Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:44 PM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

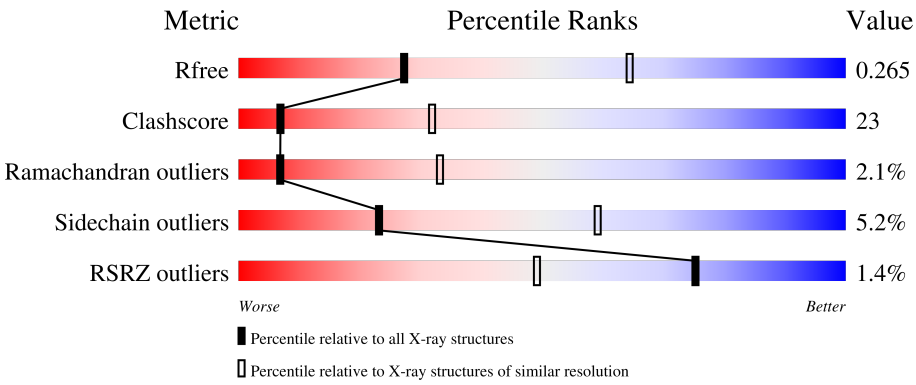
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	706	% 51% 40% • 5%
1	B	706	% 57% 35% • 5%
1	C	706	% 59% 34% • 5%
1	D	706	3% 53% 37% 5% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein transport protein TIP20.

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

There are 24 discrepancies between the modelled and reference sequences:

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

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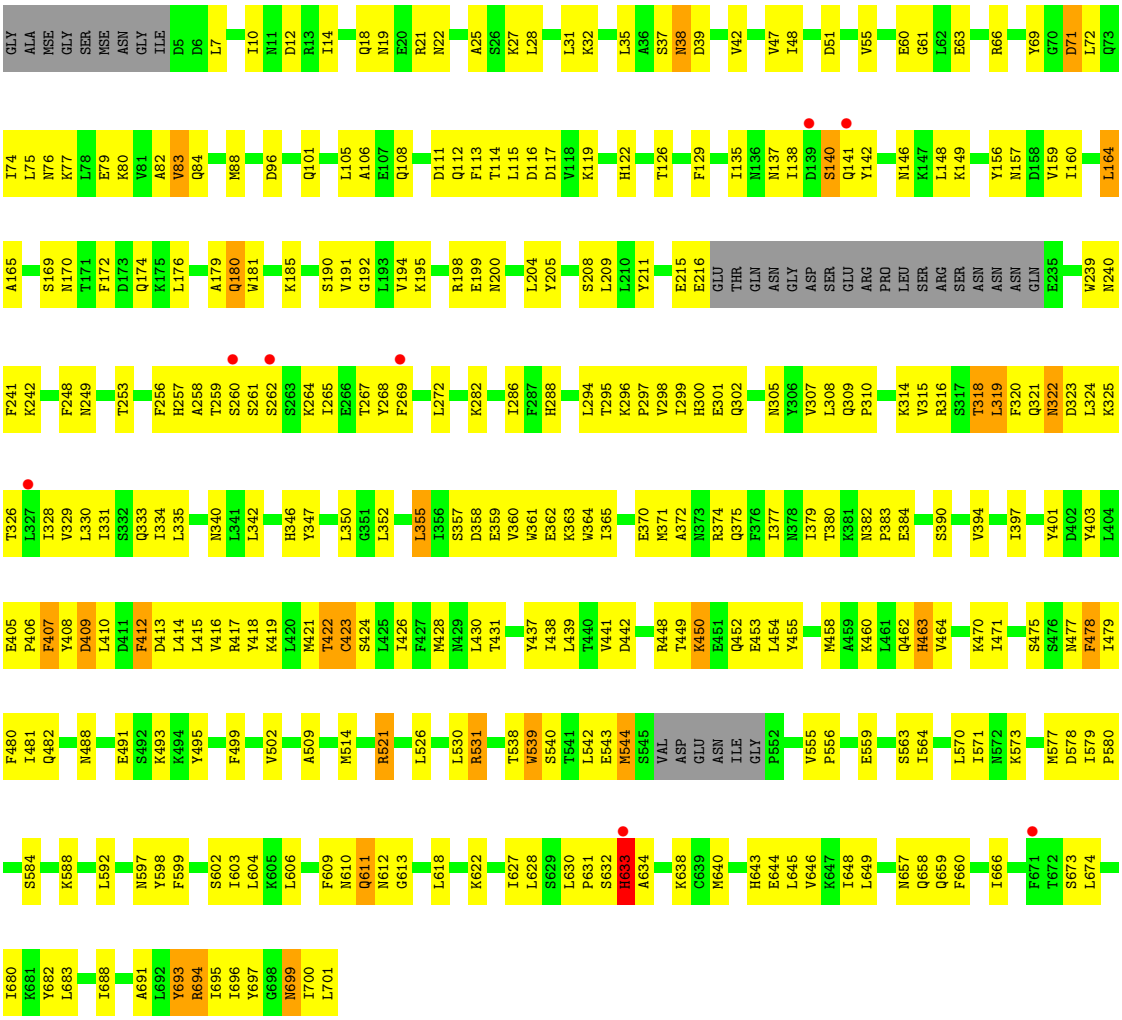
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP P33891
D	0	SER	-	EXPRESSION TAG	UNP P33891
D	1	MSE	-	EXPRESSION TAG	UNP P33891

3 Residue-property plots (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.

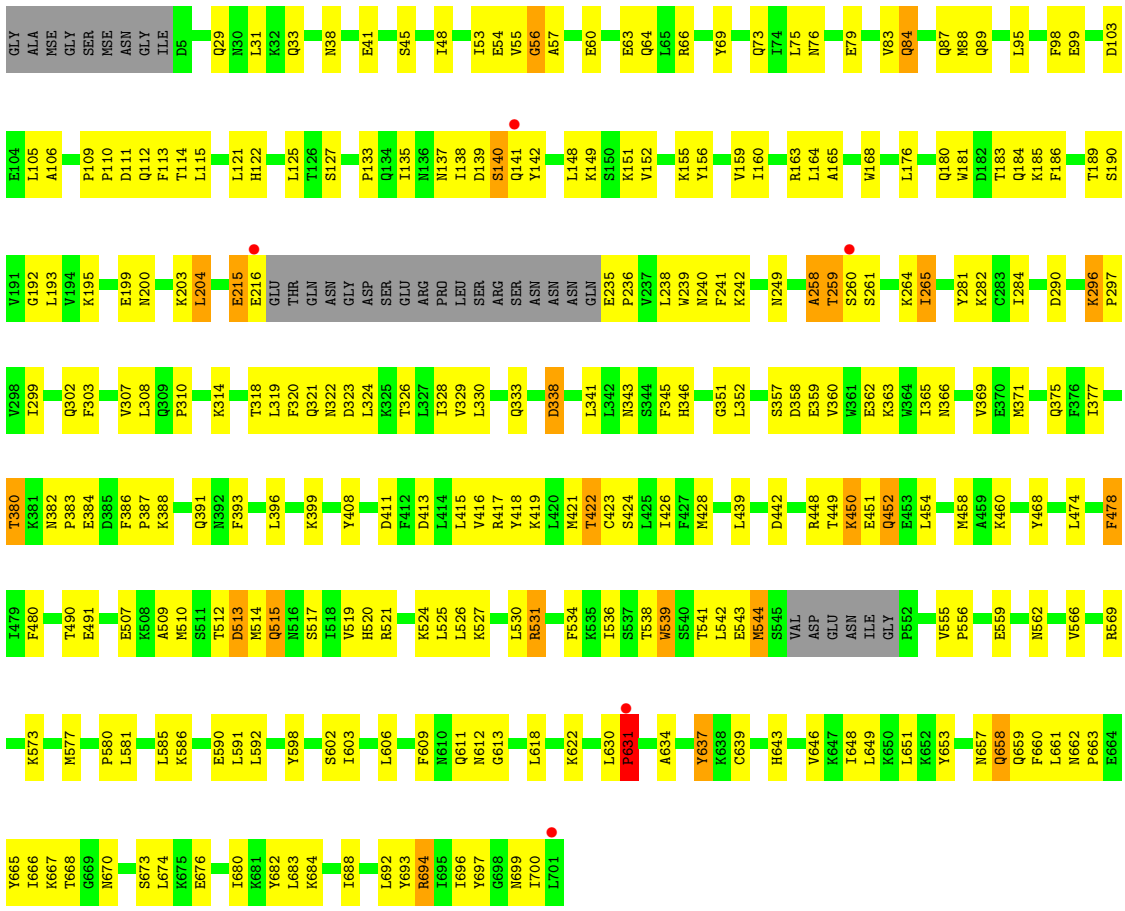
• Molecule 1: Protein transport protein TIP20

Chain A:



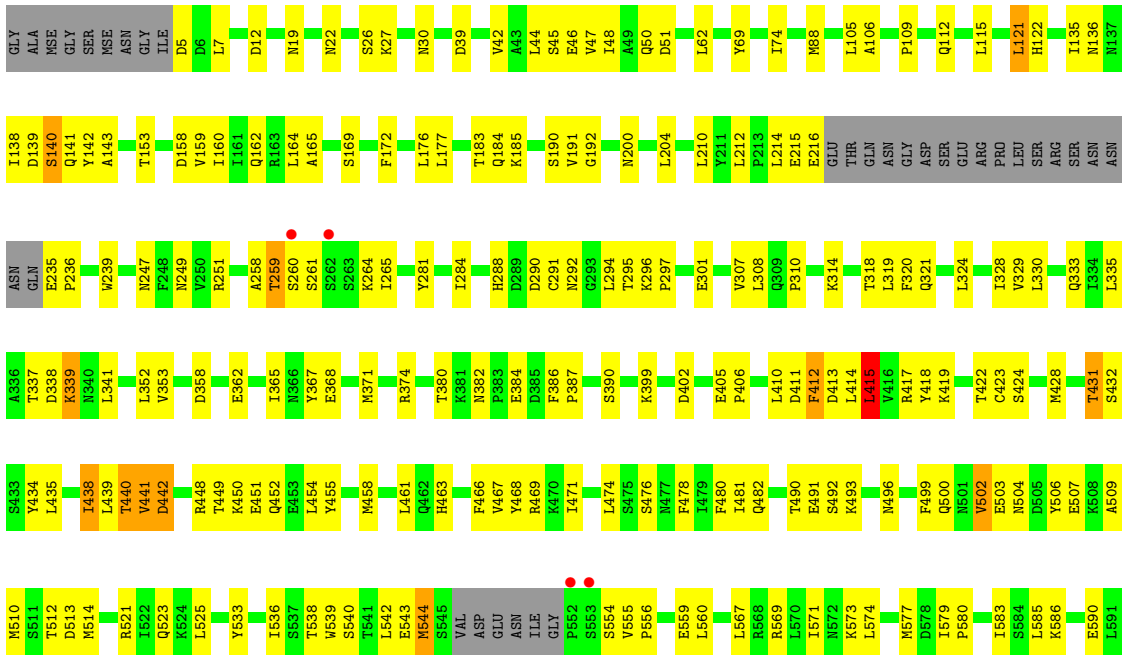
• Molecule 1: Protein transport protein TIP20

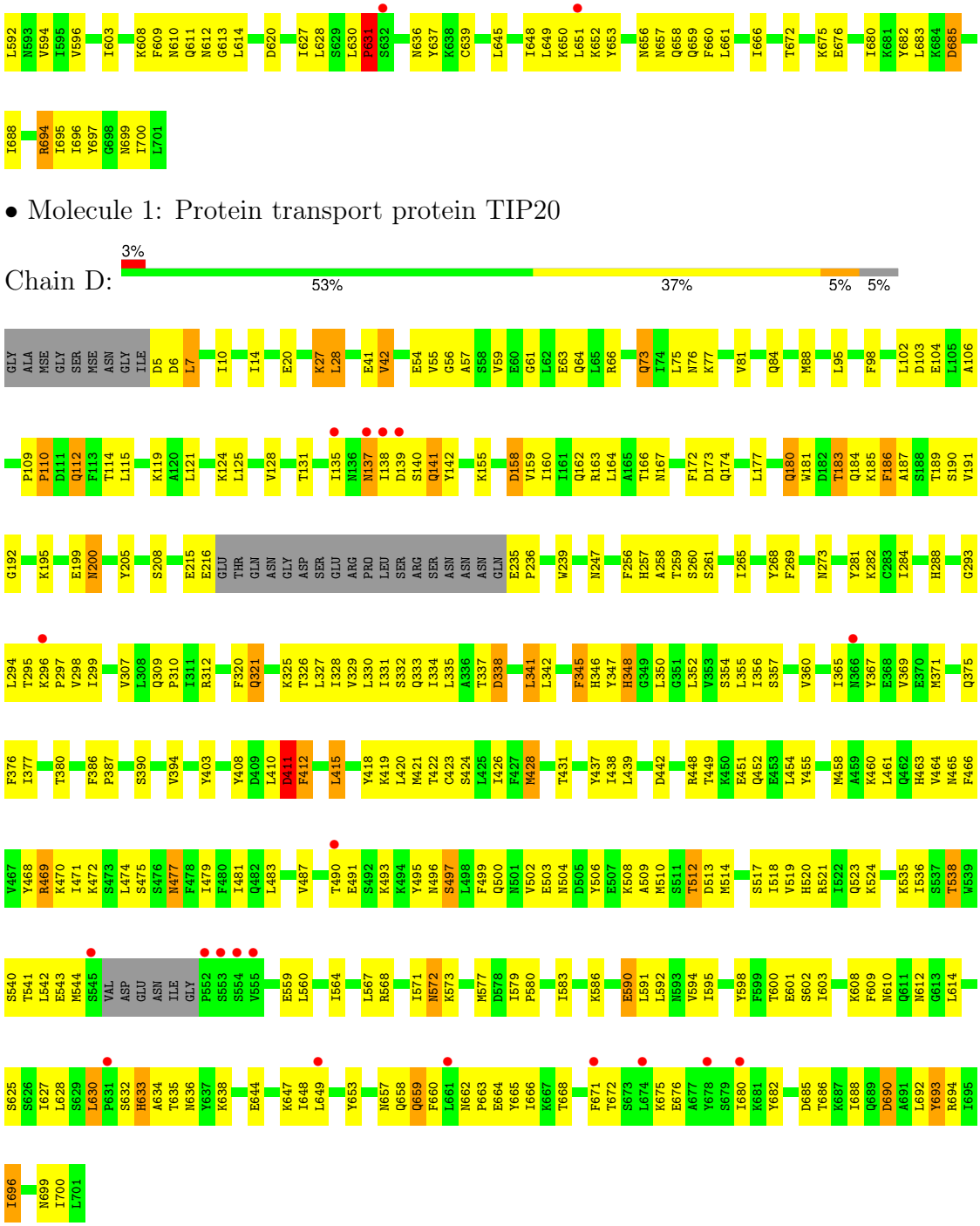
Chain B:



• Molecule 1: Protein transport protein TIP20

Chain C:




L592 N593 V594 I595 V596 I603 K608 F609 N610 Q611 N612 G613 L614 D620 I627 L628 S629 L630 P631 S632 N636 Y637 K638 C639 L645 I648 L649 K650 L651 K652 Y653 N656 N657 Q658 Q659 F660 L661 I666 T672 K675 E676 I680 K681 Y682 L683 K684 D685
I688 R694 I695 I696 Y697 G698 N699 I700 L701
• Molecule 1: Protein transport protein TIP20
Chain D:
3%
53%
37%
5%
5%
GLY ALA MSE GLY SER MSE ASN GLY ILE D5 D6 L7 I10 I14 E20 K27 L28 E41 V42 E54 V55 G56 A57 S58 V59 E60 G61 L62 E63 Q64 L65 R66 Q73 I74 L75 N76 K77 V81 Q84 M88 L95 F98 L102 D103 E104 L105 A106
P109 P110 D111 Q112 F113 T114 L115 K119 A120 L121 K124 L125 V128 T131 I135 N136 N137 I138 D139 S140 Q141 Y142 K155 D158 V159 I160 I161 Q162 R163 L164 A165 T166 N167 F172 D173 Q174 L177 Q180 W181 D182 T183 Q184 K185 F186 A187 S188 T189 S190 V191
G192 K195 E199 N200 Y205 S208 E215 E216 GLU THR GLN ASN GLY ASP SER GLU ARG PRO LEU SER ARG SER ASN ASN ASN GLN E235 P236 W239 N247 F256 H257 A258 T259 S260 S261 I265 Y268 F269 N273 Y281 K282 C283 I284 H288 G293
L294 T295 K296 P297 V298 I299 V307 L308 Q309 P310 I311 R312 F320 Q321 K325 T326 L327 I328 V329 L330 I331 S332 Q333 I334 L335 A336 T337 D338 L341 L342 F345 H346 Y347 H348 G349 L350 G351 L352 V353 S354 L355 I356 S357 V360 I365 N366 Y367 E368 V369 E370 M371 Q375
F376 I377 T380 F386 P387 S390 V394 Y403 Y408 D409 L410 D411 F412 L415 Y418 K419 L420 M421 T422 C423 S424 L425 I426 F427 M428 T431 Y437 I438 L439 D442 R448 T449 K450 E451 Q452 E453 L454 Y455 M458 A459 K460 L461 Q462 H463 V464 N465 F466
V467 Y468 R469 K470 I471 K472 S473 L474 S475 S476 N477 F478 I479 F480 I481 Q482 L483 V487 T490 E491 S492 K493 K494 Y495 N496 S497 L498 F499 Q500 N501 V502 E503 N504 D505 Y506 E507 K508 A509 M510 S511 T512 D513 M514 S517 I518 V519 H520 R521 I522 Q523 K524 K535 I536 S537 T538 W539
S540 T541 L542 E543 M544 S545 VAL ASP GLU ASN ILE GLY P552 S553 S554 V555 E559 L560 I564 L567 R568 I571 N572 K573 M577 D578 I579 P580 I583 K586 E590 L591 L592 N593 V594 I595 Y598 F599 T600 E601 S602 I603 K608 F609 N610 Q611 N612 G613 L614
S625 S626 I627 L628 S629 L630 P631 S632 H633 A634 T635 N636 Y637 K638 E644 K647 I648 L649 Y653 N657 Q658 Q659 F660 L661 N662 P663 E664 Y665 I666 K667 T668 F671 T672 S673 L674 K675 E676 A677 Y678 S679 I680 K681 Y682 D685 T686 K687 I688 Q689 D690 A691 L692 Y693 R694 I695
I696 N699 I700 L701

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.48Å 111.62Å 149.84Å 77.09° 88.12° 70.35°	Depositor
Resolution (Å)	29.90 – 3.00 48.97 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.90-3.00) 97.7 (48.97-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.265 0.220 , 0.265	Depositor DCC
R_{free} test set	5006 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	73.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22040	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.42	0/5601	0.63	1/7561 (0.0%)
1	B	0.46	1/5601 (0.0%)	0.64	0/7561
1	C	0.44	0/5601	0.63	1/7561 (0.0%)
1	D	0.40	0/5601	0.60	0/7561
All	All	0.43	1/22404 (0.0%)	0.63	2/30244 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	LYS	CE-NZ	5.25	1.62	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	PHE	N-CA-C	-5.97	94.87	111.00
1	C	415	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5510	0	5545	325	0
1	B	5510	0	5545	244	0
1	C	5510	0	5545	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5510	0	5545	275	0
All	All	22040	0	22180	1020	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 (1020) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ARG:HH21	1:B:383:PRO:HD3	1.13	1.14
1:C:183:THR:HG22	1:C:185:LYS:H	1.10	1.14
1:B:365:ILE:HD11	1:B:418:TYR:HD2	1.19	1.05
1:A:295:THR:CG2	1:A:297:PRO:HD2	1.88	1.04
1:B:183:THR:HG22	1:B:185:LYS:H	1.22	1.03
1:A:531:ARG:HH11	1:A:531:ARG:HB2	1.18	1.03
1:A:295:THR:HG22	1:A:297:PRO:CD	1.89	1.01
1:A:564:ILE:HG23	1:A:627:ILE:HD11	1.44	0.99
1:C:424:SER:HA	1:C:428:MSE:HG3	1.45	0.99
1:C:538:THR:HG22	1:C:542:LEU:HB3	1.42	0.99
1:D:583:ILE:HA	1:D:586:LYS:HD2	1.45	0.98
1:A:521:ARG:HG3	1:A:521:ARG:HH11	1.29	0.96
1:D:183:THR:HG23	1:D:185:LYS:H	1.30	0.96
1:D:544:MSE:H	1:D:612:ASN:ND2	1.64	0.95
1:C:419:LYS:O	1:C:422:THR:HG22	1.64	0.95
1:A:295:THR:HG22	1:A:297:PRO:HD2	0.96	0.95
1:B:538:THR:HG22	1:B:542:LEU:HB3	1.48	0.95
1:A:335:LEU:HD21	1:A:410:LEU:HD11	1.49	0.94
1:A:531:ARG:NH2	1:B:383:PRO:HD3	1.83	0.93
1:D:235:GLU:N	1:D:236:PRO:HA	1.85	0.92
1:A:419:LYS:O	1:A:422:THR:HG22	1.68	0.92
1:D:439:LEU:HD21	1:D:514:MSE:HE2	1.50	0.92
1:C:649:LEU:HD22	1:C:700:ILE:HD11	1.49	0.91
1:C:695:ILE:HG12	1:C:700:ILE:HD12	1.49	0.91
1:C:338:ASP:OD1	1:C:353:VAL:HG23	1.71	0.91
1:D:592:LEU:HD23	1:D:636:ASN:HD22	1.34	0.90
1:C:365:ILE:HD11	1:C:418:TYR:HB3	1.53	0.89
1:B:265:ILE:HD12	1:B:330:LEU:HD22	1.53	0.88
1:B:658:GLN:HG3	1:B:661:LEU:HD12	1.55	0.88
1:D:449:THR:HG22	1:D:451:GLU:H	1.38	0.88
1:B:419:LYS:O	1:B:422:THR:HG22	1.73	0.88
1:C:88:MSE:HE1	1:C:141:GLN:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:THR:HB	1:D:452:GLN:HG3	1.57	0.86
1:D:394:VAL:HG13	1:D:470:LYS:HG2	1.55	0.85
1:A:377:ILE:HD13	1:B:534:PHE:HZ	1.41	0.85
1:B:259:THR:HG22	1:B:260:SER:H	1.41	0.84
1:B:666:ILE:HD12	1:B:696:ILE:HD12	1.60	0.84
1:C:586:LYS:O	1:C:590:GLU:HG2	1.78	0.84
1:C:450:LYS:HD2	1:C:525:LEU:HD23	1.60	0.83
1:C:371:MSE:HE1	1:C:374:ARG:HH21	1.43	0.83
1:B:630:LEU:HB3	1:B:631:PRO:HD2	1.61	0.82
1:C:412:PHE:O	1:C:415:LEU:HD22	1.78	0.82
1:B:555:VAL:HG12	1:B:556:PRO:HD2	1.62	0.82
1:C:458:MSE:HE2	1:C:574:LEU:HD13	1.60	0.82
1:B:531:ARG:HH11	1:B:531:ARG:HB2	1.44	0.81
1:A:137:ASN:HB2	1:A:140:SER:OG	1.81	0.81
1:A:666:ILE:HD12	1:A:696:ILE:HD12	1.62	0.81
1:C:140:SER:C	1:C:142:TYR:H	1.85	0.81
1:D:544:MSE:H	1:D:612:ASN:HD22	1.27	0.81
1:C:648:ILE:HD11	1:C:680:ILE:HD13	1.61	0.81
1:A:599:PHE:HA	1:A:603:ILE:HD13	1.63	0.80
1:C:666:ILE:HD12	1:C:696:ILE:HD12	1.63	0.80
1:B:235:GLU:HB3	1:B:236:PRO:HD3	1.62	0.80
1:D:140:SER:C	1:D:142:TYR:H	1.82	0.79
1:B:365:ILE:HD11	1:B:418:TYR:CD2	2.11	0.79
1:A:215:GLU:HG2	1:A:216:GLU:HG3	1.64	0.79
1:C:358:ASP:O	1:C:362:GLU:HG2	1.83	0.79
1:D:455:TYR:HD1	1:D:458:MSE:HE2	1.48	0.79
1:B:630:LEU:HB2	1:B:634:ALA:HB3	1.64	0.79
1:D:672:THR:O	1:D:676:GLU:HG2	1.83	0.78
1:D:424:SER:HA	1:D:428:MSE:HB2	1.64	0.78
1:A:428:MSE:HE2	1:A:499:PHE:HA	1.64	0.78
1:D:455:TYR:CD1	1:D:458:MSE:HE2	2.19	0.78
1:D:487:VAL:HA	1:D:490:THR:HG22	1.65	0.77
1:B:329:VAL:O	1:B:333:GLN:HG3	1.84	0.77
1:C:672:THR:O	1:C:676:GLU:HG2	1.84	0.77
1:D:542:LEU:HD12	1:D:612:ASN:HB3	1.66	0.77
1:B:649:LEU:HD22	1:B:700:ILE:HD11	1.67	0.77
1:A:316:ARG:HH12	1:A:357:SER:HB2	1.50	0.76
1:A:261:SER:HB3	1:A:264:LYS:HG3	1.67	0.76
1:D:458:MSE:HE1	1:D:573:LYS:HB3	1.67	0.76
1:A:531:ARG:HB2	1:A:531:ARG:NH1	1.96	0.76
1:D:499:PHE:O	1:D:503:GLU:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:ILE:HD11	1:B:680:ILE:HD13	1.67	0.76
1:B:84:GLN:HG2	1:B:135:ILE:HD13	1.67	0.76
1:A:618:LEU:HD11	1:A:646:VAL:HG21	1.67	0.76
1:A:88:MSE:HE3	1:A:141:GLN:HB2	1.67	0.75
1:C:666:ILE:HD12	1:C:696:ILE:CD1	2.17	0.75
1:D:560:LEU:O	1:D:564:ILE:HG13	1.85	0.75
1:A:448:ARG:HH22	1:B:450:LYS:HE3	1.51	0.75
1:C:630:LEU:HB3	1:C:631:PRO:HD2	1.67	0.74
1:A:371:MSE:O	1:A:375:GLN:HG3	1.87	0.74
1:D:564:ILE:HG22	1:D:627:ILE:HD11	1.68	0.74
1:C:432:SER:HB3	1:C:502:VAL:HG12	1.69	0.74
1:A:521:ARG:HG3	1:A:521:ARG:NH1	1.96	0.73
1:C:7:LEU:O	1:C:7:LEU:HD23	1.89	0.73
1:A:316:ARG:NH1	1:A:357:SER:HB2	2.03	0.73
1:D:325:LYS:HG2	1:D:367:TYR:OH	1.88	0.73
1:B:450:LYS:HB2	1:B:450:LYS:NZ	2.02	0.73
1:C:503:GLU:O	1:C:507:GLU:HG3	1.88	0.73
1:C:510:MSE:HE2	1:C:583:ILE:HD12	1.71	0.73
1:A:598:TYR:CE2	1:A:603:ILE:HD11	2.24	0.72
1:A:405:GLU:HB3	1:A:406:PRO:HD3	1.71	0.72
1:C:449:THR:HB	1:C:452:GLN:HG3	1.72	0.72
1:A:454:LEU:HG	1:A:458:MSE:HE2	1.71	0.72
1:D:648:ILE:HD13	1:D:688:ILE:HG23	1.71	0.72
1:A:649:LEU:HG	1:A:700:ILE:HD11	1.71	0.72
1:A:322:ASN:ND2	1:A:323:ASP:H	1.87	0.72
1:B:362:GLU:HG2	1:B:418:TYR:HE2	1.54	0.72
1:C:555:VAL:CG1	1:C:556:PRO:HD2	2.19	0.71
1:D:474:LEU:O	1:D:477:ASN:HB2	1.89	0.71
1:A:455:TYR:CE1	1:A:573:LYS:HG3	2.26	0.71
1:D:371:MSE:O	1:D:375:GLN:HG3	1.89	0.71
1:B:140:SER:C	1:B:142:TYR:H	1.94	0.71
1:B:651:LEU:HB3	1:B:661:LEU:HD21	1.72	0.71
1:A:571:ILE:HD12	1:A:628:LEU:HA	1.72	0.70
1:C:139:ASP:OD1	1:C:143:ALA:HB2	1.90	0.70
1:C:308:LEU:HD22	1:C:352:LEU:HD21	1.72	0.70
1:D:376:PHE:O	1:D:380:THR:HG22	1.91	0.70
1:C:696:ILE:HG22	1:C:697:TYR:CD2	2.26	0.70
1:A:325:LYS:O	1:A:328:ILE:HG22	1.91	0.70
1:B:113:PHE:HB2	1:B:164:LEU:HD11	1.73	0.70
1:B:660:PHE:HD2	1:B:665:TYR:CE2	2.10	0.70
1:B:449:THR:HG23	1:B:452:GLN:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:THR:HG22	1:C:451:GLU:H	1.57	0.69
1:B:365:ILE:O	1:B:369:VAL:HG23	1.91	0.69
1:B:555:VAL:CG1	1:B:556:PRO:HD2	2.22	0.69
1:C:259:THR:HG22	1:C:260:SER:H	1.56	0.69
1:A:449:THR:HG23	1:A:452:GLN:H	1.55	0.69
1:C:685:ASP:HA	1:C:688:ILE:HD12	1.73	0.69
1:D:350:LEU:HD11	1:D:354:SER:HB3	1.72	0.69
1:D:438:ILE:HD11	1:D:463:HIS:HB3	1.75	0.69
1:A:140:SER:C	1:A:142:TYR:H	1.94	0.69
1:C:509:ALA:HB1	1:C:514:MSE:HE2	1.75	0.68
1:C:324:LEU:HD13	1:C:367:TYR:HB2	1.75	0.68
1:A:439:LEU:HD21	1:A:514:MSE:HE2	1.75	0.68
1:A:357:SER:HB3	1:A:360:VAL:HG23	1.75	0.68
1:C:183:THR:HG22	1:C:185:LYS:N	1.96	0.68
1:A:428:MSE:CE	1:A:499:PHE:HA	2.24	0.68
1:C:371:MSE:CE	1:C:374:ARG:HH21	2.06	0.68
1:A:31:LEU:O	1:A:35:LEU:HD12	1.94	0.68
1:D:592:LEU:HD23	1:D:636:ASN:ND2	2.07	0.68
1:A:648:ILE:HD11	1:A:680:ILE:HD13	1.76	0.68
1:D:183:THR:HG23	1:D:185:LYS:N	2.07	0.68
1:D:88:MSE:HE1	1:D:141:GLN:HB2	1.75	0.67
1:D:439:LEU:CD2	1:D:514:MSE:HE2	2.23	0.67
1:D:504:ASN:HB3	1:D:508:LYS:HE3	1.76	0.67
1:B:618:LEU:O	1:B:622:LYS:HG3	1.94	0.67
1:D:7:LEU:HD23	1:D:7:LEU:H	1.58	0.67
1:A:55:VAL:HG12	1:A:61:GLY:HA3	1.76	0.67
1:C:424:SER:O	1:C:428:MSE:HB2	1.94	0.67
1:A:428:MSE:HE1	1:A:502:VAL:HB	1.76	0.67
1:D:543:GLU:HA	1:D:612:ASN:ND2	2.10	0.67
1:D:259:THR:HG22	1:D:260:SER:H	1.59	0.67
1:A:478:PHE:O	1:A:481:ILE:HG12	1.94	0.67
1:C:259:THR:HG22	1:C:260:SER:N	2.10	0.67
1:D:185:LYS:HE2	1:D:185:LYS:HA	1.75	0.67
1:D:408:TYR:HA	1:D:419:LYS:HE2	1.77	0.66
1:A:322:ASN:OD1	1:A:326:THR:HG21	1.95	0.66
1:D:449:THR:HG22	1:D:451:GLU:N	2.09	0.66
1:A:282:LYS:O	1:A:286:ILE:HG13	1.95	0.66
1:B:450:LYS:HB2	1:B:450:LYS:HZ2	1.60	0.66
1:C:567:LEU:HD23	1:C:627:ILE:HD12	1.77	0.66
1:D:390:SER:O	1:D:394:VAL:HG23	1.96	0.66
1:D:55:VAL:CG1	1:D:61:GLY:HA3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:ILE:HD11	1:D:680:ILE:HG12	1.76	0.66
1:D:259:THR:HG22	1:D:260:SER:N	2.10	0.66
1:B:449:THR:HG22	1:B:452:GLN:CD	2.16	0.66
1:A:544:MSE:H	1:A:612:ASN:HB3	1.60	0.65
1:C:585:LEU:HD21	1:C:631:PRO:HD3	1.76	0.65
1:A:7:LEU:CD1	1:D:77:LYS:HB3	2.27	0.65
1:D:465:ASN:OD1	1:D:580:PRO:HD3	1.95	0.65
1:B:259:THR:HG22	1:B:260:SER:N	2.11	0.65
1:A:269:PHE:CE1	1:A:352:LEU:HD11	2.32	0.65
1:D:542:LEU:CD1	1:D:612:ASN:HB3	2.26	0.65
1:B:666:ILE:HD12	1:B:696:ILE:CD1	2.25	0.65
1:B:424:SER:HA	1:B:428:MSE:HE3	1.78	0.65
1:D:140:SER:C	1:D:142:TYR:N	2.47	0.65
1:A:564:ILE:HG23	1:A:627:ILE:CD1	2.25	0.65
1:D:55:VAL:O	1:D:57:ALA:N	2.30	0.65
1:D:487:VAL:HA	1:D:490:THR:CG2	2.26	0.65
1:A:555:VAL:HG22	1:A:556:PRO:HD2	1.79	0.65
1:B:618:LEU:HD22	1:B:646:VAL:HG11	1.79	0.65
1:C:523:GLN:HG3	1:C:594:VAL:HG11	1.78	0.64
1:C:630:LEU:HD12	1:C:630:LEU:H	1.62	0.64
1:D:579:ILE:HG23	1:D:580:PRO:HD2	1.78	0.64
1:D:662:ASN:HD21	1:D:665:TYR:HB2	1.61	0.64
1:D:140:SER:O	1:D:142:TYR:N	2.30	0.64
1:D:509:ALA:HB1	1:D:514:MSE:HE3	1.79	0.64
1:B:657:ASN:C	1:B:659:GLN:H	2.00	0.64
1:C:172:PHE:CE1	1:C:200:ASN:HB3	2.32	0.64
1:C:544:MSE:CE	1:C:554:SER:HB3	2.28	0.64
1:A:7:LEU:HD13	1:D:77:LYS:HB3	1.79	0.64
1:A:413:ASP:HA	1:A:416:VAL:HG23	1.78	0.64
1:B:630:LEU:H	1:B:630:LEU:HD12	1.62	0.64
1:D:665:TYR:O	1:D:668:THR:HB	1.98	0.64
1:A:288:HIS:CD2	1:A:296:LYS:HE3	2.32	0.64
1:B:159:VAL:HG12	1:B:160:ILE:HD12	1.80	0.64
1:A:113:PHE:HB2	1:A:164:LEU:HD11	1.80	0.63
1:A:394:VAL:HG13	1:A:470:LYS:HG2	1.80	0.63
1:C:592:LEU:HD22	1:C:639:CYS:SG	2.38	0.63
1:D:564:ILE:CG2	1:D:627:ILE:HD11	2.28	0.63
1:B:454:LEU:HG	1:B:458:MSE:HE2	1.79	0.63
1:C:265:ILE:HG21	1:C:330:LEU:HD22	1.79	0.63
1:D:428:MSE:HE3	1:D:428:MSE:HA	1.79	0.63
1:B:55:VAL:CG2	1:B:56:GLY:N	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HG12	1:C:69:TYR:CE2	2.33	0.63
1:B:536:ILE:HD11	1:B:559:GLU:HG2	1.80	0.63
1:C:424:SER:HA	1:C:428:MSE:CG	2.26	0.63
1:C:510:MSE:HA	1:C:514:MSE:HE3	1.80	0.63
1:D:491:GLU:HB3	1:D:493:LYS:NZ	2.13	0.63
1:A:454:LEU:HG	1:A:458:MSE:CE	2.28	0.63
1:C:538:THR:CG2	1:C:542:LEU:HB3	2.23	0.63
1:A:295:THR:O	1:A:298:VAL:HB	1.99	0.62
1:A:407:PHE:O	1:A:408:TYR:HB2	1.98	0.62
1:A:618:LEU:HD13	1:A:646:VAL:HG11	1.80	0.62
1:B:343:ASN:ND2	1:C:339:LYS:HD2	2.13	0.62
1:B:517:SER:O	1:B:521:ARG:HG3	1.99	0.62
1:C:109:PRO:HG2	1:C:112:GLN:HG3	1.82	0.62
1:C:140:SER:C	1:C:142:TYR:N	2.50	0.62
1:C:512:THR:HG22	1:C:513:ASP:N	2.14	0.62
1:C:215:GLU:O	1:C:216:GLU:HB2	1.97	0.62
1:A:370:GLU:O	1:A:374:ARG:HG2	2.00	0.62
1:C:544:MSE:HE1	1:C:554:SER:HB3	1.81	0.62
1:C:555:VAL:HG12	1:C:556:PRO:HD2	1.82	0.62
1:B:630:LEU:HB3	1:B:631:PRO:CD	2.29	0.62
1:D:454:LEU:O	1:D:458:MSE:HG3	1.98	0.62
1:B:66:ARG:NH2	1:B:76:ASN:OD1	2.33	0.62
1:D:215:GLU:O	1:D:216:GLU:HB2	2.00	0.62
1:A:573:LYS:O	1:A:577:MSE:HG2	2.00	0.61
1:B:648:ILE:HD13	1:B:688:ILE:HG23	1.82	0.61
1:D:269:PHE:CE2	1:D:352:LEU:HD11	2.35	0.61
1:A:14:ILE:O	1:A:18:GLN:HG3	2.00	0.61
1:C:308:LEU:HD22	1:C:352:LEU:CD2	2.30	0.61
1:C:542:LEU:HD11	1:C:613:GLY:N	2.15	0.61
1:A:401:TYR:OH	1:A:479:ILE:HD12	2.00	0.61
1:A:185:LYS:O	1:A:185:LYS:HD3	2.00	0.61
1:A:363:LYS:HA	1:B:697:TYR:HE2	1.64	0.61
1:C:542:LEU:HD11	1:C:613:GLY:CA	2.30	0.61
1:C:636:ASN:HD22	1:C:639:CYS:H	1.48	0.61
1:D:121:LEU:HD13	1:D:160:ILE:HD13	1.82	0.61
1:C:658:GLN:HG3	1:C:661:LEU:HD12	1.82	0.61
1:A:431:THR:CG2	1:A:471:ILE:HD11	2.31	0.61
1:A:431:THR:HG23	1:A:471:ILE:HD11	1.82	0.61
1:A:509:ALA:HB1	1:A:514:MSE:HE1	1.83	0.61
1:C:261:SER:HB3	1:C:264:LYS:HD2	1.83	0.61
1:A:531:ARG:HH11	1:A:531:ARG:CB	2.05	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:PHE:HD2	1:B:665:TYR:HE2	1.49	0.61
1:A:335:LEU:HD22	1:A:410:LEU:HD21	1.83	0.60
1:C:318:THR:O	1:C:321:GLN:HG2	2.01	0.60
1:D:235:GLU:N	1:D:236:PRO:CA	2.61	0.60
1:A:38:ASN:HD21	1:D:6:ASP:HB2	1.66	0.60
1:A:335:LEU:CD2	1:A:410:LEU:HD11	2.29	0.60
1:A:372:ALA:HB1	1:A:430:LEU:HD11	1.83	0.60
1:B:190:SER:HB3	1:B:193:LEU:HB3	1.82	0.60
1:D:337:THR:O	1:D:341:LEU:HB2	2.00	0.60
1:A:588:LYS:HD3	1:A:628:LEU:O	2.01	0.60
1:B:358:ASP:O	1:B:362:GLU:HG3	2.02	0.60
1:C:183:THR:HG22	1:C:184:GLN:N	2.14	0.60
1:D:158:ASP:O	1:D:162:GLN:HB3	2.01	0.60
1:B:573:LYS:O	1:B:577:MSE:HG2	2.00	0.60
1:C:630:LEU:HD12	1:C:630:LEU:N	2.15	0.60
1:A:135:ILE:HG22	1:A:137:ASN:ND2	2.17	0.60
1:C:320:PHE:CE1	1:C:321:GLN:HB3	2.36	0.60
1:A:48:ILE:HG12	1:A:69:TYR:CE2	2.36	0.60
1:A:108:GLN:HG3	1:A:112:GLN:NE2	2.17	0.60
1:D:633:HIS:CD2	1:D:634:ALA:H	2.19	0.60
1:A:72:LEU:HB2	1:A:75:LEU:HD13	1.84	0.60
1:B:180:GLN:OE1	1:B:185:LYS:HD3	2.02	0.60
1:D:420:LEU:HD23	1:D:483:LEU:HD22	1.82	0.60
1:C:183:THR:CG2	1:C:185:LYS:HG2	2.31	0.60
1:C:455:TYR:CE1	1:C:573:LYS:HG3	2.37	0.60
1:D:307:VAL:O	1:D:310:PRO:HD2	2.01	0.60
1:A:405:GLU:O	1:A:407:PHE:O	2.20	0.59
1:B:451:GLU:CD	1:B:569:ARG:HH12	2.06	0.59
1:C:695:ILE:CG1	1:C:700:ILE:HD12	2.29	0.59
1:B:371:MSE:O	1:B:375:GLN:HG3	2.02	0.59
1:B:450:LYS:HD2	1:B:525:LEU:HD23	1.84	0.59
1:D:309:GLN:OE1	1:D:312:ARG:HD2	2.03	0.59
1:A:21:ARG:NH2	1:D:28:LEU:HD21	2.17	0.59
1:A:603:ILE:N	1:A:603:ILE:HD12	2.17	0.59
1:D:390:SER:HB3	1:D:466:PHE:HD2	1.67	0.59
1:A:645:LEU:HD12	1:A:683:LEU:HD21	1.83	0.59
1:A:657:ASN:C	1:A:659:GLN:H	2.04	0.59
1:D:183:THR:CG2	1:D:185:LYS:HB2	2.32	0.59
1:D:479:ILE:HG13	1:D:483:LEU:HD12	1.83	0.59
1:D:544:MSE:N	1:D:612:ASN:ND2	2.46	0.59
1:D:520:HIS:HB3	1:D:524:LYS:NZ	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:SER:C	1:A:610:ASN:HD22	2.06	0.59
1:B:190:SER:O	1:B:192:GLY:N	2.35	0.59
1:A:449:THR:HG22	1:A:452:GLN:HG3	1.83	0.59
1:C:478:PHE:O	1:C:482:GLN:HG2	2.03	0.59
1:A:455:TYR:HD1	1:A:458:MSE:HE3	1.67	0.59
1:C:88:MSE:CE	1:C:141:GLN:HB2	2.31	0.59
1:D:320:PHE:HD1	1:D:320:PHE:O	1.86	0.59
1:B:539:TRP:O	1:B:609:PHE:HA	2.03	0.58
1:D:590:GLU:O	1:D:594:VAL:HG23	2.02	0.58
1:D:649:LEU:HD22	1:D:700:ILE:HD12	1.84	0.58
1:A:428:MSE:CE	1:A:502:VAL:HB	2.33	0.58
1:A:530:LEU:HD13	1:A:598:TYR:CE2	2.38	0.58
1:A:543:GLU:O	1:A:543:GLU:HG2	2.03	0.58
1:C:579:ILE:HG23	1:C:580:PRO:HD2	1.84	0.58
1:A:140:SER:C	1:A:142:TYR:N	2.57	0.58
1:A:666:ILE:CD1	1:A:696:ILE:HD12	2.33	0.58
1:D:538:THR:O	1:D:542:LEU:HD23	2.03	0.58
1:A:406:PRO:O	1:A:409:ASP:HB2	2.02	0.58
1:A:408:TYR:HA	1:A:419:LYS:HE2	1.84	0.58
1:B:543:GLU:O	1:B:543:GLU:HG2	2.03	0.58
1:D:190:SER:O	1:D:192:GLY:N	2.28	0.58
1:A:195:LYS:NZ	1:A:198:ARG:HH21	2.02	0.58
1:A:584:SER:O	1:A:588:LYS:HG3	2.03	0.58
1:C:105:LEU:HD13	1:C:121:LEU:HD11	1.86	0.58
1:D:394:VAL:CG1	1:D:470:LYS:HG2	2.31	0.58
1:A:449:THR:HG22	1:A:452:GLN:OE1	2.04	0.58
1:C:249:ASN:OD1	1:C:310:PRO:HB3	2.03	0.58
1:D:332:SER:O	1:D:335:LEU:HB3	2.04	0.58
1:A:571:ILE:CD1	1:A:628:LEU:HA	2.34	0.58
1:B:258:ALA:CB	1:B:264:LYS:HZ3	2.17	0.58
1:B:359:GLU:O	1:B:363:LYS:HG2	2.04	0.58
1:A:618:LEU:CD1	1:A:646:VAL:HG21	2.34	0.58
1:C:657:ASN:C	1:C:659:GLN:H	2.07	0.58
1:A:377:ILE:HD13	1:B:534:PHE:CZ	2.32	0.57
1:A:449:THR:HG22	1:A:452:GLN:CG	2.34	0.57
1:A:96:ASP:OD1	1:A:148:LEU:HD21	2.04	0.57
1:C:439:LEU:O	1:C:440:THR:HG23	2.04	0.57
1:D:124:LYS:O	1:D:128:VAL:HG23	2.04	0.57
1:A:176:LEU:HD22	1:A:181:TRP:CD1	2.39	0.57
1:B:29:GLN:O	1:B:33:GLN:HG3	2.04	0.57
1:D:512:THR:HG22	1:D:513:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ALA:HB1	1:A:514:MSE:CE	2.35	0.57
1:C:106:ALA:HB2	1:C:159:VAL:HG11	1.86	0.57
1:D:660:PHE:HD2	1:D:665:TYR:CE2	2.23	0.57
1:A:542:LEU:HD11	1:A:613:GLY:N	2.20	0.57
1:C:46:GLU:O	1:C:50:GLN:HG2	2.03	0.57
1:A:449:THR:CG2	1:A:452:GLN:HG3	2.35	0.57
1:D:649:LEU:HD13	1:D:700:ILE:HD11	1.85	0.57
1:C:7:LEU:HD23	1:C:7:LEU:C	2.24	0.57
1:D:160:ILE:O	1:D:164:LEU:HG	2.05	0.57
1:D:536:ILE:HD11	1:D:559:GLU:HG3	1.87	0.57
1:C:509:ALA:CB	1:C:514:MSE:HE2	2.35	0.57
1:A:84:GLN:NE2	1:A:135:ILE:HG21	2.19	0.57
1:A:542:LEU:HD11	1:A:613:GLY:CA	2.34	0.57
1:A:606:LEU:HD13	1:B:377:ILE:HD11	1.86	0.57
1:A:538:THR:HG22	1:A:542:LEU:HD23	1.87	0.56
1:D:609:PHE:HB2	1:D:614:LEU:HD13	1.86	0.56
1:A:406:PRO:C	1:A:407:PHE:O	2.38	0.56
1:B:555:VAL:HG12	1:B:556:PRO:CD	2.33	0.56
1:D:509:ALA:HB1	1:D:514:MSE:CE	2.35	0.56
1:A:77:LYS:HE3	1:D:7:LEU:HB3	1.86	0.56
1:C:183:THR:CG2	1:C:184:GLN:N	2.68	0.56
1:A:362:GLU:HG3	1:B:667:LYS:NZ	2.21	0.56
1:B:530:LEU:HD13	1:B:598:TYR:CE2	2.40	0.56
1:A:260:SER:HB2	1:A:318:THR:HB	1.87	0.56
1:D:496:ASN:HB2	1:D:500:GLN:NE2	2.20	0.56
1:A:648:ILE:HD12	1:A:683:LEU:HD23	1.88	0.56
1:B:140:SER:C	1:B:142:TYR:N	2.58	0.56
1:B:585:LEU:HD22	1:B:631:PRO:HD3	1.87	0.56
1:D:183:THR:CG2	1:D:185:LYS:H	2.13	0.56
1:B:103:ASP:OD1	1:B:155:LYS:HE2	2.06	0.56
1:B:541:THR:HG22	1:B:541:THR:O	2.05	0.56
1:C:533:TYR:HE2	1:C:603:ILE:HD13	1.70	0.56
1:D:591:LEU:O	1:D:595:ILE:HG13	2.06	0.56
1:A:269:PHE:CZ	1:A:352:LEU:HD11	2.40	0.55
1:D:411:ASP:O	1:D:412:PHE:O	2.24	0.55
1:D:483:LEU:O	1:D:487:VAL:HG23	2.06	0.55
1:A:412:PHE:CE1	1:A:414:LEU:HD12	2.41	0.55
1:C:367:TYR:CE1	1:C:371:MSE:HE3	2.41	0.55
1:C:442:ASP:CG	1:C:448:ARG:HH12	2.09	0.55
1:B:357:SER:OG	1:B:360:VAL:HG23	2.06	0.55
1:C:651:LEU:HD21	1:C:660:PHE:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:ASN:OD1	1:D:665:TYR:N	2.35	0.55
1:B:55:VAL:O	1:B:57:ALA:N	2.39	0.55
1:C:42:VAL:HG12	1:C:42:VAL:O	2.07	0.55
1:D:573:LYS:O	1:D:577:MSE:HG2	2.06	0.55
1:D:491:GLU:O	1:D:493:LYS:HD2	2.06	0.55
1:B:113:PHE:CB	1:B:164:LEU:HD11	2.37	0.55
1:D:538:THR:HG22	1:D:542:LEU:HB3	1.87	0.55
1:B:261:SER:HB3	1:B:264:LYS:HG3	1.89	0.55
1:C:555:VAL:HG13	1:C:556:PRO:HD2	1.87	0.55
1:D:55:VAL:HG11	1:D:61:GLY:HA3	1.89	0.55
1:C:542:LEU:HD12	1:C:542:LEU:O	2.07	0.55
1:B:160:ILE:O	1:B:164:LEU:HD23	2.07	0.55
1:B:382:ASN:HB3	1:B:384:GLU:CD	2.27	0.55
1:B:649:LEU:HD22	1:B:700:ILE:CD1	2.36	0.55
1:C:165:ALA:HB1	1:C:239:TRP:CG	2.42	0.55
1:D:510:MSE:HB3	1:D:583:ILE:CD1	2.36	0.55
1:B:559:GLU:H	1:B:559:GLU:CD	2.11	0.54
1:C:140:SER:HB2	1:C:142:TYR:HB2	1.89	0.54
1:D:59:VAL:O	1:D:63:GLU:HG2	2.07	0.54
1:D:487:VAL:CA	1:D:490:THR:HG22	2.37	0.54
1:A:648:ILE:HD11	1:A:680:ILE:CD1	2.37	0.54
1:B:168:TRP:CE3	1:B:203:LYS:HE3	2.42	0.54
1:B:538:THR:CG2	1:B:542:LEU:HB3	2.30	0.54
1:C:434:TYR:CE2	1:C:467:VAL:HG21	2.42	0.54
1:D:544:MSE:N	1:D:612:ASN:HD22	2.01	0.54
1:A:408:TYR:CE2	1:A:422:THR:HG21	2.42	0.54
1:D:422:THR:O	1:D:426:ILE:HB	2.07	0.54
1:B:338:ASP:OD1	1:B:351:GLY:HA3	2.07	0.54
1:B:658:GLN:HG3	1:B:661:LEU:CD1	2.35	0.54
1:D:666:ILE:HD12	1:D:696:ILE:HD12	1.88	0.54
1:B:490:THR:O	1:B:490:THR:HG22	2.07	0.54
1:C:435:LEU:HB2	1:C:506:TYR:CE1	2.42	0.54
1:B:83:VAL:O	1:B:87:GLN:HG3	2.07	0.54
1:D:345:PHE:O	1:D:347:TYR:N	2.40	0.54
1:A:316:ARG:HH12	1:A:357:SER:CB	2.20	0.54
1:D:84:GLN:HG3	1:D:135:ILE:HD12	1.90	0.54
1:C:160:ILE:O	1:C:164:LEU:HG	2.08	0.54
1:C:491:GLU:O	1:C:493:LYS:HG3	2.07	0.54
1:C:510:MSE:HB3	1:C:583:ILE:CD1	2.37	0.54
1:A:330:LEU:O	1:A:334:ILE:HG13	2.08	0.53
1:A:359:GLU:HG3	1:B:667:LYS:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:GLN:HG3	1:A:660:PHE:N	2.23	0.53
1:B:189:THR:O	1:B:189:THR:HG22	2.08	0.53
1:B:611:GLN:HB2	1:B:653:TYR:CE2	2.44	0.53
1:C:382:ASN:HB3	1:C:384:GLU:OE2	2.08	0.53
1:A:179:ALA:O	1:A:180:GLN:C	2.45	0.53
1:B:520:HIS:O	1:B:524:LYS:HG3	2.09	0.53
1:C:261:SER:HB3	1:C:264:LYS:CD	2.38	0.53
1:D:536:ILE:CD1	1:D:559:GLU:HG3	2.39	0.53
1:D:657:ASN:C	1:D:659:GLN:H	2.11	0.53
1:A:538:THR:CG2	1:A:542:LEU:HD23	2.38	0.53
1:B:66:ARG:HH21	1:B:76:ASN:HA	1.73	0.53
1:A:140:SER:HB2	1:A:142:TYR:HB2	1.89	0.53
1:A:610:ASN:O	1:A:613:GLY:N	2.40	0.53
1:A:438:ILE:HD13	1:A:464:VAL:HG23	1.91	0.53
1:B:422:THR:CG2	1:B:423:CYS:N	2.71	0.53
1:B:666:ILE:HD13	1:B:692:LEU:HB3	1.91	0.53
1:D:660:PHE:HD2	1:D:665:TYR:HE2	1.55	0.53
1:A:137:ASN:N	1:A:137:ASN:HD22	2.06	0.53
1:A:383:PRO:HG2	1:A:384:GLU:OE1	2.09	0.53
1:A:441:VAL:HG22	1:A:442:ASP:N	2.22	0.53
1:A:475:SER:HB3	1:A:499:PHE:HD2	1.74	0.53
1:A:695:ILE:HG12	1:A:700:ILE:HD12	1.91	0.53
1:B:84:GLN:HG2	1:B:135:ILE:CD1	2.37	0.53
1:C:694:ARG:O	1:C:699:ASN:HB2	2.09	0.53
1:D:540:SER:HA	1:D:610:ASN:ND2	2.23	0.53
1:A:315:VAL:HG11	1:A:355:LEU:HD21	1.90	0.53
1:C:542:LEU:HD12	1:C:542:LEU:C	2.28	0.53
1:A:359:GLU:HG3	1:B:667:LYS:CE	2.39	0.53
1:A:697:TYR:CE2	1:B:363:LYS:HD3	2.44	0.53
1:C:431:THR:HG23	1:C:471:ILE:HD11	1.90	0.53
1:D:121:LEU:HD13	1:D:160:ILE:CD1	2.39	0.53
1:B:55:VAL:HG23	1:B:56:GLY:N	2.24	0.53
1:D:183:THR:HG23	1:D:184:GLN:N	2.24	0.53
1:A:66:ARG:HD3	1:A:71:ASP:OD1	2.08	0.52
1:A:542:LEU:HD11	1:A:613:GLY:HA2	1.92	0.52
1:D:602:SER:C	1:D:603:ILE:HD12	2.29	0.52
1:A:455:TYR:CD1	1:A:458:MSE:HE3	2.44	0.52
1:D:106:ALA:HA	1:D:163:ARG:NH1	2.24	0.52
1:D:195:LYS:O	1:D:199:GLU:HG3	2.09	0.52
1:D:694:ARG:O	1:D:699:ASN:HB2	2.10	0.52
1:A:63:GLU:HG2	1:A:79:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ALA:O	1:A:514:MSE:HE3	2.09	0.52
1:B:326:THR:O	1:B:330:LEU:HG	2.10	0.52
1:B:388:LYS:HD3	1:B:391:GLN:NE2	2.25	0.52
1:B:509:ALA:O	1:B:514:MSE:HE3	2.10	0.52
1:D:330:LEU:O	1:D:334:ILE:HG13	2.10	0.52
1:B:510:MSE:HE1	1:B:580:PRO:CD	2.39	0.52
1:A:261:SER:HB3	1:A:264:LYS:CG	2.38	0.52
1:A:382:ASN:HA	1:B:531:ARG:HH21	1.75	0.52
1:D:461:LEU:HD23	1:D:579:ILE:HD13	1.92	0.52
1:D:490:THR:HG23	1:D:491:GLU:N	2.25	0.52
1:A:261:SER:H	1:A:264:LYS:HB2	1.74	0.52
1:A:342:LEU:O	1:A:346:HIS:HA	2.09	0.52
1:B:602:SER:C	1:B:603:ILE:HD12	2.30	0.52
1:D:103:ASP:OD1	1:D:155:LYS:HE2	2.10	0.52
1:A:538:THR:CG2	1:A:542:LEU:HB3	2.40	0.52
1:C:411:ASP:O	1:C:413:ASP:N	2.43	0.52
1:A:530:LEU:HD23	1:A:563:SER:OG	2.10	0.52
1:B:509:ALA:HB1	1:B:514:MSE:CE	2.40	0.52
1:C:510:MSE:HE1	1:C:580:PRO:CD	2.40	0.52
1:D:568:ARG:O	1:D:572:ASN:HB2	2.09	0.52
1:C:329:VAL:O	1:C:333:GLN:HG3	2.10	0.51
1:A:101:GLN:O	1:A:105:LEU:HG	2.10	0.51
1:A:190:SER:C	1:A:192:GLY:H	2.13	0.51
1:B:148:LEU:O	1:B:152:VAL:HG23	2.10	0.51
1:D:464:VAL:HG21	1:D:514:MSE:SE	2.61	0.51
1:A:335:LEU:CD2	1:A:410:LEU:HD21	2.40	0.51
1:C:165:ALA:HB1	1:C:239:TRP:CD1	2.46	0.51
1:D:177:LEU:HD23	1:D:247:ASN:OD1	2.10	0.51
1:B:531:ARG:HB2	1:B:531:ARG:NH1	2.19	0.51
1:C:45:SER:OG	1:C:48:ILE:HG13	2.10	0.51
1:C:592:LEU:O	1:C:596:VAL:HG23	2.11	0.51
1:D:284:ILE:CG2	1:D:296:LYS:HG2	2.41	0.51
1:A:477:ASN:HB3	1:A:480:PHE:HD1	1.76	0.51
1:A:555:VAL:CG2	1:A:556:PRO:HD2	2.40	0.51
1:B:637:TYR:CE2	1:B:682:TYR:HB3	2.45	0.51
1:C:696:ILE:HG22	1:C:697:TYR:HD2	1.73	0.51
1:A:66:ARG:NH2	1:A:76:ASN:OD1	2.43	0.51
1:C:454:LEU:HA	1:C:521:ARG:HD3	1.93	0.51
1:D:27:LYS:HB2	1:D:27:LYS:NZ	2.26	0.51
1:A:165:ALA:HB1	1:A:239:TRP:CG	2.45	0.51
1:B:657:ASN:HB3	1:B:660:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ILE:HD11	1:C:559:GLU:CG	2.41	0.51
1:B:106:ALA:HB2	1:B:159:VAL:HG11	1.92	0.51
1:C:190:SER:O	1:C:192:GLY:N	2.37	0.51
1:C:414:LEU:O	1:C:414:LEU:HD23	2.11	0.51
1:C:510:MSE:HB3	1:C:583:ILE:HD11	1.92	0.51
1:D:649:LEU:HB3	1:D:700:ILE:CD1	2.40	0.51
1:A:543:GLU:OE2	1:A:543:GLU:N	2.44	0.51
1:B:48:ILE:HG12	1:B:69:TYR:CD2	2.46	0.51
1:A:77:LYS:CE	1:D:7:LEU:HB3	2.41	0.50
1:A:352:LEU:HB3	1:A:355:LEU:HD23	1.94	0.50
1:D:635:THR:HG22	1:D:635:THR:O	2.11	0.50
1:C:261:SER:HB3	1:C:264:LYS:CG	2.40	0.50
1:D:428:MSE:HE2	1:D:502:VAL:HB	1.92	0.50
1:A:364:TRP:HE1	1:A:403:TYR:HH	1.59	0.50
1:C:284:ILE:O	1:C:288:HIS:HB3	2.11	0.50
1:C:653:TYR:CD1	1:C:653:TYR:N	2.79	0.50
1:D:592:LEU:CD1	1:D:625:SER:HB2	2.41	0.50
1:A:113:PHE:CB	1:A:164:LEU:HD11	2.41	0.50
1:A:371:MSE:HA	1:A:371:MSE:HE2	1.92	0.50
1:B:536:ILE:HD11	1:B:559:GLU:CG	2.42	0.50
1:C:386:PHE:N	1:C:387:PRO:HD2	2.27	0.50
1:C:450:LYS:HD2	1:C:525:LEU:CD2	2.39	0.50
1:B:88:MSE:HE1	1:B:141:GLN:C	2.31	0.50
1:C:649:LEU:CD2	1:C:700:ILE:HD11	2.33	0.50
1:D:657:ASN:O	1:D:659:GLN:N	2.44	0.50
1:A:248:PHE:CD2	1:A:307:VAL:HG13	2.47	0.50
1:B:622:LYS:HE2	1:B:643:HIS:HE1	1.76	0.50
1:C:590:GLU:O	1:C:594:VAL:HG23	2.12	0.50
1:D:690:ASP:O	1:D:694:ARG:HG3	2.12	0.50
1:A:618:LEU:HD23	1:A:622:LYS:NZ	2.27	0.50
1:A:694:ARG:HG3	1:A:699:ASN:HB2	1.94	0.50
1:B:442:ASP:OD2	1:B:448:ARG:NH1	2.39	0.50
1:D:181:TRP:HA	1:D:186:PHE:HB2	1.92	0.50
1:D:471:ILE:HG23	1:D:499:PHE:HD2	1.76	0.50
1:A:296:LYS:HB2	1:A:297:PRO:HD3	1.94	0.50
1:A:539:TRP:O	1:A:609:PHE:HA	2.12	0.50
1:D:172:PHE:CE1	1:D:200:ASN:HB3	2.46	0.50
1:D:183:THR:HG21	1:D:185:LYS:HB2	1.94	0.50
1:D:256:PHE:CD2	1:D:268:TYR:HE2	2.30	0.50
1:D:475:SER:HB2	1:D:497:SER:OG	2.12	0.50
1:D:682:TYR:CD1	1:D:682:TYR:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LYS:O	1:B:590:GLU:HG2	2.11	0.49
1:B:611:GLN:N	1:B:653:TYR:OH	2.45	0.49
1:C:510:MSE:HE1	1:C:580:PRO:HD3	1.94	0.49
1:D:295:THR:CG2	1:D:297:PRO:HD2	2.42	0.49
1:A:408:TYR:OH	1:A:422:THR:HG21	2.12	0.49
1:C:685:ASP:HA	1:C:688:ILE:CD1	2.42	0.49
1:A:170:ASN:O	1:A:174:GLN:HG3	2.12	0.49
1:A:262:SER:O	1:A:333:GLN:OE1	2.30	0.49
1:A:324:LEU:CD2	1:A:363:LYS:HE2	2.42	0.49
1:B:215:GLU:O	1:B:216:GLU:HB2	2.12	0.49
1:C:571:ILE:HG12	1:C:628:LEU:HD23	1.93	0.49
1:D:139:ASP:C	1:D:140:SER:O	2.49	0.49
1:D:331:ILE:HG23	1:D:410:LEU:HD11	1.94	0.49
1:D:411:ASP:O	1:D:412:PHE:C	2.50	0.49
1:A:579:ILE:HG23	1:A:580:PRO:HD2	1.95	0.49
1:B:422:THR:O	1:B:426:ILE:HB	2.13	0.49
1:D:98:PHE:CE2	1:D:125:LEU:HD22	2.48	0.49
1:A:657:ASN:O	1:A:659:GLN:N	2.46	0.49
1:B:181:TRP:O	1:B:282:LYS:HE2	2.12	0.49
1:B:439:LEU:HD21	1:B:514:MSE:HE2	1.94	0.49
1:C:177:LEU:HD23	1:C:247:ASN:OD1	2.12	0.49
1:D:106:ALA:HB2	1:D:159:VAL:HG11	1.94	0.49
1:A:205:TYR:CG	1:A:294:LEU:HD21	2.48	0.49
1:A:380:THR:HB	1:A:437:TYR:CE2	2.47	0.49
1:D:320:PHE:O	1:D:320:PHE:CD1	2.66	0.49
1:D:469:ARG:HG2	1:D:469:ARG:HH11	1.78	0.49
1:D:666:ILE:HG12	1:D:692:LEU:HD13	1.94	0.49
1:A:359:GLU:OE2	1:B:667:LYS:HE3	2.12	0.49
1:B:694:ARG:O	1:B:699:ASN:HB2	2.12	0.49
1:C:5:ASP:C	1:C:7:LEU:H	2.15	0.49
1:C:109:PRO:HG2	1:C:112:GLN:CG	2.42	0.49
1:A:352:LEU:N	1:A:352:LEU:HD23	2.27	0.49
1:B:45:SER:OG	1:B:48:ILE:HG13	2.13	0.49
1:B:105:LEU:HD13	1:B:121:LEU:HD11	1.93	0.49
1:C:543:GLU:HA	1:C:612:ASN:ND2	2.28	0.49
1:C:648:ILE:HD12	1:C:683:LEU:HD23	1.94	0.49
1:A:424:SER:HA	1:A:428:MSE:HB2	1.94	0.49
1:B:122:HIS:HB2	1:B:156:TYR:OH	2.12	0.49
1:B:413:ASP:O	1:B:416:VAL:HG12	2.13	0.49
1:C:26:SER:O	1:C:30:ASN:ND2	2.45	0.49
1:C:630:LEU:HB3	1:C:631:PRO:CD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:PRO:CG	1:D:583:ILE:HD12	2.43	0.49
1:A:491:GLU:O	1:A:493:LYS:HG3	2.13	0.49
1:D:109:PRO:HA	1:D:110:PRO:HD3	1.72	0.49
1:D:471:ILE:HG23	1:D:499:PHE:CD2	2.47	0.49
1:D:506:TYR:O	1:D:510:MSE:HG3	2.13	0.49
1:D:579:ILE:CG2	1:D:580:PRO:HD2	2.42	0.49
1:B:630:LEU:O	1:B:631:PRO:C	2.51	0.48
1:C:555:VAL:HG12	1:C:556:PRO:CD	2.43	0.48
1:C:573:LYS:O	1:C:577:MSE:HG2	2.13	0.48
1:D:84:GLN:HE21	1:D:135:ILE:HD13	1.78	0.48
1:D:490:THR:HG23	1:D:491:GLU:CD	2.33	0.48
1:D:540:SER:C	1:D:610:ASN:ND2	2.66	0.48
1:A:269:PHE:HE1	1:A:352:LEU:HD11	1.78	0.48
1:A:610:ASN:O	1:A:612:ASN:N	2.46	0.48
1:D:128:VAL:O	1:D:131:THR:HB	2.13	0.48
1:A:260:SER:HB2	1:A:318:THR:CB	2.43	0.48
1:C:458:MSE:HE2	1:C:574:LEU:CD1	2.40	0.48
1:D:115:LEU:O	1:D:119:LYS:HG3	2.12	0.48
1:A:42:VAL:HG12	1:A:42:VAL:O	2.13	0.48
1:B:195:LYS:O	1:B:199:GLU:HG3	2.13	0.48
1:B:408:TYR:OH	1:B:422:THR:CG2	2.61	0.48
1:C:183:THR:HG21	1:C:185:LYS:HG2	1.96	0.48
1:A:441:VAL:CG1	1:A:460:LYS:HE2	2.43	0.48
1:A:450:LYS:HE3	1:B:448:ARG:HH22	1.78	0.48
1:C:158:ASP:HA	1:C:162:GLN:HB2	1.95	0.48
1:C:235:GLU:HB2	1:C:236:PRO:HD3	1.94	0.48
1:D:166:THR:HG22	1:D:167:ASN:N	2.29	0.48
1:D:644:GLU:OE2	1:D:682:TYR:CD1	2.66	0.48
1:A:205:TYR:CE2	1:A:209:LEU:HD11	2.49	0.48
1:C:648:ILE:HD11	1:C:680:ILE:CD1	2.37	0.48
1:D:288:HIS:HA	1:D:299:ILE:HD12	1.95	0.48
1:A:129:PHE:CD2	1:A:149:LYS:HE3	2.49	0.48
1:A:438:ILE:HD11	1:A:463:HIS:HB3	1.96	0.48
1:C:284:ILE:CG2	1:C:296:LYS:HG2	2.43	0.48
1:C:496:ASN:N	1:C:500:GLN:OE1	2.35	0.48
1:A:383:PRO:HD3	1:B:531:ARG:NH2	2.29	0.48
1:B:137:ASN:O	1:B:139:ASP:N	2.47	0.48
1:B:261:SER:H	1:B:264:LYS:HD2	1.78	0.48
1:A:88:MSE:SE	1:A:142:TYR:HD1	2.47	0.48
1:A:649:LEU:CG	1:A:700:ILE:HD11	2.41	0.48
1:D:496:ASN:HB2	1:D:500:GLN:CD	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:ASP:HA	1:D:693:TYR:HB2	1.95	0.48
1:A:407:PHE:O	1:A:409:ASP:N	2.37	0.48
1:A:454:LEU:HD23	1:A:570:LEU:HD22	1.96	0.48
1:A:538:THR:HG22	1:A:542:LEU:HB3	1.95	0.48
1:A:645:LEU:O	1:A:649:LEU:HD13	2.14	0.48
1:B:468:TYR:CE1	1:B:507:GLU:HG3	2.49	0.48
1:A:47:VAL:HG13	1:A:48:ILE:N	2.29	0.47
1:A:106:ALA:HB2	1:A:159:VAL:HG11	1.96	0.47
1:A:417:ARG:O	1:A:421:MSE:HG3	2.14	0.47
1:A:441:VAL:HG12	1:A:460:LYS:HE2	1.95	0.47
1:A:604:LEU:HG	1:A:694:ARG:HH22	1.79	0.47
1:B:88:MSE:HE1	1:B:141:GLN:CB	2.44	0.47
1:A:610:ASN:O	1:A:611:GLN:C	2.53	0.47
1:D:328:ILE:HG13	1:D:403:TYR:CZ	2.49	0.47
1:D:536:ILE:HG12	1:D:559:GLU:HG3	1.96	0.47
1:A:39:ASP:HB2	1:A:74:ILE:HD12	1.95	0.47
1:B:450:LYS:NZ	1:B:450:LYS:CB	2.74	0.47
1:B:651:LEU:O	1:B:661:LEU:HD11	2.14	0.47
1:C:476:SER:HA	1:C:481:ILE:HD11	1.96	0.47
1:C:542:LEU:HD11	1:C:613:GLY:HA2	1.95	0.47
1:D:442:ASP:CG	1:D:448:ARG:HH12	2.16	0.47
1:B:109:PRO:O	1:B:111:ASP:N	2.48	0.47
1:B:544:MSE:H	1:B:612:ASN:HB3	1.79	0.47
1:C:540:SER:HB3	1:C:608:LYS:O	2.14	0.47
1:D:686:THR:O	1:D:690:ASP:OD1	2.32	0.47
1:B:303:PHE:O	1:B:307:VAL:HG23	2.14	0.47
1:D:259:THR:CG2	1:D:260:SER:H	2.26	0.47
1:A:48:ILE:HG12	1:A:69:TYR:CD2	2.50	0.47
1:A:422:THR:CG2	1:A:423:CYS:N	2.77	0.47
1:C:384:GLU:O	1:C:387:PRO:HD2	2.15	0.47
1:D:663:PRO:HG2	1:D:664:GLU:OE1	2.15	0.47
1:A:137:ASN:HB2	1:A:140:SER:HG	1.78	0.47
1:A:347:TYR:HE2	1:A:350:LEU:O	1.98	0.47
1:A:559:GLU:CD	1:A:559:GLU:H	2.17	0.47
1:A:688:ILE:O	1:A:691:ALA:HB3	2.15	0.47
1:B:258:ALA:HB3	1:B:264:LYS:HZ3	1.79	0.47
1:B:386:PHE:N	1:B:387:PRO:HD2	2.30	0.47
1:B:515:GLN:O	1:B:519:VAL:HG23	2.15	0.47
1:B:539:TRP:HB3	1:B:609:PHE:CD2	2.50	0.47
1:C:362:GLU:OE2	1:C:417:ARG:NH1	2.47	0.47
1:A:122:HIS:O	1:A:126:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD22	1:A:352:LEU:HD21	1.97	0.47
1:A:422:THR:O	1:A:426:ILE:HB	2.14	0.47
1:A:694:ARG:HD2	1:A:699:ASN:OD1	2.15	0.47
1:C:122:HIS:NE2	1:C:212:LEU:HD21	2.29	0.47
1:C:153:THR:HB	1:C:214:LEU:CD2	2.45	0.47
1:C:335:LEU:HD22	1:C:410:LEU:HD11	1.96	0.47
1:C:365:ILE:HD11	1:C:418:TYR:CB	2.33	0.47
1:D:295:THR:HB	1:D:298:VAL:HG23	1.95	0.47
1:D:657:ASN:HB3	1:D:660:PHE:CE1	2.50	0.47
1:A:195:LYS:HZ3	1:A:198:ARG:HH21	1.63	0.47
1:B:204:LEU:HD12	1:B:239:TRP:HB2	1.96	0.47
1:B:258:ALA:HB1	1:B:264:LYS:HZ3	1.80	0.47
1:B:527:LYS:NZ	1:B:598:TYR:HB2	2.30	0.47
1:A:190:SER:O	1:A:192:GLY:N	2.44	0.47
1:A:660:PHE:CD1	1:A:674:LEU:HD13	2.50	0.47
1:D:662:ASN:ND2	1:D:665:TYR:HB2	2.30	0.47
1:B:84:GLN:HE21	1:B:135:ILE:HD13	1.80	0.46
1:C:290:ASP:C	1:C:292:ASN:H	2.18	0.46
1:A:157:ASN:ND2	1:A:211:TYR:CE1	2.83	0.46
1:A:319:LEU:HD21	1:A:360:VAL:HG11	1.98	0.46
1:A:462:GLN:HG3	1:A:578:ASP:H	1.79	0.46
1:B:478:PHE:H	1:B:478:PHE:HD2	1.60	0.46
1:C:390:SER:HB2	1:C:466:PHE:HD2	1.79	0.46
1:D:420:LEU:CD2	1:D:483:LEU:HD22	2.44	0.46
1:A:408:TYR:OH	1:A:422:THR:CG2	2.63	0.46
1:B:559:GLU:CD	1:B:559:GLU:N	2.69	0.46
1:D:431:THR:HB	1:D:502:VAL:HG11	1.97	0.46
1:A:108:GLN:HG3	1:A:112:GLN:HE21	1.78	0.46
1:B:180:GLN:O	1:B:183:THR:HB	2.15	0.46
1:C:281:TYR:HA	1:C:284:ILE:HD12	1.98	0.46
1:A:355:LEU:C	1:A:355:LEU:HD12	2.36	0.46
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.72	0.46
1:D:261:SER:O	1:D:265:ILE:HG13	2.16	0.46
1:D:510:MSE:HB3	1:D:583:ILE:HD11	1.98	0.46
1:A:240:ASN:OD1	1:A:241:PHE:CD1	2.68	0.46
1:A:592:LEU:HD13	1:A:628:LEU:HD12	1.98	0.46
1:C:648:ILE:HD12	1:C:683:LEU:CD2	2.45	0.46
1:D:671:PHE:HE2	1:D:692:LEU:CD1	2.29	0.46
1:D:700:ILE:O	1:D:700:ILE:HG22	2.15	0.46
1:A:390:SER:OG	1:A:463:HIS:CG	2.68	0.46
1:B:140:SER:HB2	1:B:142:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TRP:CZ3	1:B:203:LYS:HE3	2.50	0.46
1:B:284:ILE:HA	1:B:299:ILE:HG21	1.96	0.46
1:B:296:LYS:CB	1:B:297:PRO:HD3	2.45	0.46
1:C:499:PHE:O	1:C:502:VAL:HG23	2.16	0.46
1:D:61:GLY:O	1:D:64:GLN:HB2	2.15	0.46
1:B:259:THR:CG2	1:B:260:SER:H	2.20	0.46
1:C:165:ALA:HB1	1:C:239:TRP:CD2	2.51	0.46
1:D:205:TYR:CG	1:D:294:LEU:HD21	2.51	0.46
1:A:137:ASN:ND2	1:A:137:ASN:N	2.64	0.46
1:A:438:ILE:HG22	1:A:439:LEU:HD23	1.97	0.46
1:B:451:GLU:OE2	1:B:569:ARG:NH1	2.49	0.46
1:B:693:TYR:HD2	1:B:697:TYR:CE1	2.34	0.46
1:C:371:MSE:HE1	1:C:374:ARG:NH2	2.23	0.46
1:C:658:GLN:HG3	1:C:661:LEU:CD1	2.46	0.46
1:B:543:GLU:N	1:B:543:GLU:OE2	2.48	0.45
1:B:684:LYS:O	1:B:688:ILE:HG13	2.15	0.45
1:D:259:THR:CG2	1:D:260:SER:N	2.78	0.45
1:A:308:LEU:HD22	1:A:352:LEU:CD2	2.46	0.45
1:A:331:ILE:HD12	1:A:364:TRP:CD1	2.52	0.45
1:A:604:LEU:HD12	1:A:609:PHE:CE1	2.50	0.45
1:B:55:VAL:HG22	1:B:56:GLY:H	1.81	0.45
1:B:109:PRO:HD2	1:B:112:GLN:OE1	2.16	0.45
1:B:490:THR:O	1:B:491:GLU:HG3	2.17	0.45
1:B:622:LYS:HE2	1:B:643:HIS:CE1	2.51	0.45
1:C:307:VAL:O	1:C:307:VAL:HG12	2.16	0.45
1:A:205:TYR:O	1:A:208:SER:HB2	2.16	0.45
1:A:592:LEU:HD22	1:A:630:LEU:HD12	1.98	0.45
1:A:640:MSE:HE2	1:A:640:MSE:HA	1.98	0.45
1:C:490:THR:HG22	1:C:490:THR:O	2.16	0.45
1:D:41:GLU:HG2	1:D:73:GLN:NE2	2.32	0.45
1:D:102:LEU:C	1:D:104:GLU:H	2.20	0.45
1:A:454:LEU:CG	1:A:458:MSE:HE2	2.43	0.45
1:A:531:ARG:HH21	1:B:383:PRO:CD	2.04	0.45
1:A:666:ILE:HG21	1:A:693:TYR:CE2	2.51	0.45
1:B:512:THR:OG1	1:B:513:ASP:N	2.49	0.45
1:C:585:LEU:CD2	1:C:631:PRO:HD3	2.45	0.45
1:D:106:ALA:HA	1:D:163:ARG:HH12	1.81	0.45
1:A:38:ASN:HD21	1:D:6:ASP:CB	2.29	0.45
1:B:95:LEU:HD13	1:B:149:LYS:HA	1.99	0.45
1:C:658:GLN:CG	1:C:661:LEU:HD12	2.45	0.45
1:D:431:THR:CG2	1:D:471:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HH12	1:B:450:LYS:HG3	1.81	0.45
1:A:481:ILE:HG13	1:A:482:GLN:N	2.30	0.45
1:A:694:ARG:O	1:A:699:ASN:HB2	2.16	0.45
1:D:42:VAL:HG12	1:D:42:VAL:O	2.17	0.45
1:A:116:ASP:O	1:A:119:LYS:N	2.50	0.45
1:C:543:GLU:HA	1:C:612:ASN:HD22	1.81	0.45
1:D:461:LEU:HD21	1:D:583:ILE:HG21	1.99	0.45
1:A:644:GLU:O	1:A:648:ILE:HG13	2.16	0.45
1:C:44:LEU:HD11	1:C:74:ILE:HD13	1.98	0.45
1:C:259:THR:CG2	1:C:260:SER:H	2.26	0.45
1:D:187:ALA:C	1:D:189:THR:H	2.20	0.45
1:D:365:ILE:HD12	1:D:418:TYR:HD2	1.81	0.45
1:D:415:LEU:HD13	1:D:419:LYS:HE3	1.99	0.45
1:D:468:TYR:CZ	1:D:472:LYS:HE3	2.52	0.45
1:D:644:GLU:OE2	1:D:682:TYR:HD1	1.99	0.45
1:C:438:ILE:HD11	1:C:463:HIS:HB2	1.99	0.45
1:D:5:ASP:N	1:D:7:LEU:HD21	2.31	0.45
1:D:377:ILE:HA	1:D:380:THR:CG2	2.47	0.45
1:D:428:MSE:HA	1:D:428:MSE:CE	2.47	0.45
1:D:438:ILE:CD1	1:D:463:HIS:HB3	2.46	0.45
1:D:600:THR:HG22	1:D:601:GLU:OE2	2.16	0.45
1:A:622:LYS:HE2	1:A:643:HIS:NE2	2.32	0.45
1:B:159:VAL:O	1:B:163:ARG:HD3	2.17	0.45
1:C:536:ILE:HD11	1:C:559:GLU:HG2	1.98	0.45
1:D:41:GLU:O	1:D:42:VAL:C	2.54	0.45
1:D:493:LYS:HG2	1:D:495:TYR:HE1	1.81	0.45
1:D:567:LEU:O	1:D:571:ILE:HB	2.15	0.45
1:B:666:ILE:HG22	1:B:693:TYR:CE1	2.52	0.44
1:C:135:ILE:HG22	1:C:136:ASN:N	2.32	0.44
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.78	0.44
1:C:637:TYR:CD1	1:C:682:TYR:HD2	2.35	0.44
1:A:488:ASN:HD21	1:A:495:TYR:H	1.64	0.44
1:D:580:PRO:HG2	1:D:583:ILE:HD12	2.00	0.44
1:D:647:LYS:HB2	1:D:647:LYS:HE3	1.83	0.44
1:C:320:PHE:CD1	1:C:321:GLN:N	2.85	0.44
1:D:491:GLU:HB3	1:D:493:LYS:HZ3	1.82	0.44
1:A:321:GLN:HG3	1:A:321:GLN:O	2.18	0.44
1:A:597:ASN:HD21	1:A:638:LYS:HE2	1.83	0.44
1:D:5:ASP:N	1:D:7:LEU:CD2	2.80	0.44
1:D:365:ILE:O	1:D:369:VAL:HG23	2.18	0.44
1:D:536:ILE:CG1	1:D:559:GLU:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:O	1:A:14:ILE:HG13	2.17	0.44
1:A:538:THR:O	1:A:540:SER:N	2.50	0.44
1:B:249:ASN:ND2	1:B:310:PRO:HB3	2.32	0.44
1:C:451:GLU:CD	1:C:569:ARG:HH12	2.19	0.44
1:C:468:TYR:CE1	1:C:507:GLU:HG2	2.53	0.44
1:C:539:TRP:O	1:C:609:PHE:HA	2.17	0.44
1:D:592:LEU:HD13	1:D:628:LEU:HD12	1.97	0.44
1:A:116:ASP:O	1:A:117:ASP:C	2.56	0.44
1:A:265:ILE:HA	1:A:268:TYR:CD1	2.53	0.44
1:A:328:ILE:HG23	1:A:329:VAL:N	2.33	0.44
1:A:363:LYS:HA	1:B:697:TYR:CE2	2.50	0.44
1:A:377:ILE:CD1	1:B:534:PHE:HZ	2.20	0.44
1:B:338:ASP:OD2	1:B:352:LEU:N	2.51	0.44
1:B:637:TYR:HE2	1:B:682:TYR:HB3	1.80	0.44
1:B:665:TYR:O	1:B:668:THR:HB	2.18	0.44
1:D:181:TRP:HA	1:D:186:PHE:CG	2.52	0.44
1:D:523:GLN:NE2	1:D:594:VAL:HG13	2.32	0.44
1:A:37:SER:C	1:A:39:ASP:H	2.21	0.44
1:A:521:ARG:HH11	1:A:521:ARG:CG	2.07	0.44
1:A:632:SER:O	1:A:633:HIS:C	2.55	0.44
1:D:293:GLY:O	1:D:298:VAL:HG21	2.17	0.44
1:D:365:ILE:HG21	1:D:421:MSE:HE2	1.98	0.44
1:A:542:LEU:HD12	1:A:542:LEU:O	2.17	0.44
1:A:659:GLN:HG3	1:A:660:PHE:H	1.81	0.44
1:D:338:ASP:O	1:D:342:LEU:HB2	2.18	0.44
1:D:350:LEU:HD21	1:D:354:SER:CB	2.47	0.44
1:D:386:PHE:N	1:D:387:PRO:HD2	2.33	0.44
1:A:179:ALA:O	1:A:181:TRP:N	2.51	0.43
1:B:55:VAL:CG2	1:B:56:GLY:H	2.31	0.43
1:B:240:ASN:OD1	1:B:241:PHE:N	2.51	0.43
1:B:284:ILE:HG21	1:B:296:LYS:HG3	2.00	0.43
1:B:657:ASN:HB3	1:B:660:PHE:HE1	1.83	0.43
1:A:362:GLU:HG3	1:B:667:LYS:HZ1	1.82	0.43
1:A:540:SER:C	1:A:610:ASN:ND2	2.72	0.43
1:A:597:ASN:ND2	1:A:638:LYS:HE2	2.33	0.43
1:B:422:THR:HG22	1:B:423:CYS:N	2.33	0.43
1:C:109:PRO:HG2	1:C:112:GLN:CD	2.38	0.43
1:D:535:LYS:O	1:D:535:LYS:HG2	2.19	0.43
1:A:114:THR:HG22	1:A:115:LEU:N	2.33	0.43
1:C:338:ASP:CG	1:C:352:LEU:H	2.20	0.43
1:C:533:TYR:CD1	1:C:560:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:HIS:ND1	1:D:258:ALA:N	2.66	0.43
1:D:577:MSE:HB3	1:D:579:ILE:HG13	1.99	0.43
1:A:7:LEU:HD11	1:D:77:LYS:HB3	1.99	0.43
1:A:27:LYS:HD2	1:D:20:GLU:OE2	2.19	0.43
1:A:648:ILE:HG12	1:A:680:ILE:HD11	2.01	0.43
1:B:657:ASN:O	1:B:659:GLN:N	2.50	0.43
1:C:259:THR:CG2	1:C:260:SER:N	2.79	0.43
1:D:321:GLN:HG2	1:D:321:GLN:O	2.18	0.43
1:D:662:ASN:HD21	1:D:665:TYR:CB	2.30	0.43
1:B:362:GLU:HG2	1:B:418:TYR:CE2	2.44	0.43
1:B:408:TYR:OH	1:B:422:THR:HG21	2.17	0.43
1:B:542:LEU:C	1:B:542:LEU:HD12	2.38	0.43
1:C:169:SER:HA	1:C:204:LEU:HD21	2.01	0.43
1:C:461:LEU:HD23	1:C:579:ILE:HD13	2.01	0.43
1:B:382:ASN:HB3	1:B:384:GLU:OE1	2.19	0.43
1:B:478:PHE:N	1:B:478:PHE:CD2	2.86	0.43
1:C:295:THR:OG1	1:C:297:PRO:HD2	2.18	0.43
1:D:510:MSE:HE2	1:D:583:ILE:HD12	2.01	0.43
1:A:156:TYR:O	1:A:160:ILE:HB	2.18	0.43
1:A:448:ARG:NH1	1:B:450:LYS:HG3	2.33	0.43
1:B:41:GLU:OE1	1:B:73:GLN:HB3	2.18	0.43
1:B:88:MSE:HE1	1:B:141:GLN:HB2	2.01	0.43
1:B:109:PRO:C	1:B:111:ASP:H	2.21	0.43
1:B:424:SER:CA	1:B:428:MSE:HE3	2.46	0.43
1:B:660:PHE:HE2	1:B:673:SER:HB2	1.83	0.43
1:C:320:PHE:CZ	1:C:321:GLN:NE2	2.87	0.43
1:C:405:GLU:HB3	1:C:406:PRO:CD	2.48	0.43
1:D:377:ILE:HA	1:D:380:THR:HG22	2.01	0.43
1:A:256:PHE:O	1:A:314:LYS:NZ	2.48	0.43
1:A:365:ILE:HD11	1:A:418:TYR:HB3	1.99	0.43
1:B:66:ARG:NH2	1:B:76:ASN:HA	2.33	0.43
1:C:319:LEU:HA	1:C:319:LEU:HD12	1.77	0.43
1:D:568:ARG:HA	1:D:627:ILE:HG21	2.00	0.43
1:D:598:TYR:O	1:D:602:SER:HB2	2.18	0.43
1:D:603:ILE:HD12	1:D:603:ILE:N	2.34	0.43
1:D:630:LEU:HD22	1:D:632:SER:H	1.84	0.43
1:A:80:LYS:O	1:A:83:VAL:HG12	2.19	0.43
1:A:632:SER:O	1:A:634:ALA:N	2.52	0.43
1:B:31:LEU:HD23	1:B:53:ILE:HG12	2.01	0.43
1:B:183:THR:HG22	1:B:185:LYS:N	2.07	0.43
1:B:449:THR:HG22	1:B:452:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:OD1	1:A:310:PRO:HB3	2.19	0.43
1:A:297:PRO:O	1:A:301:GLU:HB2	2.19	0.43
1:A:644:GLU:OE2	1:A:682:TYR:HD1	2.01	0.43
1:B:176:LEU:HD22	1:B:181:TRP:CD1	2.53	0.43
1:B:260:SER:HB2	1:B:318:THR:OG1	2.19	0.43
1:B:324:LEU:O	1:B:328:ILE:HG12	2.19	0.43
1:D:295:THR:HG22	1:D:297:PRO:HD2	2.00	0.43
1:D:355:LEU:HD12	1:D:356:ILE:N	2.34	0.43
1:A:431:THR:CG2	1:A:502:VAL:HG11	2.49	0.42
1:A:542:LEU:HD12	1:A:542:LEU:C	2.39	0.42
1:C:474:LEU:HD22	1:C:480:PHE:HE1	1.84	0.42
1:C:560:LEU:CD2	1:C:620:ASP:HB3	2.49	0.42
1:D:571:ILE:HD12	1:D:571:ILE:HA	1.79	0.42
1:A:657:ASN:C	1:A:659:GLN:N	2.72	0.42
1:C:510:MSE:CA	1:C:514:MSE:HE3	2.48	0.42
1:C:538:THR:HG22	1:C:538:THR:O	2.18	0.42
1:D:348:HIS:O	1:D:348:HIS:ND1	2.52	0.42
1:A:315:VAL:O	1:A:318:THR:HG22	2.19	0.42
1:B:319:LEU:O	1:B:322:ASN:HB2	2.19	0.42
1:B:365:ILE:CD1	1:B:421:MSE:SE	3.17	0.42
1:B:591:LEU:HD23	1:B:591:LEU:HA	1.79	0.42
1:C:27:LYS:HD2	1:C:27:LYS:HA	1.79	0.42
1:C:265:ILE:HG21	1:C:330:LEU:CD2	2.48	0.42
1:A:28:LEU:HG	1:A:32:LYS:NZ	2.34	0.42
1:A:240:ASN:OD1	1:A:241:PHE:HD1	2.03	0.42
1:A:269:PHE:HA	1:A:272:LEU:HB3	2.00	0.42
1:B:60:GLU:O	1:B:64:GLN:HG3	2.20	0.42
1:B:183:THR:CG2	1:B:184:GLN:N	2.82	0.42
1:B:320:PHE:CG	1:B:321:GLN:N	2.87	0.42
1:B:592:LEU:HD11	1:B:639:CYS:SG	2.59	0.42
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.88	0.42
1:C:533:TYR:CE2	1:C:603:ILE:HD13	2.52	0.42
1:D:84:GLN:HG3	1:D:135:ILE:CD1	2.49	0.42
1:D:519:VAL:HG21	1:D:590:GLU:HB3	2.02	0.42
1:A:19:ASN:O	1:A:22:ASN:N	2.52	0.42
1:A:259:THR:HG22	1:A:260:SER:N	2.35	0.42
1:A:309:GLN:HB3	1:A:310:PRO:CD	2.50	0.42
1:A:377:ILE:HD11	1:B:606:LEU:CD1	2.49	0.42
1:A:488:ASN:ND2	1:A:495:TYR:H	2.18	0.42
1:A:521:ARG:NH1	1:A:521:ARG:CG	2.67	0.42
1:B:99:GLU:OE2	1:B:151:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:O	1:B:366:ASN:HB2	2.20	0.42
1:C:39:ASP:HB2	1:C:74:ILE:HD12	2.01	0.42
1:C:115:LEU:HD12	1:C:115:LEU:O	2.19	0.42
1:D:180:GLN:O	1:D:183:THR:HG22	2.19	0.42
1:D:380:THR:OG1	1:D:437:TYR:CE2	2.72	0.42
1:A:74:ILE:HG23	1:A:75:LEU:HD12	2.01	0.42
1:B:284:ILE:CG2	1:B:296:LYS:HG3	2.49	0.42
1:D:109:PRO:HG2	1:D:112:GLN:CD	2.39	0.42
1:D:137:ASN:CB	1:D:140:SER:HB2	2.50	0.42
1:D:295:THR:HG22	1:D:297:PRO:CD	2.49	0.42
1:D:590:GLU:HA	1:D:590:GLU:OE1	2.18	0.42
1:A:428:MSE:HE3	1:A:502:VAL:CG2	2.49	0.42
1:D:357:SER:HB3	1:D:360:VAL:HG23	2.02	0.42
1:B:98:PHE:CD2	1:B:125:LEU:HD13	2.55	0.42
1:B:651:LEU:HD11	1:B:674:LEU:HD11	2.01	0.42
1:D:295:THR:HB	1:D:297:PRO:HD2	2.00	0.42
1:B:417:ARG:HG3	1:B:418:TYR:N	2.34	0.42
1:B:581:LEU:O	1:B:585:LEU:HG	2.20	0.42
1:B:659:GLN:HG3	1:B:660:PHE:N	2.34	0.42
1:D:95:LEU:O	1:D:98:PHE:N	2.51	0.42
1:D:158:ASP:C	1:D:158:ASP:OD1	2.58	0.42
1:D:460:LYS:O	1:D:464:VAL:HG23	2.19	0.42
1:B:88:MSE:HE1	1:B:141:GLN:O	2.20	0.42
1:B:204:LEU:HB3	1:B:240:ASN:HB3	2.01	0.42
1:B:302:GLN:OE1	1:B:302:GLN:HA	2.19	0.42
1:C:62:LEU:HA	1:C:62:LEU:HD23	1.85	0.42
1:D:10:ILE:O	1:D:14:ILE:HG13	2.19	0.42
1:D:195:LYS:HB2	1:D:195:LYS:NZ	2.35	0.42
1:A:631:PRO:HG2	1:A:634:ALA:CB	2.49	0.41
1:B:63:GLU:HG2	1:B:79:GLU:OE1	2.19	0.41
1:C:614:LEU:HD12	1:C:614:LEU:HA	1.92	0.41
1:D:102:LEU:C	1:D:104:GLU:N	2.73	0.41
1:A:195:LYS:O	1:A:199:GLU:HG3	2.19	0.41
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.91	0.41
1:B:542:LEU:HD11	1:B:613:GLY:N	2.34	0.41
1:B:683:LEU:HD12	1:B:683:LEU:HA	1.88	0.41
1:C:338:ASP:HA	1:C:341:LEU:HD12	2.02	0.41
1:C:431:THR:HG22	1:C:432:SER:N	2.34	0.41
1:A:302:GLN:O	1:A:305:ASN:HB3	2.21	0.41
1:A:660:PHE:CZ	1:A:673:SER:HB3	2.55	0.41
1:B:164:LEU:O	1:B:165:ALA:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:LEU:HD11	1:D:625:SER:HB2	2.01	0.41
1:A:205:TYR:CD1	1:A:294:LEU:HD21	2.55	0.41
1:A:318:THR:O	1:A:322:ASN:HB2	2.20	0.41
1:A:450:LYS:HE3	1:B:448:ARG:NH2	2.35	0.41
1:A:462:GLN:HG3	1:A:578:ASP:N	2.35	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.82	0.41
1:B:474:LEU:HD22	1:B:480:PHE:CE1	2.56	0.41
1:D:657:ASN:HB3	1:D:660:PHE:HE1	1.85	0.41
1:D:671:PHE:O	1:D:675:LYS:HB2	2.20	0.41
1:A:448:ARG:CD	1:A:453:GLU:OE1	2.68	0.41
1:A:683:LEU:HD12	1:A:683:LEU:HA	1.90	0.41
1:C:645:LEU:O	1:C:649:LEU:HG	2.21	0.41
1:D:390:SER:HB3	1:D:466:PHE:CD2	2.52	0.41
1:A:31:LEU:HG	1:A:35:LEU:HD11	2.01	0.41
1:A:358:ASP:OD1	1:A:418:TYR:OH	2.38	0.41
1:A:431:THR:HG21	1:A:471:ILE:CD1	2.51	0.41
1:A:431:THR:HG21	1:A:471:ILE:HD11	2.03	0.41
1:A:648:ILE:HD13	1:A:688:ILE:HG23	2.02	0.41
1:A:649:LEU:HG	1:A:700:ILE:CD1	2.47	0.41
1:B:377:ILE:HA	1:B:380:THR:HG22	2.02	0.41
1:C:650:LYS:C	1:C:652:LYS:H	2.23	0.41
1:D:256:PHE:CD2	1:D:268:TYR:CE2	3.08	0.41
1:D:330:LEU:HG	1:D:334:ILE:HD11	2.03	0.41
1:A:79:GLU:HA	1:A:82:ALA:HB3	2.03	0.41
1:A:172:PHE:CE1	1:A:200:ASN:HB3	2.56	0.41
1:A:542:LEU:HD12	1:A:612:ASN:HB2	2.02	0.41
1:A:693:TYR:O	1:A:697:TYR:HD1	2.04	0.41
1:B:114:THR:HG22	1:B:115:LEU:N	2.36	0.41
1:B:165:ALA:HB1	1:B:239:TRP:CG	2.56	0.41
1:B:416:VAL:HG22	1:B:416:VAL:O	2.21	0.41
1:C:172:PHE:CE2	1:C:176:LEU:HD11	2.55	0.41
1:D:657:ASN:C	1:D:659:GLN:N	2.73	0.41
1:A:571:ILE:HD11	1:A:628:LEU:HD23	2.03	0.41
1:A:638:LYS:HE3	1:A:638:LYS:HB3	1.81	0.41
1:B:308:LEU:HD22	1:B:352:LEU:HD21	2.03	0.41
1:D:512:THR:O	1:D:513:ASP:C	2.59	0.41
1:D:541:THR:O	1:D:541:THR:HG22	2.21	0.41
1:A:22:ASN:O	1:A:25:ALA:HB3	2.21	0.41
1:A:371:MSE:HA	1:A:371:MSE:CE	2.49	0.41
1:A:478:PHE:CD1	1:A:481:ILE:HD11	2.55	0.41
1:A:630:LEU:HB3	1:A:631:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:PHE:HD1	1:A:674:LEU:HD13	1.85	0.41
1:B:181:TRP:HA	1:B:186:PHE:CD1	2.56	0.41
1:B:562:ASN:O	1:B:566:VAL:HG23	2.21	0.41
1:B:668:THR:HG22	1:B:670:ASN:H	1.84	0.41
1:C:320:PHE:CG	1:C:321:GLN:N	2.89	0.41
1:C:422:THR:CG2	1:C:423:CYS:N	2.84	0.41
1:C:610:ASN:O	1:C:611:GLN:C	2.59	0.41
1:C:675:LYS:HE3	1:C:675:LYS:HB2	1.86	0.41
1:D:281:TYR:CD1	1:D:282:LYS:N	2.89	0.41
1:D:431:THR:HG23	1:D:471:ILE:HD11	2.02	0.41
1:D:490:THR:HG23	1:D:491:GLU:H	1.86	0.41
1:D:543:GLU:HG2	1:D:543:GLU:O	2.20	0.41
1:D:608:LYS:HA	1:D:699:ASN:O	2.20	0.41
1:A:165:ALA:HB1	1:A:239:TRP:CD2	2.56	0.41
1:A:699:ASN:HD22	1:A:699:ASN:HA	1.55	0.41
1:C:204:LEU:HD12	1:C:204:LEU:HA	1.87	0.41
1:D:114:THR:HG22	1:D:115:LEU:N	2.36	0.41
1:D:477:ASN:O	1:D:481:ILE:HG13	2.21	0.41
1:A:602:SER:C	1:A:603:ILE:HD12	2.41	0.40
1:B:345:PHE:O	1:B:346:HIS:HB2	2.21	0.40
1:B:393:PHE:O	1:B:396:LEU:HB3	2.21	0.40
1:B:602:SER:O	1:B:603:ILE:HD12	2.21	0.40
1:C:432:SER:HB3	1:C:502:VAL:CG1	2.46	0.40
1:D:208:SER:OG	1:D:239:TRP:HD1	2.04	0.40
1:D:329:VAL:O	1:D:333:GLN:HG3	2.20	0.40
1:D:439:LEU:HD21	1:D:514:MSE:CE	2.35	0.40
1:D:638:LYS:HE3	1:D:638:LYS:HB3	1.88	0.40
1:A:169:SER:HA	1:A:204:LEU:HD21	2.02	0.40
1:B:84:GLN:CG	1:B:135:ILE:HD13	2.45	0.40
1:A:299:ILE:O	1:A:300:HIS:C	2.58	0.40
1:A:379:ILE:HG13	1:A:380:THR:HG23	2.02	0.40
1:A:588:LYS:CB	1:A:630:LEU:HD21	2.51	0.40
1:B:281:TYR:HB2	1:C:481:ILE:HD12	2.03	0.40
1:B:649:LEU:HB3	1:B:700:ILE:HD13	2.03	0.40
1:D:671:PHE:HE2	1:D:692:LEU:HD12	1.86	0.40
1:A:7:LEU:HB2	1:D:81:VAL:HG21	2.04	0.40
1:A:407:PHE:C	1:A:409:ASP:H	2.23	0.40
1:A:540:SER:HB2	1:A:701:LEU:HD12	2.03	0.40
1:B:658:GLN:HG2	1:B:658:GLN:O	2.21	0.40
1:C:666:ILE:HD12	1:C:696:ILE:HD11	1.99	0.40
1:D:106:ALA:HB2	1:D:159:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:O	1:A:364:TRP:HB3	2.22	0.40
1:C:19:ASN:O	1:C:22:ASN:HB2	2.21	0.40
1:C:172:PHE:CD1	1:C:200:ASN:HB3	2.56	0.40
1:C:294:LEU:HD23	1:C:294:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	667/706 (94%)	589 (88%)	64 (10%)	14 (2%)	7 33
1	B	667/706 (94%)	610 (92%)	43 (6%)	14 (2%)	7 33
1	C	667/706 (94%)	606 (91%)	49 (7%)	12 (2%)	8 37
1	D	667/706 (94%)	592 (89%)	59 (9%)	16 (2%)	6 29
All	All	2668/2824 (94%)	2397 (90%)	215 (8%)	56 (2%)	7 33

All (56) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	D	512	THR
1	D	633	HIS
1	A	138	ILE
1	A	140	SER
1	A	180	GLN
1	A	191	VAL
1	A	544	MSE
1	B	544	MSE
1	C	492	SER
1	D	138	ILE
1	D	141	GLN
1	D	658	GLN
1	A	258	ALA
1	A	658	GLN
1	B	110	PRO
1	C	259	THR
1	C	685	ASP
1	D	158	ASP
1	D	321	GLN
1	D	411	ASP
1	B	258	ALA
1	B	259	THR
1	B	513	ASP
1	B	539	TRP
1	C	140	SER
1	D	685	ASP
1	A	38	ASN
1	A	319	LEU
1	A	423	CYS
1	B	140	SER
1	B	265	ILE
1	B	658	GLN
1	C	291	CYS
1	C	544	MSE
1	D	110	PRO
1	D	186	PHE
1	D	497	SER
1	B	663	PRO
1	C	191	VAL
1	C	258	ALA
1	D	191	VAL
1	C	441	VAL

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Mol	Chain	Res	Type
1	D	42	VAL
1	B	133	PRO
1	A	194	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	633/648 (98%)	601 (95%)	32 (5%)	24	60
1	B	633/648 (98%)	601 (95%)	32 (5%)	24	60
1	C	633/648 (98%)	607 (96%)	26 (4%)	30	67
1	D	633/648 (98%)	592 (94%)	41 (6%)	17	50
All	All	2532/2592 (98%)	2401 (95%)	131 (5%)	23	59

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	51	ASP
1	A	60	GLU
1	A	71	ASP
1	A	83	VAL
1	A	111	ASP
1	A	146	ASN
1	A	164	LEU
1	A	242	LYS
1	A	253	THR
1	A	257	HIS
1	A	267	THR
1	A	318	THR
1	A	320	PHE
1	A	322	ASN
1	A	340	ASN
1	A	355	LEU
1	A	397	ILE

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Mol	Chain	Res	Type
1	A	409	ASP
1	A	412	PHE
1	A	415	LEU
1	A	422	THR
1	A	450	LYS
1	A	463	HIS
1	A	478	PHE
1	A	521	ARG
1	A	526	LEU
1	A	531	ARG
1	A	633	HIS
1	A	693	TYR
1	A	694	ARG
1	A	699	ASN
1	B	38	ASN
1	B	54	GLU
1	B	75	LEU
1	B	84	GLN
1	B	89	GLN
1	B	127	SER
1	B	200	ASN
1	B	204	LEU
1	B	215	GLU
1	B	242	LYS
1	B	290	ASP
1	B	296	LYS
1	B	314	LYS
1	B	323	ASP
1	B	338	ASP
1	B	341	LEU
1	B	380	THR
1	B	399	LYS
1	B	411	ASP
1	B	415	LEU
1	B	422	THR
1	B	450	LYS
1	B	452	GLN
1	B	478	PHE
1	B	515	GLN
1	B	526	LEU
1	B	531	ARG
1	B	631	PRO

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Mol	Chain	Res	Type
1	B	637	TYR
1	B	662	ASN
1	B	676	GLU
1	B	694	ARG
1	C	12	ASP
1	C	47	VAL
1	C	51	ASP
1	C	121	LEU
1	C	251	ARG
1	C	301	GLU
1	C	314	LYS
1	C	328	ILE
1	C	337	THR
1	C	339	LYS
1	C	368	GLU
1	C	380	THR
1	C	399	LYS
1	C	402	ASP
1	C	415	LEU
1	C	431	THR
1	C	438	ILE
1	C	440	THR
1	C	441	VAL
1	C	442	ASP
1	C	469	ARG
1	C	502	VAL
1	C	504	ASN
1	C	631	PRO
1	C	656	ASN
1	C	694	ARG
1	D	7	LEU
1	D	27	LYS
1	D	28	LEU
1	D	54	GLU
1	D	66	ARG
1	D	73	GLN
1	D	75	LEU
1	D	76	ASN
1	D	112	GLN
1	D	137	ASN
1	D	173	ASP
1	D	174	GLN

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Mol	Chain	Res	Type
1	D	180	GLN
1	D	183	THR
1	D	200	ASN
1	D	273	ASN
1	D	326	THR
1	D	327	LEU
1	D	338	ASP
1	D	341	LEU
1	D	345	PHE
1	D	346	HIS
1	D	348	HIS
1	D	411	ASP
1	D	415	LEU
1	D	423	CYS
1	D	428	MSE
1	D	469	ARG
1	D	477	ASN
1	D	517	SER
1	D	518	ILE
1	D	521	ARG
1	D	538	THR
1	D	572	ASN
1	D	590	GLU
1	D	630	LEU
1	D	653	TYR
1	D	659	GLN
1	D	690	ASP
1	D	693	TYR
1	D	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	108	GLN
1	A	112	GLN
1	A	137	ASN
1	A	322	ASN
1	A	333	GLN
1	A	392	ASN
1	A	488	ASN
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	610	ASN
1	A	616	GLN
1	A	633	HIS
1	A	689	GLN
1	B	22	ASN
1	B	84	GLN
1	B	206	GLN
1	B	249	ASN
1	B	321	GLN
1	B	343	ASN
1	B	373	ASN
1	B	391	GLN
1	B	429	ASN
1	B	496	ASN
1	B	500	GLN
1	B	562	ASN
1	B	612	ASN
1	B	615	ASN
1	B	643	HIS
1	C	33	GLN
1	C	50	GLN
1	C	85	GLN
1	C	112	GLN
1	C	137	ASN
1	C	206	GLN
1	C	321	GLN
1	C	373	ASN
1	C	496	ASN
1	C	589	ASN
1	C	612	ASN
1	C	636	ASN
1	D	84	GLN
1	D	137	ASN
1	D	146	ASN
1	D	343	ASN
1	D	392	ASN
1	D	500	GLN
1	D	504	ASN
1	D	523	GLN
1	D	593	ASN
1	D	612	ASN
1	D	633	HIS

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Mol	Chain	Res	Type
1	D	636	ASN
1	D	659	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	663/706 (93%)	-0.14	8 (1%)	79	54	47, 83, 125, 155	0
1	B	663/706 (93%)	-0.15	5 (0%)	86	65	44, 70, 121, 160	0
1	C	663/706 (93%)	-0.16	6 (0%)	84	63	42, 71, 127, 161	0
1	D	663/706 (93%)	-0.10	19 (2%)	51	23	52, 86, 128, 162	0
All	All	2652/2824 (93%)	-0.14	38 (1%)	75	49	42, 77, 125, 162	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	553	SER	5.0
1	D	674	LEU	4.1
1	B	141	GLN	4.0
1	D	138	ILE	3.8
1	D	545	SER	3.8
1	A	260	SER	3.7
1	D	680	ILE	3.2
1	D	135	ILE	3.0
1	B	701	LEU	2.9
1	D	671	PHE	2.8
1	A	633	HIS	2.7
1	C	552	PRO	2.7
1	D	137	ASN	2.7
1	C	262	SER	2.6
1	D	554	SER	2.5
1	D	139	ASP	2.5
1	B	260	SER	2.5
1	C	651	LEU	2.4
1	A	269	PHE	2.4
1	A	141	GLN	2.3
1	C	260	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	678	TYR	2.3
1	A	327	LEU	2.3
1	D	296	LYS	2.3
1	C	553	SER	2.3
1	A	671	PHE	2.2
1	D	631	PRO	2.2
1	A	139	ASP	2.1
1	D	490	THR	2.1
1	B	631	PRO	2.1
1	D	552	PRO	2.1
1	C	632	SER	2.1
1	D	366	ASN	2.0
1	D	555	VAL	2.0
1	D	649	LEU	2.0
1	A	262	SER	2.0
1	B	216	GLU	2.0
1	D	661	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.