



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:04 PM GMT

PDB ID : 1RXT
Title : Crystal structure of human myristoyl-CoA:protein N-myristoyltransferase.
Authors : Yang, J.; Wang, Y.; Frey, G.; Abeles, R.H.; Petsko, G.A.; Ringe, D.
Deposited on : 2003-12-18
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

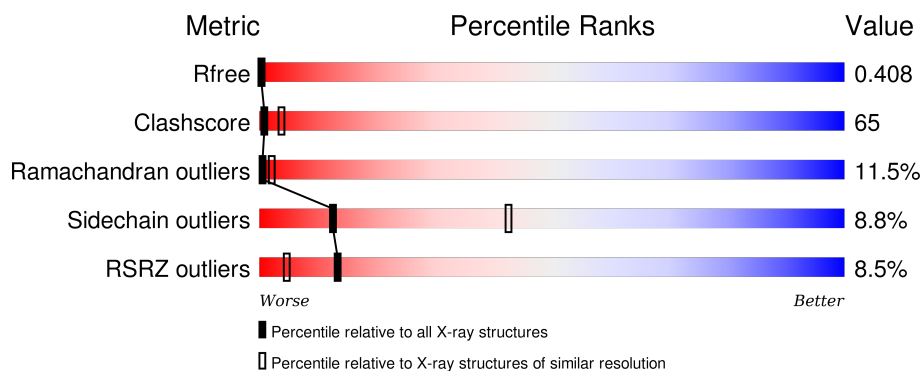
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	496	<div> <div>4%</div> <div>20%</div> <div>40%</div> <div>8%</div> <div>31%</div> </div>
1	B	496	<div> <div>4%</div> <div>21%</div> <div>39%</div> <div>9%</div> <div>31%</div> </div>
1	C	496	<div> <div>7%</div> <div>17%</div> <div>38%</div> <div>9%</div> <div>34%</div> </div>
1	D	496	<div> <div>8%</div> <div>17%</div> <div>39%</div> <div>8%</div> <div>34%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10420 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 Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2646	1724	439	471	12			
1	B	342	Total	C	N	O	S	0	0	0
			2640	1718	438	472	12			
1	C	325	Total	C	N	O	S	0	0	0
			2538	1652	424	450	12			
1	D	326	Total	C	N	O	S	0	0	0
			2523	1642	418	451	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ILE	LEU	CONFLICT	UNP P30419
B	452	ILE	LEU	CONFLICT	UNP P30419
C	452	ILE	LEU	CONFLICT	UNP P30419
D	452	ILE	LEU	CONFLICT	UNP P30419

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Co	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

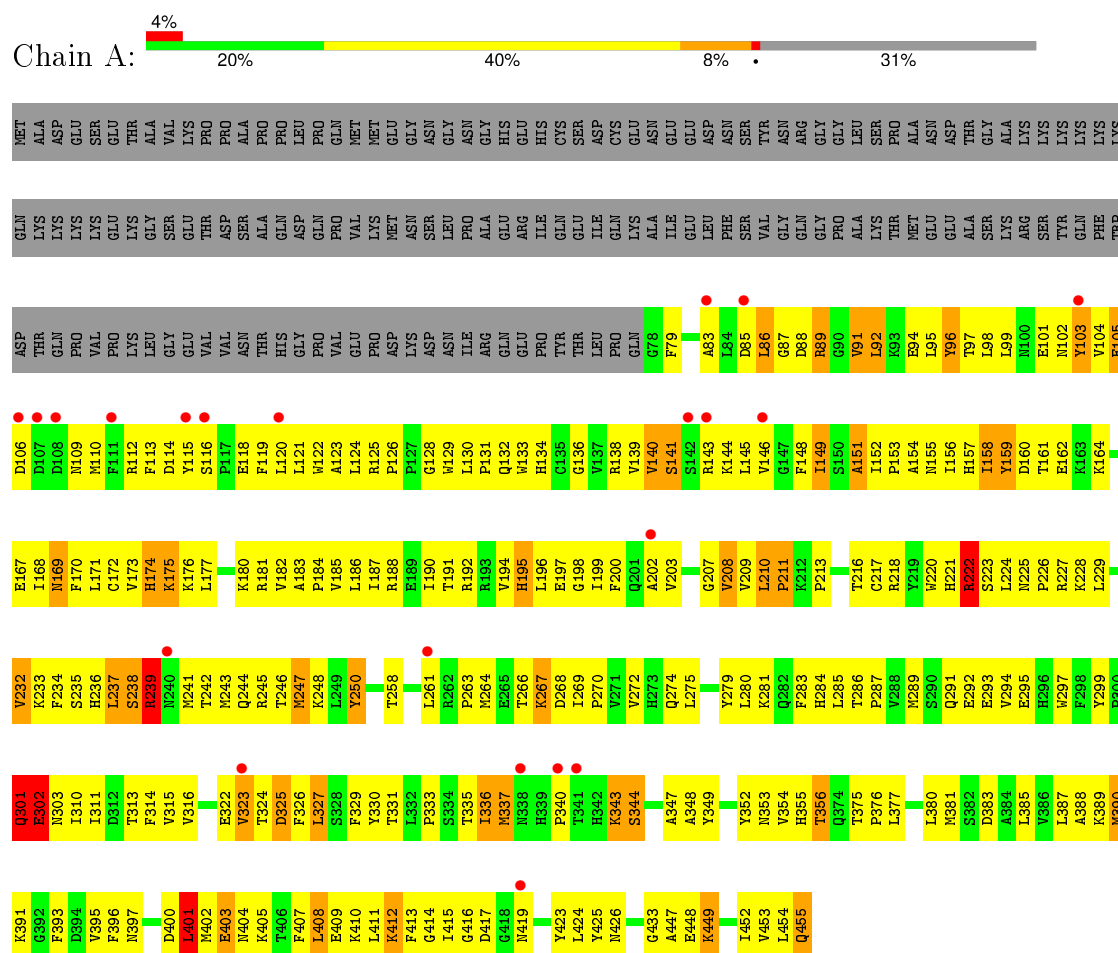
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	13	Total	O	0	0
			13	13		
4	C	10	Total	O	0	0
			10	10		
4	D	16	Total	O	0	0
			16	16		

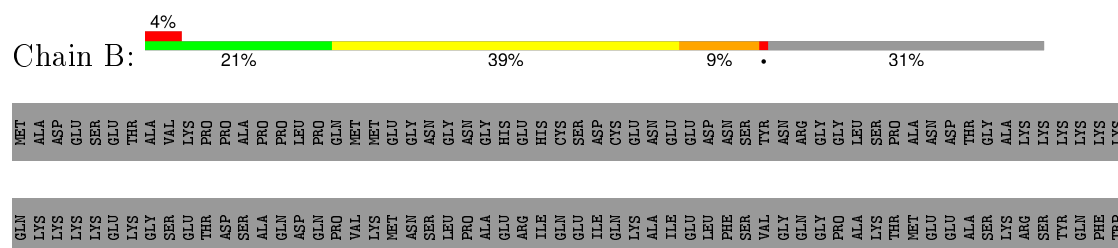
3 Residue-property plots

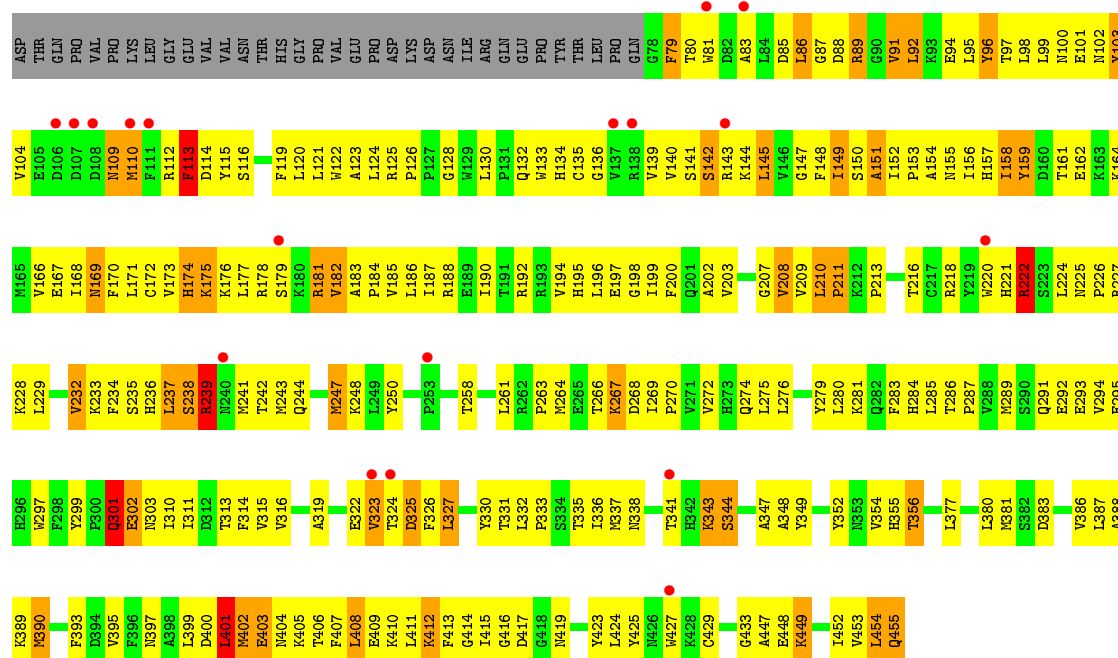
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Glycylpeptide N-tetradecanoyltransferase 1

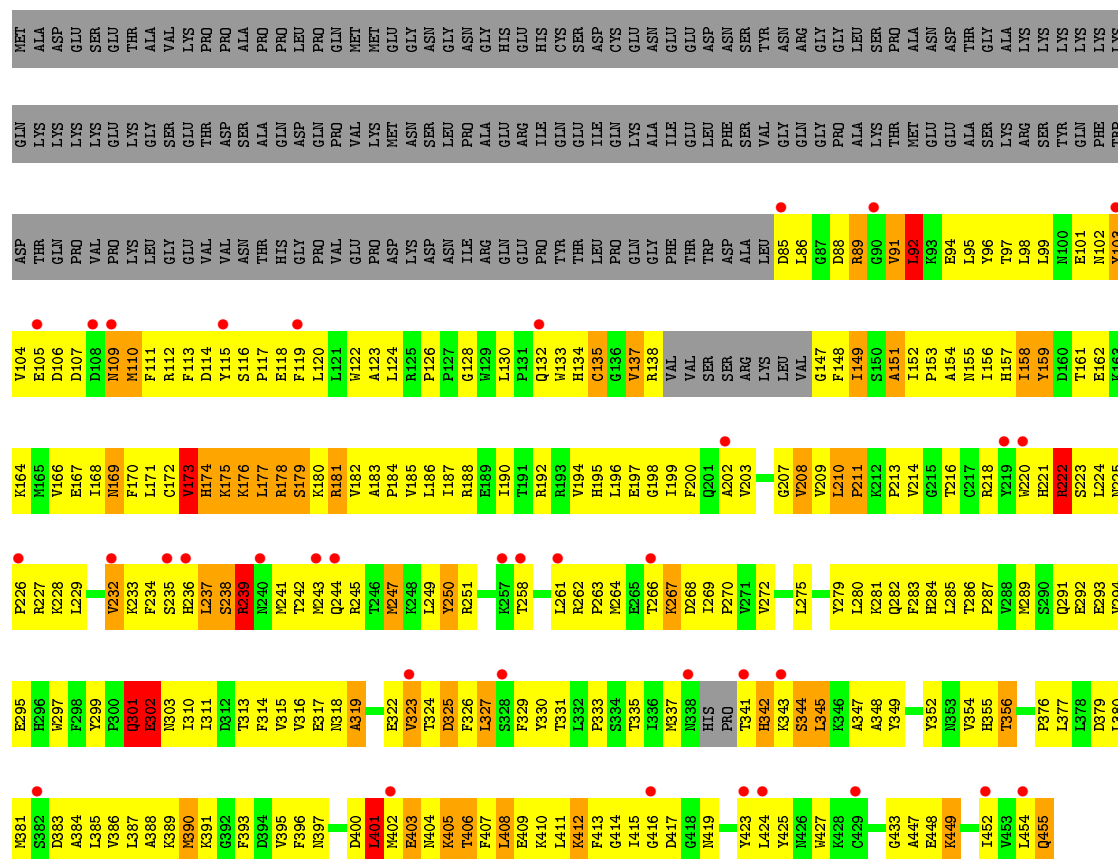
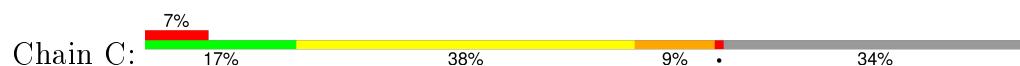


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1





• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 116.42Å 90.36Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 96.5 (29.44-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.391 0.319 , 0.408	Depositor DCC
R_{free} test set	1163 reflections (4.02%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 121.5	EDS
Estimated twinning fraction	0.380 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Outliers	0 of 28898 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.63 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7162e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CO, SO4

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	0.76	3/2718 (0.1%)	1.01	8/3715 (0.2%)
1	B	1.04	4/2712 (0.1%)	1.15	8/3709 (0.2%)
1	C	0.74	3/2605 (0.1%)	0.96	6/3551 (0.2%)
1	D	1.10	4/2592 (0.2%)	1.12	9/3542 (0.3%)
All	All	0.92	14/10627 (0.1%)	1.06	31/14517 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	3
All	All	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	LEU	C-N	-32.53	0.59	1.34
1	D	401	LEU	C-N	-32.37	0.59	1.34
1	B	401	LEU	C-N	-31.27	0.62	1.34
1	B	402	MET	C-N	28.57	1.99	1.34
1	D	302	GLU	C-N	-27.80	0.70	1.34
1	D	402	MET	C-N	27.64	1.97	1.34
1	B	302	GLU	C-N	-24.04	0.78	1.34
1	C	302	GLU	C-N	-22.49	0.82	1.34
1	C	401	LEU	C-N	-19.99	0.88	1.34
1	D	301	GLN	C-N	-15.88	0.97	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	301	GLN	C-N	-15.36	0.98	1.34
1	B	301	GLN	C-N	-14.99	0.99	1.34
1	A	301	GLN	C-N	-12.33	1.05	1.34
1	A	302	GLU	C-N	-8.16	1.15	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLN	O-C-N	-47.53	46.66	122.70
1	B	301	GLN	O-C-N	-44.79	51.04	122.70
1	C	301	GLN	O-C-N	-37.26	63.09	122.70
1	A	301	GLN	O-C-N	-29.43	75.62	122.70
1	B	401	LEU	O-C-N	-24.32	83.78	122.70
1	A	401	LEU	O-C-N	-23.70	84.78	122.70
1	D	402	MET	C-N-CA	-19.24	73.61	121.70
1	B	402	MET	C-N-CA	-19.14	73.85	121.70
1	A	302	GLU	O-C-N	-18.80	92.62	122.70
1	A	302	GLU	C-N-CA	16.06	161.84	121.70
1	C	401	LEU	O-C-N	-15.96	97.17	122.70
1	B	401	LEU	C-N-CA	14.60	158.20	121.70
1	A	302	GLU	CA-C-N	14.20	148.45	117.20
1	B	402	MET	O-C-N	13.52	144.33	122.70
1	C	302	GLU	O-C-N	-13.29	101.43	122.70
1	D	402	MET	O-C-N	13.05	143.58	122.70
1	D	401	LEU	O-C-N	-12.55	102.62	122.70
1	B	401	LEU	CA-C-N	11.55	142.60	117.20
1	C	302	GLU	C-N-CA	11.50	150.46	121.70
1	D	402	MET	CA-C-N	-10.64	93.79	117.20
1	B	402	MET	CA-C-N	-10.06	95.08	117.20
1	A	401	LEU	C-N-CA	9.36	145.10	121.70
1	A	301	GLN	CA-C-N	-8.97	97.46	117.20
1	C	302	GLU	CA-C-N	8.91	136.79	117.20
1	D	401	LEU	C-N-CA	7.64	140.81	121.70
1	A	401	LEU	CA-C-N	7.11	132.84	117.20
1	D	401	LEU	CA-C-N	6.61	131.74	117.20
1	D	302	GLU	C-N-CA	6.06	136.86	121.70
1	C	401	LEU	C-N-CA	5.83	136.28	121.70
1	B	302	GLU	C-N-CA	5.69	135.92	121.70
1	D	301	GLN	CA-C-N	5.37	129.01	117.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	GLN	Mainchain
1	A	401	LEU	Mainchain,Peptide
1	B	301	GLN	Mainchain
1	B	401	LEU	Mainchain,Peptide
1	C	301	GLN	Mainchain
1	C	302	GLU	Mainchain
1	C	401	LEU	Mainchain,Peptide
1	D	301	GLN	Mainchain
1	D	401	LEU	Mainchain,Peptide

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	2646	0	2523	316	0
1	B	2640	0	2514	336	0
1	C	2538	0	2434	338	1
1	D	2523	0	2395	332	1
2	C	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	13	0	0	3	0
4	B	13	0	0	3	0
4	C	10	0	0	4	0
4	D	16	0	0	2	0
All	All	10420	0	9866	1322	1

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 65.

All (1322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLU:CA	1:B:303:ASN:N	1.95	1.29
1:D:302:GLU:CA	1:D:303:ASN:N	1.94	1.29
1:D:302:GLU:C	1:D:303:ASN:CA	2.03	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLU:O	1:C:303:ASN:N	1.61	1.26
1:D:302:GLU:O	1:D:303:ASN:N	1.68	1.25
1:B:302:GLU:C	1:B:303:ASN:CA	2.09	1.21
1:D:402:MET:C	1:D:403:GLU:CA	2.09	1.20
1:B:402:MET:C	1:B:403:GLU:HA	1.63	1.19
1:A:402:MET:C	1:A:403:GLU:CA	2.10	1.19
1:B:402:MET:C	1:B:403:GLU:CA	2.12	1.18
1:D:402:MET:C	1:D:403:GLU:HA	1.63	1.17
1:D:402:MET:C	1:D:403:GLU:N	1.97	1.17
1:B:222:ARG:HH21	1:B:250:TYR:HA	1.10	1.16
1:B:402:MET:C	1:B:403:GLU:N	1.99	1.14
1:A:402:MET:C	1:A:403:GLU:N	2.01	1.14
1:A:222:ARG:HH21	1:A:250:TYR:HA	1.09	1.14
1:B:302:GLU:O	1:B:303:ASN:N	1.80	1.14
1:A:402:MET:C	1:A:403:GLU:HA	1.68	1.13
1:C:181:ARG:HH11	1:C:181:ARG:HA	1.11	1.12
1:D:222:ARG:HH21	1:D:250:TYR:HA	1.12	1.11
1:C:402:MET:C	1:C:403:GLU:HA	1.71	1.11
1:C:402:MET:C	1:C:403:GLU:CA	2.20	1.10
1:A:228:LYS:HZ2	1:A:343:LYS:HE2	1.13	1.09
1:C:302:GLU:C	1:C:303:ASN:CA	2.21	1.07
1:C:302:GLU:CA	1:C:303:ASN:N	2.18	1.05
1:C:222:ARG:HH21	1:C:250:TYR:HA	1.14	1.05
1:B:156:ILE:HG21	1:B:203:VAL:HG21	1.38	1.04
1:C:402:MET:C	1:C:403:GLU:N	2.12	1.02
1:A:222:ARG:HG2	1:A:412:LYS:HB2	1.40	1.02
1:A:156:ILE:HG21	1:A:203:VAL:HG21	1.40	1.00
1:D:222:ARG:HG2	1:D:412:LYS:HB2	1.40	0.99
1:B:222:ARG:HG2	1:B:412:LYS:HB2	1.43	0.98
1:C:222:ARG:HG2	1:C:412:LYS:HB2	1.47	0.97
1:C:156:ILE:HG21	1:C:203:VAL:HG21	1.44	0.96
1:D:156:ILE:HG21	1:D:203:VAL:HG21	1.48	0.95
1:D:412:LYS:H	1:D:412:LYS:HD2	1.32	0.95
1:A:412:LYS:H	1:A:412:LYS:HD2	1.31	0.95
1:D:338:ASN:HD22	1:D:338:ASN:H	0.99	0.95
1:B:412:LYS:H	1:B:412:LYS:HD2	1.32	0.94
1:A:269:ILE:HB	1:A:270:PRO:HD3	1.50	0.92
1:D:325:ASP:HB3	1:D:355:HIS:HA	1.49	0.91
1:D:331:THR:HG22	1:D:333:PRO:HD3	1.52	0.91
1:B:269:ILE:HB	1:B:270:PRO:HD3	1.51	0.91
1:B:331:THR:HG22	1:B:333:PRO:HD3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:H	1:B:343:LYS:HD3	1.35	0.91
1:C:269:ILE:HB	1:C:270:PRO:HD3	1.53	0.90
1:A:325:ASP:HB3	1:A:355:HIS:HA	1.52	0.90
1:C:331:THR:HG22	1:C:333:PRO:HD3	1.51	0.90
1:A:222:ARG:NH2	1:A:250:TYR:HA	1.87	0.90
1:A:331:THR:HG22	1:A:333:PRO:HD3	1.52	0.90
1:D:338:ASN:H	1:D:338:ASN:ND2	1.70	0.90
1:B:325:ASP:HB3	1:B:355:HIS:HA	1.51	0.90
1:A:130:LEU:HB2	1:A:132:GLN:HE22	1.37	0.89
1:D:269:ILE:HD13	1:D:295:GLU:HG3	1.54	0.89
1:C:130:LEU:HB2	1:C:132:GLN:HE22	1.38	0.87
1:C:302:GLU:C	1:C:303:ASN:N	0.82	0.87
1:D:269:ILE:HB	1:D:270:PRO:HD3	1.53	0.87
1:C:412:LYS:H	1:C:412:LYS:HD2	1.37	0.86
1:C:325:ASP:HB3	1:C:355:HIS:HA	1.58	0.86
1:C:275:LEU:HD23	1:C:326:PHE:CE1	2.11	0.85
1:B:222:ARG:NH2	1:B:250:TYR:HA	1.92	0.84
1:B:302:GLU:C	1:B:303:ASN:N	0.78	0.83
1:D:283:PHE:HB2	1:D:286:THR:CG2	2.08	0.83
1:C:275:LEU:HD23	1:C:326:PHE:HE1	1.43	0.83
1:B:388:ALA:O	1:B:393:PHE:HB2	1.79	0.83
1:D:130:LEU:HB2	1:D:132:GLN:HE22	1.41	0.83
1:A:133:TRP:HZ3	1:A:153:PRO:HG3	1.42	0.83
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.13	0.83
1:A:275:LEU:HD23	1:A:326:PHE:CE1	2.15	0.82
1:C:283:PHE:HB2	1:C:286:THR:CG2	2.10	0.82
1:B:229:LEU:HD22	1:B:234:PHE:HD2	1.44	0.82
1:D:133:TRP:HZ3	1:D:153:PRO:HG3	1.42	0.82
1:A:405:LYS:HA	1:A:408:LEU:HD12	1.60	0.82
1:B:130:LEU:HB2	1:B:132:GLN:HE22	1.43	0.82
1:C:130:LEU:CB	1:C:132:GLN:HE22	1.92	0.81
1:A:283:PHE:HB2	1:A:286:THR:CG2	2.10	0.81
1:A:122:TRP:CZ2	1:A:311:ILE:HG21	2.15	0.81
1:D:275:LEU:HD23	1:D:326:PHE:CE1	2.15	0.81
1:C:269:ILE:HD13	1:C:295:GLU:HG3	1.61	0.81
1:C:222:ARG:NH2	1:C:250:TYR:HA	1.95	0.81
1:A:130:LEU:CB	1:A:132:GLN:HE22	1.94	0.81
1:D:404:ASN:O	1:D:408:LEU:HG	1.80	0.81
1:C:343:LYS:HD2	1:C:343:LYS:H	1.44	0.81
1:C:267:LYS:H	1:C:267:LYS:HD3	1.44	0.80
1:D:130:LEU:CB	1:D:132:GLN:HE22	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TRP:HZ3	1:B:153:PRO:HG3	1.46	0.80
1:B:336:ILE:HG12	1:B:337:MET:N	1.96	0.80
1:A:302:GLU:HA	1:A:302:GLU:OE1	1.81	0.80
1:A:404:ASN:O	1:A:408:LEU:HG	1.82	0.80
1:D:221:HIS:O	1:D:413:PHE:HA	1.82	0.80
1:C:315:VAL:HG22	1:C:324:THR:OG1	1.80	0.80
1:D:181:ARG:HD3	1:D:184:PRO:HB2	1.61	0.79
1:A:229:LEU:HD22	1:A:234:PHE:HD2	1.47	0.79
1:B:404:ASN:O	1:B:408:LEU:HG	1.82	0.79
1:B:275:LEU:HD23	1:B:326:PHE:CE1	2.17	0.79
1:B:400:ASP:HB3	1:B:447:ALA:HB1	1.64	0.79
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.17	0.79
1:D:338:ASN:HD22	1:D:338:ASN:N	1.73	0.78
1:C:404:ASN:O	1:C:408:LEU:HG	1.82	0.78
1:A:222:ARG:HH21	1:A:250:TYR:CA	1.94	0.78
1:A:183:ALA:HA	1:A:186:LEU:HB3	1.65	0.78
1:B:218:ARG:HG2	1:B:419:ASN:HB3	1.66	0.78
1:D:102:ASN:HB3	1:D:172:CYS:SG	2.24	0.78
1:B:275:LEU:HD23	1:B:326:PHE:HE1	1.48	0.78
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.19	0.78
1:D:122:TRP:CZ2	1:D:311:ILE:HG21	2.19	0.77
1:A:122:TRP:NE1	1:A:311:ILE:HD13	2.00	0.77
1:B:122:TRP:CZ2	1:B:311:ILE:HG21	2.19	0.77
1:D:275:LEU:HD23	1:D:326:PHE:HE1	1.47	0.77
1:D:181:ARG:C	1:D:184:PRO:HD2	2.05	0.77
1:C:104:VAL:HG13	1:C:111:PHE:O	1.85	0.77
1:D:315:VAL:HG22	1:D:324:THR:OG1	1.83	0.77
1:D:137:VAL:HG12	1:D:137:VAL:O	1.83	0.76
1:C:122:TRP:CZ2	1:C:311:ILE:HG21	2.19	0.76
1:B:283:PHE:HB2	1:B:286:THR:CG2	2.16	0.76
1:A:218:ARG:HG2	1:A:419:ASN:HB3	1.67	0.76
1:C:401:LEU:O	1:C:402:MET:C	2.20	0.76
1:B:269:ILE:HD13	1:B:295:GLU:HG3	1.68	0.76
1:D:388:ALA:O	1:D:393:PHE:HB2	1.86	0.76
1:D:183:ALA:HA	1:D:186:LEU:HB3	1.67	0.76
1:B:412:LYS:N	1:B:412:LYS:HD2	2.01	0.76
1:D:222:ARG:NH2	1:D:250:TYR:HA	1.95	0.76
1:C:229:LEU:HD22	1:C:234:PHE:HD2	1.51	0.75
1:A:388:ALA:O	1:A:393:PHE:HB2	1.85	0.75
1:B:102:ASN:HD21	1:B:174:HIS:HA	1.51	0.75
1:B:267:LYS:H	1:B:267:LYS:HD3	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:LYS:N	1:D:412:LYS:HD2	2.02	0.75
1:A:269:ILE:HD13	1:A:295:GLU:HG3	1.67	0.75
1:B:130:LEU:CB	1:B:132:GLN:HE22	1.98	0.75
1:A:228:LYS:NZ	1:A:343:LYS:HE2	1.98	0.75
1:D:173:VAL:HG23	1:D:174:HIS:H	1.51	0.75
1:D:302:GLU:C	1:D:303:ASN:N	0.70	0.75
1:D:218:ARG:HG2	1:D:419:ASN:HB3	1.68	0.75
1:B:222:ARG:HH21	1:B:250:TYR:CA	1.96	0.75
1:C:388:ALA:O	1:C:393:PHE:HB2	1.86	0.75
1:A:275:LEU:HD23	1:A:326:PHE:HE1	1.50	0.74
1:B:336:ILE:HB	1:B:344:SER:HA	1.68	0.74
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.22	0.74
1:D:135:CYS:HB2	1:D:149:ILE:CG2	2.17	0.74
1:A:400:ASP:HB3	1:A:447:ALA:HB1	1.69	0.74
1:B:183:ALA:HA	1:B:186:LEU:HB3	1.68	0.74
1:A:267:LYS:H	1:A:267:LYS:HD3	1.52	0.74
1:A:232:VAL:HG22	1:A:233:LYS:H	1.53	0.74
1:C:405:LYS:HA	1:C:408:LEU:HD12	1.70	0.74
1:C:412:LYS:N	1:C:412:LYS:HD2	2.02	0.73
1:B:402:MET:O	1:B:403:GLU:HA	1.88	0.73
1:C:104:VAL:HG22	1:C:112:ARG:HA	1.70	0.73
1:A:315:VAL:HG22	1:A:324:THR:OG1	1.89	0.73
1:B:83:ALA:HB3	1:B:136:GLY:O	1.88	0.73
1:D:222:ARG:HH21	1:D:250:TYR:CA	1.98	0.73
1:A:343:LYS:HD3	1:A:343:LYS:H	1.54	0.73
1:B:122:TRP:NE1	1:B:311:ILE:HD13	2.04	0.73
1:A:412:LYS:N	1:A:412:LYS:HD2	2.03	0.73
1:C:222:ARG:HH21	1:C:250:TYR:CA	1.97	0.73
1:D:207:GLY:O	1:D:208:VAL:HG13	1.89	0.73
1:C:232:VAL:HG22	1:C:233:LYS:H	1.53	0.73
1:C:267:LYS:HD3	1:C:267:LYS:N	2.04	0.73
1:B:81:TRP:CZ2	1:B:140:VAL:HG22	2.24	0.73
1:B:221:HIS:O	1:B:413:PHE:HA	1.89	0.72
1:D:232:VAL:HG22	1:D:233:LYS:H	1.54	0.72
1:C:149:ILE:HD13	1:C:171:LEU:HB2	1.70	0.72
1:B:202:ALA:HB3	1:B:425:TYR:CB	2.19	0.72
1:C:221:HIS:O	1:C:413:PHE:HA	1.89	0.72
1:A:267:LYS:N	1:A:267:LYS:HD3	2.05	0.72
1:C:122:TRP:NE1	1:C:311:ILE:HD13	2.05	0.72
1:C:149:ILE:HD12	1:C:169:ASN:O	1.90	0.72
1:C:155:ASN:OD1	1:C:164:LYS:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD22	1:C:99:LEU:H	1.52	0.72
1:B:202:ALA:HB3	1:B:425:TYR:HB2	1.72	0.71
1:B:167:GLU:HB3	1:B:454:LEU:HD11	1.71	0.71
1:B:232:VAL:HG22	1:B:233:LYS:H	1.55	0.71
1:D:181:ARG:CD	1:D:184:PRO:HB2	2.20	0.71
1:B:149:ILE:HD12	1:B:169:ASN:O	1.89	0.71
1:B:405:LYS:HA	1:B:408:LEU:HD12	1.71	0.71
1:B:83:ALA:HB1	4:B:902:HOH:O	1.90	0.71
1:D:343:LYS:HD3	1:D:344:SER:N	2.04	0.71
1:C:105:GLU:CD	1:C:207:GLY:HA3	2.11	0.71
1:B:267:LYS:N	1:B:267:LYS:HD3	2.05	0.71
1:C:137:VAL:HB	1:C:147:GLY:N	2.05	0.71
1:B:158:ILE:HD12	1:B:158:ILE:H	1.54	0.71
1:A:149:ILE:HD12	1:A:169:ASN:O	1.91	0.71
1:D:400:ASP:HB3	1:D:447:ALA:HB1	1.73	0.71
1:D:111:PHE:HZ	1:D:234:PHE:HA	1.52	0.71
1:C:202:ALA:HB3	1:C:425:TYR:CB	2.21	0.71
1:D:402:MET:O	1:D:403:GLU:HA	1.92	0.70
1:C:400:ASP:HB3	1:C:447:ALA:HB1	1.73	0.70
1:B:315:VAL:HG22	1:B:324:THR:OG1	1.90	0.70
1:D:267:LYS:N	1:D:267:LYS:HD3	2.07	0.70
1:C:103:TYR:O	1:C:113:PHE:HB2	1.91	0.70
1:C:202:ALA:HB3	1:C:425:TYR:HB2	1.73	0.70
1:D:202:ALA:HB3	1:D:425:TYR:CB	2.22	0.70
1:C:302:GLU:OE1	1:C:302:GLU:HA	1.91	0.70
1:C:135:CYS:HB2	1:C:149:ILE:HG22	1.72	0.70
1:D:229:LEU:HD22	1:D:234:PHE:HD2	1.57	0.69
1:A:99:LEU:H	1:A:99:LEU:HD22	1.56	0.69
1:A:155:ASN:OD1	1:A:164:LYS:HG3	1.92	0.69
1:D:89:ARG:HA	1:D:89:ARG:CZ	2.22	0.69
1:D:149:ILE:HD13	1:D:171:LEU:HB2	1.72	0.69
1:C:207:GLY:O	1:C:208:VAL:HG13	1.92	0.69
1:A:102:ASN:HD21	1:A:174:HIS:HA	1.58	0.69
1:C:228:LYS:NZ	1:C:343:LYS:HB2	2.07	0.69
1:A:190:ILE:O	1:A:194:VAL:HG23	1.93	0.69
1:B:99:LEU:H	1:B:99:LEU:HD22	1.57	0.69
1:D:155:ASN:OD1	1:D:164:LYS:HG3	1.93	0.68
1:C:89:ARG:CZ	1:C:89:ARG:HA	2.23	0.68
1:A:221:HIS:O	1:A:413:PHE:HA	1.93	0.68
1:D:405:LYS:HA	1:D:408:LEU:HD12	1.74	0.68
1:A:99:LEU:HD12	1:A:103:TYR:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASN:OD1	1:B:164:LYS:HG3	1.93	0.68
1:D:267:LYS:HD3	1:D:267:LYS:H	1.57	0.68
1:A:222:ARG:HD3	1:A:222:ARG:O	1.92	0.68
1:D:133:TRP:CZ3	1:D:153:PRO:HG3	2.28	0.68
1:A:279:TYR:CD2	1:A:354:VAL:HG13	2.29	0.68
1:D:402:MET:CA	1:D:403:GLU:N	2.57	0.68
1:D:107:ASP:HA	1:D:111:PHE:H	1.59	0.68
1:A:228:LYS:HZ2	1:A:343:LYS:CE	1.99	0.68
1:A:126:PRO:HB3	1:A:297:TRP:CZ2	2.30	0.67
1:C:412:LYS:H	1:C:412:LYS:CD	2.07	0.67
1:B:149:ILE:HD13	1:B:171:LEU:HB2	1.75	0.67
1:C:107:ASP:HA	1:C:111:PHE:H	1.59	0.67
1:C:292:GLU:O	1:C:295:GLU:HB3	1.94	0.67
1:D:154:ALA:HB2	1:D:167:GLU:HG3	1.75	0.67
1:D:122:TRP:NE1	1:D:311:ILE:HD13	2.10	0.67
1:A:224:LEU:HD22	1:A:389:LYS:HB2	1.76	0.66
1:D:301:GLN:HB3	1:D:310:ILE:HD12	1.77	0.66
1:D:222:ARG:HD3	1:D:222:ARG:O	1.94	0.66
1:B:233:LYS:HA	1:B:236:HIS:HE1	1.60	0.66
1:B:412:LYS:H	1:B:412:LYS:CD	2.06	0.66
1:A:311:ILE:HG22	1:A:330:TYR:CB	2.25	0.66
1:B:94:GLU:HB2	1:B:145:LEU:CD1	2.25	0.66
1:A:232:VAL:HG22	1:A:233:LYS:N	2.11	0.66
1:D:355:HIS:CG	1:D:377:LEU:HB3	2.30	0.66
1:D:412:LYS:CD	1:D:412:LYS:H	2.06	0.66
1:C:311:ILE:HG22	1:C:330:TYR:CB	2.26	0.66
1:C:94:GLU:O	1:C:97:THR:HB	1.95	0.66
1:B:79:PHE:HE1	1:B:140:VAL:HG23	1.61	0.66
1:B:292:GLU:O	1:B:295:GLU:HB3	1.96	0.66
1:C:343:LYS:HD2	1:C:343:LYS:N	2.11	0.66
1:A:114:ASP:HB2	1:A:335:THR:OG1	1.96	0.66
1:A:233:LYS:HA	1:A:236:HIS:HE1	1.61	0.65
1:D:94:GLU:O	1:D:97:THR:HB	1.96	0.65
1:D:185:VAL:HG13	1:D:188:ARG:HE	1.61	0.65
1:D:224:LEU:HD22	1:D:389:LYS:HB2	1.78	0.65
1:C:218:ARG:HG2	1:C:419:ASN:HB3	1.76	0.65
1:B:156:ILE:CG2	1:B:203:VAL:HG21	2.22	0.65
1:B:268:ASP:O	1:B:272:VAL:HG23	1.96	0.65
1:C:102:ASN:ND2	1:C:174:HIS:O	2.29	0.65
1:A:202:ALA:HB3	1:A:425:TYR:CB	2.27	0.65
1:D:283:PHE:HB2	1:D:286:THR:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD21	1:B:287:PRO:HD2	1.77	0.65
1:D:269:ILE:HD13	1:D:295:GLU:CG	2.24	0.65
1:D:292:GLU:O	1:D:295:GLU:HB3	1.96	0.65
1:A:263:PRO:HG3	1:A:314:PHE:CE2	2.31	0.65
1:C:181:ARG:NH1	1:C:181:ARG:HA	1.97	0.65
1:D:99:LEU:HD22	1:D:99:LEU:H	1.60	0.65
1:A:268:ASP:O	1:A:272:VAL:HG23	1.96	0.65
1:A:123:ALA:HA	1:A:297:TRP:CZ3	2.32	0.65
1:C:355:HIS:NE2	1:C:377:LEU:HD22	2.11	0.65
1:C:222:ARG:O	1:C:222:ARG:HD3	1.95	0.65
1:B:116:SER:HB3	1:B:119:PHE:HB2	1.79	0.65
1:D:233:LYS:HA	1:D:236:HIS:HE1	1.60	0.65
1:D:126:PRO:HB3	1:D:297:TRP:CZ2	2.31	0.65
1:A:172:CYS:SG	1:A:173:VAL:N	2.71	0.65
1:C:279:TYR:CD2	1:C:354:VAL:HG13	2.32	0.65
1:A:433:GLY:H	1:A:449:LYS:HD3	1.62	0.64
1:B:220:TRP:HB3	1:B:413:PHE:HB3	1.80	0.64
1:A:232:VAL:HG13	1:A:233:LYS:N	2.12	0.64
1:D:232:VAL:HG22	1:D:233:LYS:N	2.12	0.64
1:B:133:TRP:CZ3	1:B:153:PRO:HG3	2.32	0.64
1:A:149:ILE:HD13	1:A:171:LEU:HB2	1.78	0.64
1:A:116:SER:HB3	1:A:119:PHE:HB2	1.79	0.64
1:A:133:TRP:CZ3	1:A:153:PRO:HG3	2.29	0.64
1:C:227:ARG:HB2	1:C:247:MET:HE3	1.79	0.64
1:A:192:ARG:O	1:A:196:LEU:HD13	1.97	0.64
1:C:232:VAL:HG22	1:C:233:LYS:N	2.13	0.64
1:A:174:HIS:HB3	1:A:177:LEU:CD1	2.28	0.64
1:C:183:ALA:HA	1:C:186:LEU:HB3	1.80	0.64
1:A:433:GLY:N	1:A:449:LYS:HD3	2.13	0.64
1:D:149:ILE:HD12	1:D:169:ASN:O	1.97	0.64
1:D:202:ALA:HB3	1:D:425:TYR:HB2	1.79	0.64
1:A:202:ALA:HB3	1:A:425:TYR:HB2	1.79	0.64
1:C:185:VAL:HG13	1:C:188:ARG:HE	1.62	0.64
1:A:412:LYS:H	1:A:412:LYS:CD	2.05	0.64
1:B:99:LEU:HD12	1:B:103:TYR:HB2	1.80	0.64
1:D:268:ASP:O	1:D:272:VAL:HG23	1.98	0.64
1:B:232:VAL:HG22	1:B:233:LYS:N	2.13	0.64
1:D:158:ILE:HG23	1:D:285:LEU:HD13	1.80	0.64
1:A:94:GLU:O	1:A:97:THR:HB	1.97	0.64
1:C:263:PRO:HG3	1:C:314:PHE:CE2	2.32	0.64
1:B:402:MET:CA	1:B:403:GLU:N	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:SD	1:A:272:VAL:HG21	2.39	0.63
1:B:126:PRO:HB3	1:B:297:TRP:CZ2	2.33	0.63
1:B:355:HIS:CG	1:B:377:LEU:HB3	2.33	0.63
1:B:455:GLN:N	1:B:455:GLN:HE21	1.97	0.63
1:C:355:HIS:CG	1:C:377:LEU:HB3	2.34	0.63
1:C:225:ASN:OD1	1:C:228:LYS:HB2	1.98	0.63
1:D:135:CYS:HB2	1:D:149:ILE:HG23	1.80	0.63
1:A:266:THR:O	1:A:269:ILE:HG13	1.99	0.63
1:D:99:LEU:HD12	1:D:103:TYR:HB2	1.80	0.63
1:D:315:VAL:HG22	1:D:324:THR:HG1	1.62	0.63
1:A:156:ILE:CG2	1:A:203:VAL:HG21	2.22	0.63
1:A:331:THR:HG1	1:A:393:PHE:HZ	1.47	0.63
1:C:116:SER:HB3	1:C:119:PHE:HB2	1.81	0.63
1:D:152:ILE:HG13	1:D:167:GLU:HB2	1.80	0.63
1:D:183:ALA:O	1:D:187:ILE:HG13	1.99	0.63
1:B:264:MET:SD	1:B:272:VAL:HG21	2.39	0.63
1:C:269:ILE:HD13	1:C:295:GLU:CG	2.29	0.63
1:B:158:ILE:HD13	1:B:159:TYR:H	1.63	0.63
1:C:102:ASN:O	1:C:104:VAL:N	2.32	0.63
1:B:172:CYS:SG	1:B:173:VAL:N	2.72	0.63
1:A:301:GLN:HB3	1:A:310:ILE:HD12	1.80	0.63
1:A:355:HIS:NE2	1:A:377:LEU:HD22	2.14	0.62
1:B:279:TYR:CD2	1:B:354:VAL:HG13	2.34	0.62
1:B:301:GLN:HB3	1:B:310:ILE:HD12	1.81	0.62
1:D:381:MET:HG3	1:D:407:PHE:CE2	2.34	0.62
1:B:102:ASN:O	1:B:104:VAL:N	2.32	0.62
1:D:263:PRO:HG3	1:D:314:PHE:CE2	2.34	0.62
1:C:237:LEU:HD22	1:C:241:MET:O	1.98	0.62
1:B:283:PHE:HE2	1:B:402:MET:CB	2.13	0.62
1:A:154:ALA:HB2	1:A:167:GLU:HG3	1.80	0.62
1:B:123:ALA:HA	1:B:297:TRP:CZ3	2.33	0.62
1:C:381:MET:HG3	1:C:407:PHE:CE2	2.35	0.62
1:A:102:ASN:HB3	1:A:172:CYS:SG	2.39	0.62
1:D:242:THR:C	1:D:244:GLN:H	2.02	0.62
1:A:377:LEU:HD23	1:A:377:LEU:H	1.64	0.62
1:A:280:LEU:HG	1:A:286:THR:HB	1.82	0.62
1:C:283:PHE:HB2	1:C:286:THR:HG23	1.81	0.62
1:D:311:ILE:HG22	1:D:330:TYR:CB	2.29	0.62
1:D:383:ASP:O	1:D:387:LEU:HD23	2.00	0.62
1:C:232:VAL:HG13	1:C:233:LYS:N	2.14	0.62
1:D:264:MET:SD	1:D:272:VAL:HG21	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HG13	1:B:233:LYS:N	2.15	0.62
1:C:233:LYS:HA	1:C:236:HIS:HE1	1.64	0.62
1:B:110:MET:CB	1:B:337:MET:HG3	2.30	0.62
1:C:355:HIS:CE1	1:C:377:LEU:HD22	2.35	0.61
1:B:123:ALA:HA	1:B:297:TRP:HZ3	1.65	0.61
1:D:218:ARG:HG2	1:D:419:ASN:CB	2.29	0.61
1:A:104:VAL:HG12	1:A:106:ASP:H	1.65	0.61
1:C:314:PHE:HB2	1:C:327:LEU:HD11	1.81	0.61
1:A:355:HIS:CG	1:A:377:LEU:HB3	2.35	0.61
1:C:325:ASP:OD1	1:C:356:THR:HG23	2.00	0.61
1:C:228:LYS:HE3	1:C:343:LYS:HD3	1.80	0.61
1:A:158:ILE:HD12	1:A:158:ILE:H	1.66	0.61
1:D:355:HIS:NE2	1:D:377:LEU:HD22	2.15	0.61
1:B:455:GLN:N	1:B:455:GLN:NE2	2.47	0.61
1:D:222:ARG:HD3	1:D:222:ARG:C	2.21	0.61
1:A:183:ALA:O	1:A:187:ILE:HG13	2.00	0.61
1:D:85:ASP:HA	1:D:91:VAL:HG11	1.81	0.61
1:B:315:VAL:HG22	1:B:324:THR:HG1	1.64	0.61
1:B:314:PHE:O	1:B:327:LEU:HD13	2.00	0.61
1:C:154:ALA:HB2	1:C:167:GLU:HG3	1.81	0.61
1:A:242:THR:C	1:A:244:GLN:H	2.03	0.61
1:D:232:VAL:HG13	1:D:233:LYS:N	2.16	0.61
1:D:311:ILE:HG22	1:D:330:TYR:HB3	1.83	0.61
1:C:152:ILE:HG13	1:C:167:GLU:HB2	1.83	0.61
1:B:154:ALA:HB2	1:B:167:GLU:HG3	1.81	0.61
1:A:292:GLU:O	1:A:295:GLU:HB3	2.00	0.61
1:D:116:SER:HB3	1:D:119:PHE:HB2	1.83	0.61
1:B:222:ARG:HD3	1:B:222:ARG:O	2.00	0.60
1:B:343:LYS:N	1:B:343:LYS:HD3	2.13	0.60
1:C:242:THR:C	1:C:244:GLN:H	2.04	0.60
1:C:220:TRP:HB3	1:C:413:PHE:HB3	1.83	0.60
1:C:287:PRO:HD3	1:C:452:ILE:HG12	1.83	0.60
1:C:158:ILE:H	1:C:158:ILE:HD12	1.66	0.60
1:C:268:ASP:O	1:C:272:VAL:HG23	2.01	0.60
1:B:313:THR:HA	1:B:327:LEU:O	2.01	0.60
1:D:291:GLN:O	1:D:295:GLU:HB2	2.01	0.60
1:C:311:ILE:HG22	1:C:330:TYR:HB3	1.82	0.60
1:B:135:CYS:HB2	1:B:149:ILE:CG2	2.31	0.60
1:A:174:HIS:HB3	1:A:177:LEU:HD12	1.84	0.60
1:A:355:HIS:CE1	1:A:377:LEU:HD22	2.36	0.60
1:C:264:MET:SD	1:C:272:VAL:HG21	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:PRO:HB3	1:D:297:TRP:HZ2	1.65	0.60
1:A:92:LEU:O	1:A:95:LEU:HB3	2.02	0.60
1:B:283:PHE:HB3	1:B:449:LYS:O	2.01	0.60
1:A:455:GLN:HE21	1:A:455:GLN:N	1.99	0.60
1:D:128:GLY:O	1:D:153:PRO:HG2	2.02	0.60
1:A:311:ILE:HG22	1:A:330:TYR:HB3	1.83	0.60
1:A:146:VAL:HB	1:A:177:LEU:HD11	1.83	0.60
1:D:158:ILE:HD12	1:D:158:ILE:H	1.67	0.60
1:D:158:ILE:HA	1:D:284:HIS:O	2.02	0.60
1:D:181:ARG:O	1:D:184:PRO:HD2	2.02	0.60
1:C:126:PRO:HG3	1:C:152:ILE:HB	1.84	0.60
1:C:99:LEU:HD12	1:C:103:TYR:HB2	1.83	0.60
1:B:242:THR:C	1:B:244:GLN:H	2.04	0.60
1:C:323:VAL:HG23	4:C:993:HOH:O	2.02	0.60
1:D:315:VAL:HA	1:D:326:PHE:HB3	1.84	0.60
1:A:222:ARG:HD3	1:A:222:ARG:C	2.22	0.60
1:A:123:ALA:HA	1:A:297:TRP:HZ3	1.66	0.60
1:B:218:ARG:HG2	1:B:419:ASN:CB	2.32	0.59
1:D:197:GLU:HG2	1:D:197:GLU:O	2.01	0.59
1:B:266:THR:O	1:B:269:ILE:HG13	2.01	0.59
1:B:336:ILE:HG12	1:B:337:MET:H	1.67	0.59
1:C:301:GLN:HB3	1:C:310:ILE:HD12	1.84	0.59
1:C:402:MET:HA	1:C:448:GLU:HA	1.83	0.59
1:C:313:THR:HA	1:C:327:LEU:O	2.03	0.59
1:B:167:GLU:HA	1:B:203:VAL:O	2.02	0.59
1:A:380:LEU:HD23	1:A:380:LEU:O	2.02	0.59
1:B:207:GLY:O	1:B:208:VAL:HG13	2.02	0.59
1:C:315:VAL:HA	1:C:326:PHE:HB3	1.85	0.59
1:C:390:MET:SD	1:C:391:LYS:HG3	2.42	0.59
1:B:433:GLY:N	1:B:449:LYS:HD3	2.17	0.59
1:A:402:MET:CA	1:A:403:GLU:N	2.66	0.59
1:A:126:PRO:HB3	1:A:297:TRP:HZ2	1.67	0.59
1:A:104:VAL:HG22	1:A:112:ARG:CB	2.32	0.59
1:B:315:VAL:HA	1:B:326:PHE:HB3	1.85	0.59
1:C:409:GLU:C	1:C:411:LEU:H	2.05	0.59
1:C:355:HIS:CE1	1:C:377:LEU:HD13	2.37	0.59
1:B:81:TRP:CE2	1:B:140:VAL:HG22	2.38	0.59
1:A:409:GLU:C	1:A:411:LEU:H	2.06	0.59
1:C:385:LEU:HD11	1:C:411:LEU:HD21	1.84	0.59
1:C:203:VAL:HG13	4:C:997:HOH:O	2.01	0.59
1:C:433:GLY:N	1:C:449:LYS:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TRP:CE2	1:A:311:ILE:HG21	2.38	0.58
1:A:169:ASN:HB2	4:A:907:HOH:O	2.01	0.58
1:D:455:GLN:NE2	1:D:455:GLN:N	2.51	0.58
1:A:269:ILE:HD13	1:A:295:GLU:CG	2.33	0.58
1:D:348:ALA:HB2	1:D:393:PHE:CD1	2.38	0.58
1:D:387:LEU:HA	1:D:390:MET:HG3	1.86	0.58
1:B:192:ARG:O	1:B:196:LEU:HD13	2.03	0.58
1:D:237:LEU:HD22	1:D:241:MET:O	2.03	0.58
1:C:315:VAL:HG22	1:C:324:THR:HG1	1.67	0.58
1:B:343:LYS:HG2	1:B:344:SER:H	1.68	0.58
1:A:218:ARG:HG2	1:A:419:ASN:CB	2.33	0.58
1:C:222:ARG:C	1:C:222:ARG:HD3	2.23	0.58
1:C:135:CYS:HB2	1:C:149:ILE:CG2	2.33	0.58
1:C:190:ILE:O	1:C:194:VAL:HG23	2.02	0.58
1:D:324:THR:OG1	1:D:325:ASP:N	2.36	0.58
1:A:404:ASN:HA	1:A:407:PHE:HE2	1.66	0.58
1:B:327:LEU:H	1:B:327:LEU:HD13	1.69	0.58
1:C:102:ASN:HB3	1:C:172:CYS:SG	2.42	0.58
1:A:291:GLN:O	1:A:295:GLU:HB2	2.03	0.58
1:D:377:LEU:HD23	1:D:377:LEU:H	1.69	0.58
1:B:197:GLU:HG2	1:B:197:GLU:O	2.04	0.58
1:D:301:GLN:CB	1:D:310:ILE:HD12	2.33	0.58
1:A:280:LEU:HD21	1:A:287:PRO:HD2	1.86	0.58
1:B:311:ILE:HG22	1:B:330:TYR:CB	2.33	0.58
1:D:181:ARG:HH11	1:D:185:VAL:CG2	2.17	0.58
1:C:122:TRP:CE2	1:C:311:ILE:HD13	2.38	0.58
1:C:133:TRP:HZ3	1:C:153:PRO:HG3	1.67	0.58
1:B:102:ASN:ND2	1:B:174:HIS:HA	2.17	0.58
1:B:158:ILE:CD1	1:B:159:TYR:H	2.17	0.57
1:A:99:LEU:N	1:A:99:LEU:HD22	2.19	0.57
1:C:380:LEU:HD23	1:C:380:LEU:O	2.04	0.57
1:B:222:ARG:HD3	1:B:222:ARG:C	2.25	0.57
1:C:138:ARG:H	1:C:147:GLY:N	2.01	0.57
1:B:302:GLU:CB	1:B:303:ASN:N	2.67	0.57
1:C:264:MET:HG3	1:C:268:ASP:HB2	1.87	0.57
1:D:126:PRO:HG3	1:D:152:ILE:HB	1.85	0.57
1:C:341:THR:O	1:C:342:HIS:HB2	2.03	0.57
1:D:239:ARG:N	1:D:239:ARG:HE	2.02	0.57
1:B:224:LEU:HD22	1:B:389:LYS:HB2	1.86	0.57
1:D:302:GLU:O	1:D:303:ASN:CA	2.37	0.57
1:A:122:TRP:CE2	1:A:311:ILE:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:MET:HG3	1:B:407:PHE:CE2	2.39	0.57
1:C:149:ILE:HD11	1:C:168:ILE:HG22	1.86	0.57
1:A:207:GLY:O	1:A:208:VAL:HG13	2.04	0.57
1:A:315:VAL:HA	1:A:326:PHE:HB3	1.86	0.57
1:D:409:GLU:C	1:D:411:LEU:H	2.07	0.57
1:B:98:LEU:O	1:B:102:ASN:HB2	2.04	0.57
1:A:301:GLN:CB	1:A:310:ILE:HD12	2.34	0.57
1:C:86:LEU:HA	1:C:92:LEU:HD23	1.87	0.57
1:A:197:GLU:O	1:A:197:GLU:HG2	2.04	0.57
1:C:192:ARG:O	1:C:196:LEU:HD13	2.05	0.57
1:C:194:VAL:CG1	1:C:199:ILE:HB	2.34	0.57
1:A:313:THR:HA	1:A:327:LEU:O	2.04	0.57
1:A:402:MET:O	1:A:403:GLU:HA	2.05	0.57
1:D:148:PHE:CG	1:D:149:ILE:N	2.72	0.57
1:A:104:VAL:HG12	1:A:105:GLU:N	2.20	0.57
1:A:224:LEU:HB3	1:A:389:LYS:HD3	1.86	0.57
1:D:390:MET:SD	1:D:391:LYS:HG3	2.44	0.57
1:A:157:HIS:O	1:A:285:LEU:HA	2.04	0.57
1:A:411:LEU:HD12	1:A:412:LYS:HD2	1.87	0.57
1:D:192:ARG:O	1:D:196:LEU:HD13	2.05	0.57
1:A:455:GLN:NE2	1:A:455:GLN:N	2.52	0.57
1:A:220:TRP:HB3	1:A:413:PHE:HB3	1.87	0.56
1:C:272:VAL:HG13	1:C:326:PHE:CZ	2.40	0.56
1:B:122:TRP:CE2	1:B:311:ILE:HD13	2.40	0.56
1:D:313:THR:HA	1:D:327:LEU:O	2.05	0.56
1:B:433:GLY:H	1:B:449:LYS:HD3	1.71	0.56
1:A:314:PHE:O	1:A:327:LEU:HD13	2.06	0.56
1:D:185:VAL:HA	1:D:188:ARG:HG2	1.87	0.56
1:B:92:LEU:O	1:B:95:LEU:HB3	2.05	0.56
1:A:336:ILE:CG2	1:A:344:SER:HA	2.35	0.56
1:D:280:LEU:HD21	1:D:287:PRO:HD2	1.86	0.56
1:B:377:LEU:H	1:B:377:LEU:HD23	1.71	0.56
1:C:280:LEU:HG	1:C:286:THR:HB	1.87	0.56
1:C:148:PHE:CG	1:C:149:ILE:N	2.74	0.56
1:D:225:ASN:OD1	1:D:228:LYS:HB2	2.05	0.56
1:A:355:HIS:CE1	1:A:377:LEU:HD13	2.41	0.56
1:B:409:GLU:C	1:B:411:LEU:H	2.07	0.56
1:A:167:GLU:HB3	1:A:454:LEU:HD11	1.88	0.56
1:C:383:ASP:O	1:C:387:LEU:HD23	2.04	0.56
1:B:280:LEU:CD2	1:B:286:THR:HB	2.36	0.56
1:D:233:LYS:HA	1:D:236:HIS:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PRO:HB3	1:C:297:TRP:CZ2	2.41	0.56
1:B:157:HIS:O	1:B:285:LEU:HA	2.05	0.56
1:C:227:ARG:HB2	1:C:247:MET:CE	2.34	0.56
1:C:185:VAL:HA	1:C:188:ARG:HG2	1.88	0.56
1:D:355:HIS:CE1	1:D:377:LEU:HD22	2.41	0.56
1:D:283:PHE:HB3	1:D:449:LYS:O	2.05	0.56
1:C:377:LEU:H	1:C:377:LEU:HD23	1.71	0.56
1:B:194:VAL:CG1	1:B:199:ILE:HB	2.36	0.56
1:B:239:ARG:CA	1:B:239:ARG:HE	2.19	0.56
1:A:138:ARG:HA	1:A:144:LYS:O	2.05	0.56
1:D:269:ILE:CD1	1:D:295:GLU:HG3	2.33	0.56
1:C:455:GLN:N	1:C:455:GLN:NE2	2.53	0.56
1:C:348:ALA:HB2	1:C:393:PHE:CD1	2.41	0.56
1:A:158:ILE:HD13	1:A:159:TYR:H	1.71	0.56
1:A:232:VAL:HG13	1:A:233:LYS:H	1.69	0.56
1:B:291:GLN:O	1:B:295:GLU:HB2	2.06	0.56
1:A:381:MET:HG3	1:A:407:PHE:CE2	2.41	0.56
1:B:158:ILE:H	1:B:158:ILE:CD1	2.14	0.56
1:A:102:ASN:ND2	1:A:174:HIS:HA	2.20	0.56
1:B:99:LEU:N	1:B:99:LEU:HD22	2.21	0.56
1:A:158:ILE:CD1	1:A:159:TYR:H	2.18	0.56
1:B:301:GLN:CB	1:B:310:ILE:HD12	2.36	0.56
1:D:264:MET:HG3	1:D:268:ASP:HB2	1.88	0.56
1:C:123:ALA:O	1:C:152:ILE:HG21	2.06	0.56
1:D:258:THR:HG23	1:D:261:LEU:HB2	1.88	0.56
1:B:190:ILE:O	1:B:194:VAL:HG23	2.06	0.56
1:B:185:VAL:HA	1:B:188:ARG:HG2	1.88	0.56
1:B:287:PRO:HG3	1:B:352:TYR:OH	2.05	0.56
1:D:343:LYS:HD3	1:D:344:SER:HB3	1.88	0.56
1:C:197:GLU:O	1:C:197:GLU:HG2	2.06	0.56
1:C:301:GLN:CB	1:C:310:ILE:HD12	2.36	0.55
1:B:311:ILE:HG22	1:B:330:TYR:HB3	1.88	0.55
1:B:145:LEU:O	1:B:145:LEU:HG	2.06	0.55
1:B:383:ASP:O	1:B:387:LEU:HD23	2.07	0.55
1:D:280:LEU:HG	1:D:286:THR:HB	1.88	0.55
1:D:115:TYR:CE2	1:D:170:PHE:HE2	2.22	0.55
1:A:139:VAL:O	1:A:141:SER:N	2.39	0.55
1:A:287:PRO:HD3	1:A:452:ILE:HG12	1.88	0.55
1:B:336:ILE:CG1	1:B:337:MET:N	2.69	0.55
1:C:280:LEU:HD21	1:C:287:PRO:HD2	1.88	0.55
1:D:181:ARG:NE	1:D:184:PRO:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PHE:CG	1:B:149:ILE:N	2.74	0.55
1:C:314:PHE:O	1:C:327:LEU:HD13	2.05	0.55
1:B:89:ARG:HA	1:B:89:ARG:CZ	2.37	0.55
1:B:280:LEU:HD21	1:B:286:THR:HB	1.88	0.55
1:A:327:LEU:HD13	1:A:327:LEU:H	1.72	0.55
1:A:233:LYS:HA	1:A:236:HIS:CE1	2.40	0.55
1:C:324:THR:HG1	1:C:325:ASP:N	2.05	0.55
1:A:302:GLU:CA	1:A:302:GLU:OE1	2.54	0.55
1:A:159:TYR:C	1:A:161:THR:H	2.09	0.55
1:D:227:ARG:HB2	1:D:247:MET:HE3	1.87	0.55
1:B:237:LEU:HD22	1:B:241:MET:O	2.07	0.55
1:D:180:LYS:O	1:D:181:ARG:HB2	2.05	0.55
1:B:94:GLU:O	1:B:97:THR:HB	2.07	0.55
1:D:433:GLY:N	1:D:449:LYS:HD3	2.21	0.55
1:A:411:LEU:O	1:A:413:PHE:N	2.40	0.55
1:A:336:ILE:HG23	1:A:344:SER:HA	1.87	0.55
1:B:173:VAL:HG11	1:B:179:SER:OG	2.07	0.55
1:C:158:ILE:HA	1:C:284:HIS:O	2.06	0.55
1:C:291:GLN:O	1:C:295:GLU:HB2	2.06	0.55
1:A:171:LEU:CD1	1:A:186:LEU:HD12	2.37	0.55
1:A:91:VAL:O	1:A:94:GLU:HG2	2.07	0.55
1:D:280:LEU:HD12	1:D:283:PHE:CD1	2.41	0.54
1:A:315:VAL:HG22	1:A:324:THR:HG1	1.72	0.54
1:A:123:ALA:O	1:A:152:ILE:HG21	2.07	0.54
1:B:228:LYS:HZ2	1:B:343:LYS:HE3	1.72	0.54
1:B:218:ARG:HB3	1:B:218:ARG:NH1	2.23	0.54
1:C:183:ALA:O	1:C:187:ILE:HG13	2.08	0.54
1:C:327:LEU:HD13	1:C:327:LEU:H	1.72	0.54
1:A:375:THR:HG23	4:A:908:HOH:O	2.06	0.54
1:C:179:SER:O	1:C:180:LYS:C	2.44	0.54
1:C:98:LEU:O	1:C:102:ASN:HB2	2.08	0.54
1:D:292:GLU:HA	1:D:295:GLU:OE2	2.08	0.54
1:B:227:ARG:HB2	1:B:247:MET:HE3	1.89	0.54
1:B:355:HIS:NE2	1:B:377:LEU:HD22	2.23	0.54
1:D:411:LEU:O	1:D:413:PHE:N	2.39	0.54
1:C:104:VAL:HG22	1:C:112:ARG:CA	2.36	0.54
1:D:194:VAL:CG1	1:D:199:ILE:HB	2.37	0.54
1:B:91:VAL:O	1:B:94:GLU:HG2	2.08	0.54
1:B:233:LYS:HA	1:B:236:HIS:CE1	2.42	0.54
1:B:159:TYR:C	1:B:161:THR:H	2.10	0.54
1:A:222:ARG:NH1	1:A:412:LYS:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH1	1:A:218:ARG:HB3	2.23	0.54
1:D:224:LEU:HB3	1:D:389:LYS:HD3	1.90	0.54
1:C:159:TYR:C	1:C:161:THR:H	2.10	0.54
1:B:258:THR:HG23	1:B:261:LEU:HB2	1.90	0.54
1:C:239:ARG:HE	1:C:239:ARG:CA	2.21	0.54
1:B:280:LEU:HG	1:B:286:THR:HB	1.88	0.54
1:A:327:LEU:O	1:A:327:LEU:HD22	2.08	0.54
1:C:402:MET:O	1:C:403:GLU:HA	2.07	0.54
1:A:343:LYS:CD	1:A:343:LYS:H	2.21	0.54
1:A:270:PRO:O	1:A:274:GLN:HG2	2.08	0.54
1:B:183:ALA:HB3	1:B:184:PRO:HD3	1.90	0.54
1:D:239:ARG:CA	1:D:239:ARG:HE	2.20	0.54
1:D:279:TYR:CD2	1:D:354:VAL:HG13	2.42	0.54
1:B:232:VAL:HG13	1:B:233:LYS:H	1.71	0.54
1:C:280:LEU:HD12	1:C:283:PHE:CD1	2.42	0.54
1:C:237:LEU:O	1:C:237:LEU:HD12	2.08	0.54
1:A:239:ARG:HE	1:A:239:ARG:HA	1.73	0.54
1:C:130:LEU:HB3	1:C:132:GLN:HE22	1.73	0.54
1:C:115:TYR:CE2	1:C:170:PHE:HE2	2.26	0.54
1:C:224:LEU:HD22	1:C:389:LYS:HB2	1.89	0.54
1:C:400:ASP:O	1:C:401:LEU:HB2	2.08	0.54
1:A:225:ASN:OD1	1:A:228:LYS:HB2	2.08	0.54
1:C:174:HIS:ND1	1:C:175:LYS:N	2.56	0.54
1:A:287:PRO:HG3	1:A:352:TYR:OH	2.08	0.54
1:D:122:TRP:HE1	1:D:311:ILE:HD13	1.72	0.54
1:D:159:TYR:C	1:D:161:THR:H	2.09	0.53
1:B:227:ARG:HB2	1:B:247:MET:CE	2.38	0.53
1:A:89:ARG:CZ	1:A:89:ARG:HA	2.38	0.53
1:A:283:PHE:HB3	1:A:449:LYS:O	2.08	0.53
1:A:122:TRP:HE1	1:A:311:ILE:HD13	1.72	0.53
1:B:183:ALA:O	1:B:187:ILE:HG13	2.09	0.53
1:D:194:VAL:C	1:D:196:LEU:H	2.12	0.53
1:A:194:VAL:CG1	1:A:199:ILE:HB	2.38	0.53
1:A:349:TYR:HD1	1:A:349:TYR:H	1.56	0.53
1:C:156:ILE:CG2	1:C:203:VAL:HG21	2.30	0.53
1:B:81:TRP:HZ2	1:B:140:VAL:HG13	1.74	0.53
1:A:149:ILE:HD11	1:A:168:ILE:HG22	1.91	0.53
1:C:194:VAL:C	1:C:196:LEU:H	2.12	0.53
1:A:139:VAL:HB	1:A:144:LYS:HD2	1.90	0.53
1:D:220:TRP:HB3	1:D:413:PHE:HB3	1.91	0.53
1:B:122:TRP:CE2	1:B:311:ILE:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:C	1:A:196:LEU:H	2.12	0.53
1:C:386:VAL:O	1:C:390:MET:HB3	2.08	0.53
1:B:121:LEU:H	1:B:121:LEU:HD12	1.73	0.53
1:A:126:PRO:HG3	1:A:152:ILE:HB	1.91	0.53
1:C:455:GLN:N	1:C:455:GLN:HE21	2.07	0.53
1:C:218:ARG:NH1	1:C:218:ARG:HB3	2.24	0.53
1:C:232:VAL:HG13	1:C:233:LYS:H	1.72	0.53
1:B:269:ILE:HD13	1:B:295:GLU:CG	2.36	0.53
1:B:270:PRO:O	1:B:274:GLN:HG2	2.09	0.53
1:A:102:ASN:HD21	1:A:174:HIS:CA	2.21	0.53
1:D:102:ASN:O	1:D:104:VAL:N	2.42	0.53
1:B:169:ASN:HB2	4:B:906:HOH:O	2.09	0.53
1:B:239:ARG:HE	1:B:239:ARG:HA	1.72	0.53
1:B:183:ALA:O	1:B:187:ILE:N	2.42	0.53
1:C:327:LEU:HD22	1:C:327:LEU:C	2.29	0.53
1:D:400:ASP:O	1:D:401:LEU:HB2	2.09	0.53
1:D:287:PRO:HD3	1:D:452:ILE:HG12	1.90	0.53
1:D:232:VAL:HG13	1:D:233:LYS:H	1.72	0.53
1:A:283:PHE:HB2	1:A:286:THR:HG23	1.90	0.53
1:D:269:ILE:CB	1:D:270:PRO:HD3	2.34	0.53
1:D:130:LEU:HB3	1:D:132:GLN:HE22	1.72	0.53
1:C:283:PHE:HB3	1:C:449:LYS:O	2.09	0.53
1:C:381:MET:HG3	1:C:407:PHE:CZ	2.44	0.53
1:C:151:ALA:HA	1:C:168:ILE:HA	1.91	0.53
1:B:94:GLU:HB2	1:B:145:LEU:HD13	1.91	0.53
1:C:327:LEU:HD22	1:C:327:LEU:O	2.09	0.53
1:C:194:VAL:HG12	1:C:199:ILE:HB	1.90	0.53
1:A:239:ARG:HE	1:A:239:ARG:CA	2.22	0.53
1:C:104:VAL:HG22	1:C:112:ARG:CB	2.39	0.52
1:B:181:ARG:HA	1:B:181:ARG:NE	2.24	0.52
1:D:227:ARG:HB2	1:D:247:MET:CE	2.39	0.52
1:B:269:ILE:CB	1:B:270:PRO:HD3	2.33	0.52
1:D:86:LEU:HA	1:D:92:LEU:HD23	1.91	0.52
1:C:324:THR:OG1	1:C:325:ASP:N	2.42	0.52
1:A:269:ILE:HB	1:A:270:PRO:CD	2.33	0.52
1:C:128:GLY:O	1:C:153:PRO:HG2	2.09	0.52
1:A:198:GLY:O	1:A:200:PHE:HD1	1.92	0.52
1:C:233:LYS:HA	1:C:236:HIS:CE1	2.43	0.52
1:A:148:PHE:CG	1:A:149:ILE:N	2.78	0.52
1:D:124:LEU:HD21	1:D:170:PHE:CD1	2.44	0.52
1:C:220:TRP:CZ3	1:C:409:GLU:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG12	1:A:199:ILE:HB	1.91	0.52
1:A:279:TYR:CG	1:A:354:VAL:HG13	2.44	0.52
1:C:182:VAL:CG2	1:C:183:ALA:N	2.72	0.52
1:B:194:VAL:C	1:B:196:LEU:H	2.13	0.52
1:D:455:GLN:HE21	1:D:455:GLN:N	2.08	0.52
1:B:355:HIS:CE1	1:B:377:LEU:HD13	2.45	0.52
1:A:280:LEU:HD12	1:A:283:PHE:CD1	2.45	0.52
1:D:404:ASN:HA	1:D:407:PHE:HE2	1.71	0.52
1:C:279:TYR:CG	1:C:354:VAL:HG13	2.45	0.52
1:C:239:ARG:HE	1:C:239:ARG:N	2.07	0.52
1:B:349:TYR:HD1	1:B:349:TYR:H	1.56	0.52
1:D:340:PRO:O	1:D:341:THR:HB	2.09	0.52
1:A:258:THR:HG23	1:A:261:LEU:HB2	1.90	0.52
1:D:221:HIS:ND1	1:D:397:ASN:ND2	2.58	0.52
1:A:185:VAL:HA	1:A:188:ARG:HG2	1.92	0.52
1:A:387:LEU:HA	1:A:390:MET:HG3	1.91	0.52
1:C:301:GLN:O	1:C:303:ASN:N	2.43	0.52
1:B:263:PRO:HG3	1:B:314:PHE:CE2	2.44	0.52
1:B:102:ASN:HD21	1:B:174:HIS:CA	2.22	0.52
1:A:279:TYR:CD1	1:A:354:VAL:HG22	2.44	0.52
1:B:324:THR:OG1	1:B:325:ASP:N	2.42	0.52
1:A:324:THR:OG1	1:A:325:ASP:N	2.42	0.52
1:C:175:LYS:O	1:C:176:LYS:HB2	2.10	0.52
1:C:266:THR:O	1:C:269:ILE:HG13	2.10	0.52
1:B:99:LEU:H	1:B:99:LEU:CD2	2.23	0.52
1:C:218:ARG:HG2	1:C:419:ASN:CB	2.40	0.52
1:A:128:GLY:O	1:A:153:PRO:HG2	2.10	0.52
1:A:182:VAL:HG12	1:A:183:ALA:N	2.24	0.52
1:A:102:ASN:O	1:A:104:VAL:N	2.43	0.52
1:C:97:THR:HG21	4:C:999:HOH:O	2.09	0.52
1:C:258:THR:HG23	1:C:261:LEU:HB2	1.91	0.52
1:B:228:LYS:HE3	1:B:343:LYS:HE3	1.91	0.51
1:B:123:ALA:O	1:B:152:ILE:HG21	2.09	0.51
1:D:325:ASP:OD1	1:D:356:THR:HG23	2.10	0.51
1:B:287:PRO:HD3	1:B:452:ILE:HG12	1.92	0.51
1:B:411:LEU:O	1:B:413:PHE:N	2.42	0.51
1:D:108:ASP:N	1:D:111:PHE:HD2	2.08	0.51
1:B:185:VAL:HG13	1:B:188:ARG:HE	1.74	0.51
1:B:322:GLU:O	1:B:323:VAL:C	2.49	0.51
1:B:228:LYS:CE	1:B:343:LYS:HE3	2.40	0.51
1:D:172:CYS:SG	1:D:173:VAL:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:O	1:D:102:ASN:HB2	2.09	0.51
1:D:183:ALA:O	1:D:187:ILE:N	2.43	0.51
1:C:113:PHE:HB3	1:C:115:TYR:CE1	2.45	0.51
1:A:102:ASN:O	1:A:104:VAL:HG23	2.10	0.51
1:A:390:MET:SD	1:A:391:LYS:HG3	2.50	0.51
1:D:355:HIS:HB3	1:D:380:LEU:HD13	1.92	0.51
1:D:433:GLY:H	1:D:449:LYS:HD3	1.76	0.51
1:A:221:HIS:CE1	1:A:234:PHE:HZ	2.29	0.51
1:C:85:ASP:N	1:C:91:VAL:HG11	2.25	0.51
1:C:158:ILE:CD1	1:C:159:TYR:H	2.23	0.51
1:A:225:ASN:N	1:A:226:PRO:HD3	2.26	0.51
1:C:99:LEU:HD22	1:C:99:LEU:N	2.22	0.51
1:C:264:MET:HG3	1:C:268:ASP:CB	2.41	0.51
1:D:218:ARG:NH1	1:D:218:ARG:HB3	2.26	0.51
1:D:225:ASN:N	1:D:226:PRO:HD3	2.25	0.51
1:B:336:ILE:HD12	1:B:343:LYS:O	2.11	0.51
1:C:407:PHE:HA	1:C:410:LYS:CG	2.41	0.51
1:D:237:LEU:O	1:D:237:LEU:HD12	2.10	0.51
1:B:283:PHE:HB2	1:B:286:THR:HG23	1.91	0.51
1:B:449:LYS:HD2	1:B:449:LYS:N	2.26	0.51
1:C:138:ARG:N	1:C:147:GLY:N	2.59	0.51
1:A:185:VAL:HG13	1:A:188:ARG:HE	1.76	0.51
1:D:233:LYS:HB3	4:D:459:HOH:O	2.10	0.50
1:C:293:GLU:C	1:C:295:GLU:H	2.13	0.50
1:C:452:ILE:HG22	1:C:454:LEU:HB2	1.93	0.50
1:C:122:TRP:CZ2	1:C:297:TRP:HE3	2.28	0.50
1:B:172:CYS:O	1:B:173:VAL:HG13	2.10	0.50
1:D:135:CYS:HB2	1:D:149:ILE:HG22	1.93	0.50
1:A:98:LEU:O	1:A:102:ASN:HB2	2.11	0.50
1:A:272:VAL:HG13	1:A:326:PHE:CZ	2.46	0.50
1:B:381:MET:HG3	1:B:407:PHE:CD2	2.46	0.50
1:D:190:ILE:O	1:D:194:VAL:HG23	2.11	0.50
1:C:224:LEU:HB3	1:C:389:LYS:HD3	1.92	0.50
1:B:228:LYS:HZ2	1:B:343:LYS:CE	2.24	0.50
1:C:381:MET:O	1:C:384:ALA:HB3	2.11	0.50
1:A:139:VAL:HB	1:A:144:LYS:HB2	1.93	0.50
1:B:258:THR:HG23	1:B:258:THR:O	2.12	0.50
1:A:237:LEU:HD22	1:A:241:MET:O	2.10	0.50
1:B:355:HIS:CE1	1:B:377:LEU:HD22	2.47	0.50
1:D:110:MET:O	1:D:337:MET:HB2	2.12	0.50
1:C:266:THR:HA	1:C:299:TYR:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:GLU:C	1:D:295:GLU:H	2.14	0.50
1:C:433:GLY:H	1:C:449:LYS:HD3	1.75	0.50
1:A:183:ALA:O	1:A:187:ILE:N	2.43	0.50
1:A:99:LEU:CD2	1:A:99:LEU:H	2.23	0.50
1:C:94:GLU:HA	4:C:999:HOH:O	2.12	0.50
1:D:258:THR:HG22	1:D:383:ASP:OD1	2.11	0.50
1:A:241:MET:HE1	1:A:246:THR:HA	1.93	0.50
1:C:349:TYR:H	1:C:349:TYR:HD1	1.59	0.50
1:A:221:HIS:O	1:A:412:LYS:O	2.30	0.50
1:B:171:LEU:CD1	1:B:186:LEU:HD12	2.42	0.50
1:D:202:ALA:HB3	1:D:425:TYR:HB3	1.93	0.50
1:C:157:HIS:O	1:C:285:LEU:HA	2.11	0.50
1:B:194:VAL:HG12	1:B:199:ILE:HB	1.92	0.50
1:C:114:ASP:HB2	1:C:335:THR:OG1	2.12	0.50
1:B:120:LEU:HB3	1:B:124:LEU:HD12	1.93	0.50
1:A:316:VAL:HG12	1:A:316:VAL:O	2.11	0.50
1:B:280:LEU:CG	1:B:286:THR:HB	2.42	0.50
1:A:348:ALA:HB2	1:A:393:PHE:CD1	2.47	0.50
1:D:157:HIS:O	1:D:285:LEU:HA	2.12	0.50
1:D:221:HIS:CE1	1:D:234:PHE:HZ	2.30	0.50
1:C:228:LYS:HZ2	1:C:343:LYS:HB2	1.76	0.50
1:A:183:ALA:HA	1:A:186:LEU:CB	2.39	0.50
1:A:416:GLY:O	1:A:417:ASP:C	2.51	0.50
1:D:355:HIS:CE1	1:D:377:LEU:HD13	2.47	0.50
1:D:283:PHE:HE2	1:D:402:MET:CB	2.25	0.50
1:D:270:PRO:HG3	1:D:291:GLN:CD	2.33	0.50
1:C:225:ASN:N	1:C:226:PRO:HD3	2.27	0.50
1:D:122:TRP:CE2	1:D:311:ILE:HG21	2.47	0.50
1:B:202:ALA:HB3	1:B:425:TYR:HB3	1.94	0.50
1:D:347:ALA:HB1	1:D:349:TYR:CE1	2.46	0.50
1:A:264:MET:HG3	1:A:268:ASP:HB2	1.94	0.50
1:D:151:ALA:HA	1:D:168:ILE:HA	1.93	0.50
1:A:322:GLU:O	1:A:323:VAL:C	2.50	0.50
1:B:142:SER:O	1:B:144:LYS:N	2.45	0.50
1:C:106:ASP:C	1:C:111:PHE:HB2	2.32	0.49
1:B:279:TYR:CG	1:B:354:VAL:HG13	2.46	0.49
1:C:347:ALA:HB1	1:C:349:TYR:CE1	2.47	0.49
1:B:355:HIS:HB3	1:B:380:LEU:HD13	1.93	0.49
1:A:183:ALA:N	1:A:184:PRO:CD	2.76	0.49
1:B:380:LEU:O	1:B:380:LEU:HD23	2.11	0.49
1:A:218:ARG:HB3	1:A:218:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ILE:H	1:D:158:ILE:CD1	2.25	0.49
1:C:92:LEU:O	1:C:95:LEU:HB3	2.12	0.49
1:B:225:ASN:OD1	1:B:228:LYS:HB2	2.12	0.49
1:B:158:ILE:HG21	1:B:424:LEU:HD11	1.95	0.49
1:A:85:ASP:O	1:A:86:LEU:CB	2.60	0.49
1:B:454:LEU:C	1:B:455:GLN:HE21	2.15	0.49
1:A:167:GLU:HA	1:A:203:VAL:O	2.13	0.49
1:B:182:VAL:HG12	1:B:183:ALA:N	2.26	0.49
1:D:316:VAL:O	1:D:316:VAL:HG12	2.13	0.49
1:C:316:VAL:HG12	1:C:316:VAL:O	2.11	0.49
1:C:402:MET:CA	1:C:403:GLU:N	2.75	0.49
1:D:407:PHE:HA	1:D:410:LYS:CG	2.43	0.49
1:B:85:ASP:O	1:B:86:LEU:CB	2.60	0.49
1:B:209:VAL:O	1:B:210:LEU:HD12	2.13	0.49
1:B:213:PRO:HA	1:B:423:TYR:CD2	2.48	0.49
1:C:107:ASP:C	1:C:109:ASN:H	2.16	0.49
1:B:174:HIS:CG	1:B:175:LYS:N	2.80	0.49
1:D:149:ILE:HD11	1:D:168:ILE:HG22	1.93	0.49
1:D:158:ILE:CD1	1:D:159:TYR:H	2.25	0.49
1:A:158:ILE:HG23	1:A:285:LEU:HD13	1.95	0.49
1:C:166:VAL:HB	1:C:199:ILE:HG21	1.95	0.49
1:D:279:TYR:CG	1:D:354:VAL:HG13	2.47	0.49
1:B:113:PHE:O	1:B:115:TYR:CD1	2.66	0.49
1:D:355:HIS:HE1	1:D:403:GLU:HG3	1.78	0.49
1:C:397:ASN:HD22	1:C:397:ASN:N	2.09	0.49
1:A:280:LEU:CG	1:A:286:THR:HB	2.42	0.49
1:C:270:PRO:HG3	1:C:291:GLN:CD	2.33	0.49
1:D:181:ARG:HH11	1:D:185:VAL:HG22	1.76	0.49
1:C:158:ILE:HD13	1:C:159:TYR:H	1.78	0.49
1:C:92:LEU:O	1:C:92:LEU:HD13	2.12	0.49
1:B:301:GLN:O	1:B:303:ASN:N	2.46	0.49
1:D:327:LEU:HD13	1:D:327:LEU:H	1.78	0.49
1:B:293:GLU:C	1:B:295:GLU:H	2.16	0.49
1:C:269:ILE:HB	1:C:270:PRO:CD	2.36	0.49
1:D:266:THR:HA	1:D:299:TYR:HE2	1.78	0.49
1:D:381:MET:HG3	1:D:407:PHE:CZ	2.48	0.49
1:B:237:LEU:O	1:B:237:LEU:HD12	2.12	0.49
1:B:209:VAL:HG12	1:B:210:LEU:N	2.28	0.49
1:B:87:GLY:HA3	1:B:125:ARG:NH2	2.28	0.49
1:D:449:LYS:N	1:D:449:LYS:HD2	2.28	0.49
1:B:224:LEU:HB3	1:B:389:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:O	1:D:95:LEU:HB3	2.13	0.49
1:A:383:ASP:O	1:A:387:LEU:HD23	2.12	0.49
1:D:209:VAL:HG12	1:D:210:LEU:N	2.28	0.49
1:A:397:ASN:HD22	1:A:397:ASN:N	2.10	0.48
1:C:223:SER:OG	1:C:229:LEU:HD12	2.13	0.48
1:C:287:PRO:HD3	1:C:452:ILE:HA	1.95	0.48
1:B:122:TRP:HE1	1:B:311:ILE:HD13	1.77	0.48
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.78	0.48
1:C:411:LEU:O	1:C:413:PHE:N	2.44	0.48
1:B:343:LYS:H	1:B:343:LYS:CD	2.06	0.48
1:B:145:LEU:N	1:B:145:LEU:HD23	2.28	0.48
1:C:322:GLU:O	1:C:323:VAL:C	2.52	0.48
1:B:198:GLY:O	1:B:200:PHE:HD1	1.97	0.48
1:A:293:GLU:C	1:A:295:GLU:H	2.15	0.48
1:D:381:MET:HG3	1:D:407:PHE:CD2	2.48	0.48
1:A:121:LEU:HD12	1:A:121:LEU:H	1.78	0.48
1:A:327:LEU:HD22	1:A:327:LEU:C	2.32	0.48
1:D:280:LEU:HD12	1:D:283:PHE:CE1	2.48	0.48
1:A:402:MET:HA	1:A:448:GLU:HA	1.94	0.48
1:C:287:PRO:HG3	1:C:352:TYR:OH	2.14	0.48
1:D:97:THR:HG21	4:D:469:HOH:O	2.12	0.48
1:A:158:ILE:HA	1:A:284:HIS:O	2.14	0.48
1:A:120:LEU:HB3	1:A:124:LEU:HD12	1.96	0.48
1:A:124:LEU:HD21	1:A:170:PHE:CD1	2.48	0.48
1:A:325:ASP:OD1	1:A:356:THR:HG23	2.13	0.48
1:B:269:ILE:HB	1:B:270:PRO:CD	2.34	0.48
1:C:404:ASN:HA	1:C:407:PHE:HE2	1.77	0.48
1:D:302:GLU:O	1:D:303:ASN:HA	2.12	0.48
1:C:178:ARG:O	1:C:181:ARG:CZ	2.62	0.48
1:D:92:LEU:HD13	1:D:92:LEU:O	2.14	0.48
1:D:179:SER:OG	1:D:182:VAL:HB	2.13	0.48
1:D:322:GLU:O	1:D:323:VAL:C	2.51	0.48
1:B:327:LEU:C	1:B:327:LEU:HD22	2.34	0.48
1:B:221:HIS:CE1	1:B:234:PHE:HZ	2.32	0.48
1:A:223:SER:HB2	1:A:226:PRO:HG3	1.96	0.48
1:B:225:ASN:N	1:B:226:PRO:HD3	2.27	0.48
1:C:449:LYS:N	1:C:449:LYS:HD2	2.29	0.48
1:B:95:LEU:O	1:B:98:LEU:HB3	2.13	0.48
1:A:158:ILE:CD1	1:A:158:ILE:H	2.24	0.48
1:B:88:ASP:OD2	1:B:89:ARG:N	2.47	0.48
1:C:221:HIS:O	1:C:412:LYS:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ALA:O	1:D:152:ILE:HG21	2.14	0.48
1:D:137:VAL:CG1	1:D:137:VAL:O	2.56	0.48
1:C:158:ILE:HG23	1:C:285:LEU:HD13	1.96	0.48
1:D:237:LEU:O	1:D:238:SER:O	2.31	0.48
1:B:247:MET:O	1:B:248:LYS:C	2.53	0.48
1:B:327:LEU:O	1:B:327:LEU:HD22	2.14	0.48
1:B:355:HIS:HE1	1:B:403:GLU:HG3	1.79	0.48
1:D:338:ASN:N	1:D:338:ASN:ND2	2.42	0.48
1:A:209:VAL:HG12	1:A:210:LEU:N	2.28	0.48
1:A:397:ASN:N	1:A:397:ASN:ND2	2.62	0.47
1:C:174:HIS:O	1:C:175:LYS:HB2	2.14	0.47
1:A:454:LEU:C	1:A:455:GLN:HE21	2.17	0.47
1:B:404:ASN:HA	1:B:407:PHE:HE2	1.76	0.47
1:A:174:HIS:CG	1:A:175:LYS:N	2.82	0.47
1:D:301:GLN:O	1:D:303:ASN:N	2.47	0.47
1:C:302:GLU:O	1:C:303:ASN:CA	2.49	0.47
1:C:221:HIS:ND1	1:C:397:ASN:ND2	2.62	0.47
1:B:126:PRO:HB3	1:B:297:TRP:HZ2	1.76	0.47
1:D:114:ASP:HB2	1:D:335:THR:OG1	2.13	0.47
1:B:222:ARG:NH1	1:B:412:LYS:HD3	2.29	0.47
1:A:158:ILE:HG21	1:A:424:LEU:HD11	1.97	0.47
1:B:115:TYR:CE2	1:B:170:PHE:HE2	2.32	0.47
1:C:99:LEU:CD2	1:C:99:LEU:H	2.23	0.47
1:B:347:ALA:HB1	1:B:349:TYR:CE1	2.49	0.47
1:A:237:LEU:O	1:A:237:LEU:HD12	2.15	0.47
1:B:87:GLY:HA3	4:B:905:HOH:O	2.13	0.47
1:D:352:TYR:CE2	1:D:453:VAL:HB	2.49	0.47
1:A:324:THR:HG1	1:A:325:ASP:N	2.12	0.47
1:B:348:ALA:HB2	1:B:393:PHE:CD1	2.50	0.47
1:B:411:LEU:HD12	1:B:412:LYS:HD2	1.96	0.47
1:B:266:THR:HA	1:B:299:TYR:HE2	1.79	0.47
1:D:173:VAL:HG23	1:D:174:HIS:N	2.24	0.47
1:C:218:ARG:HB3	1:C:218:ARG:HH11	1.79	0.47
1:D:349:TYR:H	1:D:349:TYR:HD1	1.61	0.47
1:C:385:LEU:CD1	1:C:411:LEU:HD21	2.45	0.47
1:B:149:ILE:HD11	1:B:168:ILE:HG22	1.96	0.47
1:C:183:ALA:HA	1:C:186:LEU:CB	2.45	0.47
1:A:347:ALA:HB1	1:A:349:TYR:CE1	2.49	0.47
1:B:316:VAL:HG12	1:B:316:VAL:O	2.14	0.47
1:D:287:PRO:HG3	1:D:352:TYR:OH	2.15	0.47
1:A:229:LEU:CB	1:A:235:SER:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:PHE:HZ	1:C:234:PHE:HD1	1.63	0.47
1:C:396:PHE:C	1:C:397:ASN:HD22	2.18	0.47
1:C:397:ASN:ND2	1:C:397:ASN:N	2.63	0.47
1:A:122:TRP:HE1	1:A:297:TRP:HA	1.79	0.47
1:C:182:VAL:HG23	1:C:183:ALA:N	2.28	0.47
1:B:166:VAL:HB	1:B:199:ILE:HG21	1.96	0.47
1:C:239:ARG:HE	1:C:239:ARG:HA	1.80	0.47
1:D:347:ALA:HB1	1:D:349:TYR:HE1	1.79	0.47
1:A:227:ARG:HB2	1:A:247:MET:HE3	1.97	0.47
1:B:355:HIS:O	1:B:356:THR:O	2.33	0.47
1:B:221:HIS:O	1:B:412:LYS:O	2.33	0.47
1:C:355:HIS:HE1	1:C:403:GLU:HG3	1.78	0.47
1:D:122:TRP:CZ2	1:D:297:TRP:HE3	2.33	0.47
1:B:280:LEU:HD12	1:B:283:PHE:CD1	2.50	0.47
1:A:209:VAL:O	1:A:210:LEU:HD12	2.15	0.47
1:C:123:ALA:HA	1:C:297:TRP:CZ3	2.50	0.47
1:C:91:VAL:O	1:C:94:GLU:HG2	2.14	0.47
1:B:264:MET:HG3	1:B:268:ASP:HB2	1.97	0.46
1:B:122:TRP:CZ2	1:B:297:TRP:HE3	2.32	0.46
1:B:181:ARG:CZ	1:B:181:ARG:HA	2.45	0.46
1:C:279:TYR:CD1	1:C:354:VAL:HG22	2.49	0.46
1:D:452:ILE:HG22	1:D:454:LEU:HB2	1.97	0.46
1:B:325:ASP:OD1	1:B:356:THR:HG23	2.16	0.46
1:B:452:ILE:HG22	1:B:454:LEU:HB2	1.97	0.46
1:A:280:LEU:HG	1:A:286:THR:CB	2.45	0.46
1:D:91:VAL:O	1:D:94:GLU:HG2	2.16	0.46
1:C:183:ALA:HB3	1:C:184:PRO:HD3	1.97	0.46
1:B:258:THR:HG22	1:B:383:ASP:OD1	2.15	0.46
1:D:213:PRO:HA	1:D:423:TYR:CD2	2.50	0.46
1:A:213:PRO:HA	1:A:423:TYR:CD2	2.51	0.46
1:D:401:LEU:HD23	1:D:402:MET:N	2.30	0.46
1:D:330:TYR:CD1	1:D:330:TYR:O	2.68	0.46
1:A:401:LEU:C	1:A:401:LEU:HD23	2.35	0.46
1:D:105:GLU:OE2	1:D:207:GLY:HA3	2.14	0.46
1:D:177:LEU:O	1:D:178:ARG:C	2.54	0.46
1:B:287:PRO:HD3	1:B:452:ILE:HA	1.98	0.46
1:A:377:LEU:H	1:A:377:LEU:CD2	2.26	0.46
1:A:355:HIS:HB3	1:A:380:LEU:HD13	1.97	0.46
1:B:229:LEU:HB3	1:B:235:SER:HB3	1.97	0.46
1:A:449:LYS:N	1:A:449:LYS:HD2	2.31	0.46
1:C:293:GLU:C	1:C:295:GLU:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:THR:O	1:C:410:LYS:HG2	2.16	0.46
1:C:126:PRO:HB3	1:C:297:TRP:HZ2	1.79	0.46
1:B:179:SER:CB	1:B:182:VAL:HB	2.45	0.46
1:C:279:TYR:O	1:C:282:GLN:HG2	2.15	0.46
1:C:161:THR:HG21	1:C:427:TRP:CH2	2.50	0.46
1:D:385:LEU:HD11	1:D:411:LEU:HD21	1.97	0.46
1:D:269:ILE:HB	1:D:270:PRO:CD	2.36	0.46
1:D:406:THR:O	1:D:410:LYS:HG2	2.16	0.46
1:D:102:ASN:ND2	1:D:174:HIS:O	2.48	0.46
1:A:104:VAL:CG1	1:A:105:GLU:N	2.78	0.46
1:C:416:GLY:O	1:C:417:ASP:C	2.54	0.46
1:B:151:ALA:HA	1:B:168:ILE:HA	1.98	0.46
1:D:314:PHE:O	1:D:327:LEU:HD13	2.15	0.46
1:C:181:ARG:N	1:C:181:ARG:HD2	2.29	0.46
1:D:107:ASP:N	1:D:111:PHE:HB2	2.31	0.46
1:A:287:PRO:HD3	1:A:452:ILE:HA	1.98	0.46
1:A:352:TYR:CE2	1:A:453:VAL:HB	2.51	0.46
1:D:88:ASP:OD2	1:D:89:ARG:N	2.49	0.46
1:C:329:PHE:CD1	1:C:329:PHE:O	2.69	0.46
1:B:327:LEU:N	1:B:327:LEU:HD13	2.30	0.46
1:D:293:GLU:C	1:D:295:GLU:N	2.68	0.46
1:C:228:LYS:HZ1	1:C:343:LYS:HB2	1.80	0.46
1:B:116:SER:HB3	1:B:119:PHE:CB	2.46	0.46
1:D:380:LEU:HD23	1:D:380:LEU:O	2.16	0.46
1:A:289:MET:HB3	1:A:293:GLU:HB2	1.97	0.46
1:D:181:ARG:HD3	1:D:181:ARG:O	2.15	0.46
1:A:400:ASP:O	1:A:401:LEU:HB2	2.16	0.46
1:B:158:ILE:N	1:B:158:ILE:HD12	2.23	0.46
1:D:239:ARG:HA	1:D:239:ARG:HE	1.81	0.46
1:D:314:PHE:HB2	1:D:327:LEU:HD11	1.98	0.46
1:D:355:HIS:O	1:D:356:THR:O	2.34	0.46
1:A:229:LEU:HB3	1:A:235:SER:HB3	1.97	0.46
1:A:145:LEU:HB3	4:A:906:HOH:O	2.16	0.46
1:D:287:PRO:HD3	1:D:452:ILE:HA	1.98	0.45
1:D:111:PHE:CZ	1:D:234:PHE:HA	2.43	0.45
1:A:266:THR:HA	1:A:299:TYR:HE2	1.81	0.45
1:C:292:GLU:HA	1:C:295:GLU:OE2	2.16	0.45
1:D:272:VAL:HG12	1:D:294:VAL:CG1	2.47	0.45
1:D:327:LEU:C	1:D:327:LEU:HD22	2.36	0.45
1:D:454:LEU:C	1:D:455:GLN:HE21	2.19	0.45
1:C:106:ASP:CB	1:C:111:PHE:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:CB	1:C:270:PRO:HD3	2.36	0.45
1:D:292:GLU:HA	1:D:295:GLU:HB3	1.98	0.45
1:D:381:MET:HE2	1:D:381:MET:HB3	1.90	0.45
1:B:128:GLY:O	1:B:153:PRO:HG2	2.16	0.45
1:C:258:THR:HG22	1:C:383:ASP:OD1	2.16	0.45
1:D:416:GLY:O	1:D:417:ASP:C	2.54	0.45
1:B:402:MET:HA	1:B:448:GLU:HA	1.98	0.45
1:C:111:PHE:CZ	1:C:234:PHE:HD1	2.34	0.45
1:D:166:VAL:HB	1:D:199:ILE:HG21	1.98	0.45
1:D:158:ILE:HD13	1:D:159:TYR:H	1.81	0.45
1:A:87:GLY:HA3	1:A:125:ARG:NH2	2.32	0.45
1:C:401:LEU:HD23	1:C:401:LEU:C	2.37	0.45
1:C:269:ILE:CD1	1:C:295:GLU:HG3	2.39	0.45
1:B:158:ILE:HG23	1:B:285:LEU:HD13	1.97	0.45
1:C:213:PRO:HA	1:C:423:TYR:CD2	2.52	0.45
1:A:151:ALA:HA	1:A:168:ILE:HA	1.99	0.45
1:B:347:ALA:HB1	1:B:349:TYR:HE1	1.81	0.45
1:B:221:HIS:ND1	1:B:397:ASN:ND2	2.65	0.45
1:A:385:LEU:HD11	1:A:411:LEU:HD21	1.98	0.45
1:C:221:HIS:CE1	1:C:234:PHE:HZ	2.35	0.45
1:C:454:LEU:C	1:C:455:GLN:HE21	2.19	0.45
1:D:123:ALA:HA	1:D:297:TRP:CZ3	2.52	0.45
1:D:183:ALA:HA	1:D:186:LEU:CB	2.43	0.45
1:B:96:TYR:CD1	1:B:96:TYR:C	2.90	0.45
1:D:264:MET:HG3	1:D:268:ASP:CB	2.45	0.45
1:B:280:LEU:HG	1:B:286:THR:CB	2.46	0.45
1:C:275:LEU:HD23	1:C:326:PHE:CD1	2.52	0.45
1:A:293:GLU:C	1:A:295:GLU:N	2.70	0.45
1:B:276:LEU:HD21	1:B:289:MET:HE3	1.99	0.45
1:D:289:MET:HB3	1:D:293:GLU:HB2	1.98	0.45
1:B:401:LEU:C	1:B:401:LEU:HD23	2.37	0.45
1:B:79:PHE:HE1	1:B:140:VAL:CG2	2.30	0.45
1:D:99:LEU:HD22	1:D:99:LEU:N	2.28	0.45
1:D:247:MET:O	1:D:248:LYS:C	2.55	0.45
1:A:115:TYR:CE2	1:A:170:PHE:HE2	2.35	0.45
1:C:172:CYS:SG	1:C:173:VAL:N	2.90	0.45
1:D:291:GLN:HG2	1:D:291:GLN:O	2.17	0.45
1:B:264:MET:HG3	1:B:268:ASP:CB	2.46	0.44
1:B:355:HIS:HB3	1:B:380:LEU:CD1	2.47	0.44
1:B:327:LEU:HB3	1:B:380:LEU:CD2	2.47	0.44
1:A:269:ILE:HD13	1:A:295:GLU:CD	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD12	1:C:283:PHE:CE1	2.52	0.44
1:C:120:LEU:HB3	1:C:124:LEU:HD12	1.99	0.44
1:C:183:ALA:O	1:C:187:ILE:N	2.43	0.44
1:D:327:LEU:HA	1:D:353:ASN:OD1	2.17	0.44
1:D:377:LEU:CD2	1:D:377:LEU:H	2.30	0.44
1:D:276:LEU:HD21	1:D:289:MET:HE3	1.99	0.44
1:D:194:VAL:HG12	1:D:199:ILE:O	2.17	0.44
1:B:239:ARG:N	1:B:239:ARG:HE	2.15	0.44
1:B:349:TYR:N	1:B:349:TYR:CD1	2.86	0.44
1:A:227:ARG:HB2	1:A:247:MET:CE	2.47	0.44
1:A:180:LYS:O	1:A:184:PRO:HG2	2.16	0.44
1:C:122:TRP:CE2	1:C:311:ILE:HG21	2.50	0.44
1:C:113:PHE:HB3	1:C:115:TYR:HE1	1.82	0.44
1:A:347:ALA:HB1	1:A:349:TYR:HE1	1.82	0.44
1:A:275:LEU:HD23	1:A:326:PHE:CD1	2.52	0.44
1:A:221:HIS:ND1	1:A:397:ASN:ND2	2.65	0.44
1:C:178:ARG:O	1:C:181:ARG:NH1	2.50	0.44
1:B:270:PRO:HG3	1:B:291:GLN:CD	2.38	0.44
1:B:289:MET:HB3	1:B:293:GLU:HB2	1.98	0.44
1:D:269:ILE:HD13	1:D:295:GLU:CD	2.36	0.44
1:B:386:VAL:O	1:B:390:MET:HB3	2.17	0.44
1:A:96:TYR:C	1:A:96:TYR:CD1	2.91	0.44
1:C:337:MET:O	1:C:337:MET:HG3	2.17	0.44
1:D:376:PRO:O	1:D:379:ASP:OD1	2.34	0.44
1:B:397:ASN:ND2	1:B:397:ASN:N	2.65	0.44
1:C:291:GLN:O	1:C:291:GLN:HG2	2.18	0.44
1:B:218:ARG:HB3	1:B:218:ARG:HH11	1.80	0.44
1:B:150:SER:O	1:B:151:ALA:HB2	2.18	0.44
1:D:292:GLU:C	1:D:295:GLU:HB3	2.37	0.44
1:A:407:PHE:HA	1:A:410:LYS:CG	2.48	0.44
1:C:122:TRP:HE1	1:C:311:ILE:HD13	1.81	0.44
1:B:169:ASN:HA	1:B:169:ASN:HD22	1.61	0.44
1:D:214:VAL:HG21	1:D:424:LEU:HG	2.00	0.44
1:B:377:LEU:H	1:B:377:LEU:CD2	2.31	0.44
1:A:220:TRP:CZ3	1:A:409:GLU:HG2	2.52	0.44
1:C:107:ASP:C	1:C:109:ASN:N	2.71	0.44
1:A:129:TRP:O	1:A:130:LEU:HD23	2.18	0.44
1:B:330:TYR:O	1:B:330:TYR:CD1	2.71	0.44
1:B:124:LEU:HD21	1:B:170:PHE:CD1	2.53	0.44
1:D:121:LEU:HD12	1:D:121:LEU:H	1.83	0.44
1:D:402:MET:HA	1:D:448:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:MET:N	1:D:403:GLU:N	2.66	0.44
1:B:314:PHE:HB2	1:B:327:LEU:HD11	1.98	0.44
1:C:107:ASP:OD2	1:C:110:MET:N	2.51	0.44
1:C:269:ILE:HD13	1:C:295:GLU:CD	2.38	0.44
1:B:400:ASP:O	1:B:401:LEU:HB2	2.17	0.44
1:A:171:LEU:HD13	1:A:186:LEU:HD12	1.98	0.44
1:D:99:LEU:H	1:D:99:LEU:CD2	2.29	0.44
1:D:242:THR:C	1:D:244:GLN:N	2.70	0.44
1:A:191:THR:O	1:A:195:HIS:ND1	2.51	0.44
1:D:191:THR:O	1:D:195:HIS:ND1	2.51	0.44
1:D:280:LEU:HG	1:D:286:THR:CB	2.48	0.44
1:A:314:PHE:HB2	1:A:327:LEU:HD11	1.98	0.44
1:D:118:GLU:O	1:D:119:PHE:C	2.55	0.44
1:B:86:LEU:HA	1:B:92:LEU:HD23	1.99	0.44
1:A:237:LEU:O	1:A:238:SER:O	2.36	0.44
1:B:216:THR:HG22	1:B:216:THR:O	2.18	0.44
1:D:245:ARG:HG3	1:D:245:ARG:HH11	1.82	0.44
1:B:416:GLY:O	1:B:417:ASP:C	2.56	0.44
1:A:232:VAL:HG13	1:A:234:PHE:H	1.83	0.43
1:C:280:LEU:HG	1:C:286:THR:CB	2.47	0.43
1:B:139:VAL:C	1:B:141:SER:H	2.21	0.43
1:D:113:PHE:CE2	1:D:332:LEU:HD22	2.53	0.43
1:C:194:VAL:O	1:C:196:LEU:N	2.51	0.43
1:C:381:MET:HG3	1:C:407:PHE:CD2	2.53	0.43
1:B:92:LEU:HD13	1:B:92:LEU:O	2.17	0.43
1:A:336:ILE:HB	1:A:337:MET:H	1.47	0.43
1:A:245:ARG:HG3	1:A:245:ARG:HH11	1.83	0.43
1:C:198:GLY:O	1:C:200:PHE:HD1	2.01	0.43
1:D:220:TRP:CZ3	1:D:409:GLU:HG2	2.53	0.43
1:A:223:SER:CB	1:A:226:PRO:HG3	2.48	0.43
1:B:293:GLU:C	1:B:295:GLU:N	2.71	0.43
1:D:213:PRO:HB3	1:D:423:TYR:CE2	2.54	0.43
1:C:214:VAL:HG21	1:C:424:LEU:HG	2.00	0.43
1:B:272:VAL:HG13	1:B:326:PHE:CZ	2.53	0.43
1:D:270:PRO:HA	1:D:273:HIS:HB3	2.00	0.43
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.83	0.43
1:D:135:CYS:O	1:D:148:PHE:HA	2.18	0.43
1:D:103:TYR:O	1:D:113:PHE:CB	2.66	0.43
1:D:232:VAL:O	1:D:233:LYS:HD3	2.19	0.43
1:D:181:ARG:CZ	1:D:184:PRO:HB2	2.47	0.43
1:B:181:ARG:HH12	1:B:184:PRO:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD21	1:C:170:PHE:CD1	2.54	0.43
1:C:88:ASP:OD2	1:C:89:ARG:N	2.51	0.43
1:C:237:LEU:O	1:C:238:SER:O	2.36	0.43
1:A:242:THR:C	1:A:244:GLN:N	2.70	0.43
1:A:88:ASP:OD2	1:A:89:ARG:N	2.51	0.43
1:D:294:VAL:HG12	1:D:294:VAL:O	2.19	0.43
1:D:337:MET:O	1:D:338:ASN:C	2.57	0.43
1:B:79:PHE:CZ	1:B:139:VAL:HA	2.53	0.43
1:C:242:THR:C	1:C:244:GLN:N	2.71	0.43
1:A:280:LEU:CD2	1:A:286:THR:HB	2.49	0.43
1:B:109:ASN:ND2	1:B:110:MET:H	2.16	0.43
1:B:119:PHE:O	1:B:122:TRP:HB3	2.18	0.43
1:A:355:HIS:HE1	1:A:403:GLU:HG3	1.82	0.43
1:C:411:LEU:HD12	1:C:412:LYS:HD2	2.01	0.43
1:A:452:ILE:HG22	1:A:454:LEU:HB2	2.00	0.43
1:C:343:LYS:H	1:C:343:LYS:CD	2.22	0.43
1:A:118:GLU:OE1	1:A:310:ILE:HD13	2.19	0.43
1:D:179:SER:HA	1:D:182:VAL:CG2	2.48	0.43
1:A:329:PHE:O	1:A:329:PHE:CD1	2.71	0.43
1:B:402:MET:N	1:B:403:GLU:N	2.67	0.43
1:D:397:ASN:N	1:D:397:ASN:HD22	2.15	0.43
1:B:158:ILE:HA	1:B:284:HIS:O	2.19	0.43
1:A:216:THR:HG22	1:A:216:THR:O	2.19	0.43
1:C:294:VAL:HG12	1:C:294:VAL:O	2.19	0.43
1:B:232:VAL:HG13	1:B:234:PHE:H	1.84	0.43
1:B:292:GLU:HA	1:B:295:GLU:OE2	2.19	0.43
1:C:292:GLU:C	1:C:295:GLU:HB3	2.39	0.43
1:C:452:ILE:CG2	1:C:454:LEU:HB2	2.49	0.43
1:B:79:PHE:HZ	1:B:139:VAL:HA	1.83	0.43
1:A:113:PHE:HB3	1:A:115:TYR:CE1	2.54	0.43
1:A:247:MET:O	1:A:248:LYS:C	2.56	0.43
1:B:130:LEU:HB3	1:B:132:GLN:HE22	1.80	0.42
1:A:194:VAL:C	1:A:196:LEU:N	2.73	0.42
1:C:194:VAL:C	1:C:196:LEU:N	2.72	0.42
1:C:262:ARG:NH2	1:C:317:GLU:HB2	2.34	0.42
1:D:96:TYR:CD1	1:D:96:TYR:C	2.93	0.42
1:A:396:PHE:C	1:A:397:ASN:HD22	2.22	0.42
1:A:381:MET:HG3	1:A:407:PHE:CZ	2.55	0.42
1:D:123:ALA:HA	1:D:297:TRP:HZ3	1.84	0.42
1:A:294:VAL:O	1:A:294:VAL:HG12	2.19	0.42
1:C:376:PRO:O	1:C:379:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:LEU:HB3	1:D:380:LEU:CD2	2.49	0.42
1:A:355:HIS:HB3	1:A:380:LEU:CD1	2.49	0.42
1:C:409:GLU:C	1:C:411:LEU:N	2.73	0.42
1:B:332:LEU:N	1:B:333:PRO:HD3	2.35	0.42
1:C:122:TRP:HE1	1:C:297:TRP:HA	1.84	0.42
1:B:267:LYS:H	1:B:267:LYS:CD	2.24	0.42
1:C:116:SER:HB3	1:C:119:PHE:CB	2.49	0.42
1:C:347:ALA:HB1	1:C:349:TYR:HE1	1.81	0.42
1:C:109:ASN:O	1:C:110:MET:CB	2.67	0.42
1:C:155:ASN:HA	1:C:164:LYS:HA	2.01	0.42
1:D:343:LYS:HD3	1:D:343:LYS:C	2.40	0.42
1:B:161:THR:HG21	1:B:427:TRP:CH2	2.54	0.42
1:A:194:VAL:O	1:A:196:LEU:N	2.53	0.42
1:A:86:LEU:HA	1:A:92:LEU:HD23	2.01	0.42
1:B:242:THR:C	1:B:244:GLN:N	2.70	0.42
1:A:258:THR:HG23	1:A:258:THR:O	2.19	0.42
1:B:397:ASN:N	1:B:397:ASN:HD22	2.16	0.42
1:A:232:VAL:CG2	1:A:233:LYS:H	2.22	0.42
1:D:181:ARG:NH1	1:D:185:VAL:HG22	2.33	0.42
1:B:407:PHE:HA	1:B:410:LYS:CG	2.50	0.42
1:C:123:ALA:HA	1:C:297:TRP:HZ3	1.84	0.42
1:A:116:SER:HB3	1:A:119:PHE:CB	2.48	0.42
1:B:232:VAL:O	1:B:233:LYS:HD3	2.20	0.42
1:B:220:TRP:CZ3	1:B:409:GLU:HG2	2.54	0.42
1:D:232:VAL:HG13	1:D:234:PHE:H	1.85	0.42
1:C:229:LEU:CB	1:C:235:SER:HB3	2.50	0.42
1:A:330:TYR:CD1	1:A:330:TYR:O	2.72	0.42
1:C:280:LEU:CG	1:C:286:THR:HB	2.49	0.42
1:D:119:PHE:O	1:D:122:TRP:HB3	2.19	0.42
1:A:174:HIS:HB3	1:A:177:LEU:HG	2.02	0.42
1:A:110:MET:CB	1:A:337:MET:HG3	2.50	0.42
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.85	0.42
1:D:279:TYR:O	1:D:282:GLN:HG2	2.19	0.42
1:C:209:VAL:HG12	1:C:210:LEU:N	2.34	0.42
1:D:272:VAL:HG13	1:D:326:PHE:CZ	2.54	0.42
1:D:280:LEU:CD2	1:D:286:THR:HB	2.50	0.42
1:B:348:ALA:HB3	1:B:395:VAL:O	2.20	0.42
1:A:279:TYR:C	1:A:281:LYS:N	2.73	0.42
1:A:139:VAL:O	1:A:140:VAL:C	2.57	0.42
1:C:245:ARG:HG3	1:C:245:ARG:NH1	2.35	0.42
1:D:324:THR:HG1	1:D:325:ASP:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:CG1	1:B:337:MET:H	2.29	0.42
1:C:287:PRO:HD3	1:C:452:ILE:CG1	2.50	0.42
1:D:174:HIS:CG	1:D:175:LYS:N	2.87	0.42
1:B:139:VAL:HG12	1:B:141:SER:H	1.84	0.42
1:B:237:LEU:O	1:B:238:SER:O	2.36	0.42
1:B:229:LEU:CB	1:B:235:SER:HB3	2.49	0.42
1:D:266:THR:O	1:D:269:ILE:HG13	2.20	0.42
1:B:102:ASN:HB3	1:B:172:CYS:SG	2.59	0.42
1:B:427:TRP:HD1	1:B:429:CYS:HG	1.64	0.42
1:D:329:PHE:HB2	1:D:349:TYR:O	2.19	0.42
1:D:397:ASN:ND2	1:D:397:ASN:N	2.68	0.42
1:B:381:MET:HB3	1:B:381:MET:HE2	1.85	0.42
1:C:169:ASN:HD22	1:C:169:ASN:HA	1.56	0.42
1:A:301:GLN:O	1:A:303:ASN:N	2.45	0.42
1:D:179:SER:CB	1:D:182:VAL:HB	2.50	0.42
1:A:83:ALA:HB3	1:A:136:GLY:CA	2.50	0.42
1:A:264:MET:HG3	1:A:268:ASP:CB	2.50	0.41
1:D:270:PRO:O	1:D:274:GLN:HG2	2.20	0.41
1:A:353:ASN:ND2	1:A:381:MET:SD	2.92	0.41
1:A:381:MET:HG3	1:A:407:PHE:CD2	2.54	0.41
1:D:207:GLY:O	1:D:208:VAL:CG1	2.65	0.41
1:C:327:LEU:N	1:C:327:LEU:HD13	2.34	0.41
1:C:158:ILE:H	1:C:158:ILE:CD1	2.26	0.41
1:D:243:MET:O	1:D:247:MET:HE2	2.20	0.41
1:B:213:PRO:HB3	1:B:423:TYR:CE2	2.55	0.41
1:B:399:LEU:HD12	1:B:399:LEU:N	2.35	0.41
1:D:275:LEU:HD23	1:D:326:PHE:CD1	2.53	0.41
1:C:267:LYS:H	1:C:267:LYS:CD	2.17	0.41
1:D:149:ILE:HA	1:D:170:PHE:O	2.20	0.41
1:A:425:TYR:CD2	1:A:426:ASN:ND2	2.89	0.41
1:C:315:VAL:HG22	1:C:316:VAL:H	1.85	0.41
1:A:311:ILE:HA	1:A:330:TYR:HA	2.02	0.41
1:A:139:VAL:C	1:A:141:SER:N	2.73	0.41
1:D:280:LEU:CG	1:D:286:THR:HB	2.49	0.41
1:B:232:VAL:CG2	1:B:233:LYS:N	2.80	0.41
1:C:292:GLU:HA	1:C:295:GLU:HB3	2.02	0.41
1:B:279:TYR:C	1:B:281:LYS:N	2.72	0.41
1:A:375:THR:HA	1:A:376:PRO:HD3	1.97	0.41
1:C:221:HIS:ND1	1:C:395:VAL:HG21	2.35	0.41
1:A:292:GLU:HA	1:A:295:GLU:OE2	2.20	0.41
1:C:202:ALA:HB3	1:C:425:TYR:HB3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:C	1:A:411:LEU:N	2.74	0.41
1:C:138:ARG:HG3	1:C:138:ARG:O	2.21	0.41
1:D:411:LEU:HD12	1:D:412:LYS:HD2	2.01	0.41
1:C:385:LEU:HD11	1:C:411:LEU:CD2	2.51	0.41
1:C:250:TYR:CE2	1:C:412:LYS:HB3	2.55	0.41
1:B:352:TYR:CE2	1:B:453:VAL:HB	2.56	0.41
1:C:289:MET:HB3	1:C:293:GLU:HB2	2.02	0.41
1:D:116:SER:HA	1:D:117:PRO:HD3	1.96	0.41
1:C:96:TYR:CD1	1:C:96:TYR:C	2.93	0.41
1:D:280:LEU:HG	1:D:286:THR:CG2	2.51	0.41
1:B:327:LEU:HB3	1:B:380:LEU:HD23	2.01	0.41
1:A:221:HIS:ND1	1:A:395:VAL:HG21	2.35	0.41
1:A:130:LEU:HA	1:A:131:PRO:HD3	1.84	0.41
1:A:122:TRP:CZ2	1:A:297:TRP:HE3	2.39	0.41
1:B:174:HIS:HB3	1:B:177:LEU:HG	2.03	0.41
1:D:199:ILE:O	1:D:199:ILE:HG22	2.20	0.41
1:A:400:ASP:CB	1:A:447:ALA:HB1	2.43	0.41
1:C:116:SER:HA	1:C:117:PRO:HD3	1.95	0.41
1:B:198:GLY:HA2	1:B:200:PHE:HE1	1.85	0.41
1:D:452:ILE:CG2	1:D:454:LEU:HB2	2.51	0.41
1:A:327:LEU:HD13	1:A:327:LEU:N	2.34	0.41
1:D:221:HIS:O	1:D:412:LYS:O	2.39	0.41
1:C:401:LEU:O	1:C:403:GLU:N	2.54	0.41
1:C:232:VAL:HG13	1:C:234:PHE:H	1.86	0.41
1:C:330:TYR:O	1:C:330:TYR:CD1	2.73	0.41
1:B:177:LEU:O	1:B:177:LEU:HD12	2.20	0.41
1:C:149:ILE:HA	1:C:170:PHE:O	2.21	0.41
1:B:159:TYR:C	1:B:161:THR:N	2.74	0.41
1:C:183:ALA:N	1:C:184:PRO:CD	2.83	0.41
1:A:118:GLU:HA	1:A:121:LEU:HD13	2.01	0.41
1:D:258:THR:O	1:D:258:THR:HG23	2.20	0.41
1:C:198:GLY:HA2	1:C:200:PHE:HE1	1.86	0.41
1:C:344:SER:O	1:C:345:LEU:HB2	2.20	0.41
1:D:432:MET:CB	1:D:449:LYS:HD3	2.51	0.41
1:B:283:PHE:CE2	1:B:402:MET:CB	3.00	0.41
1:A:327:LEU:HB3	1:A:380:LEU:CD2	2.51	0.41
1:A:402:MET:C	1:A:403:GLU:C	2.75	0.41
1:B:395:VAL:HG13	1:B:397:ASN:HD21	1.85	0.41
1:C:138:ARG:HB3	1:C:177:LEU:HD11	2.02	0.41
1:C:177:LEU:O	1:C:178:ARG:CB	2.68	0.41
1:C:355:HIS:O	1:C:356:THR:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:VAL:CG2	1:C:233:LYS:H	2.23	0.41
1:A:336:ILE:O	1:A:337:MET:HG2	2.21	0.41
1:B:275:LEU:HD21	1:B:324:THR:O	2.20	0.40
1:B:292:GLU:HA	1:B:295:GLU:HB3	2.03	0.40
1:D:299:TYR:HA	1:D:300:PRO:HD3	1.88	0.40
1:A:381:MET:HB3	1:A:381:MET:HE2	1.85	0.40
1:C:280:LEU:CD2	1:C:286:THR:HB	2.51	0.40
1:D:102:ASN:CB	1:D:172:CYS:SG	3.03	0.40
1:D:194:VAL:C	1:D:196:LEU:N	2.73	0.40
1:D:194:VAL:HG12	1:D:199:ILE:HB	2.02	0.40
1:A:159:TYR:C	1:A:161:THR:N	2.74	0.40
1:C:199:ILE:HG22	1:C:199:ILE:O	2.20	0.40
1:B:185:VAL:HA	1:B:188:ARG:CG	2.50	0.40
1:D:198:GLY:O	1:D:200:PHE:HD1	2.05	0.40
1:C:318:ASN:ND2	1:C:319:ALA:H	2.18	0.40
1:B:156:ILE:HG22	1:B:452:ILE:HD11	2.02	0.40
1:A:232:VAL:O	1:A:233:LYS:HD3	2.20	0.40
1:B:291:GLN:HG2	1:B:291:GLN:O	2.21	0.40
1:B:152:ILE:HA	1:B:153:PRO:HD3	1.85	0.40
1:D:181:ARG:HH11	1:D:185:VAL:HG23	1.83	0.40
1:C:152:ILE:HA	1:C:153:PRO:HD3	1.85	0.40
1:D:159:TYR:C	1:D:161:THR:N	2.74	0.40
1:C:211:PRO:O	1:C:213:PRO:HD3	2.21	0.40
1:B:341:THR:HG22	1:B:341:THR:O	2.20	0.40
1:B:294:VAL:O	1:B:294:VAL:HG12	2.21	0.40
1:B:114:ASP:HB2	1:B:335:THR:OG1	2.21	0.40
1:D:315:VAL:HG22	1:D:316:VAL:H	1.86	0.40
1:A:222:ARG:CZ	1:A:412:LYS:HD3	2.52	0.40
1:B:311:ILE:HA	1:B:330:TYR:HA	2.04	0.40
1:B:171:LEU:HD13	1:B:186:LEU:HD12	2.02	0.40
1:D:120:LEU:HB3	1:D:124:LEU:HD12	2.03	0.40
1:A:217:CYS:HB3	1:A:400:ASP:HB2	2.03	0.40
1:A:335:THR:HG22	1:A:336:ILE:N	2.36	0.40
1:D:198:GLY:HA2	1:D:200:PHE:HE1	1.85	0.40
1:C:249:LEU:C	1:C:251:ARG:H	2.24	0.40
1:D:249:LEU:C	1:D:251:ARG:H	2.24	0.40
1:D:222:ARG:NH1	1:D:412:LYS:HD3	2.36	0.40
1:C:316:VAL:N	1:C:324:THR:OG1	2.50	0.40
1:A:181:ARG:NH1	1:A:184:PRO:HG2	2.36	0.40
1:D:135:CYS:SG	1:D:190:ILE:HB	2.61	0.40
1:D:155:ASN:HA	1:D:164:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ILE:O	1:B:199:ILE:HG22	2.21	0.40
1:B:96:TYR:O	1:B:100:ASN:HB2	2.22	0.40
1:B:292:GLU:C	1:B:295:GLU:HB3	2.41	0.40
1:D:311:ILE:HA	1:D:330:TYR:HA	2.04	0.40
1:C:118:GLU:O	1:C:119:PHE:C	2.58	0.40
1:D:349:TYR:N	1:D:349:TYR:CD1	2.90	0.40
1:D:375:THR:HA	1:D:376:PRO:HD3	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:O	1:D:196:LEU:O[1_655]	2.17	0.03

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	338/496 (68%)	224 (66%)	80 (24%)	34 (10%)	1	3
1	B	340/496 (68%)	226 (66%)	73 (22%)	41 (12%)	0	2
1	C	317/496 (64%)	212 (67%)	65 (20%)	40 (13%)	0	1
1	D	322/496 (65%)	213 (66%)	73 (23%)	36 (11%)	0	2
All	All	1317/1984 (66%)	875 (66%)	291 (22%)	151 (12%)	0	2

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	151	ALA
1	A	232	VAL

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Mol	Chain	Res	Type
1	A	238	SER
1	A	239	ARG
1	A	337	MET
1	A	344	SER
1	A	356	THR
1	A	408	LEU
1	A	412	LYS
1	B	86	LEU
1	B	109	ASN
1	B	110	MET
1	B	112	ARG
1	B	113	PHE
1	B	143	ARG
1	B	145	LEU
1	B	151	ALA
1	B	182	VAL
1	B	232	VAL
1	B	238	SER
1	B	239	ARG
1	B	356	THR
1	B	408	LEU
1	B	412	LYS
1	C	109	ASN
1	C	175	LYS
1	C	178	ARG
1	C	179	SER
1	C	232	VAL
1	C	238	SER
1	C	239	ARG
1	C	344	SER
1	C	345	LEU
1	C	356	THR
1	C	412	LYS
1	D	107	ASP
1	D	178	ARG
1	D	181	ARG
1	D	232	VAL
1	D	238	SER
1	D	239	ARG
1	D	338	ASN
1	D	344	SER
1	D	356	THR

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Mol	Chain	Res	Type
1	D	412	LYS
1	A	86	LEU
1	A	103	TYR
1	A	140	VAL
1	A	176	LYS
1	A	195	HIS
1	A	222	ARG
1	A	323	VAL
1	B	103	TYR
1	B	147	GLY
1	B	174	HIS
1	B	175	LYS
1	B	176	LYS
1	B	178	ARG
1	B	181	ARG
1	B	323	VAL
1	B	338	ASN
1	B	344	SER
1	C	103	TYR
1	C	110	MET
1	C	137	VAL
1	C	149	ILE
1	C	151	ALA
1	C	176	LYS
1	C	195	HIS
1	C	401	LEU
1	C	408	LEU
1	D	103	TYR
1	D	109	ASN
1	D	149	ILE
1	D	151	ALA
1	D	175	LYS
1	D	323	VAL
1	D	343	LYS
1	D	408	LEU
1	A	109	ASN
1	A	159	TYR
1	A	174	HIS
1	A	211	PRO
1	A	340	PRO
1	A	401	LEU
1	B	149	ILE

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Mol	Chain	Res	Type
1	B	159	TYR
1	B	195	HIS
1	B	211	PRO
1	B	222	ARG
1	B	401	LEU
1	C	135	CYS
1	C	159	TYR
1	C	173	VAL
1	C	216	THR
1	C	222	ARG
1	C	323	VAL
1	D	92	LEU
1	D	135	CYS
1	D	159	TYR
1	D	195	HIS
1	D	222	ARG
1	D	345	LEU
1	A	149	ILE
1	A	175	LYS
1	A	243	MET
1	A	336	ILE
1	B	80	THR
1	B	243	MET
1	B	454	LEU
1	C	174	HIS
1	C	211	PRO
1	C	250	TYR
1	C	281	LYS
1	C	319	ALA
1	C	414	GLY
1	D	91	VAL
1	D	176	LYS
1	D	211	PRO
1	D	243	MET
1	D	250	TYR
1	D	401	LEU
1	A	143	ARG
1	A	160	ASP
1	A	414	GLY
1	B	142	SER
1	B	414	GLY
1	C	92	LEU

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Mol	Chain	Res	Type
1	C	208	VAL
1	C	243	MET
1	C	342	HIS
1	C	405	LYS
1	C	406	THR
1	D	319	ALA
1	D	414	GLY
1	A	91	VAL
1	A	250	TYR
1	B	319	ALA
1	B	406	THR
1	B	415	ILE
1	C	91	VAL
1	D	208	VAL
1	D	216	THR
1	D	415	ILE
1	A	208	VAL
1	B	91	VAL
1	B	208	VAL
1	D	173	VAL
1	A	415	ILE
1	C	415	ILE

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	272/443 (61%)	247 (91%)	25 (9%)	11	40
1	B	271/443 (61%)	247 (91%)	24 (9%)	12	42
1	C	263/443 (59%)	240 (91%)	23 (9%)	13	43
1	D	259/443 (58%)	237 (92%)	22 (8%)	13	45
All	All	1065/1772 (60%)	971 (91%)	94 (9%)	12	42

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	PHE
1	A	89	ARG
1	A	92	LEU
1	A	96	TYR
1	A	101	GLU
1	A	105	GLU
1	A	134	HIS
1	A	158	ILE
1	A	162	GLU
1	A	169	ASN
1	A	210	LEU
1	A	211	PRO
1	A	222	ARG
1	A	237	LEU
1	A	239	ARG
1	A	247	MET
1	A	267	LYS
1	A	302	GLU
1	A	325	ASP
1	A	327	LEU
1	A	343	LYS
1	A	390	MET
1	A	403	GLU
1	A	449	LYS
1	A	455	GLN
1	B	79	PHE
1	B	89	ARG
1	B	92	LEU
1	B	96	TYR
1	B	101	GLU
1	B	113	PHE
1	B	134	HIS
1	B	158	ILE
1	B	162	GLU
1	B	169	ASN
1	B	210	LEU
1	B	211	PRO
1	B	222	ARG
1	B	237	LEU
1	B	239	ARG
1	B	247	MET
1	B	267	LYS
1	B	325	ASP

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Mol	Chain	Res	Type
1	B	327	LEU
1	B	343	LYS
1	B	390	MET
1	B	403	GLU
1	B	449	LYS
1	B	455	GLN
1	C	89	ARG
1	C	92	LEU
1	C	101	GLU
1	C	134	HIS
1	C	158	ILE
1	C	162	GLU
1	C	169	ASN
1	C	173	VAL
1	C	177	LEU
1	C	181	ARG
1	C	210	LEU
1	C	222	ARG
1	C	237	LEU
1	C	239	ARG
1	C	247	MET
1	C	267	LYS
1	C	302	GLU
1	C	325	ASP
1	C	327	LEU
1	C	390	MET
1	C	403	GLU
1	C	449	LYS
1	C	455	GLN
1	D	89	ARG
1	D	92	LEU
1	D	96	TYR
1	D	101	GLU
1	D	113	PHE
1	D	134	HIS
1	D	158	ILE
1	D	162	GLU
1	D	169	ASN
1	D	211	PRO
1	D	222	ARG
1	D	237	LEU
1	D	239	ARG

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Mol	Chain	Res	Type
1	D	247	MET
1	D	267	LYS
1	D	325	ASP
1	D	327	LEU
1	D	338	ASN
1	D	390	MET
1	D	403	GLU
1	D	449	LYS
1	D	455	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	169	ASN
1	A	236	HIS
1	A	244	GLN
1	A	397	ASN
1	A	426	ASN
1	A	455	GLN
1	B	102	ASN
1	B	132	GLN
1	B	169	ASN
1	B	236	HIS
1	B	244	GLN
1	B	273	HIS
1	B	397	ASN
1	B	426	ASN
1	B	455	GLN
1	C	132	GLN
1	C	169	ASN
1	C	236	HIS
1	C	244	GLN
1	C	273	HIS
1	C	338	ASN
1	C	397	ASN
1	C	426	ASN
1	C	455	GLN
1	D	132	GLN
1	D	169	ASN
1	D	236	HIS
1	D	244	GLN

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Mol	Chain	Res	Type
1	D	338	ASN
1	D	397	ASN
1	D	426	ASN
1	D	455	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	902	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	A	903	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	B	901	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	C	904	-	4,4,4	0.22	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	902	-	-	0/0/0/0	0/0/0/0
3	SO4	A	903	-	-	0/0/0/0	0/0/0/0
3	SO4	B	901	-	-	0/0/0/0	0/0/0/0
3	SO4	C	904	-	-	0/0/0/0	0/0/0/0

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 [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	342/496 (68%)	0.28	21 (6%) 25 9	0, 32, 106, 190	0
1	B	342/496 (68%)	0.26	18 (5%) 30 12	0, 30, 100, 197	0
1	C	325/496 (65%)	0.83	36 (11%) 7 3	3, 47, 131, 191	0
1	D	326/496 (65%)	0.81	39 (11%) 6 2	1, 50, 129, 197	0
All	All	1335/1984 (67%)	0.54	114 (8%) 13 5	0, 39, 122, 197	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	ASP	10.5
1	A	341	THR	8.2
1	C	236	HIS	7.9
1	A	107	ASP	7.8
1	D	340	PRO	7.6
1	D	108	ASP	7.5
1	A	108	ASP	6.2
1	A	142	SER	6.1
1	D	132	GLN	5.7
1	C	323	VAL	5.6
1	C	108	ASP	5.6
1	D	236	HIS	5.5
1	D	172	CYS	5.4
1	D	323	VAL	5.1
1	A	85	ASP	5.0
1	B	341	THR	4.8
1	C	132	GLN	4.7
1	D	240	ASN	4.4
1	A	83	ALA	4.3
1	B	143	ARG	4.3
1	C	429	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	111	PHE	4.1
1	C	338	ASN	4.0
1	C	240	ASN	4.0
1	B	108	ASP	4.0
1	A	143	ARG	4.0
1	C	202	ALA	3.9
1	C	109	ASN	3.8
1	D	85	ASP	3.7
1	D	165	MET	3.7
1	A	106	ASP	3.5
1	C	232	VAL	3.5
1	C	105	GLU	3.4
1	D	313	THR	3.4
1	C	103	TYR	3.3
1	C	261	LEU	3.3
1	D	431	SER	3.2
1	B	138	ARG	3.2
1	D	114	ASP	3.2
1	B	253	PRO	3.2
1	D	427	TRP	3.1
1	D	328	SER	3.1
1	C	452	ILE	3.1
1	C	328	SER	3.1
1	C	257	LYS	3.0
1	C	226	PRO	3.0
1	D	277	THR	3.0
1	B	323	VAL	3.0
1	A	146	VAL	3.0
1	D	430	PRO	2.9
1	D	159	TYR	2.9
1	D	375	THR	2.9
1	C	402	MET	2.9
1	A	338	ASN	2.9
1	D	402	MET	2.8
1	B	137	VAL	2.8
1	C	424	LEU	2.8
1	C	115	TYR	2.8
1	D	113	PHE	2.8
1	B	240	ASN	2.7
1	C	423	TYR	2.7
1	C	243	MET	2.7
1	D	244	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	341	THR	2.7
1	B	106	ASP	2.6
1	C	454	LEU	2.6
1	C	416	GLY	2.6
1	A	111	PHE	2.6
1	D	107	ASP	2.6
1	D	90	GLY	2.5
1	D	432	MET	2.5
1	A	202	ALA	2.5
1	C	119	PHE	2.5
1	D	317	GLU	2.5
1	C	343	LYS	2.5
1	D	429	CYS	2.5
1	D	418	GLY	2.5
1	A	323	VAL	2.5
1	A	115	TYR	2.4
1	C	235	SER	2.4
1	D	409	GLU	2.4
1	D	286	THR	2.4
1	D	320	ASN	2.4
1	D	261	LEU	2.4
1	C	258	THR	2.4
1	C	266	THR	2.4
1	A	261	LEU	2.4
1	C	219	TYR	2.3
1	B	220	TRP	2.3
1	B	427	TRP	2.3
1	A	116	SER	2.3
1	A	120	LEU	2.2
1	B	179	SER	2.2
1	B	107	ASP	2.2
1	A	340	PRO	2.2
1	D	268	ASP	2.2
1	C	382	SER	2.2
1	D	424	LEU	2.2
1	C	220	TRP	2.2
1	D	103	TYR	2.2
1	C	244	GLN	2.2
1	B	83	ALA	2.1
1	A	419	ASN	2.1
1	D	300	PRO	2.1
1	A	240	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	220	TRP	2.1
1	D	266	THR	2.1
1	B	81	TRP	2.1
1	D	341	THR	2.1
1	B	110	MET	2.1
1	D	382	SER	2.0
1	C	90	GLY	2.0
1	B	324	THR	2.0
1	A	103	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	901	5/5	0.77	0.24	0.58	69,72,75,77	0
2	CO	C	990	1/1	0.88	0.29	-0.32	61,61,61,61	0
3	SO4	A	902	5/5	0.81	0.30	-	106,108,111,112	0
3	SO4	A	903	5/5	0.87	0.19	-	80,84,86,86	0
3	SO4	C	904	5/5	0.56	0.32	-	104,105,109,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.