.61
1:D:522:ASN:O	1:D:526:ARG:HG3	1.99	0.61
1:A:245:ILE:HG21	1:A:311:LEU:CD2	2.31	0.61
1:B:501:THR:HG23	1:D:29:SER:HB2	1.83	0.61
1:C:172:GLN:CB	1:C:188:LYS:HZ2	2.13	0.61
1:D:595:ILE:HD12	1:D:595:ILE:N	2.16	0.61
1:B:595:ILE:HD12	1:B:595:ILE:N	2.15	0.61
1:C:245:ILE:HG21	1:C:311:LEU:CD2	2.31	0.61
1:C:595:ILE:N	1:C:595:ILE:HD12	2.16	0.61
1:C:690:VAL:CG1	1:C:691:LYS:N	2.63	0.61
1:D:172:GLN:CB	1:D:188:LYS:HZ2	2.13	0.61
1:D:282:LEU:HB3	1:D:287:LEU:HD12	1.82	0.61
1:D:690:VAL:CG1	1:D:691:LYS:N	2.63	0.60
1:A:500:GLU:HB2	1:A:507:PHE:CZ	2.37	0.60
1:B:282:LEU:HB3	1:B:287:LEU:HD12	1.82	0.60
1:C:187:LYS:HD3	1:C:197:LEU:HD11	1.82	0.60
1:C:500:GLU:HB2	1:C:507:PHE:CZ	2.36	0.60
1:A:595:ILE:N	1:A:595:ILE:HD12	2.16	0.60
1:C:522:ASN:O	1:C:526:ARG:HG3	2.00	0.60
1:B:351:LEU:HB3	1:B:366:LEU:HB3	1.83	0.60
1:C:282:LEU:HB3	1:C:287:LEU:HD12	1.83	0.60
1:D:70:TYR:HA	1:D:80:THR:O	2.00	0.60
1:D:434:MET:HE3	1:D:442:TYR:CD1	2.33	0.60
1:D:500:GLU:HB2	1:D:507:PHE:CZ	2.37	0.60
1:D:601:PHE:O	1:D:602:ILE:C	2.44	0.60
1:A:351:LEU:HB3	1:A:366:LEU:HB3	1.84	0.60
1:C:601:PHE:O	1:C:602:ILE:C	2.44	0.60
1:A:601:PHE:O	1:A:602:ILE:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PHE:O	1:B:602:ILE:C	2.44	0.59
1:C:457:PHE:CD2	1:C:477:GLN:HG2	2.37	0.59
1:D:188:LYS:NZ	1:D:188:LYS:HB3	2.18	0.59
1:A:304:LEU:O	1:A:305:VAL:HG23	2.02	0.59
1:D:173:PHE:HE2	1:D:248:LEU:HD13	1.65	0.59
1:D:342:LEU:HD13	1:D:379:ILE:CD1	2.25	0.59
1:A:457:PHE:CD2	1:A:477:GLN:HG2	2.36	0.59
1:B:190:ASP:CG	1:B:191:GLY:H	2.11	0.59
1:B:188:LYS:HB3	1:B:188:LYS:NZ	2.17	0.59
1:B:229:PHE:HB2	1:B:235:ILE:HD11	1.85	0.59
1:B:259:MET:HE1	1:B:313:TYR:CE2	2.37	0.59
1:C:188:LYS:NZ	1:C:188:LYS:HB3	2.18	0.59
1:C:304:LEU:O	1:C:305:VAL:HG23	2.02	0.59
1:D:457:PHE:CD2	1:D:477:GLN:HG2	2.38	0.59
1:C:342:LEU:HD13	1:C:379:ILE:CD1	2.25	0.59
1:A:61:LEU:HD12	1:A:62:LEU:H	1.68	0.59
1:A:190:ASP:CG	1:A:191:GLY:H	2.11	0.59
1:B:457:PHE:CD2	1:B:477:GLN:HG2	2.37	0.59
1:A:229:PHE:HB2	1:A:235:ILE:HD11	1.85	0.59
1:B:304:LEU:O	1:B:305:VAL:HG23	2.03	0.59
1:C:101:SER:HA	1:C:123:LEU:HA	1.85	0.59
1:A:563:GLU:HB3	1:A:565:THR:HG22	1.85	0.58
1:C:563:GLU:HB3	1:C:565:THR:HG22	1.86	0.58
1:A:342:LEU:HD13	1:A:379:ILE:CD1	2.26	0.58
1:B:342:LEU:HD13	1:B:379:ILE:CD1	2.26	0.58
1:D:229:PHE:HB2	1:D:235:ILE:HD11	1.86	0.58
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.18	0.58
1:D:563:GLU:HB3	1:D:565:THR:HG22	1.86	0.58
1:A:188:LYS:HZ2	1:A:188:LYS:HB3	1.68	0.58
1:B:61:LEU:HD12	1:B:62:LEU:H	1.69	0.58
1:C:351:LEU:HB3	1:C:366:LEU:HB3	1.84	0.58
1:D:304:LEU:O	1:D:305:VAL:HG23	2.03	0.58
1:B:563:GLU:HB3	1:B:565:THR:HG22	1.85	0.58
1:D:258:ASP:OD2	1:D:260:VAL:HG22	2.03	0.58
1:A:101:SER:HA	1:A:123:LEU:HA	1.85	0.58
1:B:265:SER:O	1:B:267:PRO:HD3	2.03	0.58
1:C:190:ASP:CG	1:C:191:GLY:H	2.11	0.58
1:C:725:ARG:O	1:C:729:ILE:HG22	2.04	0.58
1:D:188:LYS:HZ2	1:D:188:LYS:HB3	1.69	0.58
1:C:61:LEU:HD12	1:C:62:LEU:H	1.67	0.58
1:C:229:PHE:HB2	1:C:235:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ILE:H	1:C:328:ILE:HD12	1.67	0.58
1:B:623:LEU:HD12	1:B:664:LEU:HD23	1.83	0.57
1:D:328:ILE:HD12	1:D:328:ILE:H	1.67	0.57
1:D:351:LEU:HB3	1:D:366:LEU:HB3	1.85	0.57
1:A:328:ILE:HD12	1:A:328:ILE:H	1.68	0.57
1:C:172:GLN:HB3	1:C:188:LYS:NZ	2.20	0.57
1:D:101:SER:HA	1:D:123:LEU:HA	1.86	0.57
1:D:163:PRO:HA	1:D:178:LEU:HD23	1.86	0.57
1:D:172:GLN:HB3	1:D:188:LYS:NZ	2.20	0.57
1:B:101:SER:HA	1:B:123:LEU:HA	1.86	0.57
1:D:404:VAL:HG11	1:D:438:GLU:HG2	1.86	0.57
1:C:163:PRO:HA	1:C:178:LEU:HD23	1.86	0.57
1:D:190:ASP:CG	1:D:191:GLY:H	2.11	0.57
1:B:188:LYS:HZ2	1:B:188:LYS:HB3	1.69	0.57
1:A:169:VAL:HB	1:A:173:PHE:O	2.05	0.57
1:A:270:PHE:C	1:A:270:PHE:HD2	2.13	0.57
1:B:328:ILE:HD12	1:B:328:ILE:H	1.68	0.57
1:B:169:VAL:HB	1:B:173:PHE:O	2.05	0.57
1:C:434:MET:HE3	1:C:442:TYR:CD1	2.37	0.57
1:A:163:PRO:HA	1:A:178:LEU:HD23	1.87	0.56
1:A:434:MET:HE3	1:A:442:TYR:CD1	2.37	0.56
1:C:262:GLN:HE22	1:C:315:PHE:HB2	1.69	0.56
1:A:113:VAL:HG11	1:A:118:LEU:HD22	1.87	0.56
1:C:169:VAL:HB	1:C:173:PHE:O	2.05	0.56
1:D:169:VAL:HB	1:D:173:PHE:O	2.05	0.56
1:D:209:THR:CG2	1:D:211:PHE:CD2	2.89	0.56
1:D:247:ASP:HB2	1:D:254:ILE:CG1	2.34	0.56
1:A:443:LEU:C	1:A:443:LEU:HD23	2.29	0.56
1:C:209:THR:CG2	1:C:211:PHE:CD2	2.89	0.56
1:C:443:LEU:C	1:C:443:LEU:HD23	2.30	0.56
1:C:113:VAL:HG11	1:C:118:LEU:HD22	1.87	0.56
1:C:177:PHE:CD1	1:C:183:LEU:HD22	2.41	0.56
1:C:188:LYS:HZ2	1:C:188:LYS:HB3	1.71	0.56
1:C:488:THR:OG1	1:C:491:GLU:HG3	2.06	0.56
1:D:61:LEU:HD12	1:D:62:LEU:H	1.69	0.56
1:D:81:PHE:O	1:D:92:THR:HA	2.05	0.56
1:D:177:PHE:CD1	1:D:183:LEU:HD22	2.41	0.56
1:A:442:TYR:O	1:A:445:ASN:N	2.31	0.56
1:B:163:PRO:HA	1:B:178:LEU:HD23	1.88	0.56
1:D:172:GLN:CD	1:D:172:GLN:H	2.13	0.56
1:D:725:ARG:O	1:D:729:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:CG2	1:B:211:PHE:CD2	2.88	0.56
1:B:81:PHE:O	1:B:92:THR:HA	2.06	0.56
1:A:623:LEU:HD12	1:A:664:LEU:HD23	1.86	0.56
1:B:113:VAL:HG11	1:B:118:LEU:HD22	1.88	0.56
1:B:442:TYR:O	1:B:445:ASN:N	2.31	0.56
1:D:443:LEU:C	1:D:443:LEU:HD23	2.31	0.56
1:A:1:MET:HE3	1:A:1:MET:HA	1.87	0.55
1:A:172:GLN:H	1:A:172:GLN:CD	2.13	0.55
1:C:1:MET:HE3	1:C:1:MET:HA	1.87	0.55
1:A:169:VAL:HG13	1:A:228:LEU:CD2	2.35	0.55
1:B:177:PHE:CD1	1:B:183:LEU:HD22	2.41	0.55
1:B:701:TYR:O	1:B:704:SER:HB3	2.07	0.55
1:D:349:LEU:HB2	1:D:368:VAL:CG2	2.36	0.55
1:B:260:VAL:HG11	1:B:270:PHE:CE1	2.40	0.55
1:C:293:LEU:CD1	1:C:297:LEU:HD12	2.34	0.55
1:D:270:PHE:C	1:D:270:PHE:CD2	2.83	0.55
1:A:177:PHE:CD1	1:A:183:LEU:HD22	2.41	0.55
1:B:245:ILE:HG21	1:B:311:LEU:CD2	2.36	0.55
1:D:1:MET:HE3	1:D:1:MET:HA	1.87	0.55
1:D:169:VAL:HG13	1:D:228:LEU:CD2	2.37	0.55
1:A:172:GLN:HB3	1:A:188:LYS:NZ	2.20	0.55
1:B:209:THR:CG2	1:B:211:PHE:HD2	2.20	0.55
1:B:288:VAL:HG12	1:B:300:MET:CB	2.31	0.55
1:B:568:LYS:HE3	1:B:572:ASP:OD2	2.06	0.55
1:C:81:PHE:O	1:C:92:THR:HA	2.07	0.55
1:C:169:VAL:HG13	1:C:228:LEU:CD2	2.37	0.55
1:C:172:GLN:CD	1:C:172:GLN:H	2.14	0.55
1:D:293:LEU:CD1	1:D:297:LEU:HD12	2.34	0.55
1:D:694:ASN:HD21	1:D:697:GLN:HE21	1.55	0.55
1:A:293:LEU:CD1	1:A:297:LEU:HD12	2.35	0.55
1:B:172:GLN:HB3	1:B:188:LYS:NZ	2.20	0.55
1:C:53:GLY:HA3	1:C:71:HIS:HB3	1.88	0.55
1:A:81:PHE:O	1:A:92:THR:HA	2.06	0.55
1:A:595:ILE:HD12	1:A:595:ILE:H	1.72	0.55
1:C:349:LEU:HB2	1:C:368:VAL:CG2	2.37	0.55
1:D:250:SER:O	1:D:251:PHE:HB2	2.07	0.55
1:A:349:LEU:HB2	1:A:368:VAL:CG2	2.37	0.55
1:B:209:THR:HG21	1:B:211:PHE:HD2	1.72	0.55
1:B:349:LEU:HB2	1:B:368:VAL:CG2	2.37	0.55
1:A:209:THR:CG2	1:A:211:PHE:CD2	2.89	0.55
1:B:293:LEU:CD1	1:B:297:LEU:HD12	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LEU:HD23	1:B:443:LEU:C	2.31	0.54
1:C:701:TYR:O	1:C:704:SER:HB3	2.07	0.54
1:D:568:LYS:HE3	1:D:572:ASP:OD2	2.07	0.54
1:B:209:THR:HG22	1:B:211:PHE:CD2	2.42	0.54
1:D:701:TYR:O	1:D:704:SER:HB3	2.08	0.54
1:A:488:THR:OG1	1:A:491:GLU:HG3	2.07	0.54
1:A:701:TYR:O	1:A:704:SER:HB3	2.08	0.54
1:D:95:ILE:CD1	1:D:133:LEU:HD11	2.37	0.54
1:D:113:VAL:HG11	1:D:118:LEU:HD22	1.89	0.54
1:A:329:TRP:HB3	1:A:355:TRP:HB3	1.90	0.54
1:A:725:ARG:O	1:A:729:ILE:HG22	2.07	0.54
1:B:169:VAL:HG13	1:B:228:LEU:CD2	2.37	0.54
1:B:595:ILE:HD12	1:B:595:ILE:H	1.73	0.54
1:D:349:LEU:HB2	1:D:368:VAL:HG21	1.90	0.54
1:C:209:THR:HG22	1:C:211:PHE:CD2	2.43	0.54
1:C:568:LYS:HE3	1:C:572:ASP:OD2	2.08	0.54
1:D:53:GLY:HA3	1:D:71:HIS:HB3	1.90	0.54
1:D:209:THR:CG2	1:D:211:PHE:HD2	2.21	0.54
1:D:209:THR:HG21	1:D:211:PHE:HD2	1.72	0.54
1:A:103:ASN:HB3	1:A:107:THR:HG23	1.90	0.54
1:A:209:THR:CG2	1:A:211:PHE:HD2	2.21	0.54
1:A:209:THR:HG21	1:A:211:PHE:HD2	1.72	0.54
1:B:329:TRP:HB3	1:B:355:TRP:HB3	1.90	0.54
1:C:209:THR:CG2	1:C:211:PHE:HD2	2.21	0.54
1:D:488:THR:OG1	1:D:491:GLU:HG3	2.08	0.54
1:C:93:ILE:CD1	1:C:138:LEU:HD23	2.38	0.54
1:C:209:THR:HG21	1:C:211:PHE:HD2	1.72	0.54
1:C:490:VAL:HG22	1:C:590:GLN:HG3	1.89	0.54
1:D:209:THR:HG22	1:D:211:PHE:CD2	2.43	0.54
1:A:490:VAL:HG22	1:A:590:GLN:HG3	1.90	0.54
1:B:172:GLN:CD	1:B:172:GLN:H	2.15	0.54
1:A:95:ILE:CD1	1:A:133:LEU:HD11	2.37	0.53
1:C:103:ASN:HB3	1:C:107:THR:HG23	1.90	0.53
1:A:93:ILE:CD1	1:A:138:LEU:HD23	2.38	0.53
1:B:1:MET:HE3	1:B:1:MET:HA	1.89	0.53
1:B:103:ASN:HB3	1:B:107:THR:HG23	1.90	0.53
1:D:457:PHE:HA	1:D:477:GLN:HB2	1.90	0.53
1:C:623:LEU:HD12	1:C:664:LEU:HD23	1.86	0.53
1:C:694:ASN:HD21	1:C:697:GLN:HE21	1.56	0.53
1:A:53:GLY:HA3	1:A:71:HIS:HB3	1.89	0.53
1:A:466:TYR:HB3	1:A:470:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:TRP:CH2	1:B:506:LEU:HD23	2.44	0.53
1:D:466:TYR:HB3	1:D:470:ILE:HB	1.89	0.53
1:A:209:THR:HG22	1:A:211:PHE:CD2	2.43	0.53
1:B:540:LEU:HD22	1:B:544:MET:HE1	1.90	0.53
1:C:270:PHE:C	1:C:270:PHE:HD2	2.16	0.53
1:C:349:LEU:HB2	1:C:368:VAL:HG21	1.91	0.53
1:C:540:LEU:HD22	1:C:544:MET:HE1	1.91	0.53
1:D:397:ILE:O	1:D:397:ILE:HG22	2.08	0.53
1:D:623:LEU:HD12	1:D:664:LEU:HD23	1.85	0.53
1:A:247:ASP:HB2	1:A:254:ILE:CG1	2.39	0.53
1:A:716:GLU:OE2	1:A:725:ARG:HD3	2.07	0.53
1:C:329:TRP:HB3	1:C:355:TRP:HB3	1.90	0.53
1:C:340:LEU:HG	1:C:341:GLU:H	1.74	0.53
1:D:103:ASN:HB3	1:D:107:THR:HG23	1.91	0.53
1:D:329:TRP:HB3	1:D:355:TRP:HB3	1.90	0.53
1:C:466:TYR:HB3	1:C:470:ILE:HB	1.90	0.53
1:B:95:ILE:CD1	1:B:133:LEU:HD11	2.37	0.53
1:D:340:LEU:HG	1:D:341:GLU:H	1.74	0.53
1:B:490:VAL:HG22	1:B:590:GLN:HG3	1.90	0.53
1:D:540:LEU:HD22	1:D:544:MET:HE1	1.91	0.53
1:A:493:TRP:CH2	1:A:506:LEU:HD23	2.44	0.53
1:A:540:LEU:HD22	1:A:544:MET:HE1	1.91	0.53
1:A:568:LYS:HE3	1:A:572:ASP:OD2	2.08	0.53
1:C:457:PHE:HA	1:C:477:GLN:HB2	1.91	0.53
1:C:493:TRP:CH2	1:C:506:LEU:HD23	2.44	0.53
1:A:457:PHE:CG	1:A:477:GLN:HG2	2.44	0.52
1:B:725:ARG:O	1:B:729:ILE:HG22	2.09	0.52
1:C:595:ILE:HD12	1:C:595:ILE:H	1.73	0.52
1:D:93:ILE:CD1	1:D:138:LEU:HD23	2.40	0.52
1:A:366:LEU:HD13	1:A:378:TRP:CE2	2.44	0.52
1:B:366:LEU:HD13	1:B:378:TRP:CE2	2.44	0.52
1:B:716:GLU:OE2	1:B:725:ARG:HD3	2.08	0.52
1:D:218:SER:C	1:D:220:TYR:H	2.18	0.52
1:D:366:LEU:HD13	1:D:378:TRP:CE2	2.44	0.52
1:B:53:GLY:HA3	1:B:71:HIS:HB3	1.90	0.52
1:A:218:SER:C	1:A:220:TYR:H	2.17	0.52
1:A:694:ASN:ND2	1:A:697:GLN:NE2	2.57	0.52
1:A:694:ASN:HD21	1:A:697:GLN:HE21	1.56	0.52
1:B:272:LYS:O	1:B:272:LYS:HG3	2.09	0.52
1:B:340:LEU:HG	1:B:341:GLU:H	1.74	0.52
1:B:466:TYR:HB3	1:B:470:ILE:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:CD1	1:C:133:LEU:HD11	2.38	0.52
1:C:272:LYS:O	1:C:272:LYS:HG3	2.08	0.52
1:C:716:GLU:OE2	1:C:725:ARG:HD3	2.09	0.52
1:B:93:ILE:CD1	1:B:138:LEU:HD23	2.39	0.52
1:B:349:LEU:HB2	1:B:368:VAL:HG21	1.91	0.52
1:D:490:VAL:HG22	1:D:590:GLN:HG3	1.91	0.52
1:A:272:LYS:O	1:A:272:LYS:HG3	2.09	0.52
1:A:721:MET:HB3	1:B:721:MET:HE2	1.90	0.52
1:D:493:TRP:CH2	1:D:506:LEU:HD23	2.44	0.52
1:C:218:SER:C	1:C:220:TYR:H	2.18	0.52
1:C:366:LEU:HD13	1:C:378:TRP:CE2	2.44	0.52
1:C:397:ILE:HG22	1:C:397:ILE:O	2.09	0.52
1:B:218:SER:C	1:B:220:TYR:H	2.17	0.52
1:C:457:PHE:CG	1:C:477:GLN:HG2	2.45	0.52
1:A:499:SER:O	1:A:500:GLU:C	2.52	0.52
1:B:247:ASP:HB2	1:B:254:ILE:CG1	2.40	0.52
1:C:1:MET:HE2	1:C:380:GLU:HG3	1.92	0.52
1:D:1:MET:HE2	1:D:380:GLU:HG3	1.92	0.52
1:A:340:LEU:HG	1:A:341:GLU:H	1.75	0.52
1:A:397:ILE:O	1:A:397:ILE:HG22	2.08	0.52
1:C:602:ILE:HB	1:C:691:LYS:O	2.10	0.52
1:B:397:ILE:HG22	1:B:397:ILE:O	2.09	0.51
1:B:457:PHE:CG	1:B:477:GLN:HG2	2.45	0.51
1:D:595:ILE:HD12	1:D:595:ILE:H	1.73	0.51
1:D:694:ASN:ND2	1:D:697:GLN:NE2	2.57	0.51
1:A:163:PRO:CA	1:A:178:LEU:HD23	2.41	0.51
1:B:229:PHE:CB	1:B:235:ILE:HD11	2.41	0.51
1:B:457:PHE:HA	1:B:477:GLN:HB2	1.91	0.51
1:C:609:GLY:O	1:C:613:ILE:HG22	2.10	0.51
1:D:272:LYS:O	1:D:272:LYS:HG3	2.09	0.51
1:A:29:SER:CB	1:C:501:THR:HG23	2.40	0.51
1:A:349:LEU:HB2	1:A:368:VAL:HG21	1.91	0.51
1:B:1:MET:HE2	1:B:380:GLU:HG3	1.92	0.51
1:B:499:SER:O	1:B:500:GLU:C	2.53	0.51
1:D:716:GLU:OE2	1:D:725:ARG:HD3	2.10	0.51
1:A:255:GLN:HB3	1:A:257:TYR:CE2	2.46	0.51
1:A:260:VAL:HG11	1:A:270:PHE:CE1	2.46	0.51
1:B:59:CYS:HB2	1:B:464:THR:OG1	2.10	0.51
1:B:163:PRO:CA	1:B:178:LEU:HD23	2.41	0.51
1:D:457:PHE:CG	1:D:477:GLN:HG2	2.46	0.51
1:D:602:ILE:HB	1:D:691:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ILE:HB	1:A:691:LYS:O	2.10	0.51
1:B:602:ILE:HB	1:B:691:LYS:O	2.10	0.51
1:A:1:MET:HE2	1:A:380:GLU:HG3	1.92	0.51
1:C:499:SER:O	1:C:500:GLU:C	2.52	0.51
1:C:690:VAL:CG1	1:C:691:LYS:H	2.24	0.51
1:C:694:ASN:ND2	1:C:697:GLN:NE2	2.57	0.51
1:D:168:TYR:HA	1:D:174:SER:HB2	1.92	0.51
1:D:499:SER:O	1:D:500:GLU:C	2.53	0.51
1:D:668:TYR:CZ	1:D:672:LYS:HE3	2.45	0.51
1:A:229:PHE:CB	1:A:235:ILE:HD11	2.41	0.51
1:A:457:PHE:HA	1:A:477:GLN:HB2	1.92	0.51
1:B:488:THR:OG1	1:B:491:GLU:HG3	2.11	0.51
1:C:260:VAL:HG11	1:C:270:PHE:CE1	2.45	0.51
1:A:253:LEU:HD11	1:A:255:GLN:O	2.11	0.51
1:C:163:PRO:CA	1:C:178:LEU:HD23	2.40	0.51
1:C:255:GLN:HB3	1:C:257:TYR:CE2	2.46	0.51
1:C:647:PHE:O	1:C:651:ILE:HG13	2.11	0.51
1:D:163:PRO:CA	1:D:178:LEU:HD23	2.40	0.51
1:A:173:PHE:HE2	1:A:248:LEU:HD13	1.76	0.50
1:A:288:VAL:HG12	1:A:300:MET:CB	2.31	0.50
1:A:609:GLY:O	1:A:613:ILE:HG22	2.10	0.50
1:B:694:ASN:ND2	1:B:697:GLN:NE2	2.59	0.50
1:C:168:TYR:HA	1:C:174:SER:HB2	1.92	0.50
1:B:690:VAL:CG1	1:B:691:LYS:H	2.24	0.50
1:C:125:ASP:OD1	1:C:127:SER:N	2.44	0.50
1:D:229:PHE:HB2	1:D:235:ILE:CD1	2.42	0.50
1:D:255:GLN:HB3	1:D:257:TYR:CE2	2.47	0.50
1:D:325:ALA:O	1:D:326:SER:CB	2.59	0.50
1:A:325:ALA:O	1:A:326:SER:CB	2.59	0.50
1:B:168:TYR:HA	1:B:174:SER:HB2	1.92	0.50
1:B:325:ALA:O	1:B:326:SER:CB	2.59	0.50
1:D:125:ASP:OD1	1:D:127:SER:N	2.44	0.50
1:D:690:VAL:CG1	1:D:691:LYS:H	2.24	0.50
1:A:103:ASN:H	1:A:107:THR:HG21	1.76	0.50
1:B:164:HIS:HB3	1:B:179:GLU:HG2	1.93	0.50
1:B:229:PHE:HB2	1:B:235:ILE:CD1	2.41	0.50
1:B:255:GLN:HB3	1:B:257:TYR:CE2	2.46	0.50
1:C:253:LEU:HD11	1:C:255:GLN:O	2.11	0.50
1:A:690:VAL:CG1	1:A:691:LYS:H	2.24	0.50
1:C:164:HIS:HB3	1:C:179:GLU:HG2	1.93	0.50
1:D:229:PHE:CB	1:D:235:ILE:HD11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:ILE:CB	1:D:691:LYS:HB2	2.41	0.50
1:A:164:HIS:HB3	1:A:179:GLU:HG2	1.93	0.50
1:A:168:TYR:HA	1:A:174:SER:HB2	1.92	0.50
1:B:694:ASN:HD21	1:B:697:GLN:HE21	1.58	0.50
1:B:609:GLY:O	1:B:613:ILE:HG22	2.11	0.50
1:C:258:ASP:OD2	1:C:260:VAL:HG22	2.12	0.50
1:C:325:ALA:O	1:C:326:SER:CB	2.59	0.50
1:A:229:PHE:HB2	1:A:235:ILE:CD1	2.42	0.50
1:B:253:LEU:HD11	1:B:255:GLN:O	2.12	0.50
1:C:229:PHE:HB2	1:C:235:ILE:CD1	2.42	0.50
1:C:229:PHE:CB	1:C:235:ILE:HD11	2.42	0.49
1:B:125:ASP:OD1	1:B:127:SER:N	2.45	0.49
1:C:173:PHE:HE2	1:C:248:LEU:HD13	1.77	0.49
1:C:602:ILE:CB	1:C:691:LYS:HB2	2.41	0.49
1:D:103:ASN:H	1:D:107:THR:HG21	1.77	0.49
1:B:158:PHE:CD1	1:B:163:PRO:HD3	2.48	0.49
1:B:300:MET:SD	1:B:373:PHE:HD2	2.35	0.49
1:B:668:TYR:CZ	1:B:672:LYS:HE3	2.47	0.49
1:C:668:TYR:CZ	1:C:672:LYS:HE3	2.46	0.49
1:A:59:CYS:HB2	1:A:464:THR:OG1	2.12	0.49
1:A:162:VAL:O	1:A:179:GLU:HG3	2.12	0.49
1:D:288:VAL:HG12	1:D:300:MET:CB	2.29	0.49
1:A:125:ASP:OD1	1:A:127:SER:N	2.45	0.49
1:A:300:MET:SD	1:A:373:PHE:HD2	2.36	0.49
1:D:253:LEU:HD11	1:D:255:GLN:O	2.12	0.49
1:A:721:MET:HE2	1:B:721:MET:HB3	1.93	0.49
1:C:407:GLY:O	1:C:411:LEU:HG	2.12	0.49
1:D:164:HIS:HB3	1:D:179:GLU:HG2	1.93	0.49
1:C:162:VAL:O	1:C:179:GLU:HG3	2.13	0.49
1:D:531:LYS:CB	1:D:553:ILE:HG12	2.43	0.49
1:D:609:GLY:O	1:D:613:ILE:HG22	2.12	0.49
1:B:605:ILE:HD12	1:B:606:LYS:HB2	1.94	0.49
1:B:647:PHE:O	1:B:651:ILE:HG13	2.12	0.49
1:C:103:ASN:H	1:C:107:THR:HG21	1.77	0.49
1:B:162:VAL:O	1:B:179:GLU:HG3	2.13	0.49
1:A:125:ASP:OD1	1:A:125:ASP:C	2.56	0.48
1:A:407:GLY:O	1:A:411:LEU:HG	2.12	0.48
1:C:288:VAL:HG12	1:C:300:MET:CB	2.30	0.48
1:D:103:ASN:H	1:D:107:THR:CG2	2.26	0.48
1:D:173:PHE:CE2	1:D:248:LEU:HD13	2.45	0.48
1:A:103:ASN:H	1:A:107:THR:CG2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CD1	1:A:163:PRO:HD3	2.49	0.48
1:A:668:TYR:CZ	1:A:672:LYS:HE3	2.48	0.48
1:B:103:ASN:H	1:B:107:THR:HG21	1.78	0.48
1:C:22:ASN:HD21	1:C:91:LYS:HB2	1.77	0.48
1:C:158:PHE:CD1	1:C:163:PRO:HD3	2.48	0.48
1:D:300:MET:SD	1:D:373:PHE:HD2	2.35	0.48
1:A:293:LEU:O	1:A:294:GLU:HB3	2.14	0.48
1:B:125:ASP:OD1	1:B:125:ASP:C	2.57	0.48
1:B:407:GLY:O	1:B:411:LEU:HG	2.13	0.48
1:D:647:PHE:O	1:D:651:ILE:HG13	2.13	0.48
1:A:647:PHE:O	1:A:651:ILE:HG13	2.13	0.48
1:B:293:LEU:O	1:B:294:GLU:HB3	2.14	0.48
1:B:508:LYS:O	1:B:512:THR:HG23	2.14	0.48
1:D:162:VAL:O	1:D:179:GLU:HG3	2.14	0.48
1:B:238:THR:OG1	1:B:242:HIS:HB2	2.13	0.48
1:B:623:LEU:HD23	1:B:623:LEU:HA	1.67	0.48
1:C:300:MET:SD	1:C:373:PHE:HD2	2.36	0.48
1:C:103:ASN:H	1:C:107:THR:CG2	2.26	0.48
1:D:605:ILE:HD12	1:D:606:LYS:HB2	1.95	0.48
1:B:103:ASN:H	1:B:107:THR:CG2	2.26	0.47
1:C:93:ILE:HD12	1:C:138:LEU:HD23	1.95	0.47
1:C:293:LEU:O	1:C:294:GLU:HB3	2.13	0.47
1:A:238:THR:OG1	1:A:242:HIS:HB2	2.13	0.47
1:D:125:ASP:OD1	1:D:125:ASP:C	2.56	0.47
1:B:500:GLU:HB2	1:B:507:PHE:CE2	2.49	0.47
1:C:540:LEU:CD2	1:C:544:MET:HE1	2.44	0.47
1:D:172:GLN:HB2	1:D:188:LYS:HB3	1.96	0.47
1:D:245:ILE:HG21	1:D:311:LEU:CD2	2.39	0.47
1:D:334:LEU:HD12	1:D:334:LEU:C	2.39	0.47
1:A:233:TYR:CD1	1:A:311:LEU:HD22	2.49	0.47
1:D:259:MET:HE2	1:D:259:MET:HA	1.97	0.47
1:D:293:LEU:O	1:D:294:GLU:HB3	2.14	0.47
1:D:407:GLY:O	1:D:411:LEU:HG	2.14	0.47
1:A:259:MET:HE2	1:A:259:MET:HA	1.96	0.47
1:B:259:MET:HA	1:B:259:MET:HE2	1.96	0.47
1:D:368:VAL:HG23	1:D:368:VAL:O	2.14	0.47
1:D:397:ILE:O	1:D:397:ILE:CG2	2.62	0.47
1:D:508:LYS:O	1:D:512:THR:HG23	2.15	0.47
1:A:605:ILE:HD12	1:A:606:LYS:HB2	1.96	0.47
1:B:368:VAL:HG23	1:B:368:VAL:O	2.13	0.47
1:C:531:LYS:CB	1:C:553:ILE:HG12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ASN:HD21	1:D:91:LYS:HB2	1.78	0.47
1:D:158:PHE:CD1	1:D:163:PRO:HD3	2.50	0.47
1:D:335:VAL:CG1	1:D:352:ILE:HB	2.42	0.47
1:D:384:LYS:NZ	1:D:392:GLU:OE2	2.44	0.47
1:A:531:LYS:CB	1:A:553:ILE:HG12	2.45	0.47
1:B:209:THR:C	1:B:211:PHE:H	2.23	0.47
1:C:172:GLN:HB2	1:C:188:LYS:HB3	1.97	0.47
1:C:508:LYS:O	1:C:512:THR:HG23	2.15	0.47
1:D:93:ILE:HD12	1:D:138:LEU:HD23	1.95	0.47
1:D:540:LEU:CD2	1:D:544:MET:HE1	2.45	0.47
1:B:531:LYS:CB	1:B:553:ILE:HG12	2.45	0.47
1:C:238:THR:OG1	1:C:242:HIS:HB2	2.14	0.47
1:C:316:GLN:O	1:C:317:ASN:HB2	2.15	0.47
1:C:335:VAL:CG1	1:C:352:ILE:HB	2.42	0.47
1:C:506:LEU:HD11	1:C:586:LEU:HB2	1.96	0.47
1:C:623:LEU:CD1	1:C:664:LEU:CD2	2.86	0.47
1:A:209:THR:C	1:A:211:PHE:H	2.23	0.47
1:A:500:GLU:HB2	1:A:507:PHE:CE2	2.50	0.47
1:A:540:LEU:CD2	1:A:544:MET:HE1	2.44	0.47
1:B:92:THR:HG21	1:B:479:TYR:HH	1.80	0.47
1:C:384:LYS:NZ	1:C:392:GLU:OE2	2.43	0.47
1:D:238:THR:OG1	1:D:242:HIS:HB2	2.14	0.47
1:A:247:ASP:O	1:A:251:PHE:N	2.47	0.47
1:A:405:GLU:OE2	1:B:405:GLU:OE2	2.32	0.47
1:A:172:GLN:HB2	1:A:188:LYS:HB3	1.96	0.46
1:A:334:LEU:C	1:A:334:LEU:HD12	2.39	0.46
1:C:334:LEU:C	1:C:334:LEU:HD12	2.40	0.46
1:B:93:ILE:HD12	1:B:138:LEU:HD23	1.96	0.46
1:B:404:VAL:HG11	1:B:437:ASN:O	2.15	0.46
1:C:368:VAL:HG23	1:C:368:VAL:O	2.14	0.46
1:C:605:ILE:HD12	1:C:606:LYS:HB2	1.96	0.46
1:C:690:VAL:HG21	1:C:701:TYR:CE1	2.50	0.46
1:D:690:VAL:HG21	1:D:701:TYR:CE1	2.49	0.46
1:A:289:THR:N	1:A:299:GLN:O	2.48	0.46
1:B:172:GLN:HB2	1:B:188:LYS:HB3	1.96	0.46
1:B:316:GLN:O	1:B:317:ASN:HB2	2.15	0.46
1:B:326:SER:O	1:B:327:ALA:HB3	2.16	0.46
1:C:109:THR:HG21	1:C:120:ASN:HB2	1.94	0.46
1:C:259:MET:HE2	1:C:259:MET:HA	1.98	0.46
1:C:729:ILE:HG23	1:C:729:ILE:OXT	2.15	0.46
1:D:59:CYS:HB2	1:D:464:THR:OG1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD12	1:A:138:LEU:HD23	1.95	0.46
1:A:368:VAL:HG23	1:A:368:VAL:O	2.14	0.46
1:B:540:LEU:CD2	1:B:544:MET:HE1	2.45	0.46
1:C:500:GLU:HB2	1:C:507:PHE:CE2	2.50	0.46
1:D:248:LEU:O	1:D:251:PHE:CE1	2.69	0.46
1:D:316:GLN:O	1:D:317:ASN:HB2	2.16	0.46
1:D:342:LEU:CD1	1:D:379:ILE:HD12	2.28	0.46
1:D:623:LEU:CD1	1:D:664:LEU:CD2	2.86	0.46
1:A:316:GLN:O	1:A:317:ASN:HB2	2.15	0.46
1:B:346:ALA:CB	1:B:369:ASN:HD22	2.28	0.46
1:C:25:ASP:OD1	1:C:94:ASN:HB2	2.15	0.46
1:C:342:LEU:CD1	1:C:379:ILE:HD12	2.28	0.46
1:D:500:GLU:HB2	1:D:507:PHE:CE2	2.50	0.46
1:A:326:SER:O	1:A:327:ALA:HB3	2.16	0.46
1:A:508:LYS:O	1:A:512:THR:HG23	2.15	0.46
1:B:334:LEU:HD12	1:B:334:LEU:C	2.40	0.46
1:B:690:VAL:HG21	1:B:701:TYR:CE1	2.51	0.46
1:C:125:ASP:OD1	1:C:125:ASP:C	2.58	0.46
1:C:346:ALA:CB	1:C:369:ASN:HD22	2.28	0.46
1:C:397:ILE:O	1:C:397:ILE:CG2	2.63	0.46
1:A:183:LEU:HD11	1:A:246:TRP:NE1	2.31	0.46
1:D:111:GLN:HG3	1:D:168:TYR:CG	2.51	0.46
1:D:125:ASP:OD1	1:D:126:GLY:N	2.49	0.46
1:A:346:ALA:CB	1:A:369:ASN:HD22	2.28	0.46
1:B:283:TYR:OH	1:B:338:ARG:HD2	2.16	0.46
1:C:111:GLN:HG3	1:C:168:TYR:CG	2.51	0.46
1:C:184:LEU:HD12	1:C:198:LEU:HD21	1.98	0.46
1:D:442:TYR:O	1:D:443:LEU:C	2.58	0.46
1:A:25:ASP:OD1	1:A:94:ASN:HB2	2.16	0.46
1:A:690:VAL:HG21	1:A:701:TYR:CE1	2.51	0.46
1:A:706:ASN:C	1:A:706:ASN:HD22	2.24	0.46
1:A:729:ILE:HG23	1:A:729:ILE:OXT	2.16	0.46
1:B:111:GLN:HG3	1:B:168:TYR:CG	2.50	0.46
1:B:637:PHE:O	1:C:210:ARG:NH1	2.48	0.46
1:D:723:PHE:O	1:D:724:PHE:C	2.58	0.46
1:A:111:GLN:HG3	1:A:168:TYR:CG	2.51	0.45
1:A:125:ASP:OD1	1:A:126:GLY:N	2.49	0.45
1:A:623:LEU:HD23	1:A:623:LEU:HA	1.66	0.45
1:C:4:LEU:N	1:C:4:LEU:HD12	2.32	0.45
1:D:62:LEU:HD13	1:D:135:LEU:CD1	2.39	0.45
1:D:404:VAL:CG1	1:D:438:GLU:HG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:H	1:A:595:ILE:CD1	2.28	0.45
1:B:183:LEU:HD11	1:B:246:TRP:NE1	2.32	0.45
1:B:270:PHE:C	1:B:270:PHE:HD2	2.22	0.45
1:B:384:LYS:NZ	1:B:392:GLU:OE2	2.43	0.45
1:D:25:ASP:OD1	1:D:94:ASN:HB2	2.16	0.45
1:D:109:THR:HG21	1:D:120:ASN:HB2	1.95	0.45
1:B:620:HIS:NE2	1:B:669:ARG:NH2	2.64	0.45
1:C:326:SER:O	1:C:327:ALA:HB3	2.16	0.45
1:D:209:THR:C	1:D:211:PHE:H	2.23	0.45
1:A:442:TYR:O	1:A:443:LEU:C	2.59	0.45
1:A:620:HIS:NE2	1:A:669:ARG:NH2	2.64	0.45
1:B:18:PRO:HD3	1:B:417:THR:HG21	1.99	0.45
1:C:283:TYR:OH	1:C:338:ARG:HD2	2.16	0.45
1:D:283:TYR:OH	1:D:338:ARG:HD2	2.15	0.45
1:D:326:SER:O	1:D:327:ALA:HB3	2.17	0.45
1:D:706:ASN:C	1:D:706:ASN:HD22	2.23	0.45
1:A:163:PRO:HA	1:A:178:LEU:HA	1.98	0.45
1:A:283:TYR:OH	1:A:338:ARG:HD2	2.17	0.45
1:A:723:PHE:O	1:A:724:PHE:C	2.59	0.45
1:B:25:ASP:OD1	1:B:94:ASN:HB2	2.16	0.45
1:B:335:VAL:CG1	1:B:352:ILE:HB	2.40	0.45
1:C:209:THR:C	1:C:211:PHE:H	2.23	0.45
1:C:442:TYR:O	1:C:443:LEU:C	2.59	0.45
1:C:499:SER:O	1:C:501:THR:N	2.50	0.45
1:D:4:LEU:N	1:D:4:LEU:HD12	2.32	0.45
1:D:163:PRO:HA	1:D:178:LEU:HA	1.98	0.45
1:D:346:ALA:CB	1:D:369:ASN:HD22	2.29	0.45
1:A:397:ILE:O	1:A:397:ILE:CG2	2.63	0.45
1:D:184:LEU:HD12	1:D:198:LEU:HD21	1.99	0.45
1:D:386:LEU:HD12	1:D:390:GLN:HG3	1.99	0.45
1:B:125:ASP:OD1	1:B:126:GLY:N	2.50	0.45
1:B:233:TYR:CD1	1:B:311:LEU:HD22	2.52	0.45
1:B:565:THR:HG23	1:B:566:ASN:N	2.32	0.45
1:A:602:ILE:CB	1:A:691:LYS:HB2	2.41	0.45
1:B:250:SER:O	1:B:251:PHE:HB2	2.17	0.45
1:B:637:PHE:CD2	1:B:642:LEU:HD12	2.52	0.45
1:C:431:LYS:HA	1:C:431:LYS:HD3	1.81	0.45
1:B:184:LEU:HD12	1:B:198:LEU:HD21	1.99	0.45
1:B:595:ILE:H	1:B:595:ILE:CD1	2.29	0.45
1:C:62:LEU:HD13	1:C:135:LEU:CD1	2.39	0.45
1:C:183:LEU:HD11	1:C:246:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LEU:O	1:D:300:MET:HA	2.17	0.45
1:A:270:PHE:HD2	1:A:271:ARG:N	2.15	0.45
1:A:499:SER:O	1:A:501:THR:N	2.50	0.45
1:B:442:TYR:O	1:B:443:LEU:C	2.60	0.45
1:B:602:ILE:CB	1:B:691:LYS:HB2	2.41	0.45
1:D:95:ILE:HD13	1:D:131:LEU:HD13	1.98	0.45
1:A:335:VAL:CG1	1:A:352:ILE:HB	2.41	0.44
1:A:342:LEU:CD1	1:A:379:ILE:HD12	2.29	0.44
1:C:59:CYS:HB2	1:C:464:THR:OG1	2.16	0.44
1:D:183:LEU:HD11	1:D:246:TRP:NE1	2.31	0.44
1:D:499:SER:O	1:D:501:THR:N	2.51	0.44
1:D:585:ASP:OD1	1:D:589:ASN:ND2	2.41	0.44
1:D:729:ILE:HG23	1:D:729:ILE:OXT	2.17	0.44
1:B:404:VAL:HG11	1:B:438:GLU:HG2	1.99	0.44
1:C:595:ILE:H	1:C:595:ILE:CD1	2.29	0.44
1:C:620:HIS:NE2	1:C:669:ARG:NH2	2.64	0.44
1:C:706:ASN:C	1:C:706:ASN:HD22	2.24	0.44
1:A:226:CYS:SG	1:A:234:LEU:HD11	2.57	0.44
1:A:506:LEU:HD11	1:A:586:LEU:HB2	1.98	0.44
1:B:163:PRO:HA	1:B:178:LEU:HA	1.99	0.44
1:B:342:LEU:CD1	1:B:379:ILE:HD12	2.28	0.44
1:B:354:LEU:HD21	1:B:460:ALA:HB1	2.00	0.44
1:C:125:ASP:OD1	1:C:126:GLY:N	2.50	0.44
1:D:506:LEU:HD11	1:D:586:LEU:HB2	1.99	0.44
1:D:620:HIS:NE2	1:D:669:ARG:NH2	2.64	0.44
1:A:184:LEU:HD12	1:A:198:LEU:HD21	1.99	0.44
1:B:95:ILE:HD13	1:B:131:LEU:HD13	2.00	0.44
1:B:706:ASN:C	1:B:706:ASN:HD22	2.26	0.44
1:C:287:LEU:O	1:C:300:MET:HA	2.18	0.44
1:C:289:THR:N	1:C:299:GLN:O	2.48	0.44
1:C:637:PHE:CD2	1:C:642:LEU:HD12	2.53	0.44
1:A:384:LYS:NZ	1:A:392:GLU:OE2	2.44	0.44
1:C:226:CYS:SG	1:C:234:LEU:HD11	2.57	0.44
1:C:571:PHE:O	1:C:575:ASN:OD1	2.36	0.44
1:D:595:ILE:H	1:D:595:ILE:CD1	2.29	0.44
1:B:729:ILE:OXT	1:B:729:ILE:HG23	2.18	0.44
1:C:163:PRO:HA	1:C:178:LEU:HA	1.99	0.44
1:C:386:LEU:HD12	1:C:390:GLN:HG3	2.00	0.44
1:D:431:LYS:HA	1:D:431:LYS:HD3	1.82	0.44
1:B:397:ILE:O	1:B:397:ILE:CG2	2.64	0.44
1:C:250:SER:O	1:C:251:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:632:GLN:O	1:D:635:LEU:HB3	2.18	0.44
1:A:189:VAL:HG21	1:A:195:GLU:OE2	2.17	0.44
1:A:291:LEU:HA	1:A:292:PRO:HD3	1.73	0.44
1:B:189:VAL:HG21	1:B:195:GLU:OE2	2.17	0.44
1:B:222:SER:O	1:B:239:GLN:HG3	2.18	0.44
1:B:386:LEU:HD12	1:B:390:GLN:HG3	2.00	0.44
1:C:222:SER:O	1:C:239:GLN:HG3	2.18	0.44
1:C:663:LEU:HD11	1:C:729:ILE:HD12	2.00	0.44
1:B:288:VAL:HG13	1:B:336:LEU:HD22	2.00	0.44
1:B:499:SER:O	1:B:501:THR:N	2.51	0.44
1:B:506:LEU:HD11	1:B:586:LEU:HB2	1.99	0.44
1:D:73:SER:HB3	1:D:78:LEU:HB3	2.00	0.44
1:A:596:PHE:C	1:A:598:LYS:H	2.26	0.43
1:A:637:PHE:CD2	1:A:642:LEU:HD12	2.53	0.43
1:B:224:ILE:HD12	1:B:279:TYR:CD2	2.53	0.43
1:C:95:ILE:HD13	1:C:131:LEU:HD13	1.99	0.43
1:C:439:ASP:O	1:C:442:TYR:HB3	2.18	0.43
1:D:289:THR:N	1:D:299:GLN:O	2.48	0.43
1:D:571:PHE:O	1:D:575:ASN:OD1	2.36	0.43
1:D:692:PHE:O	1:D:692:PHE:CD2	2.71	0.43
1:A:436:HIS:CD2	1:A:438:GLU:H	2.36	0.43
1:D:565:THR:HG23	1:D:566:ASN:N	2.33	0.43
1:A:287:LEU:O	1:A:300:MET:HA	2.17	0.43
1:B:18:PRO:HB2	1:B:418:GLN:HA	2.00	0.43
1:B:723:PHE:O	1:B:724:PHE:C	2.61	0.43
1:C:565:THR:HG23	1:C:566:ASN:N	2.33	0.43
1:B:287:LEU:O	1:B:300:MET:HA	2.17	0.43
1:B:571:PHE:O	1:B:575:ASN:OD1	2.36	0.43
1:C:493:TRP:HH2	1:C:506:LEU:HD23	1.83	0.43
1:D:337:THR:OG1	1:D:338:ARG:N	2.52	0.43
1:D:439:ASP:O	1:D:442:TYR:HB3	2.19	0.43
1:D:493:TRP:HH2	1:D:506:LEU:HD23	1.83	0.43
1:D:637:PHE:CD2	1:D:642:LEU:HD12	2.54	0.43
1:A:386:LEU:HD12	1:A:390:GLN:HG3	2.01	0.43
1:A:579:ILE:HB	1:A:580:PRO:HD3	2.01	0.43
1:B:596:PHE:C	1:B:598:LYS:H	2.27	0.43
1:C:579:ILE:HB	1:C:580:PRO:HD3	2.00	0.43
1:D:222:SER:O	1:D:239:GLN:HG3	2.19	0.43
1:A:22:ASN:HD21	1:A:91:LYS:HB2	1.78	0.43
1:A:61:LEU:HD12	1:A:62:LEU:N	2.34	0.43
1:A:222:SER:O	1:A:239:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:C	1:A:232:ARG:H	2.26	0.43
1:A:354:LEU:HD21	1:A:460:ALA:HB1	2.01	0.43
1:A:18:PRO:HB2	1:A:418:GLN:HA	2.01	0.43
1:A:439:ASP:O	1:A:442:TYR:HB3	2.18	0.43
1:B:372:SER:C	1:B:374:LYS:H	2.27	0.43
1:B:439:ASP:O	1:B:442:TYR:HB3	2.18	0.43
1:C:692:PHE:O	1:C:692:PHE:CD2	2.72	0.43
1:D:189:VAL:HG21	1:D:195:GLU:OE2	2.18	0.43
1:D:595:ILE:N	1:D:595:ILE:CD1	2.82	0.43
1:A:218:SER:O	1:A:220:TYR:N	2.50	0.43
1:A:224:ILE:HD12	1:A:279:TYR:CD2	2.54	0.43
1:A:372:SER:C	1:A:374:LYS:H	2.27	0.43
1:B:595:ILE:N	1:B:595:ILE:CD1	2.81	0.43
1:D:18:PRO:HB2	1:D:418:GLN:HA	2.00	0.43
1:A:288:VAL:HG13	1:A:336:LEU:HD22	2.01	0.43
1:A:721:MET:HE3	1:A:721:MET:HA	2.01	0.43
1:B:61:LEU:HD12	1:B:62:LEU:N	2.34	0.43
1:B:579:ILE:HB	1:B:580:PRO:HD3	2.01	0.43
1:B:620:HIS:CD2	1:B:668:TYR:CD2	3.07	0.43
1:B:632:GLN:O	1:B:635:LEU:HB3	2.19	0.43
1:C:61:LEU:HD12	1:C:62:LEU:N	2.32	0.43
1:C:189:VAL:HG21	1:C:195:GLU:OE2	2.18	0.43
1:C:237:LEU:HD11	1:C:241:CYS:HA	2.01	0.43
1:C:595:ILE:N	1:C:595:ILE:CD1	2.82	0.43
1:A:565:THR:HG23	1:A:566:ASN:N	2.34	0.43
1:C:247:ASP:O	1:C:251:PHE:N	2.51	0.43
1:C:623:LEU:HA	1:C:623:LEU:HD23	1.64	0.43
1:A:265:SER:O	1:A:267:PRO:HD3	2.19	0.42
1:C:337:THR:OG1	1:C:338:ARG:N	2.52	0.42
1:D:237:LEU:HD11	1:D:241:CYS:HA	2.01	0.42
1:A:93:ILE:HD12	1:A:138:LEU:CD2	2.49	0.42
1:A:595:ILE:N	1:A:595:ILE:CD1	2.82	0.42
1:C:346:ALA:HB1	1:C:369:ASN:HD22	1.84	0.42
1:A:4:LEU:N	1:A:4:LEU:HD12	2.33	0.42
1:A:101:SER:O	1:A:124:LYS:HG3	2.20	0.42
1:A:620:HIS:CD2	1:A:668:TYR:CD2	3.07	0.42
1:B:22:ASN:HD21	1:B:91:LYS:HB2	1.78	0.42
1:B:230:HIS:C	1:B:232:ARG:H	2.27	0.42
1:B:248:LEU:O	1:B:251:PHE:CE1	2.72	0.42
1:B:431:LYS:HA	1:B:431:LYS:HD3	1.81	0.42
1:C:93:ILE:HD12	1:C:138:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LYS:O	1:C:273:VAL:C	2.62	0.42
1:C:723:PHE:O	1:C:724:PHE:C	2.61	0.42
1:D:272:LYS:O	1:D:273:VAL:C	2.62	0.42
1:C:230:HIS:C	1:C:232:ARG:H	2.26	0.42
1:C:328:ILE:H	1:C:328:ILE:CD1	2.29	0.42
1:D:328:ILE:H	1:D:328:ILE:CD1	2.29	0.42
1:D:372:SER:C	1:D:374:LYS:H	2.27	0.42
1:A:272:LYS:O	1:A:273:VAL:C	2.62	0.42
1:B:282:LEU:HD23	1:B:282:LEU:H	1.84	0.42
1:C:596:PHE:C	1:C:598:LYS:H	2.27	0.42
1:D:230:HIS:C	1:D:232:ARG:H	2.27	0.42
1:A:95:ILE:HD13	1:A:131:LEU:HD13	2.02	0.42
1:B:93:ILE:HD12	1:B:138:LEU:CD2	2.50	0.42
1:C:73:SER:HB3	1:C:78:LEU:HB3	2.01	0.42
1:C:165:PHE:HB3	1:C:177:PHE:HB2	2.01	0.42
1:C:354:LEU:HD21	1:C:460:ALA:HB1	2.01	0.42
1:C:372:SER:C	1:C:374:LYS:H	2.27	0.42
1:C:632:GLN:O	1:C:635:LEU:HB3	2.20	0.42
1:D:516:PHE:CG	1:D:570:LEU:HD22	2.54	0.42
1:A:237:LEU:HD11	1:A:241:CYS:HA	2.01	0.42
1:A:516:PHE:CG	1:A:570:LEU:HD22	2.54	0.42
1:A:663:LEU:HD11	1:A:729:ILE:HD12	2.01	0.42
1:B:101:SER:HB2	1:B:107:THR:OG1	2.20	0.42
1:B:226:CYS:SG	1:B:234:LEU:HD11	2.59	0.42
1:B:291:LEU:HA	1:B:292:PRO:HD3	1.73	0.42
1:B:337:THR:OG1	1:B:338:ARG:N	2.52	0.42
1:B:346:ALA:HB1	1:B:369:ASN:HD22	1.84	0.42
1:C:18:PRO:HB2	1:C:418:GLN:HA	2.01	0.42
1:D:291:LEU:HA	1:D:292:PRO:HD3	1.73	0.42
1:A:109:THR:HG21	1:A:120:ASN:HB2	1.94	0.42
1:B:73:SER:HB3	1:B:78:LEU:HB3	2.01	0.42
1:C:370:ASP:OD1	1:C:372:SER:O	2.38	0.42
1:C:516:PHE:CB	1:C:570:LEU:HD22	2.50	0.42
1:C:516:PHE:CG	1:C:570:LEU:HD22	2.54	0.42
1:C:721:MET:HE3	1:C:721:MET:HA	2.01	0.42
1:D:122:ILE:HG12	1:D:128:PHE:HD1	1.85	0.42
1:A:73:SER:HB3	1:A:78:LEU:HB3	2.01	0.42
1:A:399:THR:O	1:A:526:ARG:NH2	2.52	0.42
1:A:692:PHE:O	1:A:692:PHE:CD2	2.73	0.42
1:B:497:MET:HE3	1:B:514:ASN:HB2	2.01	0.42
1:B:663:LEU:HD11	1:B:729:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:SER:O	1:C:124:LYS:HG3	2.19	0.42
1:C:233:TYR:CD1	1:C:311:LEU:HD22	2.54	0.42
1:C:282:LEU:H	1:C:282:LEU:HD23	1.84	0.42
1:D:354:LEU:HD21	1:D:460:ALA:HB1	2.01	0.42
1:D:596:PHE:C	1:D:598:LYS:H	2.27	0.42
1:D:602:ILE:CG2	1:D:691:LYS:HB2	2.50	0.42
1:A:431:LYS:HA	1:A:431:LYS:HD3	1.82	0.42
1:B:237:LEU:HD11	1:B:241:CYS:HA	2.01	0.42
1:B:399:THR:O	1:B:526:ARG:NH2	2.52	0.42
1:C:304:LEU:HD12	1:C:305:VAL:N	2.35	0.42
1:D:226:CYS:SG	1:D:234:LEU:HD11	2.60	0.42
1:D:469:GLU:OE2	1:D:694:ASN:HB2	2.20	0.42
1:A:290:LEU:HD13	1:A:298:PHE:CZ	2.55	0.41
1:A:571:PHE:O	1:A:575:ASN:OD1	2.37	0.41
1:B:272:LYS:O	1:B:273:VAL:C	2.63	0.41
1:C:101:SER:HB2	1:C:107:THR:OG1	2.20	0.41
1:C:291:LEU:HA	1:C:292:PRO:HD3	1.72	0.41
1:C:585:ASP:OD1	1:C:589:ASN:ND2	2.41	0.41
1:C:602:ILE:CG2	1:C:691:LYS:HB2	2.50	0.41
1:D:282:LEU:HD23	1:D:282:LEU:H	1.84	0.41
1:A:62:LEU:HD13	1:A:135:LEU:CD1	2.39	0.41
1:A:165:PHE:HB3	1:A:177:PHE:HB2	2.01	0.41
1:A:602:ILE:CG2	1:A:691:LYS:HB2	2.50	0.41
1:B:4:LEU:HD12	1:B:4:LEU:N	2.35	0.41
1:B:101:SER:O	1:B:124:LYS:HG3	2.21	0.41
1:B:122:ILE:HG12	1:B:128:PHE:HD1	1.85	0.41
1:D:101:SER:HB2	1:D:107:THR:OG1	2.20	0.41
1:D:288:VAL:HA	1:D:299:GLN:O	2.20	0.41
1:D:317:ASN:OD1	1:D:318:ASN:N	2.54	0.41
1:A:337:THR:OG1	1:A:338:ARG:N	2.52	0.41
1:A:346:ALA:HB1	1:A:369:ASN:HD22	1.85	0.41
1:C:229:PHE:O	1:C:230:HIS:C	2.62	0.41
1:D:101:SER:O	1:D:124:LYS:HG3	2.20	0.41
1:D:165:PHE:HB3	1:D:177:PHE:HB2	2.01	0.41
1:D:172:GLN:CD	1:D:172:GLN:N	2.78	0.41
1:D:534:ASP:HA	1:D:537:THR:OG1	2.21	0.41
1:D:579:ILE:HB	1:D:580:PRO:HD3	2.02	0.41
1:B:129:LEU:HD12	1:B:130:THR:H	1.85	0.41
1:B:605:ILE:HD12	1:B:606:LYS:CB	2.50	0.41
1:D:93:ILE:HD12	1:D:138:LEU:CD2	2.50	0.41
1:D:129:LEU:HD12	1:D:130:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:HD12	1:D:305:VAL:N	2.36	0.41
1:D:346:ALA:HB1	1:D:369:ASN:HD22	1.85	0.41
1:D:516:PHE:CB	1:D:570:LEU:HD22	2.50	0.41
1:A:370:ASP:OD1	1:A:372:SER:O	2.38	0.41
1:B:62:LEU:HD13	1:B:135:LEU:CD1	2.40	0.41
1:B:317:ASN:OD1	1:B:318:ASN:N	2.53	0.41
1:B:501:THR:HG23	1:D:29:SER:CB	2.50	0.41
1:C:399:THR:O	1:C:526:ARG:NH2	2.50	0.41
1:D:18:PRO:HD3	1:D:417:THR:HG21	2.03	0.41
1:D:342:LEU:HD22	1:D:379:ILE:HD13	2.03	0.41
1:D:370:ASP:OD1	1:D:372:SER:O	2.39	0.41
1:A:229:PHE:O	1:A:230:HIS:C	2.63	0.41
1:A:282:LEU:H	1:A:282:LEU:HD23	1.85	0.41
1:B:165:PHE:HB3	1:B:177:PHE:HB2	2.01	0.41
1:B:602:ILE:CG2	1:B:691:LYS:HB2	2.50	0.41
1:B:692:PHE:CD2	1:B:692:PHE:O	2.73	0.41
1:C:152:LEU:HD23	1:C:152:LEU:HA	1.93	0.41
1:C:288:VAL:HA	1:C:299:GLN:O	2.20	0.41
1:D:229:PHE:O	1:D:230:HIS:C	2.63	0.41
1:A:101:SER:HB2	1:A:107:THR:OG1	2.21	0.41
1:A:304:LEU:HD12	1:A:305:VAL:N	2.36	0.41
1:C:218:SER:OG	1:C:219:ASP:N	2.53	0.41
1:C:221:ASP:OD1	1:C:238:THR:HB	2.21	0.41
1:D:61:LEU:HD12	1:D:62:LEU:N	2.34	0.41
1:D:218:SER:O	1:D:220:TYR:N	2.51	0.41
1:D:659:TYR:OH	1:D:725:ARG:HD2	2.21	0.41
1:D:663:LEU:HD11	1:D:729:ILE:HD12	2.03	0.41
1:B:229:PHE:O	1:B:230:HIS:C	2.63	0.41
1:B:290:LEU:HD13	1:B:298:PHE:CZ	2.56	0.41
1:B:493:TRP:HH2	1:B:506:LEU:HD23	1.83	0.41
1:C:3:CYS:C	1:C:4:LEU:HD12	2.46	0.41
1:C:86:ASP:O	1:C:90:GLY:HA3	2.20	0.41
1:C:129:LEU:HD12	1:C:130:THR:H	1.86	0.41
1:C:172:GLN:CD	1:C:172:GLN:N	2.79	0.41
1:C:293:LEU:O	1:C:294:GLU:CB	2.68	0.41
1:C:342:LEU:HD22	1:C:379:ILE:HD13	2.03	0.41
1:C:469:GLU:OE2	1:C:694:ASN:HB2	2.21	0.41
1:D:86:ASP:O	1:D:90:GLY:HA3	2.20	0.41
1:D:264:ASP:O	1:D:266:ASP:N	2.53	0.41
1:A:18:PRO:HD3	1:A:417:THR:HG21	2.03	0.41
1:A:382:VAL:HG21	1:A:495:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:MET:HE3	1:A:514:ASN:HB2	2.02	0.41
1:B:109:THR:HG21	1:B:120:ASN:HB2	1.96	0.41
1:C:218:SER:O	1:C:220:TYR:N	2.51	0.41
1:C:497:MET:HE3	1:C:514:ASN:HB2	2.02	0.41
1:C:729:ILE:OXT	1:C:729:ILE:CG2	2.69	0.41
1:D:3:CYS:C	1:D:4:LEU:HD12	2.46	0.41
1:D:233:TYR:CD1	1:D:311:LEU:HD22	2.55	0.41
1:A:122:ILE:HG12	1:A:128:PHE:HD1	1.86	0.40
1:A:218:SER:OG	1:A:219:ASP:N	2.53	0.40
1:B:516:PHE:CG	1:B:570:LEU:HD22	2.55	0.40
1:C:122:ILE:HG12	1:C:128:PHE:HD1	1.86	0.40
1:C:290:LEU:HD13	1:C:298:PHE:CZ	2.56	0.40
1:C:317:ASN:OD1	1:C:318:ASN:N	2.55	0.40
1:D:295:ASN:ND2	1:D:329:TRP:O	2.54	0.40
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.86	0.40
1:A:248:LEU:O	1:A:251:PHE:CE1	2.74	0.40
1:A:288:VAL:HA	1:A:299:GLN:O	2.21	0.40
1:A:293:LEU:O	1:A:294:GLU:CB	2.68	0.40
1:A:632:GLN:O	1:A:635:LEU:HB3	2.22	0.40
1:B:64:ASN:O	1:B:65:SER:HB2	2.21	0.40
1:B:342:LEU:HD22	1:B:379:ILE:HD13	2.03	0.40
1:B:516:PHE:CB	1:B:570:LEU:HD22	2.50	0.40
1:D:721:MET:HE3	1:D:721:MET:HA	2.03	0.40
1:B:71:HIS:CE1	1:B:478:PRO:HA	2.57	0.40
1:B:167:PHE:O	1:B:174:SER:HB2	2.21	0.40
1:B:614:ILE:HD13	1:B:614:ILE:HA	1.94	0.40
1:C:167:PHE:O	1:C:174:SER:HB2	2.21	0.40
1:C:545:THR:OG1	1:C:548:GLU:HG3	2.22	0.40
1:A:71:HIS:CE1	1:A:478:PRO:HA	2.57	0.40
1:A:469:GLU:OE2	1:A:694:ASN:HB2	2.21	0.40
1:B:218:SER:OG	1:B:219:ASP:N	2.53	0.40
1:B:247:ASP:O	1:B:251:PHE:N	2.50	0.40
1:B:304:LEU:HD12	1:B:305:VAL:N	2.37	0.40
1:B:370:ASP:OD1	1:B:372:SER:O	2.39	0.40
1:C:224:ILE:HD12	1:C:279:TYR:CD2	2.55	0.40
1:C:659:TYR:OH	1:C:725:ARG:HD2	2.22	0.40
1:D:152:LEU:HD23	1:D:152:LEU:HA	1.93	0.40
1:D:167:PHE:O	1:D:174:SER:HB2	2.22	0.40
1:D:218:SER:OG	1:D:219:ASP:N	2.54	0.40
1:D:293:LEU:O	1:D:294:GLU:CB	2.69	0.40
1:A:129:LEU:HD12	1:A:130:THR:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:HD12	1:A:328:ILE:N	2.36	0.40
1:A:729:ILE:OXT	1:A:729:ILE:CG2	2.70	0.40
1:B:192:VAL:O	1:B:192:VAL:HG12	2.21	0.40
1:B:288:VAL:HA	1:B:299:GLN:O	2.21	0.40
1:B:296:GLY:HA2	1:B:321:THR:CG2	2.51	0.40
1:C:64:ASN:O	1:C:65:SER:HB2	2.21	0.40
1:C:248:LEU:O	1:C:251:PHE:CE1	2.74	0.40
1:C:614:ILE:HD13	1:C:614:ILE:HA	1.93	0.40
1:D:224:ILE:HD12	1:D:279:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/729 (95%)	599 (86%)	72 (10%)	24 (4%)	3	4
1	B	695/729 (95%)	599 (86%)	70 (10%)	26 (4%)	2	3
1	C	695/729 (95%)	597 (86%)	73 (10%)	25 (4%)	2	4
1	D	695/729 (95%)	596 (86%)	74 (11%)	25 (4%)	2	4
All	All	2780/2916 (95%)	2391 (86%)	289 (10%)	100 (4%)	2	4

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	SER
1	A	403	ASP
1	A	600	ASP
1	A	602	ILE
1	B	403	ASP
1	B	600	ASP

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Mol	Chain	Res	Type
1	B	602	ILE
1	C	403	ASP
1	C	600	ASP
1	C	602	ILE
1	D	268	SER
1	D	403	ASP
1	D	600	ASP
1	D	602	ILE
1	A	113	VAL
1	A	231	GLU
1	A	315	PHE
1	B	113	VAL
1	B	231	GLU
1	B	268	SER
1	B	315	PHE
1	C	113	VAL
1	C	231	GLU
1	C	265	SER
1	C	315	PHE
1	D	113	VAL
1	D	231	GLU
1	D	315	PHE
1	A	11	LEU
1	A	190	ASP
1	A	346	ALA
1	A	500	GLU
1	B	11	LEU
1	B	190	ASP
1	B	346	ALA
1	B	500	GLU
1	C	11	LEU
1	C	190	ASP
1	C	268	SER
1	C	346	ALA
1	C	500	GLU
1	C	593	PRO
1	D	11	LEU
1	D	265	SER
1	D	346	ALA
1	D	500	GLU
1	A	219	ASP
1	A	230	HIS

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Mol	Chain	Res	Type
1	A	326	SER
1	A	499	SER
1	A	593	PRO
1	A	598	LYS
1	A	671	ASP
1	B	100	ALA
1	B	230	HIS
1	B	326	SER
1	B	499	SER
1	B	593	PRO
1	B	598	LYS
1	B	671	ASP
1	C	100	ALA
1	C	219	ASP
1	C	230	HIS
1	C	326	SER
1	C	499	SER
1	C	598	LYS
1	C	671	ASP
1	D	100	ALA
1	D	190	ASP
1	D	230	HIS
1	D	326	SER
1	D	499	SER
1	D	593	PRO
1	D	598	LYS
1	D	671	ASP
1	A	100	ALA
1	B	73	SER
1	B	219	ASP
1	B	265	SER
1	D	73	SER
1	D	219	ASP
1	D	284	ASN
1	A	73	SER
1	A	284	ASN
1	A	579	ILE
1	B	284	ASN
1	B	579	ILE
1	C	73	SER
1	C	284	ASN
1	C	579	ILE

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Mol	Chain	Res	Type
1	D	579	ILE
1	A	155	PRO
1	B	155	PRO
1	C	155	PRO
1	D	155	PRO
1	A	191	GLY
1	B	191	GLY
1	C	191	GLY
1	D	191	GLY
1	B	273	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	657/682 (96%)	630 (96%)	27 (4%)	27	54
1	B	657/682 (96%)	631 (96%)	26 (4%)	28	55
1	C	657/682 (96%)	629 (96%)	28 (4%)	26	51
1	D	657/682 (96%)	627 (95%)	30 (5%)	24	49
All	All	2628/2728 (96%)	2517 (96%)	111 (4%)	26	52

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	172	GLN
1	A	183	LEU
1	A	186	LEU
1	A	188	LYS
1	A	235	ILE
1	A	270	PHE
1	A	287	LEU
1	A	305	VAL
1	A	314	THR
1	A	318	ASN

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Mol	Chain	Res	Type
1	A	328	ILE
1	A	335	VAL
1	A	338	ARG
1	A	341	GLU
1	A	363	LEU
1	A	404	VAL
1	A	422	ARG
1	A	490	VAL
1	A	499	SER
1	A	513	LEU
1	A	574	LEU
1	A	613	ILE
1	A	638	VAL
1	A	644	THR
1	A	703	ASP
1	A	721	MET
1	B	151	HIS
1	B	172	GLN
1	B	183	LEU
1	B	186	LEU
1	B	188	LYS
1	B	235	ILE
1	B	259	MET
1	B	270	PHE
1	B	287	LEU
1	B	305	VAL
1	B	314	THR
1	B	318	ASN
1	B	328	ILE
1	B	335	VAL
1	B	338	ARG
1	B	341	GLU
1	B	363	LEU
1	B	404	VAL
1	B	490	VAL
1	B	499	SER
1	B	513	LEU
1	B	574	LEU
1	B	613	ILE
1	B	638	VAL
1	B	644	THR
1	B	703	ASP

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Mol	Chain	Res	Type
1	C	151	HIS
1	C	172	GLN
1	C	183	LEU
1	C	186	LEU
1	C	188	LYS
1	C	235	ILE
1	C	250	SER
1	C	259	MET
1	C	266	ASP
1	C	270	PHE
1	C	287	LEU
1	C	305	VAL
1	C	314	THR
1	C	318	ASN
1	C	328	ILE
1	C	335	VAL
1	C	338	ARG
1	C	341	GLU
1	C	363	LEU
1	C	404	VAL
1	C	422	ARG
1	C	490	VAL
1	C	499	SER
1	C	513	LEU
1	C	574	LEU
1	C	613	ILE
1	C	638	VAL
1	C	644	THR
1	D	151	HIS
1	D	172	GLN
1	D	183	LEU
1	D	186	LEU
1	D	188	LYS
1	D	235	ILE
1	D	250	SER
1	D	259	MET
1	D	266	ASP
1	D	269	HIS
1	D	270	PHE
1	D	287	LEU
1	D	305	VAL
1	D	314	THR

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Mol	Chain	Res	Type
1	D	318	ASN
1	D	328	ILE
1	D	335	VAL
1	D	338	ARG
1	D	341	GLU
1	D	363	LEU
1	D	404	VAL
1	D	422	ARG
1	D	490	VAL
1	D	499	SER
1	D	513	LEU
1	D	574	LEU
1	D	613	ILE
1	D	638	VAL
1	D	644	THR
1	D	721	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	89	HIS
1	A	115	GLN
1	A	116	GLN
1	A	132	GLN
1	A	240	ASN
1	A	242	HIS
1	A	255	GLN
1	A	295	ASN
1	A	299	GLN
1	A	318	ASN
1	A	369	ASN
1	A	425	GLN
1	A	514	ASN
1	A	575	ASN
1	A	584	ASN
1	A	588	ASN
1	A	632	GLN
1	A	670	GLN
1	A	697	GLN
1	B	22	ASN
1	B	115	GLN

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Mol	Chain	Res	Type
1	B	116	GLN
1	B	132	GLN
1	B	240	ASN
1	B	242	HIS
1	B	255	GLN
1	B	295	ASN
1	B	299	GLN
1	B	318	ASN
1	B	369	ASN
1	B	425	GLN
1	B	514	ASN
1	B	560	ASN
1	B	575	ASN
1	B	584	ASN
1	B	588	ASN
1	B	632	GLN
1	B	670	GLN
1	B	697	GLN
1	C	115	GLN
1	C	116	GLN
1	C	132	GLN
1	C	240	ASN
1	C	242	HIS
1	C	255	GLN
1	C	262	GLN
1	C	295	ASN
1	C	299	GLN
1	C	318	ASN
1	C	369	ASN
1	C	425	GLN
1	C	514	ASN
1	C	575	ASN
1	C	584	ASN
1	C	588	ASN
1	C	632	GLN
1	C	670	GLN
1	C	697	GLN
1	D	115	GLN
1	D	116	GLN
1	D	132	GLN
1	D	240	ASN
1	D	242	HIS

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Mol	Chain	Res	Type
1	D	255	GLN
1	D	295	ASN
1	D	299	GLN
1	D	318	ASN
1	D	369	ASN
1	D	425	GLN
1	D	514	ASN
1	D	575	ASN
1	D	584	ASN
1	D	588	ASN
1	D	632	GLN
1	D	670	GLN
1	D	697	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	701/729 (96%)	-1.23	0 100 100	35, 73, 116, 143	0
1	B	701/729 (96%)	-1.25	0 100 100	36, 73, 116, 143	0
1	C	701/729 (96%)	-1.24	0 100 100	36, 73, 116, 140	0
1	D	701/729 (96%)	-1.22	0 100 100	35, 73, 116, 140	0
All	All	2804/2916 (96%)	-1.23	0 100 100	35, 73, 117, 143	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HG	B	802	1/1	0.94	0.11	201,201,201,201	0
2	HG	C	802	1/1	0.97	0.08	201,201,201,201	0
2	HG	A	802	1/1	0.98	0.13	201,201,201,201	0
2	HG	D	802	1/1	0.98	0.07	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	B	803	1/1	0.99	0.02	90,90,90,90	0
2	HG	B	801	1/1	0.99	0.05	198,198,198,198	0
2	HG	D	801	1/1	0.99	0.07	191,191,191,191	0
2	HG	A	801	1/1	0.99	0.05	185,185,185,185	0
2	HG	D	803	1/1	0.99	0.02	88,88,88,88	0
2	HG	C	801	1/1	1.00	0.07	187,187,187,187	0
2	HG	A	803	1/1	1.00	0.02	90,90,90,90	0
2	HG	C	803	1/1	1.00	0.02	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.