Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:39 PM EDT

PDB ID	:	3NL2 / pdb_00003nl2
Title	:	The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosyhthesis of Eukaryotes
Authors	:	Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.
Deposited on	:	2010-06-21
Resolution	:	3.08 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:

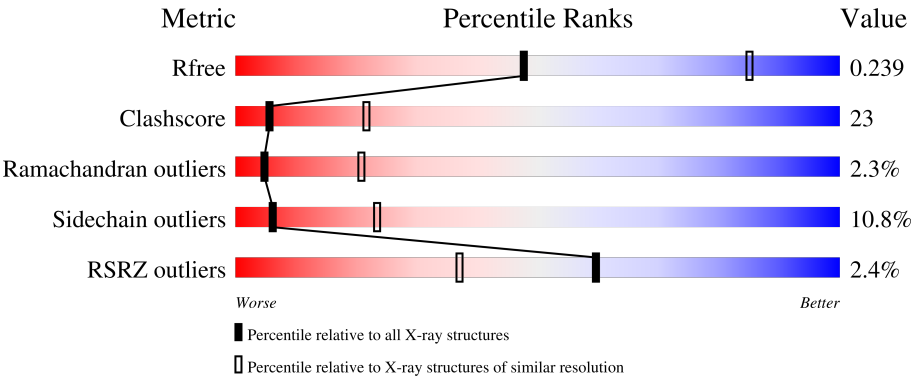
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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 <=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	540	56% 30% 7% • 6%
1	B	540	2% 53% 32% 7% • 6%
1	C	540	3% 55% 30% 7% 8%
1	D	540	3% 55% 30% 8% 7%
1	E	540	56% 30% 7% 7%

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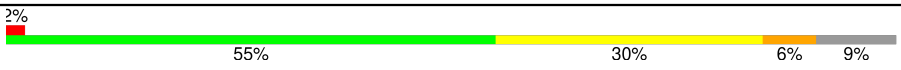
Mol	Chain	Length	Quality of chain
1	F	540	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22460 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 Thiamine biosynthetic bifunctional enzyme.

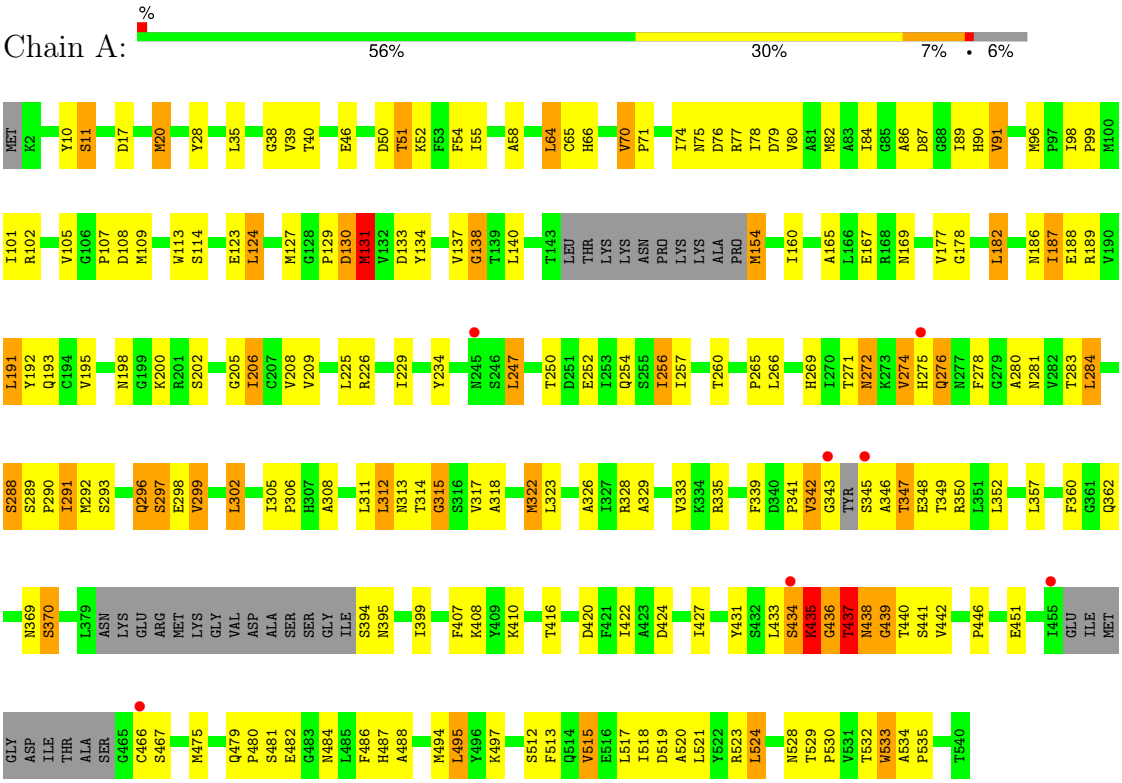
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3764	2376	634	733	21			
1	B	505	Total	C	N	O	S	0	0	0
			3766	2382	635	728	21			
1	C	498	Total	C	N	O	S	0	0	0
			3727	2356	626	724	21			
1	D	501	Total	C	N	O	S	0	0	0
			3739	2360	630	727	22			
1	E	503	Total	C	N	O	S	0	0	0
			3767	2383	634	728	22			
1	F	494	Total	C	N	O	S	0	0	0
			3697	2342	623	711	21			

3 Residue-property plots (i)

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.

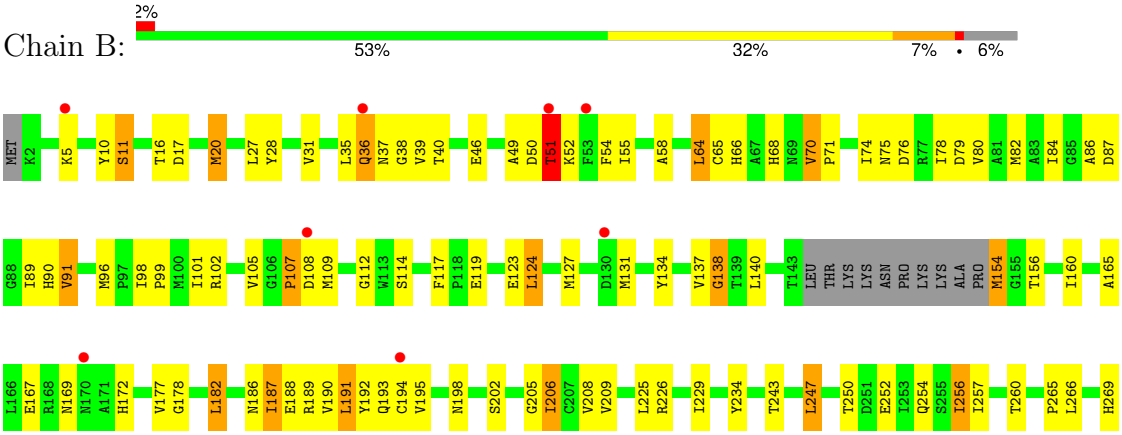
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

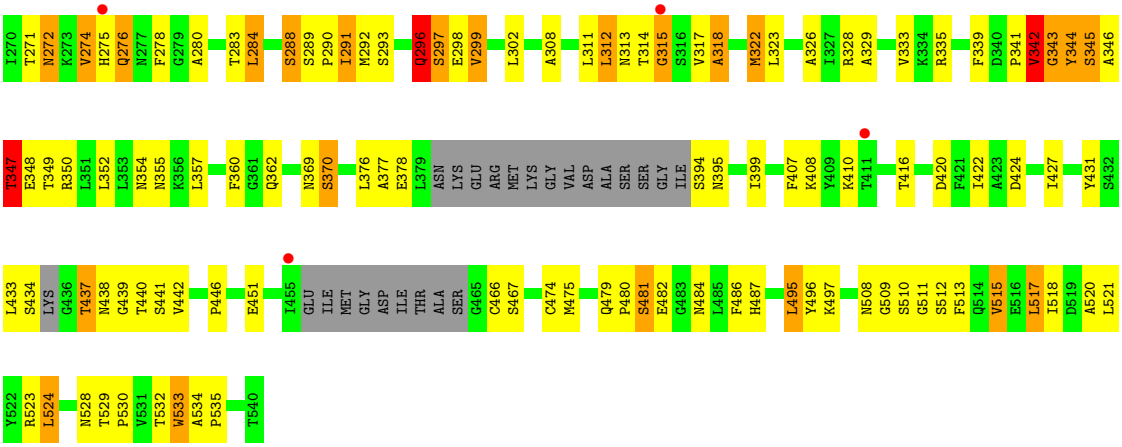
Chain A:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

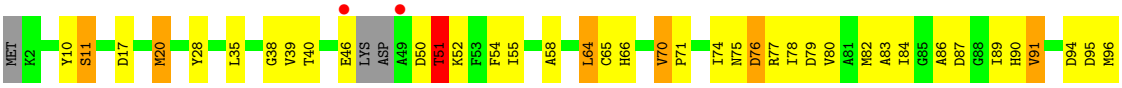
Chain B:

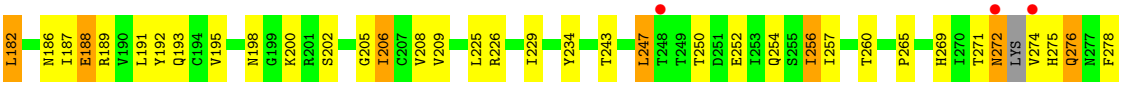


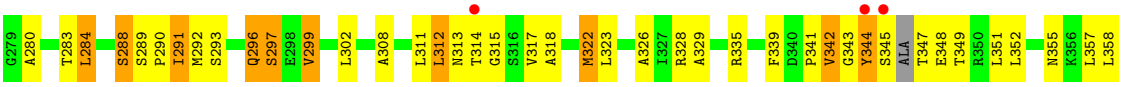


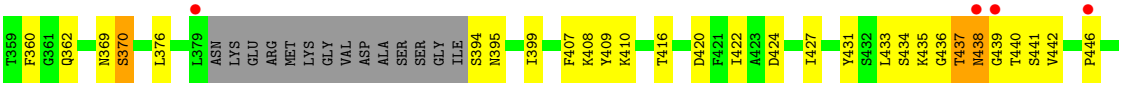
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

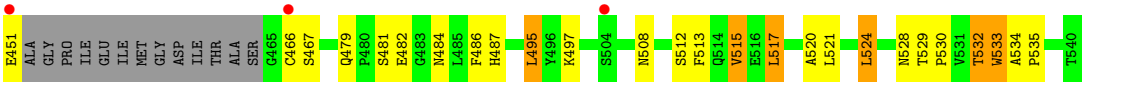
Chain C:

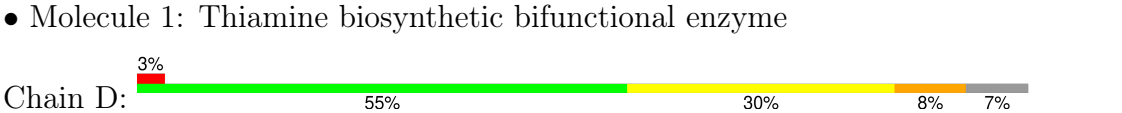


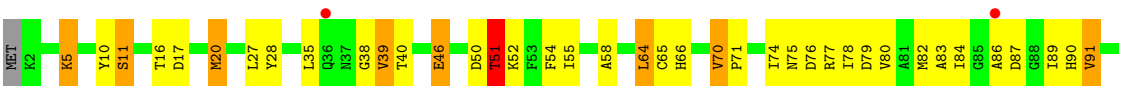


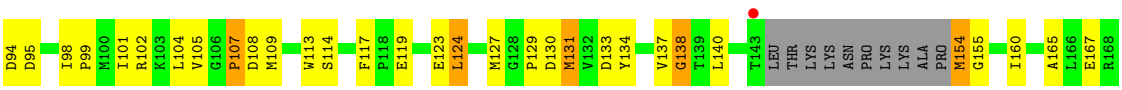






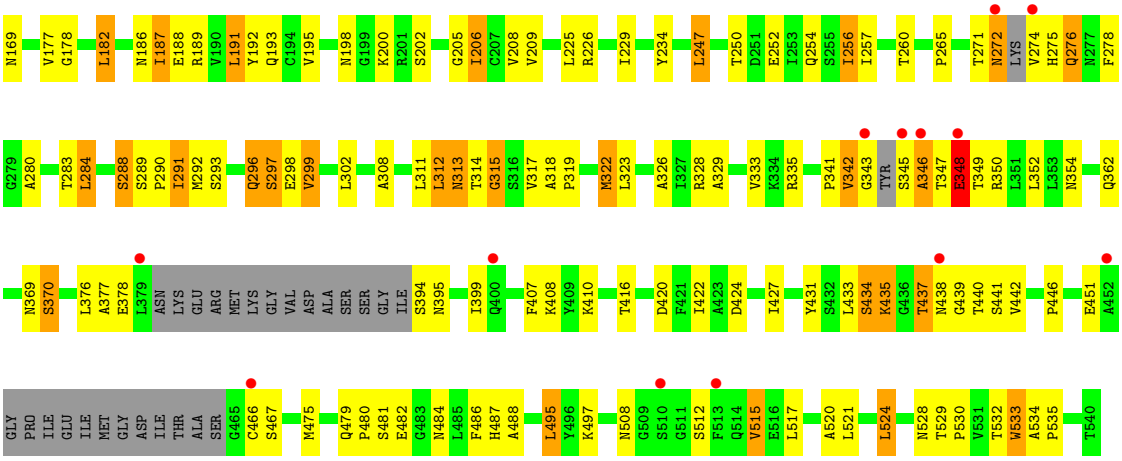






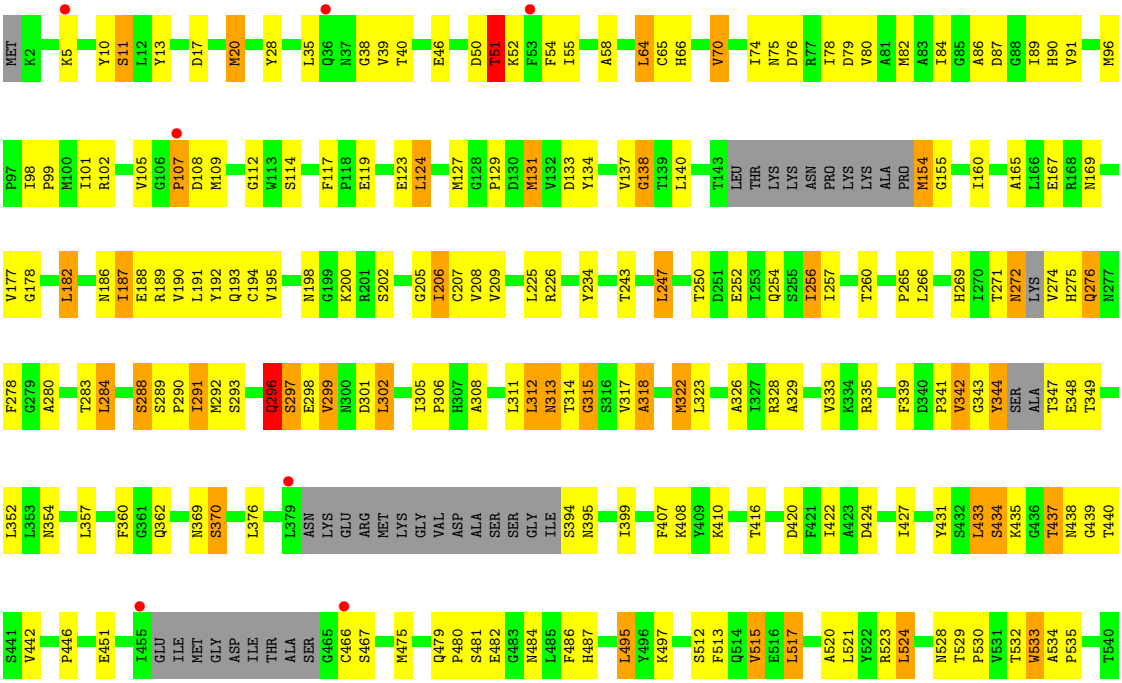
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain D:



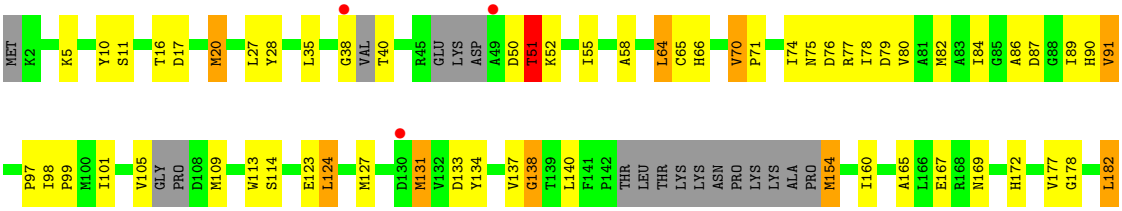
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

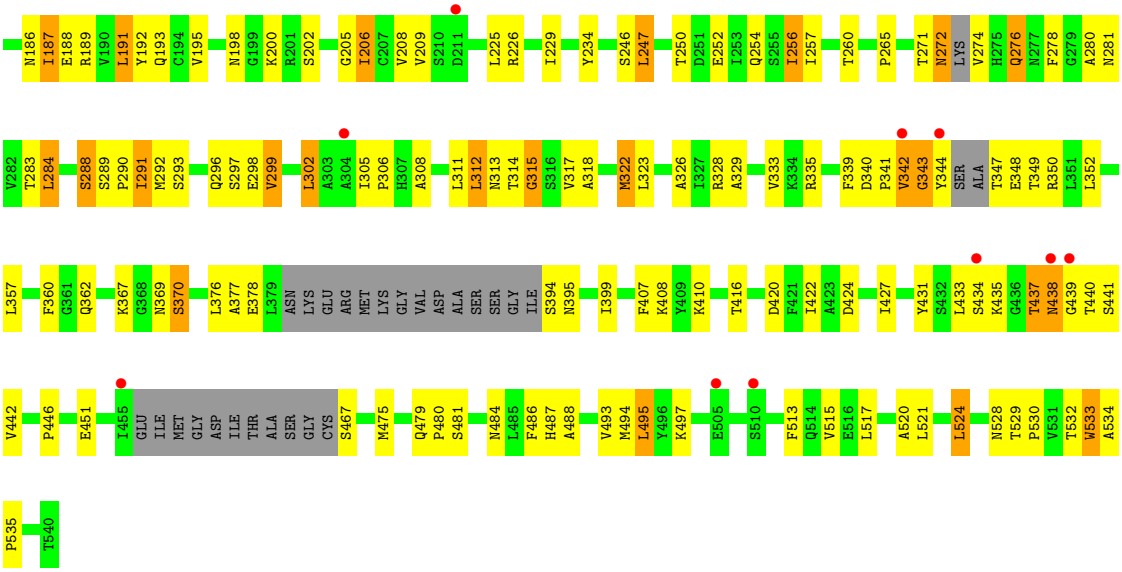
Chain E:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F:




N186 I187 E188 R189 V190 L191 Y192 Q193 C194 V195 N198 G199 K200 R201 S202 G205 I206 C207 V208 V209 S210 D211 L225 R226 I229 Y234 S246 L247 T250 D251 E252 I253 Q254 S255 I256 I257 T260 P265 T271 N272 LYS V274 H275 Q276 N277 F278 G279 A280 N281
V282 T283 L284 S288 S289 P290 I291 M292 S293 Q296 S297 E298 V299 L302 A303 A304 I305 P306 H307 A308 L311 L312 N313 T314 G315 S316 V317 A318 M322 L323 A326 I327 R328 A329 V333 K334 R335 F339 D340 P341 V342 G343 Y344 SER ALA T347 E348 T349 R350 L351 L352
L357 F360 G361 Q362 K367 G368 N369 S370 L376 A377 E378 L379 ASN LYS GLU ARG MET LYS GLY VAL ASP ALA SER SER GLY ILE S394 N395 I399 F407 K408 Y409 K410 T416 D420 F421 I422 A423 D424 I427 Y431 S432 L433 S434 K435 G436 T437 N438 G439 T440 S441
V442 P446 E451 I455 GLU ILE MET GLY ASP ILE THR ALA SER GLY CYS S467 M475 Q479 P480 S481 N484 L485 F486 H487 A488 V493 M494 L495 Y496 K497 E505 S510 F513 Q514 V515 E516 L517 A520 L521 L524 N528 T529 P530 V531 T532 W533 A534
P535 T540

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.47Å 153.01Å 146.75Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	37.00 – 3.08 37.00 – 3.08	Depositor EDS
% Data completeness (in resolution range)	85.8 (37.00-3.08) 93.2 (37.00-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.244 0.213 , 0.239	Depositor DCC
R_{free} test set	3826 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22460	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/3823	0.98	15/5189 (0.3%)
1	B	0.53	0/3826	0.94	10/5192 (0.2%)
1	C	0.54	0/3784	0.90	3/5131 (0.1%)
1	D	0.54	0/3796	0.92	11/5149 (0.2%)
1	E	0.54	0/3826	0.93	9/5188 (0.2%)
1	F	0.53	0/3752	0.90	5/5083 (0.1%)
All	All	0.54	0/22807	0.93	53/30932 (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	4
1	B	0	1
1	D	0	1
1	E	0	2
All	All	0	8

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	434	SER	CB-CA-C	-11.65	92.96	111.48
1	A	437	THR	N-CA-C	10.43	133.02	110.80
1	E	434	SER	N-CA-C	-9.72	102.67	112.97
1	D	345	SER	N-CA-CB	-9.37	94.57	110.50
1	A	434	SER	N-CA-C	7.91	122.28	112.47
1	A	435	LYS	N-CA-C	-7.54	96.14	108.12
1	D	434	SER	CB-CA-C	-7.46	95.58	110.42
1	A	274	VAL	N-CA-C	6.53	116.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	438	ASN	N-CA-C	6.48	120.38	108.58
1	D	435	LYS	N-CA-CB	6.44	121.38	110.49
1	A	435	LYS	N-CA-CB	6.38	121.75	111.04
1	E	433	LEU	O-C-N	-6.21	116.10	123.06
1	D	434	SER	N-CA-C	6.11	123.82	110.80
1	D	533	TRP	N-CA-C	6.07	119.26	110.28
1	E	533	TRP	N-CA-C	5.97	119.12	110.28
1	B	274	VAL	N-CA-C	5.85	116.03	110.53
1	D	346	ALA	N-CA-C	-5.85	105.40	113.18
1	E	296	GLN	N-CA-C	5.81	117.61	111.28
1	B	533	TRP	N-CA-C	5.70	118.72	110.28
1	B	345	SER	N-CA-C	5.67	122.87	110.80
1	B	315	GLY	N-CA-C	-5.63	107.47	115.30
1	C	533	TRP	N-CA-C	5.63	118.61	110.28
1	B	117	PHE	CA-C-N	5.49	125.15	119.05
1	B	117	PHE	C-N-CA	5.49	125.15	119.05
1	A	533	TRP	N-CA-C	5.49	118.41	110.28
1	C	532	THR	N-CA-C	5.48	117.25	111.28
1	F	434	SER	CB-CA-C	-5.45	99.58	110.42
1	F	533	TRP	N-CA-C	5.40	118.28	110.28
1	D	117	PHE	CA-C-N	5.39	125.03	119.05
1	D	117	PHE	C-N-CA	5.39	125.03	119.05
1	E	117	PHE	CA-C-N	5.37	124.83	119.24
1	E	117	PHE	C-N-CA	5.37	124.83	119.24
1	E	315	GLY	N-CA-C	-5.34	107.87	115.30
1	A	436	GLY	CA-C-N	5.32	131.70	121.54
1	A	436	GLY	C-N-CA	5.32	131.70	121.54
1	D	315	GLY	N-CA-C	-5.32	107.91	115.30
1	B	296	GLN	N-CA-C	5.25	117.00	111.28
1	D	296	GLN	N-CA-C	5.23	116.67	111.07
1	F	434	SER	N-CA-C	5.23	121.93	110.80
1	A	315	GLY	N-CA-C	-5.22	108.05	115.30
1	E	318	ALA	CA-C-N	5.20	125.74	120.38
1	E	318	ALA	C-N-CA	5.20	125.74	120.38
1	C	434	SER	CB-CA-C	-5.17	100.12	110.42
1	F	532	THR	N-CA-C	5.15	116.90	111.28
1	A	438	ASN	CA-C-N	5.15	131.50	121.41
1	A	438	ASN	C-N-CA	5.15	131.50	121.41
1	A	532	THR	N-CA-C	5.10	116.84	111.28
1	B	318	ALA	CA-C-N	5.09	125.62	120.38
1	B	318	ALA	C-N-CA	5.09	125.62	120.38
1	A	435	LYS	CA-C-O	5.07	122.64	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	315	GLY	N-CA-C	-5.07	108.26	115.30
1	D	532	THR	N-CA-C	5.04	116.77	111.28
1	B	49	ALA	N-CA-C	5.02	114.92	108.34

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	PRO	Peptide
1	A	435	LYS	Peptide
1	A	436	GLY	Peptide
1	A	438	ASN	Peptide
1	B	347	THR	Peptide
1	D	46	GLU	Peptide
1	E	343	GLY	Peptide
1	E	433	LEU	Peptide

5.2 Too-close contacts (i)

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	3764	0	3745	178	0
1	B	3766	0	3751	201	0
1	C	3727	0	3706	193	0
1	D	3739	0	3715	204	0
1	E	3767	0	3765	172	0
1	F	3697	0	3690	163	0
All	All	22460	0	22372	1052	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 23.

All (1052) 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:F:339:PHE:CE2	1:F:341:PRO:HG3	1.66	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:CE2	1:A:341:PRO:HG3	1.76	1.19
1:C:265:PRO:HD2	1:C:288:SER:HB3	1.39	1.04
1:B:345:SER:HA	1:B:347:THR:N	1.73	1.03
1:D:274:VAL:HG13	1:E:292:MET:HG3	1.42	1.01
1:F:265:PRO:HD2	1:F:288:SER:HB3	1.40	1.00
1:A:346:ALA:O	1:A:347:THR:HG23	1.60	1.00
1:D:265:PRO:HD2	1:D:288:SER:HB3	1.44	0.99
1:B:265:PRO:HD2	1:B:288:SER:HB3	1.42	0.99
1:C:52:LYS:HB3	1:D:94:ASP:O	1.62	0.99
1:E:265:PRO:HD2	1:E:288:SER:HB3	1.43	0.99
1:A:265:PRO:HD2	1:A:288:SER:HB3	1.43	0.98
1:D:342:VAL:O	1:D:342:VAL:HG22	1.68	0.92
1:B:292:MET:HG3	1:C:274:VAL:HG13	1.55	0.88
1:F:339:PHE:CE2	1:F:341:PRO:CG	2.57	0.88
1:A:272:ASN:O	1:A:276:GLN:HG2	1.75	0.86
1:E:344:TYR:OH	1:E:376:LEU:HG	1.76	0.86
1:D:292:MET:HG3	1:F:274:VAL:HG13	1.57	0.85
1:C:272:ASN:O	1:C:276:GLN:HG2	1.78	0.84
1:F:437:THR:HG23	1:F:440:THR:H	1.43	0.83
1:A:167:GLU:HG2	1:A:198:ASN:HD21	1.44	0.83
1:B:272:ASN:O	1:B:276:GLN:HG2	1.78	0.83
1:F:308:ALA:O	1:F:335:ARG:HD3	1.79	0.83
1:E:272:ASN:O	1:E:276:GLN:HG2	1.79	0.82
1:A:274:VAL:HG13	1:C:292:MET:HG3	1.61	0.81
1:D:272:ASN:O	1:D:276:GLN:HG2	1.79	0.81
1:E:78:ILE:HG22	1:E:82:MET:HE2	1.61	0.81
1:D:35:LEU:HD22	1:D:70:VAL:HG11	1.63	0.81
1:B:167:GLU:HG2	1:B:198:ASN:HD21	1.46	0.80
1:E:35:LEU:HD22	1:E:70:VAL:HG11	1.62	0.80
1:F:272:ASN:O	1:F:276:GLN:HG2	1.80	0.80
1:D:167:GLU:HG2	1:D:198:ASN:HD21	1.47	0.80
1:B:208:VAL:HG11	1:B:225:LEU:HD13	1.63	0.80
1:C:296:GLN:HG3	1:C:322:MET:HB2	1.64	0.80
1:D:78:ILE:HG22	1:D:82:MET:HE2	1.64	0.79
1:E:208:VAL:HG11	1:E:225:LEU:HD13	1.63	0.79
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.64	0.79
1:D:343:GLY:O	1:D:350:ARG:HD3	1.80	0.79
1:D:346:ALA:O	1:D:347:THR:CG2	2.30	0.79
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.64	0.79
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.65	0.79
1:C:208:VAL:HG11	1:C:225:LEU:HD13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:THR:HG23	1:C:440:THR:H	1.47	0.78
1:B:78:ILE:H	1:B:78:ILE:HD12	1.48	0.78
1:F:167:GLU:HG2	1:F:198:ASN:HD21	1.49	0.78
1:D:77:ARG:HE	1:D:80:VAL:CG2	1.95	0.78
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.48	0.77
1:A:296:GLN:HG3	1:A:322:MET:HB2	1.65	0.77
1:F:35:LEU:HD22	1:F:70:VAL:HG11	1.66	0.77
1:C:89:ILE:HD11	1:C:101:ILE:HG21	1.67	0.77
1:A:437:THR:HG23	1:A:440:THR:H	1.48	0.77
1:C:104:LEU:HD21	1:D:83:ALA:HA	1.67	0.76
1:C:437:THR:O	1:C:438:ASN:C	2.28	0.76
1:D:208:VAL:HG11	1:D:225:LEU:HD13	1.65	0.76
1:F:296:GLN:HG3	1:F:322:MET:HB2	1.65	0.76
1:D:296:GLN:HG3	1:D:322:MET:HB2	1.68	0.76
1:F:89:ILE:HD11	1:F:101:ILE:HG21	1.67	0.76
1:C:167:GLU:HG2	1:C:198:ASN:HD21	1.51	0.76
1:D:308:ALA:O	1:D:335:ARG:HD3	1.85	0.76
1:C:193:GLN:NE2	1:C:362:GLN:HE21	1.81	0.76
1:E:296:GLN:HG3	1:E:322:MET:HB2	1.65	0.76
1:D:437:THR:HG23	1:D:440:THR:H	1.50	0.75
1:F:208:VAL:HG11	1:F:225:LEU:HD13	1.67	0.75
1:C:95:ASP:C	1:D:52:LYS:HB2	2.12	0.75
1:A:193:GLN:NE2	1:A:362:GLN:HE21	1.83	0.75
1:C:308:ALA:O	1:C:335:ARG:HD3	1.86	0.75
1:B:296:GLN:HG3	1:B:322:MET:HB2	1.67	0.74
1:A:208:VAL:HG11	1:A:225:LEU:HD13	1.68	0.74
1:A:298:GLU:HG3	1:B:349:THR:HB	1.70	0.74
1:F:78:ILE:HG22	1:F:82:MET:HE2	1.67	0.74
1:F:101:ILE:O	1:F:105:VAL:HG22	1.85	0.74
1:F:437:THR:O	1:F:438:ASN:C	2.31	0.74
1:B:437:THR:HG23	1:B:440:THR:H	1.52	0.74
1:E:167:GLU:HG2	1:E:198:ASN:HD21	1.52	0.74
1:F:193:GLN:NE2	1:F:362:GLN:HE21	1.85	0.74
1:A:90:HIS:HD2	1:A:134:TYR:OH	1.71	0.74
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.53	0.74
1:B:193:GLN:NE2	1:B:362:GLN:HE21	1.86	0.73
1:D:78:ILE:H	1:D:78:ILE:HD12	1.51	0.73
1:E:193:GLN:NE2	1:E:362:GLN:HE21	1.87	0.73
1:B:297:SER:HB2	1:C:349:THR:OG1	1.87	0.73
1:D:347:THR:O	1:D:349:THR:N	2.21	0.73
1:A:78:ILE:HG22	1:A:82:MET:HE2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HD11	1:A:101:ILE:HG21	1.70	0.73
1:E:89:ILE:HD11	1:E:101:ILE:HG21	1.71	0.73
1:F:343:GLY:HA3	1:F:350:ARG:HD3	1.71	0.73
1:C:78:ILE:HG22	1:C:82:MET:HE2	1.71	0.73
1:E:308:ALA:O	1:E:335:ARG:HD3	1.88	0.73
1:B:78:ILE:HG22	1:B:82:MET:HE2	1.70	0.73
1:B:101:ILE:O	1:B:105:VAL:HG22	1.89	0.73
1:B:407:PHE:CE2	1:B:427:ILE:HD11	2.24	0.73
1:B:90:HIS:HD2	1:B:134:TYR:OH	1.72	0.73
1:D:89:ILE:HD11	1:D:101:ILE:HG21	1.71	0.73
1:D:346:ALA:O	1:D:347:THR:HG22	1.89	0.72
1:B:345:SER:HA	1:B:346:ALA:C	2.15	0.72
1:A:308:ALA:O	1:A:335:ARG:HD3	1.89	0.72
1:D:193:GLN:NE2	1:D:362:GLN:HE21	1.87	0.72
1:C:96:MET:HE2	1:D:55:ILE:HD11	1.72	0.71
1:B:75:ASN:ND2	1:B:76:ASP:HB3	2.05	0.71
1:C:95:ASP:O	1:D:52:LYS:HB2	1.89	0.71
1:A:79:ASP:HB2	1:E:96:MET:HE1	1.70	0.71
1:A:75:ASN:ND2	1:A:76:ASP:HB3	2.06	0.71
1:B:35:LEU:HD22	1:B:70:VAL:HG11	1.72	0.71
1:B:75:ASN:HD22	1:B:76:ASP:HB3	1.56	0.71
1:C:344:TYR:O	1:C:345:SER:CB	2.39	0.71
1:B:292:MET:HG3	1:C:274:VAL:CG1	2.19	0.71
1:B:308:ALA:O	1:B:335:ARG:HD3	1.90	0.71
1:E:407:PHE:CE2	1:E:427:ILE:HD11	2.26	0.70
1:E:437:THR:HG23	1:E:440:THR:H	1.54	0.70
1:A:313:ASN:ND2	1:A:342:VAL:HG21	2.06	0.70
1:C:193:GLN:HE21	1:C:362:GLN:HE21	1.39	0.70
1:E:528:ASN:C	1:E:530:PRO:HD3	2.16	0.70
1:E:90:HIS:HD2	1:E:134:TYR:OH	1.75	0.70
1:B:528:ASN:C	1:B:530:PRO:HD3	2.16	0.70
1:F:75:ASN:ND2	1:F:76:ASP:HB3	2.07	0.70
1:A:78:ILE:HD12	1:A:78:ILE:H	1.56	0.70
1:E:78:ILE:HD12	1:E:78:ILE:H	1.56	0.69
1:A:101:ILE:O	1:A:105:VAL:HG22	1.92	0.69
1:C:97:PRO:HD3	1:D:52:LYS:HG3	1.74	0.69
1:E:75:ASN:HD22	1:E:76:ASP:HB3	1.57	0.69
1:F:90:HIS:HD2	1:F:134:TYR:OH	1.74	0.69
1:D:528:ASN:C	1:D:530:PRO:HD3	2.18	0.69
1:E:75:ASN:ND2	1:E:76:ASP:HB3	2.07	0.69
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:ALA:C	1:D:347:THR:HG23	2.17	0.68
1:F:89:ILE:HD11	1:F:101:ILE:CG2	2.23	0.68
1:A:407:PHE:CE2	1:A:427:ILE:HD11	2.29	0.68
1:D:437:THR:HG21	1:D:440:THR:O	1.94	0.68
1:D:5:LYS:HE3	1:D:133:ASP:OD2	1.92	0.68
1:D:90:HIS:HD2	1:D:134:TYR:OH	1.75	0.68
1:A:437:THR:HG21	1:A:440:THR:O	1.93	0.68
1:A:528:ASN:C	1:A:530:PRO:HD3	2.19	0.68
1:D:274:VAL:CG1	1:E:292:MET:HG3	2.20	0.68
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.08	0.68
1:D:342:VAL:O	1:D:342:VAL:CG2	2.42	0.68
1:D:407:PHE:CE2	1:D:427:ILE:HD11	2.28	0.67
1:F:528:ASN:C	1:F:530:PRO:HD3	2.19	0.67
1:B:137:VAL:CG2	1:B:178:GLY:HA2	2.25	0.67
1:C:528:ASN:C	1:C:530:PRO:HD3	2.19	0.67
1:A:75:ASN:HD22	1:A:76:ASP:HB3	1.57	0.67
1:F:78:ILE:HD12	1:F:78:ILE:H	1.59	0.67
1:D:484:ASN:HD22	1:D:487:HIS:H	1.42	0.67
1:F:75:ASN:HD22	1:F:76:ASP:HB3	1.58	0.67
1:A:346:ALA:C	1:A:347:THR:HG23	2.19	0.67
1:B:86:ALA:O	1:B:109:MET:HE2	1.94	0.67
1:D:347:THR:OG1	1:E:298:GLU:HG2	1.95	0.67
1:F:437:THR:HG21	1:F:440:THR:O	1.95	0.67
1:B:422:ILE:HG22	1:B:486:PHE:HE1	1.59	0.66
1:D:75:ASN:ND2	1:D:76:ASP:HB3	2.10	0.66
1:F:193:GLN:HE21	1:F:362:GLN:HE21	1.39	0.66
1:C:52:LYS:CB	1:D:94:ASP:O	2.42	0.66
1:A:193:GLN:HE21	1:A:362:GLN:HE21	1.41	0.66
1:B:193:GLN:HE21	1:B:362:GLN:HE21	1.42	0.66
1:E:90:HIS:HE1	1:E:114:SER:OG	1.79	0.66
1:E:422:ILE:HG22	1:E:486:PHE:HE1	1.60	0.66
1:C:101:ILE:O	1:C:105:VAL:HG22	1.94	0.66
1:F:407:PHE:CE2	1:F:427:ILE:HD11	2.31	0.66
1:F:484:ASN:HD22	1:F:487:HIS:H	1.42	0.66
1:A:130:ASP:HB2	1:A:133:ASP:OD1	1.96	0.66
1:C:89:ILE:HD11	1:C:101:ILE:CG2	2.26	0.66
1:B:17:ASP:HB3	1:B:20:MET:HE2	1.77	0.66
1:D:193:GLN:HE21	1:D:362:GLN:HE21	1.44	0.66
1:A:339:PHE:CE2	1:A:341:PRO:CG	2.67	0.65
1:E:290:PRO:HB2	1:E:292:MET:CE	2.27	0.65
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:HD2	1:C:134:TYR:OH	1.79	0.65
1:C:257:ILE:HD11	1:C:533:TRP:HH2	1.61	0.65
1:B:345:SER:HA	1:B:347:THR:CA	2.26	0.65
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.30	0.65
1:B:89:ILE:HD11	1:B:101:ILE:CG2	2.26	0.65
1:C:343:GLY:O	1:C:345:SER:N	2.30	0.65
1:A:343:GLY:O	1:A:345:SER:N	2.30	0.65
1:F:322:MET:O	1:F:322:MET:HE3	1.97	0.65
1:C:343:GLY:O	1:C:344:TYR:C	2.39	0.65
1:E:193:GLN:HE21	1:E:362:GLN:HE21	1.45	0.65
1:E:484:ASN:HD22	1:E:487:HIS:H	1.43	0.65
1:C:422:ILE:HG22	1:C:486:PHE:HE1	1.63	0.64
1:D:283:THR:HG22	1:D:288:SER:O	1.96	0.64
1:A:90:HIS:HE1	1:A:114:SER:OG	1.79	0.64
1:C:90:HIS:HE1	1:C:114:SER:OG	1.79	0.64
1:B:345:SER:N	1:B:346:ALA:HB3	2.12	0.64
1:E:347:THR:HG21	1:F:302:LEU:HD13	1.79	0.64
1:D:35:LEU:CD2	1:D:70:VAL:HG11	2.27	0.64
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.62	0.64
1:F:339:PHE:CD2	1:F:341:PRO:HG3	2.31	0.64
1:A:283:THR:HG22	1:A:288:SER:O	1.97	0.64
1:F:283:THR:HG22	1:F:288:SER:O	1.98	0.64
1:E:101:ILE:O	1:E:105:VAL:HG22	1.98	0.64
1:E:137:VAL:CG2	1:E:178:GLY:HA2	2.28	0.64
1:B:46:GLU:HA	1:B:46:GLU:OE1	1.97	0.63
1:D:46:GLU:HB2	1:D:54:PHE:CE2	2.32	0.63
1:B:90:HIS:HE1	1:B:114:SER:OG	1.82	0.63
1:D:484:ASN:ND2	1:D:487:HIS:H	1.96	0.63
1:E:89:ILE:HD11	1:E:101:ILE:CG2	2.29	0.63
1:E:437:THR:HG21	1:E:440:THR:O	1.99	0.63
1:B:257:ILE:HD11	1:B:533:TRP:HH2	1.63	0.63
1:B:484:ASN:HD22	1:B:487:HIS:H	1.45	0.63
1:A:484:ASN:HD22	1:A:487:HIS:H	1.45	0.63
1:E:257:ILE:HD11	1:E:533:TRP:HH2	1.63	0.63
1:D:346:ALA:C	1:D:347:THR:CG2	2.72	0.63
1:E:86:ALA:O	1:E:109:MET:HE2	1.98	0.63
1:E:484:ASN:ND2	1:E:487:HIS:H	1.96	0.63
1:F:90:HIS:HE1	1:F:114:SER:OG	1.81	0.63
1:B:484:ASN:ND2	1:B:487:HIS:H	1.96	0.63
1:B:283:THR:HG22	1:B:288:SER:O	1.99	0.63
1:D:101:ILE:O	1:D:105:VAL:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:ALA:O	1:E:524:LEU:HB2	1.99	0.62
1:F:167:GLU:CG	1:F:198:ASN:HD21	2.12	0.62
1:C:17:ASP:HB3	1:C:20:MET:HE2	1.81	0.62
1:D:90:HIS:HE1	1:D:114:SER:OG	1.81	0.62
1:D:75:ASN:HD22	1:D:76:ASP:HB3	1.63	0.62
1:B:290:PRO:HB2	1:B:292:MET:CE	2.29	0.62
1:D:17:ASP:HB3	1:D:20:MET:HE2	1.81	0.62
1:B:46:GLU:HB2	1:B:54:PHE:CE2	2.34	0.61
1:C:437:THR:HG21	1:C:440:THR:O	2.01	0.61
1:D:89:ILE:HD11	1:D:101:ILE:CG2	2.29	0.61
1:D:257:ILE:HD11	1:D:533:TRP:HH2	1.65	0.61
1:F:484:ASN:ND2	1:F:487:HIS:H	1.98	0.61
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.35	0.61
1:F:17:ASP:HB3	1:F:20:MET:HE2	1.82	0.61
1:A:167:GLU:CG	1:A:198:ASN:HD21	2.13	0.61
1:B:407:PHE:HE2	1:B:427:ILE:HD11	1.64	0.61
1:D:290:PRO:HB2	1:D:292:MET:CE	2.31	0.61
1:A:484:ASN:ND2	1:A:487:HIS:H	1.98	0.61
1:B:437:THR:HG21	1:B:440:THR:O	2.01	0.61
1:C:78:ILE:HD12	1:C:78:ILE:H	1.64	0.61
1:D:46:GLU:HA	1:D:46:GLU:OE1	2.00	0.61
1:E:46:GLU:OE1	1:E:46:GLU:HA	2.00	0.61
1:A:17:ASP:HB3	1:A:20:MET:HE2	1.82	0.61
1:A:96:MET:HE1	1:E:79:ASP:HB2	1.82	0.61
1:B:35:LEU:CD1	1:B:64:LEU:HD22	2.31	0.61
1:F:137:VAL:CG2	1:F:178:GLY:HA2	2.31	0.61
1:A:346:ALA:O	1:A:347:THR:CG2	2.44	0.61
1:D:137:VAL:CG2	1:D:178:GLY:HA2	2.30	0.61
1:E:138:GLY:HA3	1:E:154:MET:HE2	1.82	0.61
1:C:484:ASN:ND2	1:C:487:HIS:H	1.99	0.61
1:D:422:ILE:HG22	1:D:486:PHE:HE1	1.65	0.61
1:E:17:ASP:HB3	1:E:20:MET:HE2	1.83	0.61
1:C:290:PRO:HB2	1:C:292:MET:CE	2.30	0.61
1:F:290:PRO:HB2	1:F:292:MET:CE	2.31	0.61
1:B:339:PHE:CE2	1:B:341:PRO:HG3	2.36	0.60
1:D:54:PHE:CE2	1:D:77:ARG:HD3	2.35	0.60
1:D:292:MET:HG3	1:F:274:VAL:CG1	2.29	0.60
1:F:257:ILE:HD11	1:F:533:TRP:HH2	1.66	0.60
1:D:167:GLU:CG	1:D:198:ASN:HD21	2.14	0.60
1:A:137:VAL:CG2	1:A:178:GLY:HA2	2.31	0.60
1:A:290:PRO:HB2	1:A:292:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ASN:HD22	1:C:487:HIS:H	1.49	0.60
1:E:46:GLU:HB2	1:E:54:PHE:CE2	2.36	0.60
1:C:424:ASP:HB3	1:C:446:PRO:HG2	1.84	0.60
1:A:75:ASN:HD22	1:A:76:ASP:CB	2.15	0.60
1:C:265:PRO:CD	1:C:288:SER:HB3	2.25	0.60
1:D:86:ALA:O	1:D:109:MET:HE2	2.02	0.60
1:D:347:THR:O	1:D:348:GLU:C	2.44	0.59
1:D:77:ARG:HE	1:D:80:VAL:HG21	1.65	0.59
1:E:283:THR:HG22	1:E:288:SER:O	2.02	0.59
1:A:35:LEU:CD2	1:A:70:VAL:HG11	2.32	0.59
1:E:529:THR:N	1:E:530:PRO:HD3	2.17	0.59
1:B:75:ASN:HD22	1:B:76:ASP:CB	2.15	0.59
1:F:437:THR:HG23	1:F:440:THR:N	2.16	0.59
1:C:137:VAL:CG2	1:C:178:GLY:HA2	2.32	0.59
1:D:38:GLY:O	1:D:39:VAL:C	2.46	0.59
1:B:523:ARG:HH11	1:C:508:ASN:HB3	1.66	0.59
1:F:339:PHE:HE2	1:F:341:PRO:HG3	1.58	0.59
1:D:424:ASP:HB3	1:D:446:PRO:HG2	1.85	0.59
1:A:297:SER:HB2	1:B:349:THR:OG1	2.02	0.59
1:E:322:MET:HE3	1:E:322:MET:O	2.03	0.59
1:A:529:THR:N	1:A:530:PRO:HD3	2.18	0.59
1:E:58:ALA:HB1	1:E:84:ILE:HD13	1.85	0.59
1:E:75:ASN:HD22	1:E:76:ASP:CB	2.16	0.59
1:E:407:PHE:HE2	1:E:427:ILE:HD11	1.67	0.58
1:A:422:ILE:HG22	1:A:486:PHE:HE1	1.67	0.58
1:B:345:SER:CA	1:B:347:THR:N	2.60	0.58
1:A:86:ALA:O	1:A:109:MET:HE2	2.04	0.58
1:A:187:ILE:HG23	1:A:206:ILE:CD1	2.33	0.58
1:B:529:THR:N	1:B:530:PRO:HD3	2.18	0.58
1:D:107:PRO:O	1:D:108:ASP:HB2	2.03	0.58
1:A:38:GLY:O	1:A:39:VAL:C	2.47	0.58
1:A:46:GLU:HB2	1:A:54:PHE:CE2	2.38	0.58
1:C:35:LEU:CD2	1:C:70:VAL:HG11	2.34	0.58
1:C:283:THR:HG22	1:C:288:SER:O	2.02	0.58
1:D:322:MET:HE3	1:D:322:MET:O	2.03	0.58
1:D:346:ALA:O	1:D:347:THR:HG23	2.01	0.58
1:A:58:ALA:HB1	1:A:84:ILE:HD13	1.86	0.58
1:F:344:TYR:HE2	1:F:376:LEU:HA	1.69	0.58
1:C:96:MET:HG3	1:D:55:ILE:HD12	1.86	0.58
1:B:523:ARG:NH1	1:C:508:ASN:HB3	2.19	0.58
1:B:137:VAL:HG23	1:B:178:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:HB2	1:C:54:PHE:CE2	2.38	0.58
1:F:424:ASP:HB3	1:F:446:PRO:HG2	1.85	0.58
1:F:529:THR:N	1:F:530:PRO:HD3	2.19	0.58
1:A:107:PRO:O	1:A:108:ASP:HB2	2.03	0.58
1:A:124:LEU:C	1:A:124:LEU:HD23	2.29	0.58
1:E:339:PHE:CE2	1:E:341:PRO:HG3	2.39	0.58
1:A:339:PHE:CD2	1:A:341:PRO:HG3	2.35	0.57
1:B:520:ALA:O	1:B:524:LEU:HB2	2.04	0.57
1:D:129:PRO:O	1:D:130:ASP:HB2	2.03	0.57
1:A:407:PHE:HE2	1:A:427:ILE:HD11	1.69	0.57
1:B:424:ASP:HB3	1:B:446:PRO:HG2	1.86	0.57
1:D:5:LYS:HE3	1:D:133:ASP:CG	2.28	0.57
1:E:137:VAL:HG23	1:E:178:GLY:HA2	1.86	0.57
1:B:278:PHE:CE2	1:B:467:SER:OG	2.57	0.57
1:A:252:GLU:O	1:A:256:ILE:HG12	2.05	0.57
1:A:424:ASP:HB3	1:A:446:PRO:HG2	1.86	0.57
1:D:75:ASN:HD22	1:D:76:ASP:CB	2.18	0.57
1:F:278:PHE:CE2	1:F:467:SER:OG	2.57	0.57
1:E:51:THR:O	1:E:55:ILE:HG13	2.04	0.57
1:C:344:TYR:OH	1:C:355:ASN:ND2	2.30	0.57
1:F:75:ASN:HD22	1:F:76:ASP:CB	2.16	0.57
1:B:35:LEU:CD2	1:B:70:VAL:HG11	2.35	0.57
1:C:107:PRO:O	1:C:108:ASP:HB2	2.05	0.57
1:C:437:THR:O	1:C:437:THR:CG2	2.52	0.57
1:D:529:THR:N	1:D:530:PRO:HD3	2.20	0.57
1:E:35:LEU:CD2	1:E:70:VAL:HG11	2.33	0.57
1:B:107:PRO:O	1:B:108:ASP:HB2	2.03	0.57
1:B:298:GLU:HG2	1:C:347:THR:CB	2.35	0.57
1:B:420:ASP:OD2	1:B:497:LYS:HD3	2.05	0.57
1:D:349:THR:OG1	1:E:297:SER:HB2	2.05	0.57
1:E:252:GLU:O	1:E:256:ILE:HG12	2.04	0.57
1:C:529:THR:N	1:C:530:PRO:HD3	2.20	0.57
1:D:124:LEU:C	1:D:124:LEU:HD23	2.30	0.57
1:F:35:LEU:CD2	1:F:70:VAL:HG11	2.33	0.57
1:A:278:PHE:CE2	1:A:467:SER:OG	2.58	0.56
1:C:167:GLU:CG	1:C:198:ASN:HD21	2.18	0.56
1:B:51:THR:O	1:B:55:ILE:HG13	2.05	0.56
1:B:322:MET:HE3	1:B:322:MET:O	2.05	0.56
1:E:291:ILE:HG22	1:E:293:SER:H	1.70	0.56
1:F:58:ALA:HB1	1:F:84:ILE:HD13	1.87	0.56
1:B:124:LEU:C	1:B:124:LEU:HD23	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:TYR:CE1	1:C:351:LEU:HD12	2.40	0.56
1:D:167:GLU:HG2	1:D:198:ASN:ND2	2.20	0.56
1:E:278:PHE:CE2	1:E:467:SER:OG	2.57	0.56
1:F:420:ASP:OD2	1:F:497:LYS:HD3	2.05	0.56
1:C:52:LYS:HB2	1:D:95:ASP:C	2.30	0.56
1:D:51:THR:O	1:D:55:ILE:HG13	2.06	0.56
1:B:58:ALA:HB1	1:B:84:ILE:HD13	1.87	0.56
1:A:322:MET:HG3	1:A:323:LEU:N	2.21	0.56
1:B:298:GLU:HG2	1:C:347:THR:HG21	1.87	0.56
1:D:407:PHE:HE2	1:D:427:ILE:HD11	1.69	0.56
1:A:420:ASP:OD2	1:A:497:LYS:HD3	2.06	0.56
1:C:75:ASN:HD22	1:C:76:ASP:CB	2.19	0.55
1:D:278:PHE:CE2	1:D:467:SER:OG	2.59	0.55
1:E:424:ASP:HB3	1:E:446:PRO:HG2	1.88	0.55
1:A:520:ALA:O	1:A:524:LEU:HB2	2.05	0.55
1:B:167:GLU:CG	1:B:198:ASN:HD21	2.16	0.55
1:C:38:GLY:O	1:C:40:THR:HG23	2.06	0.55
1:E:313:ASN:ND2	1:E:342:VAL:HG21	2.21	0.55
1:F:422:ILE:HG22	1:F:486:PHE:HE1	1.70	0.55
1:B:123:GLU:O	1:B:127:MET:HG3	2.06	0.55
1:C:58:ALA:HB1	1:C:84:ILE:HD13	1.88	0.55
1:C:520:ALA:O	1:C:524:LEU:HB2	2.06	0.55
1:F:123:GLU:O	1:F:127:MET:HG3	2.06	0.55
1:A:322:MET:O	1:A:322:MET:HE3	2.07	0.55
1:D:520:ALA:O	1:D:524:LEU:HB2	2.05	0.55
1:E:5:LYS:HE3	1:E:133:ASP:OD1	2.07	0.55
1:E:265:PRO:CD	1:E:288:SER:HB3	2.29	0.55
1:F:86:ALA:O	1:F:109:MET:HE2	2.06	0.55
1:C:278:PHE:CE2	1:C:467:SER:OG	2.58	0.55
1:D:10:TYR:O	1:D:205:GLY:HA3	2.06	0.55
1:A:167:GLU:HG2	1:A:198:ASN:ND2	2.18	0.55
1:C:187:ILE:HG23	1:C:206:ILE:CD1	2.37	0.55
1:B:28:TYR:CZ	1:B:64:LEU:HG	2.41	0.55
1:C:75:ASN:HD22	1:C:76:ASP:HB3	1.72	0.55
1:E:192:TYR:HA	1:E:431:TYR:HB3	1.89	0.55
1:A:343:GLY:HA3	1:A:350:ARG:HD3	1.88	0.54
1:E:38:GLY:O	1:E:40:THR:HG23	2.07	0.54
1:D:187:ILE:HG23	1:D:206:ILE:CD1	2.38	0.54
1:E:28:TYR:CZ	1:E:64:LEU:HG	2.42	0.54
1:E:127:MET:HE3	1:E:131:MET:HB3	1.88	0.54
1:C:91:VAL:HG11	1:C:101:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:VAL:HG11	1:C:101:ILE:CD1	2.37	0.54
1:C:252:GLU:O	1:C:256:ILE:HG12	2.08	0.54
1:A:74:ILE:HD11	1:A:84:ILE:HD11	1.89	0.54
1:E:137:VAL:HG22	1:E:177:VAL:O	2.08	0.54
1:C:437:THR:O	1:C:437:THR:HG22	2.08	0.54
1:D:58:ALA:HB1	1:D:84:ILE:HD13	1.89	0.54
1:E:107:PRO:O	1:E:108:ASP:HB2	2.07	0.54
1:C:86:ALA:O	1:C:109:MET:HE2	2.06	0.54
1:D:127:MET:HE3	1:D:131:MET:HB3	1.90	0.54
1:D:314:THR:O	1:D:342:VAL:CG1	2.55	0.54
1:A:291:ILE:HG22	1:A:293:SER:H	1.72	0.54
1:F:195:VAL:HG12	1:F:202:SER:HB3	1.90	0.54
1:A:518:ILE:HG22	1:B:510:SER:HB2	1.90	0.54
1:C:193:GLN:NE2	1:C:362:GLN:NE2	2.54	0.54
1:E:160:ILE:HD11	1:E:193:GLN:O	2.08	0.54
1:E:420:ASP:OD2	1:E:497:LYS:HD3	2.08	0.54
1:B:74:ILE:HD11	1:B:84:ILE:HD11	1.90	0.54
1:B:347:THR:O	1:B:348:GLU:HG2	2.07	0.54
1:F:192:TYR:HA	1:F:431:TYR:HB3	1.90	0.54
1:B:38:GLY:O	1:B:40:THR:HG23	2.08	0.53
1:C:98:ILE:HD11	1:C:113:TRP:CD1	2.43	0.53
1:D:38:GLY:O	1:D:40:THR:HG23	2.08	0.53
1:D:297:SER:HB2	1:F:349:THR:OG1	2.08	0.53
1:B:167:GLU:HG2	1:B:198:ASN:ND2	2.20	0.53
1:F:291:ILE:HG22	1:F:293:SER:H	1.74	0.53
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.07	0.53
1:B:160:ILE:HD11	1:B:193:GLN:O	2.09	0.53
1:B:280:ALA:O	1:B:284:LEU:HB2	2.08	0.53
1:D:51:THR:HB	1:D:77:ARG:CZ	2.38	0.53
1:D:195:VAL:HG12	1:D:202:SER:HB3	1.90	0.53
1:E:187:ILE:HG12	1:E:206:ILE:HD13	1.91	0.53
1:B:187:ILE:HG12	1:B:206:ILE:HD13	1.91	0.53
1:D:77:ARG:HE	1:D:80:VAL:HG23	1.71	0.53
1:F:20:MET:HE1	1:F:209:VAL:HG12	1.91	0.53
1:B:137:VAL:HG22	1:B:177:VAL:O	2.08	0.53
1:C:38:GLY:O	1:C:39:VAL:C	2.49	0.53
1:C:407:PHE:HE2	1:C:427:ILE:HD11	1.73	0.53
1:A:271:THR:HA	1:A:313:ASN:HB2	1.90	0.53
1:B:138:GLY:HA3	1:B:154:MET:CE	2.39	0.53
1:C:51:THR:O	1:C:55:ILE:HG13	2.09	0.53
1:E:127:MET:HB3	1:E:131:MET:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:VAL:HG12	1:E:202:SER:HB3	1.91	0.53
1:E:344:TYR:CD1	1:E:354:ASN:ND2	2.76	0.53
1:F:437:THR:O	1:F:437:THR:CG2	2.56	0.53
1:C:75:ASN:HD22	1:C:76:ASP:CA	2.21	0.53
1:C:75:ASN:ND2	1:C:76:ASP:HB3	2.24	0.53
1:B:265:PRO:CD	1:B:288:SER:HB3	2.29	0.52
1:C:123:GLU:O	1:C:127:MET:HG3	2.09	0.52
1:C:127:MET:HE3	1:C:131:MET:CB	2.39	0.52
1:F:124:LEU:C	1:F:124:LEU:HD23	2.34	0.52
1:B:66:HIS:HE1	1:B:87:ASP:OD1	1.92	0.52
1:B:291:ILE:HG22	1:B:293:SER:H	1.74	0.52
1:C:254:GLN:HG3	1:C:528:ASN:HB3	1.91	0.52
1:A:515:VAL:HG23	1:B:511:GLY:C	2.34	0.52
1:E:66:HIS:HE1	1:E:87:ASP:OD1	1.92	0.52
1:F:137:VAL:HG23	1:F:178:GLY:HA2	1.92	0.52
1:A:38:GLY:O	1:A:40:THR:HG23	2.10	0.52
1:A:91:VAL:HG11	1:A:101:ILE:CD1	2.40	0.52
1:A:91:VAL:HG11	1:A:101:ILE:HD13	1.92	0.52
1:C:124:LEU:HD23	1:C:124:LEU:C	2.35	0.52
1:C:160:ILE:HD11	1:C:193:GLN:O	2.10	0.52
1:D:252:GLU:O	1:D:256:ILE:HG12	2.09	0.52
1:F:74:ILE:HD11	1:F:84:ILE:HD11	1.91	0.52
1:F:127:MET:HE3	1:F:131:MET:HB3	1.91	0.52
1:D:192:TYR:HA	1:D:431:TYR:HB3	1.91	0.52
1:D:271:THR:HA	1:D:313:ASN:HB2	1.92	0.52
1:F:407:PHE:HE2	1:F:427:ILE:HD11	1.72	0.52
1:A:192:TYR:HA	1:A:431:TYR:HB3	1.91	0.52
1:D:420:ASP:OD2	1:D:497:LYS:HD3	2.09	0.52
1:E:167:GLU:CG	1:E:198:ASN:HD21	2.21	0.52
1:B:192:TYR:CZ	1:B:410:LYS:HB3	2.45	0.52
1:D:137:VAL:HG23	1:D:178:GLY:HA2	1.92	0.52
1:F:252:GLU:O	1:F:256:ILE:HG12	2.09	0.52
1:C:192:TYR:HA	1:C:431:TYR:HB3	1.91	0.52
1:D:91:VAL:HG11	1:D:101:ILE:HD13	1.92	0.52
1:B:272:ASN:N	1:B:272:ASN:ND2	2.58	0.51
1:D:265:PRO:CD	1:D:288:SER:HB3	2.29	0.51
1:F:138:GLY:HA3	1:F:154:MET:CE	2.40	0.51
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.92	0.51
1:C:271:THR:HA	1:C:313:ASN:HB2	1.92	0.51
1:C:322:MET:HE3	1:C:322:MET:O	2.11	0.51
1:D:276:GLN:HE21	1:D:276:GLN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:THR:HA	1:E:313:ASN:HB2	1.93	0.51
1:F:167:GLU:HG2	1:F:198:ASN:ND2	2.21	0.51
1:B:437:THR:HG23	1:B:440:THR:N	2.23	0.51
1:A:265:PRO:CD	1:A:288:SER:HB3	2.29	0.51
1:A:437:THR:HG23	1:A:440:THR:N	2.20	0.51
1:B:192:TYR:HA	1:B:431:TYR:HB3	1.92	0.51
1:D:127:MET:HB3	1:D:131:MET:HG3	1.93	0.51
1:F:344:TYR:CD2	1:F:376:LEU:HG	2.46	0.51
1:A:123:GLU:O	1:A:127:MET:HG3	2.09	0.51
1:E:124:LEU:C	1:E:124:LEU:HD23	2.36	0.51
1:F:140:LEU:HD12	1:F:182:LEU:HD11	1.93	0.51
1:A:195:VAL:HG12	1:A:202:SER:HB3	1.93	0.51
1:A:312:LEU:HD21	1:A:323:LEU:HD22	1.91	0.51
1:C:77:ARG:HH11	1:C:77:ARG:CG	2.24	0.51
1:D:437:THR:O	1:D:439:GLY:N	2.44	0.51
1:E:138:GLY:HA3	1:E:154:MET:CE	2.41	0.51
1:F:193:GLN:NE2	1:F:362:GLN:NE2	2.57	0.51
1:B:271:THR:HA	1:B:313:ASN:HB2	1.93	0.51
1:B:298:GLU:HG2	1:C:347:THR:OG1	2.10	0.51
1:B:495:LEU:HD22	1:B:521:LEU:HD23	1.92	0.51
1:C:291:ILE:HG22	1:C:293:SER:H	1.76	0.51
1:D:75:ASN:HD22	1:D:76:ASP:CA	2.24	0.51
1:D:298:GLU:HG2	1:F:347:THR:HG21	1.93	0.51
1:F:271:THR:HA	1:F:313:ASN:HB2	1.91	0.51
1:B:138:GLY:HA3	1:B:154:MET:HE2	1.92	0.51
1:F:265:PRO:CD	1:F:288:SER:HB3	2.27	0.51
1:F:313:ASN:ND2	1:F:342:VAL:HG21	2.26	0.51
1:F:437:THR:O	1:F:437:THR:HG22	2.11	0.51
1:A:28:TYR:CZ	1:A:64:LEU:HG	2.45	0.51
1:B:369:ASN:O	1:B:370:SER:C	2.54	0.51
1:C:195:VAL:HG12	1:C:202:SER:HB3	1.93	0.51
1:E:274:VAL:HG13	1:F:292:MET:HG3	1.93	0.51
1:F:254:GLN:HG3	1:F:528:ASN:HB3	1.93	0.51
1:D:91:VAL:HG11	1:D:101:ILE:CD1	2.41	0.51
1:D:343:GLY:O	1:D:350:ARG:CD	2.58	0.51
1:E:437:THR:O	1:E:439:GLY:N	2.44	0.51
1:B:38:GLY:O	1:B:39:VAL:C	2.53	0.50
1:B:252:GLU:O	1:B:256:ILE:HG12	2.10	0.50
1:C:322:MET:HG3	1:C:323:LEU:N	2.23	0.50
1:F:520:ALA:O	1:F:524:LEU:HB2	2.10	0.50
1:D:312:LEU:HD21	1:D:323:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:HG3	1:A:528:ASN:HB3	1.93	0.50
1:E:140:LEU:HD12	1:E:182:LEU:HD11	1.93	0.50
1:F:187:ILE:HG23	1:F:206:ILE:CD1	2.41	0.50
1:B:20:MET:CE	1:B:209:VAL:HG12	2.40	0.50
1:B:35:LEU:HD12	1:B:64:LEU:HD22	1.91	0.50
1:B:195:VAL:HG12	1:B:202:SER:HB3	1.92	0.50
1:C:46:GLU:OE1	1:C:46:GLU:HA	2.11	0.50
1:E:123:GLU:O	1:E:127:MET:HG3	2.11	0.50
1:A:160:ILE:HD11	1:A:193:GLN:O	2.12	0.50
1:B:344:TYR:OH	1:B:355:ASN:ND2	2.45	0.50
1:E:91:VAL:HG11	1:E:101:ILE:CD1	2.41	0.50
1:E:200:LYS:O	1:E:435:LYS:O	2.29	0.50
1:C:96:MET:HE2	1:D:55:ILE:CD1	2.41	0.50
1:E:495:LEU:HD22	1:E:521:LEU:HD23	1.92	0.50
1:B:322:MET:HG3	1:B:323:LEU:N	2.25	0.50
1:F:20:MET:CE	1:F:209:VAL:HG12	2.41	0.50
1:F:322:MET:HG3	1:F:323:LEU:N	2.24	0.50
1:B:313:ASN:ND2	1:B:342:VAL:HG21	2.27	0.50
1:B:20:MET:HE1	1:B:209:VAL:HG12	1.94	0.50
1:B:91:VAL:HG11	1:B:101:ILE:HD13	1.93	0.50
1:B:192:TYR:CD1	1:B:234:TYR:HD2	2.30	0.50
1:C:96:MET:HG3	1:D:55:ILE:CD1	2.42	0.50
1:B:187:ILE:HG23	1:B:206:ILE:CD1	2.41	0.49
1:D:291:ILE:HG22	1:D:293:SER:H	1.76	0.49
1:D:322:MET:HG3	1:D:323:LEU:N	2.25	0.49
1:F:98:ILE:HD11	1:F:113:TRP:CD1	2.47	0.49
1:A:138:GLY:HA3	1:A:154:MET:CE	2.42	0.49
1:A:192:TYR:CD1	1:A:234:TYR:HD2	2.30	0.49
1:A:272:ASN:N	1:A:272:ASN:ND2	2.59	0.49
1:B:254:GLN:HG3	1:B:528:ASN:HB3	1.94	0.49
1:C:312:LEU:HD21	1:C:323:LEU:HD22	1.93	0.49
1:E:38:GLY:O	1:E:39:VAL:C	2.55	0.49
1:D:275:HIS:CD2	1:D:466:CYS:HB2	2.48	0.49
1:E:167:GLU:HG2	1:E:198:ASN:ND2	2.23	0.49
1:F:296:GLN:CG	1:F:322:MET:HB2	2.38	0.49
1:A:140:LEU:HD12	1:A:182:LEU:HD11	1.95	0.49
1:B:91:VAL:HG11	1:B:101:ILE:CD1	2.43	0.49
1:D:394:SER:OG	1:D:395:ASN:N	2.45	0.49
1:E:75:ASN:HD22	1:E:76:ASP:CA	2.26	0.49
1:F:495:LEU:HD22	1:F:521:LEU:HD23	1.95	0.49
1:A:51:THR:O	1:A:55:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PHE:HE2	1:D:77:ARG:HD3	1.78	0.49
1:F:51:THR:O	1:F:55:ILE:HG13	2.12	0.49
1:F:192:TYR:CZ	1:F:410:LYS:HB3	2.47	0.49
1:A:75:ASN:HD22	1:A:76:ASP:CA	2.25	0.49
1:A:127:MET:HB3	1:A:131:MET:HG3	1.94	0.49
1:A:137:VAL:HG23	1:A:178:GLY:HA2	1.94	0.49
1:C:187:ILE:CD1	1:C:225:LEU:HD22	2.43	0.49
1:D:123:GLU:O	1:D:127:MET:HG3	2.13	0.49
1:F:91:VAL:HG11	1:F:101:ILE:HD13	1.94	0.49
1:B:193:GLN:NE2	1:B:362:GLN:NE2	2.58	0.49
1:C:137:VAL:HG23	1:C:178:GLY:HA2	1.95	0.49
1:C:369:ASN:O	1:C:370:SER:C	2.56	0.49
1:D:254:GLN:HG3	1:D:528:ASN:HB3	1.95	0.49
1:D:369:ASN:O	1:D:370:SER:C	2.55	0.49
1:E:437:THR:HG23	1:E:440:THR:N	2.24	0.49
1:A:20:MET:CE	1:A:209:VAL:HG12	2.43	0.49
1:B:36:GLN:HG2	1:B:68:HIS:NE2	2.27	0.49
1:C:275:HIS:CD2	1:C:466:CYS:HB2	2.48	0.49
1:B:275:HIS:CD2	1:B:466:CYS:HB2	2.48	0.49
1:C:416:THR:HA	1:C:420:ASP:OD1	2.13	0.49
1:D:20:MET:HE1	1:D:209:VAL:HG12	1.94	0.49
1:D:437:THR:HG23	1:D:440:THR:N	2.24	0.49
1:F:78:ILE:HG13	1:F:89:ILE:HD12	1.95	0.49
1:D:74:ILE:HD11	1:D:84:ILE:HD11	1.93	0.48
1:E:312:LEU:HD21	1:E:323:LEU:HD22	1.95	0.48
1:E:349:THR:HB	1:F:298:GLU:HG3	1.95	0.48
1:D:200:LYS:O	1:D:435:LYS:O	2.31	0.48
1:E:254:GLN:HG3	1:E:528:ASN:HB3	1.95	0.48
1:F:38:GLY:O	1:F:40:THR:HG23	2.13	0.48
1:F:312:LEU:HD21	1:F:323:LEU:HD22	1.94	0.48
1:F:479:GLN:HE21	1:F:484:ASN:H	1.61	0.48
1:E:276:GLN:HA	1:E:276:GLN:HE21	1.78	0.48
1:B:65:CYS:HB3	1:B:70:VAL:O	2.14	0.48
1:C:20:MET:HE1	1:C:209:VAL:HG12	1.95	0.48
1:C:167:GLU:HG2	1:C:198:ASN:ND2	2.24	0.48
1:C:437:THR:HG23	1:C:440:THR:N	2.20	0.48
1:E:275:HIS:CD2	1:E:466:CYS:HB2	2.48	0.48
1:E:534:ALA:N	1:E:535:PRO:HD2	2.28	0.48
1:F:28:TYR:CZ	1:F:64:LEU:HG	2.49	0.48
1:F:187:ILE:HG12	1:F:206:ILE:HD13	1.94	0.48
1:C:28:TYR:CZ	1:C:64:LEU:HG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLY:HA3	1:C:154:MET:CE	2.43	0.48
1:C:192:TYR:CZ	1:C:410:LYS:HB3	2.47	0.48
1:F:189:ARG:O	1:F:193:GLN:HG2	2.14	0.48
1:A:20:MET:HE1	1:A:209:VAL:HG12	1.95	0.48
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.44	0.48
1:B:10:TYR:O	1:B:205:GLY:HA3	2.14	0.48
1:D:479:GLN:HA	1:D:480:PRO:HD3	1.72	0.48
1:B:312:LEU:HD21	1:B:323:LEU:HD22	1.94	0.48
1:C:79:ASP:HB3	1:D:79:ASP:H	1.78	0.48
1:D:50:ASP:O	1:D:52:LYS:N	2.46	0.48
1:E:257:ILE:HG12	1:E:475:MET:HE1	1.96	0.48
1:E:280:ALA:O	1:E:284:LEU:HB2	2.14	0.48
1:F:91:VAL:HG11	1:F:101:ILE:CD1	2.44	0.48
1:A:138:GLY:HA3	1:A:154:MET:HE2	1.96	0.48
1:B:50:ASP:O	1:B:52:LYS:N	2.47	0.48
1:C:138:GLY:HA3	1:C:154:MET:HE2	1.96	0.48
1:A:280:ALA:O	1:A:284:LEU:HB2	2.14	0.48
1:E:369:ASN:O	1:E:370:SER:C	2.56	0.48
1:F:75:ASN:HD22	1:F:76:ASP:CA	2.26	0.48
1:F:280:ALA:O	1:F:284:LEU:HB2	2.14	0.48
1:F:369:ASN:O	1:F:370:SER:C	2.56	0.48
1:A:349:THR:OG1	1:C:297:SER:HB2	2.13	0.47
1:B:98:ILE:N	1:B:99:PRO:HD2	2.29	0.47
1:C:10:TYR:O	1:C:205:GLY:HA3	2.14	0.47
1:C:102:ARG:HH11	1:C:107:PRO:HA	1.79	0.47
1:C:200:LYS:O	1:C:435:LYS:O	2.31	0.47
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.68	0.47
1:D:66:HIS:HE1	1:D:87:ASP:OD1	1.98	0.47
1:B:75:ASN:HD22	1:B:76:ASP:CA	2.26	0.47
1:D:191:LEU:HD12	1:D:191:LEU:HA	1.73	0.47
1:F:66:HIS:HE1	1:F:87:ASP:OD1	1.97	0.47
1:F:534:ALA:N	1:F:535:PRO:HD2	2.29	0.47
1:A:275:HIS:CD2	1:A:466:CYS:HB2	2.49	0.47
1:A:369:ASN:O	1:A:370:SER:C	2.57	0.47
1:B:433:LEU:O	1:B:434:SER:CB	2.62	0.47
1:C:40:THR:HG21	1:C:226:ARG:HH21	1.78	0.47
1:E:190:VAL:O	1:E:194:CYS:HB2	2.13	0.47
1:E:202:SER:OG	1:E:434:SER:HA	2.14	0.47
1:A:479:GLN:HE21	1:A:484:ASN:H	1.62	0.47
1:C:102:ARG:NE	1:C:130:ASP:O	2.46	0.47
1:C:276:GLN:HE21	1:C:276:GLN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:TYR:CZ	1:D:64:LEU:HG	2.49	0.47
1:E:272:ASN:N	1:E:272:ASN:ND2	2.61	0.47
1:E:394:SER:OG	1:E:395:ASN:N	2.46	0.47
1:B:190:VAL:O	1:B:194:CYS:HB2	2.14	0.47
1:C:65:CYS:HB3	1:C:70:VAL:O	2.14	0.47
1:C:420:ASP:OD2	1:C:497:LYS:HD3	2.14	0.47
1:D:187:ILE:CD1	1:D:225:LEU:HD22	2.45	0.47
1:D:265:PRO:O	1:D:288:SER:HB2	2.14	0.47
1:D:272:ASN:N	1:D:272:ASN:ND2	2.61	0.47
1:D:280:ALA:O	1:D:284:LEU:HB2	2.15	0.47
1:A:10:TYR:O	1:A:205:GLY:HA3	2.15	0.47
1:B:276:GLN:HA	1:B:276:GLN:HE21	1.79	0.47
1:D:165:ALA:O	1:D:169:ASN:HB2	2.15	0.47
1:E:192:TYR:CD1	1:E:234:TYR:HD2	2.33	0.47
1:B:534:ALA:N	1:B:535:PRO:HD2	2.30	0.47
1:C:495:LEU:HD22	1:C:521:LEU:HD23	1.96	0.47
1:D:46:GLU:HB2	1:D:54:PHE:CD2	2.50	0.47
1:D:65:CYS:HB3	1:D:70:VAL:O	2.15	0.47
1:E:247:LEU:HD12	1:E:247:LEU:HA	1.66	0.47
1:F:200:LYS:O	1:F:435:LYS:O	2.31	0.47
1:A:165:ALA:O	1:A:169:ASN:HB2	2.14	0.47
1:D:75:ASN:HD22	1:D:76:ASP:N	2.13	0.47
1:D:160:ILE:HD11	1:D:193:GLN:O	2.15	0.47
1:E:74:ILE:HD11	1:E:84:ILE:HD11	1.96	0.47
1:E:322:MET:HG3	1:E:323:LEU:N	2.30	0.47
1:F:192:TYR:CD1	1:F:234:TYR:HD2	2.33	0.47
1:A:296:GLN:CG	1:A:322:MET:HB2	2.41	0.47
1:A:416:THR:HA	1:A:420:ASP:OD1	2.14	0.47
1:B:40:THR:HG21	1:B:226:ARG:HH21	1.80	0.47
1:B:78:ILE:H	1:B:78:ILE:CD1	2.24	0.47
1:B:437:THR:O	1:B:439:GLY:N	2.48	0.47
1:C:339:PHE:CD2	1:C:341:PRO:HG3	2.50	0.47
1:D:187:ILE:HG12	1:D:206:ILE:HD13	1.97	0.47
1:D:347:THR:O	1:D:350:ARG:N	2.44	0.47
1:E:5:LYS:HE3	1:E:133:ASP:CG	2.40	0.47
1:E:91:VAL:HG11	1:E:101:ILE:HD13	1.95	0.47
1:A:187:ILE:HG12	1:A:206:ILE:HD13	1.96	0.46
1:C:79:ASP:HB3	1:D:79:ASP:N	2.29	0.46
1:D:20:MET:CE	1:D:209:VAL:HG12	2.45	0.46
1:D:192:TYR:CD1	1:D:234:TYR:HD2	2.32	0.46
1:F:10:TYR:O	1:F:205:GLY:HA3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:HD21	1:D:83:ALA:CA	2.43	0.46
1:C:517:LEU:O	1:C:517:LEU:HD23	2.15	0.46
1:E:65:CYS:HB3	1:E:70:VAL:O	2.15	0.46
1:A:200:LYS:O	1:A:435:LYS:O	2.33	0.46
1:B:127:MET:HE3	1:B:131:MET:CB	2.46	0.46
1:C:77:ARG:HD3	1:C:80:VAL:HG21	1.97	0.46
1:C:102:ARG:NH1	1:C:107:PRO:HA	2.30	0.46
1:E:20:MET:CE	1:E:209:VAL:HG12	2.46	0.46
1:C:192:TYR:CD1	1:C:234:TYR:HD2	2.34	0.46
1:D:51:THR:HB	1:D:77:ARG:NH2	2.30	0.46
1:E:55:ILE:HG12	1:E:80:VAL:HG13	1.98	0.46
1:F:138:GLY:HA3	1:F:154:MET:HE2	1.97	0.46
1:C:20:MET:CE	1:C:209:VAL:HG12	2.44	0.46
1:F:65:CYS:HB3	1:F:70:VAL:O	2.16	0.46
1:B:89:ILE:O	1:B:89:ILE:HG13	2.16	0.46
1:E:416:THR:HA	1:E:420:ASP:OD1	2.16	0.46
1:F:127:MET:HB3	1:F:131:MET:HG3	1.97	0.46
1:F:160:ILE:HD11	1:F:193:GLN:O	2.16	0.46
1:A:256:ILE:CG2	1:A:475:MET:HE3	2.46	0.46
1:E:50:ASP:O	1:E:52:LYS:N	2.49	0.46
1:C:66:HIS:HE1	1:C:87:ASP:OD1	1.98	0.46
1:D:98:ILE:N	1:D:99:PRO:HD2	2.31	0.46
1:D:533:TRP:C	1:D:535:PRO:HD2	2.41	0.46
1:E:20:MET:HE1	1:E:209:VAL:HG12	1.98	0.46
1:A:437:THR:O	1:A:439:GLY:HA2	2.16	0.46
1:B:189:ARG:O	1:B:193:GLN:HG2	2.16	0.46
1:C:198:ASN:HA	1:C:441:SER:HB2	1.98	0.46
1:F:272:ASN:N	1:F:272:ASN:ND2	2.63	0.46
1:F:494:MET:HE3	1:F:494:MET:HB3	1.82	0.46
1:C:314:THR:HG22	1:C:315:GLY:N	2.31	0.46
1:E:529:THR:O	1:E:532:THR:HB	2.16	0.46
1:F:339:PHE:CZ	1:F:341:PRO:HG3	2.37	0.46
1:F:299:VAL:HG21	1:F:326:ALA:HB2	1.98	0.45
1:B:357:LEU:HD23	1:B:360:PHE:CD1	2.51	0.45
1:B:495:LEU:HD22	1:B:521:LEU:CD2	2.46	0.45
1:D:138:GLY:HA3	1:D:154:MET:CE	2.46	0.45
1:D:495:LEU:HD22	1:D:521:LEU:HD23	1.99	0.45
1:F:40:THR:HG21	1:F:226:ARG:HH21	1.80	0.45
1:B:112:GLY:HA2	1:B:134:TYR:O	2.16	0.45
1:B:229:ILE:CG2	1:B:433:LEU:HD11	2.47	0.45
1:B:272:ASN:ND2	1:B:272:ASN:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASP:O	1:D:52:LYS:HB3	2.15	0.45
1:C:96:MET:CE	1:D:55:ILE:HD11	2.44	0.45
1:E:165:ALA:O	1:E:169:ASN:HB2	2.17	0.45
1:A:10:TYR:O	1:A:11:SER:C	2.59	0.45
1:A:512:SER:HA	1:A:515:VAL:HG13	1.99	0.45
1:B:346:ALA:O	1:B:348:GLU:N	2.48	0.45
1:B:513:PHE:C	1:B:513:PHE:CD2	2.93	0.45
1:C:50:ASP:O	1:C:52:LYS:N	2.49	0.45
1:C:52:LYS:HB3	1:D:94:ASP:C	2.38	0.45
1:D:138:GLY:HA3	1:D:154:MET:HE2	1.98	0.45
1:E:193:GLN:NE2	1:E:362:GLN:NE2	2.60	0.45
1:B:165:ALA:O	1:B:169:ASN:HB2	2.16	0.45
1:B:266:LEU:HD11	1:B:291:ILE:HG13	1.98	0.45
1:B:318:ALA:HB1	1:B:322:MET:HG2	1.98	0.45
1:E:187:ILE:HG23	1:E:206:ILE:CD1	2.46	0.45
1:F:394:SER:OG	1:F:395:ASN:N	2.49	0.45
1:A:55:ILE:HG12	1:A:80:VAL:HG13	1.98	0.45
1:A:80:VAL:O	1:A:84:ILE:HG12	2.17	0.45
1:A:534:ALA:N	1:A:535:PRO:HD2	2.32	0.45
1:B:10:TYR:O	1:B:11:SER:C	2.59	0.45
1:B:226:ARG:HA	1:B:226:ARG:HD3	1.70	0.45
1:B:427:ILE:HG22	1:B:427:ILE:O	2.17	0.45
1:C:70:VAL:HA	1:C:71:PRO:HD3	1.85	0.45
1:E:40:THR:HG21	1:E:226:ARG:HH21	1.81	0.45
1:E:98:ILE:N	1:E:99:PRO:HD2	2.31	0.45
1:C:394:SER:OG	1:C:395:ASN:N	2.50	0.45
1:E:318:ALA:HB1	1:E:322:MET:HG2	1.99	0.45
1:F:165:ALA:O	1:F:169:ASN:HB2	2.16	0.45
1:F:299:VAL:HG13	1:F:329:ALA:CB	2.46	0.45
1:F:333:VAL:O	1:F:333:VAL:HG12	2.17	0.45
1:F:533:TRP:C	1:F:535:PRO:HD2	2.42	0.45
1:A:276:GLN:HE21	1:A:276:GLN:HA	1.81	0.45
1:A:346:ALA:C	1:A:347:THR:CG2	2.89	0.45
1:E:154:MET:HG3	1:E:155:GLY:N	2.30	0.45
1:F:55:ILE:HG12	1:F:80:VAL:HG13	1.98	0.45
1:F:479:GLN:HA	1:F:480:PRO:HD3	1.70	0.45
1:B:299:VAL:HG21	1:B:326:ALA:HB2	1.99	0.45
1:B:339:PHE:CD2	1:B:341:PRO:HG3	2.52	0.45
1:C:98:ILE:N	1:C:99:PRO:HD2	2.32	0.45
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.70	0.45
1:C:229:ILE:CG2	1:C:433:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:TYR:CZ	1:D:410:LYS:HB3	2.52	0.45
1:B:89:ILE:O	1:B:89:ILE:CG1	2.66	0.45
1:B:479:GLN:HE21	1:B:484:ASN:H	1.65	0.45
1:C:165:ALA:O	1:C:169:ASN:HB2	2.17	0.45
1:C:280:ALA:O	1:C:284:LEU:HB2	2.17	0.45
1:D:137:VAL:HG22	1:D:177:VAL:O	2.17	0.45
1:D:296:GLN:CG	1:D:322:MET:HB2	2.44	0.45
1:E:314:THR:HG21	1:E:354:ASN:OD1	2.16	0.45
1:F:314:THR:HG22	1:F:315:GLY:N	2.32	0.45
1:B:16:THR:HB	1:B:27:LEU:HD11	1.99	0.44
1:B:55:ILE:HG12	1:B:80:VAL:HG13	1.98	0.44
1:C:140:LEU:HD12	1:C:182:LEU:HD11	1.99	0.44
1:F:50:ASP:O	1:F:52:LYS:N	2.50	0.44
1:F:276:GLN:HA	1:F:276:GLN:HE21	1.82	0.44
1:F:377:ALA:O	1:F:378:GLU:HB2	2.17	0.44
1:A:102:ARG:NH1	1:A:107:PRO:HA	2.32	0.44
1:B:78:ILE:HD12	1:B:78:ILE:N	2.27	0.44
1:B:407:PHE:O	1:B:410:LYS:NZ	2.45	0.44
1:B:416:THR:HA	1:B:420:ASP:OD1	2.17	0.44
1:E:189:ARG:O	1:E:193:GLN:HG2	2.17	0.44
1:E:192:TYR:CZ	1:E:410:LYS:HB3	2.52	0.44
1:F:191:LEU:HD12	1:F:191:LEU:HA	1.77	0.44
1:A:75:ASN:HA	1:A:76:ASP:HA	1.82	0.44
1:A:313:ASN:ND2	1:A:342:VAL:CG2	2.79	0.44
1:B:36:GLN:H	1:B:36:GLN:HG3	1.52	0.44
1:B:140:LEU:HD12	1:B:182:LEU:HD11	1.99	0.44
1:B:345:SER:C	1:B:347:THR:N	2.74	0.44
1:B:533:TRP:C	1:B:535:PRO:HD2	2.43	0.44
1:E:187:ILE:HD12	1:E:225:LEU:HD22	2.00	0.44
1:F:339:PHE:CD2	1:F:341:PRO:CG	2.96	0.44
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.71	0.44
1:A:479:GLN:HA	1:A:480:PRO:HD3	1.70	0.44
1:B:52:LYS:HB2	1:F:97:PRO:HD3	2.00	0.44
1:D:187:ILE:HD12	1:D:225:LEU:HD22	1.99	0.44
1:D:229:ILE:CG2	1:D:433:LEU:HD11	2.47	0.44
1:D:333:VAL:HG12	1:D:333:VAL:O	2.17	0.44
1:F:416:THR:HA	1:F:420:ASP:OD1	2.17	0.44
1:A:50:ASP:O	1:A:52:LYS:N	2.51	0.44
1:B:266:LEU:CD1	1:B:291:ILE:HG13	2.48	0.44
1:B:341:PRO:HG2	1:B:376:LEU:HD11	1.99	0.44
1:B:343:GLY:O	1:B:350:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ALA:HA	1:D:104:LEU:HD21	2.00	0.44
1:C:512:SER:HA	1:C:515:VAL:HG13	2.00	0.44
1:D:318:ALA:HB1	1:D:322:MET:HG2	1.99	0.44
1:D:534:ALA:N	1:D:535:PRO:HD2	2.32	0.44
1:A:102:ARG:HH11	1:A:107:PRO:HA	1.81	0.44
1:A:394:SER:OG	1:A:395:ASN:N	2.50	0.44
1:B:187:ILE:CD1	1:B:225:LEU:HD22	2.47	0.44
1:C:74:ILE:HD11	1:C:84:ILE:HD11	1.98	0.44
1:F:495:LEU:HD22	1:F:521:LEU:CD2	2.48	0.44
1:B:314:THR:HG21	1:B:354:ASN:OD1	2.17	0.44
1:C:137:VAL:HG22	1:C:177:VAL:O	2.17	0.44
1:D:50:ASP:C	1:D:52:LYS:H	2.26	0.44
1:F:437:THR:O	1:F:439:GLY:N	2.50	0.44
1:F:524:LEU:HD12	1:F:524:LEU:HA	1.69	0.44
1:A:78:ILE:HG13	1:A:89:ILE:HD12	1.99	0.44
1:B:394:SER:OG	1:B:395:ASN:N	2.50	0.44
1:C:299:VAL:HG13	1:C:329:ALA:CB	2.48	0.44
1:E:266:LEU:HD11	1:E:291:ILE:HG13	2.00	0.44
1:A:127:MET:HE3	1:A:131:MET:HB3	1.99	0.44
1:A:494:MET:HE3	1:A:494:MET:HB3	1.85	0.44
1:A:533:TRP:C	1:A:535:PRO:HD2	2.43	0.44
1:C:318:ALA:HB1	1:C:322:MET:HG2	2.00	0.44
1:D:46:GLU:HB2	1:D:54:PHE:CZ	2.52	0.44
1:A:299:VAL:HG13	1:A:329:ALA:CB	2.47	0.43
1:B:102:ARG:HH11	1:B:107:PRO:HA	1.83	0.43
1:B:191:LEU:HD12	1:B:191:LEU:HA	1.70	0.43
1:C:104:LEU:HD11	1:D:83:ALA:HB2	2.00	0.43
1:D:512:SER:HA	1:D:515:VAL:HG13	2.00	0.43
1:A:40:THR:HG21	1:A:226:ARG:HH21	1.83	0.43
1:A:90:HIS:CD2	1:A:134:TYR:OH	2.61	0.43
1:A:98:ILE:N	1:A:99:PRO:HD2	2.33	0.43
1:A:187:ILE:HD12	1:A:225:LEU:HD22	2.00	0.43
1:A:192:TYR:CZ	1:A:410:LYS:HB3	2.53	0.43
1:A:314:THR:HG22	1:A:315:GLY:N	2.33	0.43
1:D:70:VAL:HA	1:D:71:PRO:HD3	1.86	0.43
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.79	0.43
1:F:257:ILE:HG12	1:F:475:MET:HE1	1.98	0.43
1:A:299:VAL:HG21	1:A:326:ALA:HB2	2.00	0.43
1:A:343:GLY:C	1:A:345:SER:N	2.76	0.43
1:B:70:VAL:HA	1:B:71:PRO:HD3	1.86	0.43
1:B:529:THR:O	1:B:532:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:THR:N	1:E:530:PRO:CD	2.81	0.43
1:F:70:VAL:HA	1:F:71:PRO:HD3	1.85	0.43
1:F:187:ILE:HD12	1:F:225:LEU:HD22	2.00	0.43
1:A:187:ILE:CD1	1:A:225:LEU:HD22	2.48	0.43
1:A:513:PHE:CD2	1:A:513:PHE:C	2.96	0.43
1:B:278:PHE:CE1	1:B:518:ILE:HD11	2.54	0.43
1:B:298:GLU:HG2	1:C:347:THR:CG2	2.47	0.43
1:C:533:TRP:C	1:C:535:PRO:HD2	2.42	0.43
1:D:40:THR:HG21	1:D:226:ARG:HH21	1.82	0.43
1:D:129:PRO:C	1:D:131:MET:H	2.26	0.43
1:D:154:MET:HG3	1:D:155:GLY:N	2.33	0.43
1:E:13:TYR:O	1:E:207:CYS:HA	2.19	0.43
1:E:89:ILE:O	1:E:89:ILE:HG13	2.18	0.43
1:B:134:TYR:CD1	1:B:134:TYR:C	2.95	0.43
1:B:299:VAL:HG13	1:B:329:ALA:CB	2.48	0.43
1:B:314:THR:HG22	1:B:315:GLY:N	2.34	0.43
1:C:534:ALA:N	1:C:535:PRO:HD2	2.33	0.43
1:E:266:LEU:CD1	1:E:291:ILE:HG13	2.48	0.43
1:E:479:GLN:HA	1:E:480:PRO:HD3	1.69	0.43
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.67	0.43
1:C:89:ILE:HG13	1:C:89:ILE:O	2.17	0.43
1:E:10:TYR:O	1:E:11:SER:C	2.61	0.43
1:A:189:ARG:O	1:A:193:GLN:HG2	2.19	0.43
1:B:46:GLU:HB2	1:B:54:PHE:CD2	2.54	0.43
1:B:102:ARG:NH1	1:B:107:PRO:HA	2.33	0.43
1:B:243:THR:HG23	1:B:446:PRO:HG3	2.01	0.43
1:C:479:GLN:HE21	1:C:484:ASN:H	1.65	0.43
1:D:299:VAL:HG13	1:D:329:ALA:CB	2.48	0.43
1:E:299:VAL:HG13	1:E:329:ALA:CB	2.49	0.43
1:F:265:PRO:O	1:F:288:SER:HB2	2.19	0.43
1:F:357:LEU:HD23	1:F:360:PHE:CD1	2.54	0.43
1:A:65:CYS:HB3	1:A:70:VAL:O	2.19	0.43
1:A:519:ASP:OD1	1:B:509:GLY:C	2.62	0.43
1:B:80:VAL:O	1:B:84:ILE:HG12	2.19	0.43
1:B:90:HIS:CD2	1:B:134:TYR:OH	2.62	0.43
1:B:187:ILE:HD12	1:B:225:LEU:HD22	2.01	0.43
1:B:517:LEU:HD23	1:B:517:LEU:O	2.18	0.43
1:D:318:ALA:HA	1:D:319:PRO:HD3	1.82	0.43
1:E:79:ASP:OD1	1:E:80:VAL:N	2.50	0.43
1:E:427:ILE:HG22	1:E:427:ILE:O	2.19	0.43
1:E:533:TRP:C	1:E:535:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:HB1	1:A:322:MET:HG2	2.00	0.43
1:B:344:TYR:CD2	1:B:354:ASN:ND2	2.81	0.43
1:C:154:MET:HG3	1:C:155:GLY:N	2.33	0.43
1:C:272:ASN:N	1:C:272:ASN:ND2	2.63	0.43
1:D:16:THR:HB	1:D:27:LEU:HD11	1.99	0.43
1:D:508:ASN:HB3	1:E:523:ARG:HH11	1.82	0.43
1:E:127:MET:HE3	1:E:131:MET:HG3	2.01	0.43
1:E:187:ILE:CD1	1:E:225:LEU:HD22	2.49	0.43
1:E:357:LEU:HD23	1:E:360:PHE:CD1	2.54	0.43
1:A:137:VAL:HG22	1:A:177:VAL:O	2.19	0.43
1:A:333:VAL:O	1:A:333:VAL:HG12	2.18	0.43
1:B:529:THR:N	1:B:530:PRO:CD	2.82	0.43
1:E:512:SER:HA	1:E:515:VAL:HG13	2.01	0.43
1:F:198:ASN:HA	1:F:441:SER:HB2	2.01	0.43
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.75	0.42
1:B:75:ASN:HA	1:B:76:ASP:HA	1.81	0.42
1:C:313:ASN:ND2	1:C:342:VAL:HG21	2.33	0.42
1:D:75:ASN:HD22	1:D:75:ASN:C	2.27	0.42
1:E:89:ILE:O	1:E:89:ILE:CG1	2.66	0.42
1:E:119:GLU:H	1:E:119:GLU:CD	2.27	0.42
1:F:187:ILE:CD1	1:F:225:LEU:HD22	2.48	0.42
1:A:274:VAL:CG1	1:C:292:MET:HG3	2.42	0.42
1:A:313:ASN:HD22	1:A:342:VAL:HG21	1.80	0.42
1:C:341:PRO:HG2	1:C:376:LEU:HD11	2.00	0.42
1:C:512:SER:O	1:C:513:PHE:C	2.62	0.42
1:D:80:VAL:O	1:D:84:ILE:HG12	2.18	0.42
1:D:347:THR:C	1:D:349:THR:N	2.77	0.42
1:E:112:GLY:HA2	1:E:134:TYR:O	2.19	0.42
1:E:299:VAL:HG21	1:E:326:ALA:HB2	2.01	0.42
1:A:134:TYR:CD1	1:A:134:TYR:C	2.97	0.42
1:B:198:ASN:HA	1:B:441:SER:HB2	2.01	0.42
1:C:76:ASP:O	1:C:78:ILE:HD12	2.20	0.42
1:C:187:ILE:HD12	1:C:225:LEU:HD22	2.00	0.42
1:D:140:LEU:HD12	1:D:182:LEU:HD11	2.00	0.42
1:E:75:ASN:ND2	1:E:75:ASN:C	2.77	0.42
1:F:134:TYR:CD1	1:F:134:TYR:C	2.97	0.42
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.71	0.42
1:B:283:THR:HG23	1:B:474:CYS:SG	2.59	0.42
1:B:512:SER:HA	1:B:515:VAL:HG13	2.01	0.42
1:D:102:ARG:NH1	1:D:107:PRO:HA	2.35	0.42
1:D:189:ARG:O	1:D:193:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:PRO:HG3	1:D:376:LEU:HD11	2.01	0.42
1:E:302:LEU:HD12	1:E:302:LEU:HA	1.85	0.42
1:E:333:VAL:HG12	1:E:333:VAL:O	2.20	0.42
1:B:75:ASN:ND2	1:B:76:ASP:CB	2.78	0.42
1:B:269:HIS:HB2	1:B:292:MET:SD	2.59	0.42
1:B:296:GLN:CG	1:B:322:MET:HB2	2.45	0.42
1:E:134:TYR:CD1	1:E:134:TYR:C	2.98	0.42
1:F:513:PHE:CD2	1:F:513:PHE:C	2.98	0.42
1:A:229:ILE:CG2	1:A:433:LEU:HD11	2.49	0.42
1:A:357:LEU:HD23	1:A:360:PHE:CD1	2.55	0.42
1:A:519:ASP:OD1	1:B:511:GLY:N	2.53	0.42
1:C:524:LEU:HD12	1:C:524:LEU:HA	1.80	0.42
1:F:229:ILE:CG2	1:F:433:LEU:HD11	2.49	0.42
1:F:344:TYR:CE2	1:F:376:LEU:HA	2.51	0.42
1:A:427:ILE:O	1:A:427:ILE:HG22	2.20	0.42
1:A:434:SER:OG	1:A:434:SER:O	2.36	0.42
1:B:50:ASP:C	1:B:52:LYS:H	2.28	0.42
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.70	0.42
1:D:193:GLN:NE2	1:D:362:GLN:NE2	2.61	0.42
1:A:198:ASN:HA	1:A:441:SER:HB2	2.02	0.42
1:B:119:GLU:H	1:B:119:GLU:CD	2.28	0.42
1:C:357:LEU:HD23	1:C:360:PHE:CD1	2.54	0.42
1:D:134:TYR:CD1	1:D:134:TYR:C	2.97	0.42
1:D:257:ILE:HG12	1:D:475:MET:HE1	2.01	0.42
1:A:529:THR:N	1:A:530:PRO:CD	2.83	0.42
1:C:52:LYS:HB2	1:D:95:ASP:O	2.20	0.42
1:C:182:LEU:HD12	1:C:182:LEU:HA	1.88	0.42
1:D:75:ASN:ND2	1:D:75:ASN:C	2.75	0.42
1:E:46:GLU:HB2	1:E:54:PHE:CZ	2.55	0.42
1:B:422:ILE:HG22	1:B:486:PHE:CE1	2.49	0.42
1:C:407:PHE:O	1:C:410:LYS:NZ	2.44	0.42
1:D:416:THR:HA	1:D:420:ASP:OD1	2.19	0.42
1:E:75:ASN:ND2	1:E:76:ASP:CB	2.79	0.42
1:C:296:GLN:CG	1:C:322:MET:HB2	2.43	0.41
1:D:119:GLU:CD	1:D:119:GLU:H	2.28	0.41
1:E:269:HIS:HB2	1:E:292:MET:SD	2.60	0.41
1:F:89:ILE:O	1:F:89:ILE:HG13	2.19	0.41
1:A:345:SER:OG	1:A:346:ALA:N	2.51	0.41
1:B:31:VAL:O	1:B:35:LEU:HG	2.20	0.41
1:C:265:PRO:O	1:C:288:SER:HB2	2.19	0.41
1:D:256:ILE:HD12	1:D:488:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:THR:HG23	1:E:446:PRO:HG3	2.02	0.41
1:E:513:PHE:CD2	1:E:513:PHE:C	2.98	0.41
1:F:5:LYS:HE3	1:F:133:ASP:CG	2.45	0.41
1:A:89:ILE:O	1:A:89:ILE:HG13	2.20	0.41
1:B:74:ILE:CD1	1:B:84:ILE:HD11	2.50	0.41
1:C:75:ASN:HA	1:C:76:ASP:HA	1.62	0.41
1:C:134:TYR:CD1	1:C:134:TYR:C	2.98	0.41
1:D:314:THR:HG22	1:D:315:GLY:N	2.34	0.41
1:E:75:ASN:HD22	1:E:76:ASP:N	2.18	0.41
1:B:79:ASP:OD1	1:B:80:VAL:N	2.51	0.41
1:C:50:ASP:C	1:C:52:LYS:H	2.29	0.41
1:C:79:ASP:HB3	1:D:79:ASP:HB3	2.02	0.41
1:C:529:THR:O	1:C:532:THR:HB	2.20	0.41
1:D:495:LEU:HD22	1:D:521:LEU:CD2	2.50	0.41
1:E:102:ARG:NH1	1:E:107:PRO:HA	2.35	0.41
1:F:16:THR:HB	1:F:27:LEU:HD11	2.03	0.41
1:F:99:PRO:HA	1:F:131:MET:HE3	2.01	0.41
1:F:254:GLN:O	1:F:528:ASN:ND2	2.54	0.41
1:F:493:VAL:O	1:F:497:LYS:HB2	2.20	0.41
1:B:333:VAL:HG12	1:B:333:VAL:O	2.21	0.41
1:C:46:GLU:HB2	1:C:54:PHE:CZ	2.54	0.41
1:C:358:LEU:HD13	1:C:409:TYR:CE2	2.55	0.41
1:D:10:TYR:O	1:D:11:SER:C	2.63	0.41
1:D:276:GLN:HA	1:D:276:GLN:NE2	2.34	0.41
1:E:226:ARG:HA	1:E:226:ARG:HD3	1.71	0.41
1:E:339:PHE:CD2	1:E:341:PRO:HG3	2.55	0.41
1:F:75:ASN:HA	1:F:76:ASP:HA	1.84	0.41
1:F:90:HIS:CD2	1:F:134:TYR:OH	2.64	0.41
1:A:66:HIS:HE1	1:A:87:ASP:OD1	2.03	0.41
1:A:292:MET:HG3	1:B:274:VAL:HG13	2.02	0.41
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.89	0.41
1:B:96:MET:HE1	1:F:79:ASP:HB2	2.03	0.41
1:B:256:ILE:CG2	1:B:475:MET:HE3	2.50	0.41
1:D:78:ILE:HG13	1:D:89:ILE:HD12	2.01	0.41
1:D:98:ILE:HD11	1:D:113:TRP:CD1	2.56	0.41
1:E:58:ALA:HB1	1:E:84:ILE:CD1	2.50	0.41
1:F:98:ILE:N	1:F:99:PRO:HD2	2.36	0.41
1:F:318:ALA:HB1	1:F:322:MET:HG2	2.02	0.41
1:A:269:HIS:HB2	1:A:292:MET:SD	2.61	0.41
1:C:427:ILE:HG22	1:C:427:ILE:O	2.21	0.41
1:F:40:THR:CG2	1:F:226:ARG:HH21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:ILE:HD12	1:F:488:ALA:HA	2.02	0.41
1:A:256:ILE:HD12	1:A:488:ALA:HA	2.02	0.41
1:A:305:ILE:HG23	1:A:306:PRO:HD2	2.02	0.41
1:B:156:THR:HG22	1:B:194:CYS:SG	2.61	0.41
1:C:75:ASN:HD22	1:C:76:ASP:N	2.19	0.41
1:C:187:ILE:HG12	1:C:206:ILE:HD13	2.03	0.41
1:C:269:HIS:HB2	1:C:292:MET:SD	2.60	0.41
1:C:299:VAL:HG21	1:C:326:ALA:HB2	2.02	0.41
1:E:58:ALA:CB	1:E:84:ILE:HD13	2.51	0.41
1:E:102:ARG:HH11	1:E:107:PRO:HA	1.85	0.41
1:F:137:VAL:HG22	1:F:177:VAL:O	2.21	0.41
1:A:107:PRO:O	1:A:108:ASP:CB	2.68	0.41
1:A:272:ASN:ND2	1:A:272:ASN:H	2.19	0.41
1:B:377:ALA:O	1:B:378:GLU:HB2	2.20	0.41
1:C:79:ASP:OD1	1:C:80:VAL:N	2.51	0.41
1:C:189:ARG:O	1:C:193:GLN:HG2	2.21	0.41
1:D:82:MET:HE3	1:D:82:MET:HB2	1.95	0.41
1:D:247:LEU:HD12	1:D:247:LEU:HA	1.66	0.41
1:D:299:VAL:HG21	1:D:326:ALA:HB2	2.02	0.41
1:D:377:ALA:O	1:D:378:GLU:HB2	2.21	0.41
1:E:341:PRO:HG2	1:E:376:LEU:HD11	2.02	0.41
1:E:495:LEU:HD22	1:E:521:LEU:CD2	2.51	0.41
1:E:517:LEU:O	1:E:517:LEU:HD23	2.21	0.41
1:F:80:VAL:O	1:F:84:ILE:HG12	2.20	0.41
1:B:467:SER:HB2	1:B:496:TYR:CE1	2.56	0.41
1:C:247:LEU:HD12	1:C:247:LEU:HA	1.66	0.41
1:D:78:ILE:H	1:D:78:ILE:CD1	2.26	0.41
1:D:198:ASN:HA	1:D:441:SER:HB2	2.03	0.41
1:E:50:ASP:C	1:E:52:LYS:H	2.29	0.41
1:A:98:ILE:HD11	1:A:113:TRP:CD1	2.56	0.40
1:A:523:ARG:NH1	1:B:508:ASN:O	2.48	0.40
1:B:40:THR:CG2	1:B:226:ARG:HH21	2.34	0.40
1:C:437:THR:O	1:C:439:GLY:N	2.54	0.40
1:D:102:ARG:HH11	1:D:107:PRO:HA	1.86	0.40
1:E:305:ILE:HG23	1:E:306:PRO:HD2	2.02	0.40
1:A:50:ASP:C	1:A:52:LYS:H	2.29	0.40
1:A:70:VAL:HA	1:A:71:PRO:HD3	1.87	0.40
1:B:480:PRO:O	1:B:481:SER:C	2.64	0.40
1:C:10:TYR:O	1:C:11:SER:C	2.64	0.40
1:C:529:THR:N	1:C:530:PRO:CD	2.84	0.40
1:D:256:ILE:CG2	1:D:475:MET:HE3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:LEU:HD12	1:F:247:LEU:HA	1.67	0.40
1:F:340:ASP:CG	1:F:367:LYS:HE3	2.46	0.40
1:C:435:LYS:CB	1:C:436:GLY:HA2	2.51	0.40
1:D:314:THR:HG21	1:D:354:ASN:OD1	2.21	0.40
1:D:529:THR:N	1:D:530:PRO:CD	2.84	0.40
1:E:10:TYR:O	1:E:205:GLY:HA3	2.22	0.40
1:E:78:ILE:H	1:E:78:ILE:CD1	2.29	0.40
1:F:77:ARG:HH11	1:F:77:ARG:HG2	1.86	0.40
1:F:246:SER:O	1:F:247:LEU:C	2.64	0.40
1:A:266:LEU:CD1	1:A:291:ILE:HG13	2.50	0.40
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.73	0.40
1:B:46:GLU:HB2	1:B:54:PHE:CZ	2.55	0.40
1:C:188:GLU:H	1:C:188:GLU:HG2	1.63	0.40
1:C:243:THR:HG23	1:C:446:PRO:HG3	2.03	0.40
1:D:127:MET:HE3	1:D:131:MET:HG3	2.03	0.40
1:D:226:ARG:HD3	1:D:226:ARG:HA	1.71	0.40
1:E:129:PRO:C	1:E:131:MET:H	2.30	0.40
1:F:305:ILE:HG23	1:F:306:PRO:HD2	2.03	0.40
1:A:193:GLN:NE2	1:A:362:GLN:NE2	2.59	0.40
1:A:266:LEU:HD11	1:A:291:ILE:HG13	2.03	0.40
1:C:254:GLN:O	1:C:528:ASN:ND2	2.55	0.40
1:D:347:THR:HB	1:E:301:ASP:HB2	2.03	0.40
1:E:75:ASN:HA	1:E:76:ASP:HA	1.82	0.40
1:E:314:THR:HG22	1:E:315:GLY:N	2.36	0.40
1:E:347:THR:CG2	1:F:302:LEU:HD13	2.47	0.40
1:F:281:ASN:HD22	1:F:281:ASN:HA	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/540 (92%)	445 (90%)	41 (8%)	9 (2%)	6	26
1	B	495/540 (92%)	439 (89%)	41 (8%)	15 (3%)	3	17
1	C	484/540 (90%)	434 (90%)	38 (8%)	12 (2%)	4	19
1	D	489/540 (91%)	440 (90%)	36 (7%)	13 (3%)	4	18
1	E	491/540 (91%)	444 (90%)	38 (8%)	9 (2%)	6	26
1	F	476/540 (88%)	434 (91%)	32 (7%)	10 (2%)	5	22
All	All	2930/3240 (90%)	2636 (90%)	226 (8%)	68 (2%)	5	21

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	MET
1	A	347	THR
1	A	370	SER
1	B	370	SER
1	C	344	TYR
1	C	370	SER
1	D	348	GLU
1	D	370	SER
1	E	370	SER
1	F	370	SER
1	A	11	SER
1	A	20	MET
1	A	138	GLY
1	B	11	SER
1	B	20	MET
1	B	138	GLY
1	B	172	HIS
1	B	438	ASN
1	C	20	MET
1	C	131	MET
1	C	138	GLY
1	D	20	MET
1	D	138	GLY
1	D	438	ASN
1	E	11	SER
1	E	20	MET
1	E	138	GLY
1	E	438	ASN
1	F	20	MET
1	A	186	ASN

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Mol	Chain	Res	Type
1	B	186	ASN
1	C	11	SER
1	C	186	ASN
1	C	438	ASN
1	D	5	LYS
1	D	11	SER
1	D	186	ASN
1	E	186	ASN
1	F	11	SER
1	F	138	GLY
1	F	172	HIS
1	F	186	ASN
1	A	276	GLN
1	B	276	GLN
1	B	347	THR
1	C	276	GLN
1	E	276	GLN
1	F	343	GLY
1	F	438	ASN
1	A	439	GLY
1	B	37	ASN
1	C	51	THR
1	C	172	HIS
1	D	51	THR
1	D	276	GLN
1	D	434	SER
1	E	51	THR
1	F	51	THR
1	F	276	GLN
1	B	5	LYS
1	B	51	THR
1	B	343	GLY
1	E	107	PRO
1	B	107	PRO
1	D	107	PRO
1	C	107	PRO
1	B	342	VAL
1	D	39	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	408/449 (91%)	363 (89%)	45 (11%)	6	23
1	B	406/449 (90%)	362 (89%)	44 (11%)	6	23
1	C	404/449 (90%)	361 (89%)	43 (11%)	6	24
1	D	404/449 (90%)	360 (89%)	44 (11%)	6	23
1	E	409/449 (91%)	364 (89%)	45 (11%)	6	23
1	F	399/449 (89%)	357 (90%)	42 (10%)	6	24
All	All	2430/2694 (90%)	2167 (89%)	263 (11%)	6	23

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	64	LEU
1	A	70	VAL
1	A	91	VAL
1	A	124	LEU
1	A	130	ASP
1	A	131	MET
1	A	154	MET
1	A	182	LEU
1	A	187	ILE
1	A	188	GLU
1	A	191	LEU
1	A	206	ILE
1	A	247	LEU
1	A	250	THR
1	A	256	ILE
1	A	260	THR
1	A	272	ASN
1	A	284	LEU
1	A	288	SER
1	A	289	SER
1	A	291	ILE

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	297	SER
1	A	299	VAL
1	A	302	LEU
1	A	311	LEU
1	A	312	LEU
1	A	317	VAL
1	A	322	MET
1	A	328	ARG
1	A	342	VAL
1	A	348	GLU
1	A	352	LEU
1	A	399	ILE
1	A	408	LYS
1	A	437	THR
1	A	442	VAL
1	A	451	GLU
1	A	481	SER
1	A	482	GLU
1	A	495	LEU
1	A	515	VAL
1	A	517	LEU
1	A	524	LEU
1	B	36	GLN
1	B	51	THR
1	B	64	LEU
1	B	70	VAL
1	B	91	VAL
1	B	124	LEU
1	B	154	MET
1	B	182	LEU
1	B	187	ILE
1	B	188	GLU
1	B	191	LEU
1	B	206	ILE
1	B	247	LEU
1	B	250	THR
1	B	256	ILE
1	B	260	THR
1	B	272	ASN
1	B	284	LEU
1	B	288	SER

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Mol	Chain	Res	Type
1	B	289	SER
1	B	291	ILE
1	B	296	GLN
1	B	297	SER
1	B	299	VAL
1	B	302	LEU
1	B	311	LEU
1	B	312	LEU
1	B	317	VAL
1	B	322	MET
1	B	328	ARG
1	B	342	VAL
1	B	344	TYR
1	B	352	LEU
1	B	399	ILE
1	B	408	LYS
1	B	437	THR
1	B	442	VAL
1	B	451	GLU
1	B	481	SER
1	B	482	GLU
1	B	495	LEU
1	B	515	VAL
1	B	517	LEU
1	B	524	LEU
1	C	51	THR
1	C	64	LEU
1	C	70	VAL
1	C	76	ASP
1	C	91	VAL
1	C	124	LEU
1	C	154	MET
1	C	182	LEU
1	C	188	GLU
1	C	191	LEU
1	C	206	ILE
1	C	247	LEU
1	C	250	THR
1	C	256	ILE
1	C	260	THR
1	C	272	ASN
1	C	284	LEU

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Mol	Chain	Res	Type
1	C	288	SER
1	C	289	SER
1	C	291	ILE
1	C	296	GLN
1	C	297	SER
1	C	299	VAL
1	C	302	LEU
1	C	311	LEU
1	C	312	LEU
1	C	317	VAL
1	C	322	MET
1	C	328	ARG
1	C	342	VAL
1	C	348	GLU
1	C	352	LEU
1	C	399	ILE
1	C	408	LYS
1	C	437	THR
1	C	442	VAL
1	C	451	GLU
1	C	481	SER
1	C	482	GLU
1	C	495	LEU
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU
1	D	51	THR
1	D	64	LEU
1	D	70	VAL
1	D	91	VAL
1	D	124	LEU
1	D	131	MET
1	D	154	MET
1	D	182	LEU
1	D	187	ILE
1	D	188	GLU
1	D	191	LEU
1	D	206	ILE
1	D	247	LEU
1	D	250	THR
1	D	256	ILE
1	D	260	THR

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Mol	Chain	Res	Type
1	D	272	ASN
1	D	284	LEU
1	D	288	SER
1	D	289	SER
1	D	291	ILE
1	D	297	SER
1	D	299	VAL
1	D	302	LEU
1	D	311	LEU
1	D	312	LEU
1	D	313	ASN
1	D	317	VAL
1	D	322	MET
1	D	328	ARG
1	D	342	VAL
1	D	348	GLU
1	D	352	LEU
1	D	399	ILE
1	D	408	LYS
1	D	437	THR
1	D	442	VAL
1	D	451	GLU
1	D	481	SER
1	D	482	GLU
1	D	495	LEU
1	D	515	VAL
1	D	517	LEU
1	D	524	LEU
1	E	51	THR
1	E	64	LEU
1	E	70	VAL
1	E	124	LEU
1	E	131	MET
1	E	154	MET
1	E	182	LEU
1	E	187	ILE
1	E	188	GLU
1	E	191	LEU
1	E	206	ILE
1	E	247	LEU
1	E	250	THR
1	E	256	ILE

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Mol	Chain	Res	Type
1	E	260	THR
1	E	272	ASN
1	E	284	LEU
1	E	288	SER
1	E	289	SER
1	E	291	ILE
1	E	296	GLN
1	E	297	SER
1	E	299	VAL
1	E	302	LEU
1	E	311	LEU
1	E	312	LEU
1	E	313	ASN
1	E	317	VAL
1	E	322	MET
1	E	328	ARG
1	E	342	VAL
1	E	344	TYR
1	E	348	GLU
1	E	352	LEU
1	E	399	ILE
1	E	408	LYS
1	E	437	THR
1	E	442	VAL
1	E	451	GLU
1	E	481	SER
1	E	482	GLU
1	E	495	LEU
1	E	515	VAL
1	E	517	LEU
1	E	524	LEU
1	F	51	THR
1	F	64	LEU
1	F	70	VAL
1	F	91	VAL
1	F	124	LEU
1	F	131	MET
1	F	154	MET
1	F	182	LEU
1	F	187	ILE
1	F	188	GLU
1	F	191	LEU

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Mol	Chain	Res	Type
1	F	206	ILE
1	F	247	LEU
1	F	250	THR
1	F	256	ILE
1	F	260	THR
1	F	272	ASN
1	F	284	LEU
1	F	288	SER
1	F	289	SER
1	F	291	ILE
1	F	297	SER
1	F	299	VAL
1	F	302	LEU
1	F	311	LEU
1	F	312	LEU
1	F	317	VAL
1	F	322	MET
1	F	328	ARG
1	F	342	VAL
1	F	348	GLU
1	F	352	LEU
1	F	399	ILE
1	F	408	LYS
1	F	437	THR
1	F	442	VAL
1	F	451	GLU
1	F	481	SER
1	F	495	LEU
1	F	515	VAL
1	F	517	LEU
1	F	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	66	HIS
1	A	75	ASN
1	A	90	HIS
1	A	193	GLN
1	A	269	HIS
1	A	276	GLN

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Mol	Chain	Res	Type
1	A	281	ASN
1	A	307	HIS
1	A	313	ASN
1	A	355	ASN
1	A	479	GLN
1	A	484	ASN
1	B	43	GLN
1	B	66	HIS
1	B	75	ASN
1	B	90	HIS
1	B	169	ASN
1	B	193	GLN
1	B	269	HIS
1	B	276	GLN
1	B	281	ASN
1	B	307	HIS
1	B	313	ASN
1	B	355	ASN
1	B	479	GLN
1	B	484	ASN
1	B	514	GLN
1	C	43	GLN
1	C	66	HIS
1	C	75	ASN
1	C	90	HIS
1	C	193	GLN
1	C	269	HIS
1	C	276	GLN
1	C	281	ASN
1	C	313	ASN
1	C	355	ASN
1	C	479	GLN
1	C	484	ASN
1	C	514	GLN
1	D	43	GLN
1	D	66	HIS
1	D	75	ASN
1	D	90	HIS
1	D	169	ASN
1	D	193	GLN
1	D	269	HIS
1	D	276	GLN

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Mol	Chain	Res	Type
1	D	281	ASN
1	D	307	HIS
1	D	355	ASN
1	D	479	GLN
1	D	484	ASN
1	E	43	GLN
1	E	66	HIS
1	E	75	ASN
1	E	90	HIS
1	E	169	ASN
1	E	193	GLN
1	E	269	HIS
1	E	276	GLN
1	E	281	ASN
1	E	307	HIS
1	E	313	ASN
1	E	355	ASN
1	E	479	GLN
1	E	484	ASN
1	E	514	GLN
1	F	43	GLN
1	F	66	HIS
1	F	75	ASN
1	F	90	HIS
1	F	193	GLN
1	F	269	HIS
1	F	276	GLN
1	F	281	ASN
1	F	307	HIS
1	F	313	ASN
1	F	355	ASN
1	F	479	GLN
1	F	484	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	505/540 (93%)	0.06	7 (1%)	73	51	51, 76, 110, 138	0
1	B	505/540 (93%)	0.23	12 (2%)	59	37	39, 77, 112, 137	0
1	C	498/540 (92%)	0.12	16 (3%)	50	28	52, 75, 108, 136	0
1	D	501/540 (92%)	0.11	16 (3%)	50	28	20, 75, 108, 139	0
1	E	503/540 (93%)	0.11	7 (1%)	73	51	39, 76, 111, 138	0
1	F	494/540 (91%)	0.11	13 (2%)	57	34	37, 75, 106, 134	0
All	All	3006/3240 (92%)	0.12	71 (2%)	59	37	20, 76, 110, 139	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	GLY	5.5
1	A	343	GLY	5.5
1	F	38	GLY	5.2
1	D	345	SER	4.4
1	F	438	ASN	4.4
1	F	455	ILE	4.1
1	C	446	PRO	3.9
1	C	466	CYS	3.9
1	A	345	SER	3.8
1	C	438	ASN	3.8
1	C	345	SER	3.7
1	A	434	SER	3.7
1	D	510	SER	3.7
1	A	455	ILE	3.6
1	D	466	CYS	3.5
1	D	272	ASN	3.5
1	F	130	ASP	3.3
1	C	439	GLY	3.3
1	F	49	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	348	GLU	3.1
1	B	130	ASP	3.1
1	F	439	GLY	3.1
1	D	452	ALA	3.0
1	B	5	LYS	3.0
1	E	466	CYS	3.0
1	F	505	GLU	2.9
1	B	36	GLN	2.9
1	C	122	ASP	2.8
1	C	379	LEU	2.8
1	A	466	CYS	2.8
1	D	513	PHE	2.8
1	C	272	ASN	2.7
1	D	274	VAL	2.7
1	F	434	SER	2.7
1	D	346	ALA	2.6
1	D	438	ASN	2.6
1	B	51	THR	2.6
1	E	455	ILE	2.6
1	F	304	ALA	2.5
1	E	53	PHE	2.5
1	C	504	SER	2.5
1	C	274	VAL	2.5
1	D	143	THR	2.4
1	F	344	TYR	2.4
1	A	245	ASN	2.3
1	B	53	PHE	2.3
1	E	107	PRO	2.3
1	D	86	ALA	2.3
1	D	400	GLN	2.3
1	F	510	SER	2.3
1	B	108	ASP	2.3
1	A	275	HIS	2.2
1	E	5	LYS	2.2
1	C	344	TYR	2.2
1	E	379	LEU	2.2
1	B	275	HIS	2.2
1	C	314	THR	2.2
1	B	411	THR	2.1
1	B	315	GLY	2.1
1	D	379	LEU	2.1
1	C	49	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	46	GLU	2.1
1	C	248	THR	2.1
1	B	170	ASN	2.1
1	B	194	CYS	2.1
1	F	342	VAL	2.0
1	B	455	ILE	2.0
1	F	211	ASP	2.0
1	D	36	GLN	2.0
1	E	36	GLN	2.0
1	C	451	GLU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.