Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:41 AM GMT

PDB ID	:	3FN9
Title	:	Crystal structure of putative beta-galactosidase from bacteroides fragilis
Authors	:	Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-12-23
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

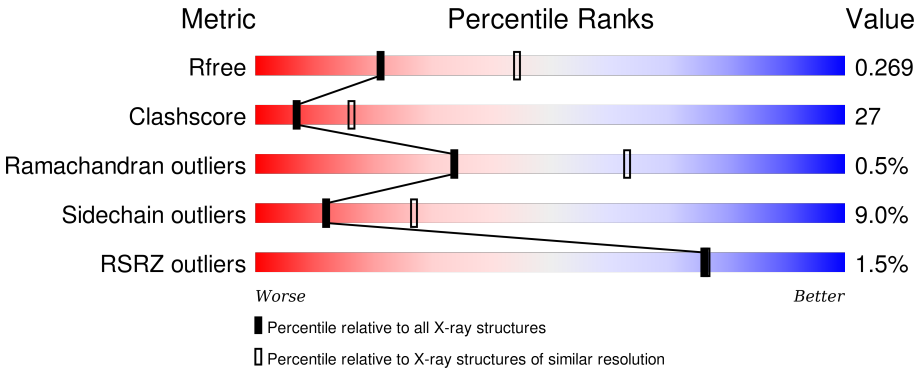
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	692	60% 34%
1	B	692	50% 40% 7%
1	C	692	64% 30%
1	D	692	58% 34%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21740 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 Putative beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5426	3469	926	1013	18			
1	B	672	Total	C	N	O	S	0	0	0
			5410	3463	923	1006	18			
1	C	673	Total	C	N	O	S	0	0	0
			5431	3471	927	1015	18			
1	D	666	Total	C	N	O	S	0	0	0
			5374	3439	916	1001	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	EXPRESSION TAG	UNP Q5LJ68
A	21	SER	-	EXPRESSION TAG	UNP Q5LJ68
A	22	LEU	-	EXPRESSION TAG	UNP Q5LJ68
A	704	GLU	-	EXPRESSION TAG	UNP Q5LJ68
A	705	GLY	-	EXPRESSION TAG	UNP Q5LJ68
A	706	HIS	-	EXPRESSION TAG	UNP Q5LJ68
A	707	HIS	-	EXPRESSION TAG	UNP Q5LJ68
A	708	HIS	-	EXPRESSION TAG	UNP Q5LJ68
A	709	HIS	-	EXPRESSION TAG	UNP Q5LJ68
A	710	HIS	-	EXPRESSION TAG	UNP Q5LJ68
A	711	HIS	-	EXPRESSION TAG	UNP Q5LJ68
B	20	MET	-	EXPRESSION TAG	UNP Q5LJ68
B	21	SER	-	EXPRESSION TAG	UNP Q5LJ68
B	22	LEU	-	EXPRESSION TAG	UNP Q5LJ68
B	704	GLU	-	EXPRESSION TAG	UNP Q5LJ68
B	705	GLY	-	EXPRESSION TAG	UNP Q5LJ68
B	706	HIS	-	EXPRESSION TAG	UNP Q5LJ68
B	707	HIS	-	EXPRESSION TAG	UNP Q5LJ68
B	708	HIS	-	EXPRESSION TAG	UNP Q5LJ68
B	709	HIS	-	EXPRESSION TAG	UNP Q5LJ68
B	710	HIS	-	EXPRESSION TAG	UNP Q5LJ68

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Chain	Residue	Modelled	Actual	Comment	Reference
B	711	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	20	MET	-	EXPRESSION TAG	UNP Q5LJ68
C	21	SER	-	EXPRESSION TAG	UNP Q5LJ68
C	22	LEU	-	EXPRESSION TAG	UNP Q5LJ68
C	704	GLU	-	EXPRESSION TAG	UNP Q5LJ68
C	705	GLY	-	EXPRESSION TAG	UNP Q5LJ68
C	706	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	707	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	708	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	709	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	710	HIS	-	EXPRESSION TAG	UNP Q5LJ68
C	711	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	20	MET	-	EXPRESSION TAG	UNP Q5LJ68
D	21	SER	-	EXPRESSION TAG	UNP Q5LJ68
D	22	LEU	-	EXPRESSION TAG	UNP Q5LJ68
D	704	GLU	-	EXPRESSION TAG	UNP Q5LJ68
D	705	GLY	-	EXPRESSION TAG	UNP Q5LJ68
D	706	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	707	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	708	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	709	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	710	HIS	-	EXPRESSION TAG	UNP Q5LJ68
D	711	HIS	-	EXPRESSION TAG	UNP Q5LJ68

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	D	3	Total Cl 3 3	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	B	18	Total O 18 18	0	0

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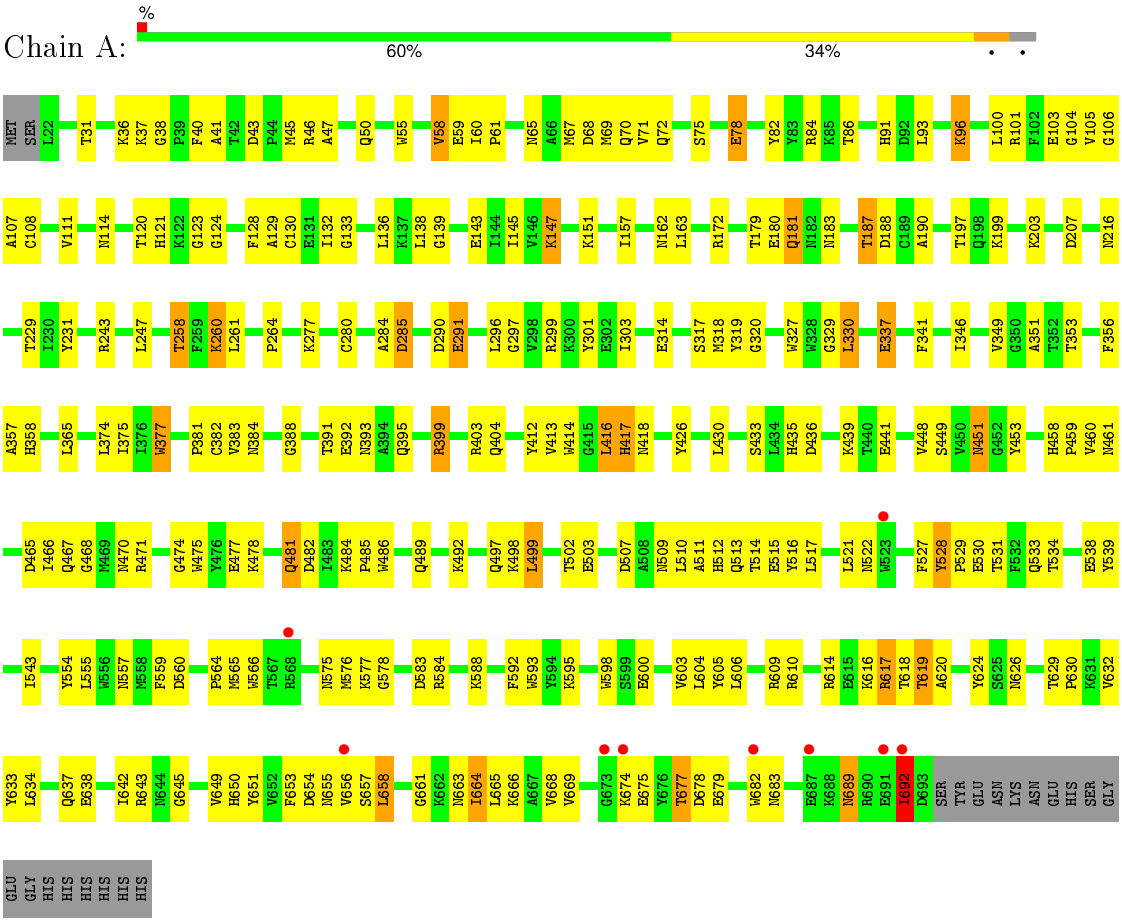
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	23	Total O 23 23	0	0
3	D	20	Total O 20 20	0	0

3 Residue-property plots (i)

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

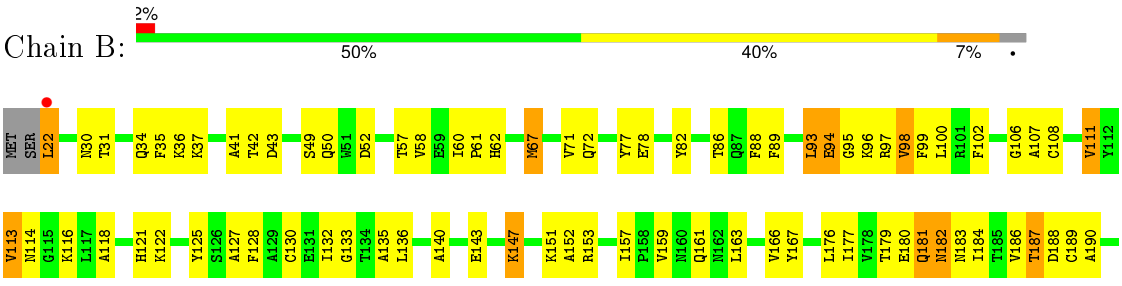
- Molecule 1: Putative beta-galactosidase

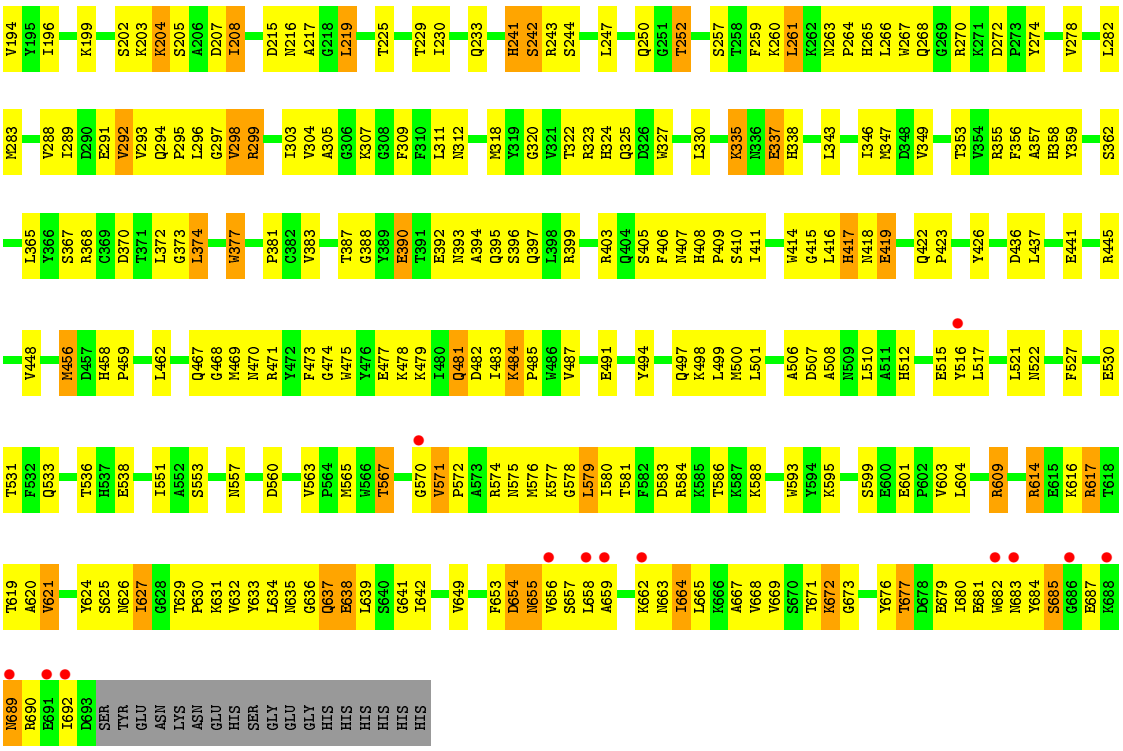
Chain A:



- Molecule 1: Putative beta-galactosidase

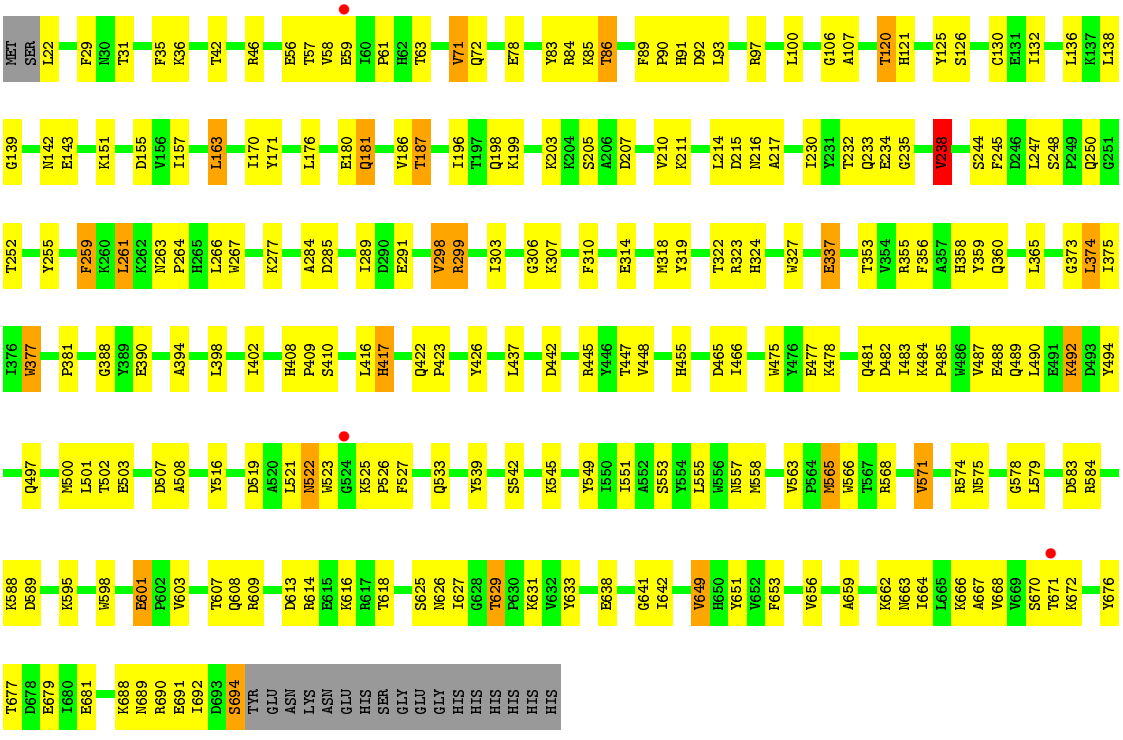
Chain B:





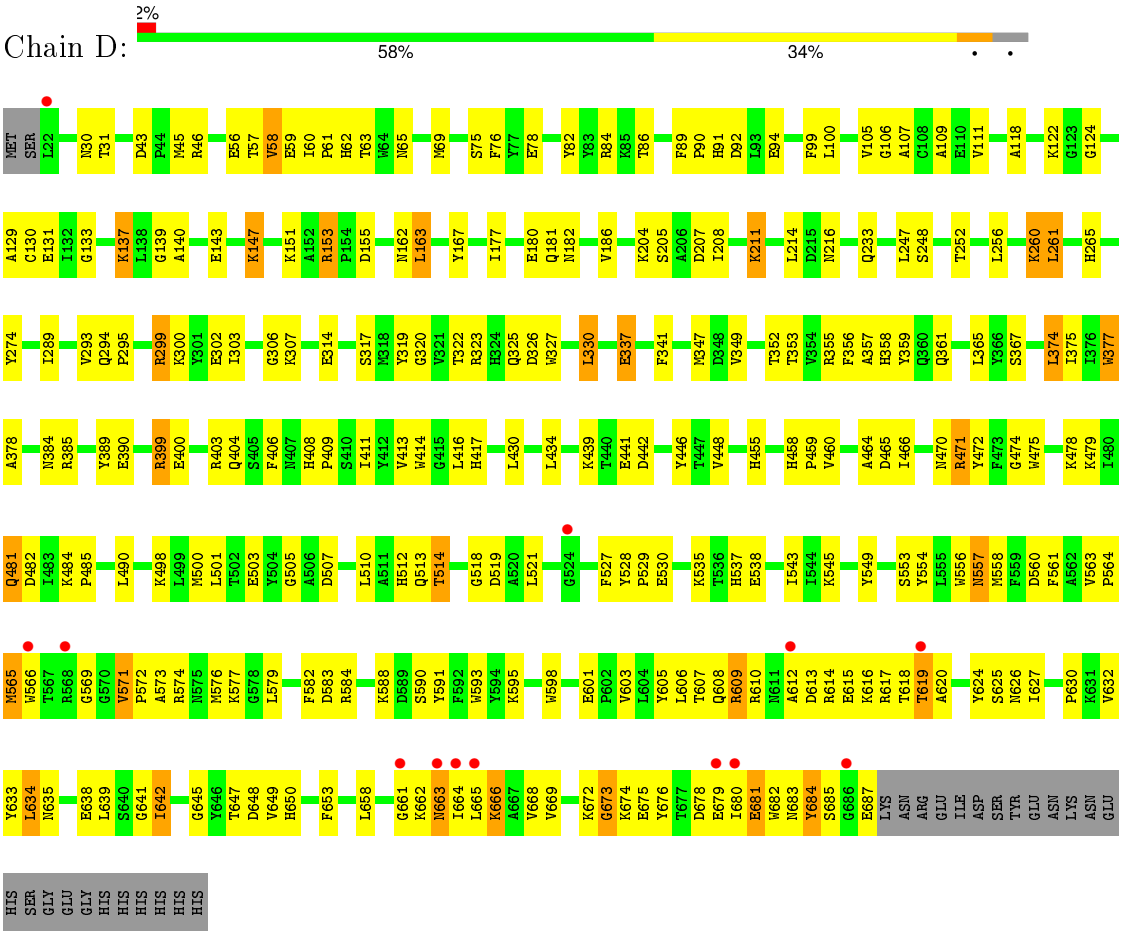
• Molecule 1: Putative beta-galactosidase

Chain C:



• Molecule 1: Putative beta-galactosidase

Chain D:


2%
58%
34%
MET SER L22 N30 T31 D43 P44 M45 R46 E56 T57 V58 E59 I60 P61 H62 T63 W64 N65 M69 S75 F76 Y77 E78 Y82 Y83 R84 K85 T86 F89 P90 H91 D92 L93 E94 F99 L100 V105 G106 A107 C108 A109 E110 V111 A118 K122 G123 G124
A129 C130 E131 I132 G133 K137 L138 G139 A140 E143 K147 K151 A152 R153 P154 D155 N162 L163 Y167 I177 E180 Q181 N182 V186 K204 S205 A206 D207 I208 K211 L214 D215 N216 Q233 L247 S248 T252 L256 K260 L261 H265
Y274 I289 V293 Q294 F295 R299 K300 Y301 E302 I303 G306 K307 E314 S317 K318 Y319 G320 Y321 T322 R323 H324 Q325 D326 W327 I330 E337 F341 N347 D348 V349 T352 T353 V354 R355 F356 A357 H358 Y359 Q360 Q361 L365 Y366 S367 L374 I375 I376 W377
A378 N384 R385 Y389 E390 R399 E400 R403 Q404 S405 F406 N407 H408 P409 S410 I411 Y412 V413 W414 G415 L416 H417 L430 L434 K439 T440 E441 D442 Y446 T447 V448 H455 H458 P459 V460 A464 D465 I466 N470 R471 Y472 F473 G474 W475 K478 K479 I480
Q481 D482 I483 K484 P485 L490 K498 L499 M500 L501 T502 E503 Y504 G505 A506 D507 L510 A511 H512 Q513 T514 G518 D519 A520 L521 G524 F527 Y528 P529 E530 K535 T536 H537 E538 I543 I544 K545 Y549 S553 Y554 L555 W556 N557 M558 F559 D560 F561 A562 V563 P564
M565 W566 T567 R568 G569 G570 V571 P572 A573 R574 N575 M576 K577 G578 L579 F582 D583 R584 K588 D589 S590 Y591 F592 W593 Y594 K595 W598 E601 P602 V603 L604 Y605 L606 T607 Q608 R609 R610 W611 A612 D613 R614 E615 K616 R617 T618 T619 A620 Y624 S625 N626 I627 P630 K631 V632
Y633 L634 N635 E638 L639 S640 G641 I642 G645 Y646 T647 D648 V649 H650 F653 L658 G661 K662 N663 I664 L665 K666 A667 V668 V669 K672 G673 K674 E675 Y676 T677 D678 E679 I680 E681 W682 N683 Y684 S685 G686 E687 LYS ASN ARG GLU ILE ASP SER TYR GLU ASN LYS ASN GLU
HIS SER GLY GLU GLY HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.45Å 133.07Å 221.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.70 46.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.39-2.70) 99.9 (46.28-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.201 , 0.270 0.205 , 0.269	Depositor DCC
R_{free} test set	4414 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 89139 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21740	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	1/5577 (0.0%)	0.67	0/7579
1	B	0.54	0/5561	0.67	0/7558
1	C	0.55	0/5582	0.66	0/7586
1	D	0.54	0/5525	0.67	0/7509
All	All	0.55	1/22245 (0.0%)	0.67	0/30232

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.66	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5426	0	5216	274	0
1	B	5410	0	5189	372	0
1	C	5431	0	5219	205	0
1	D	5374	0	5167	287	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	1	0
3	A	31	0	0	4	0
3	B	18	0	0	1	0
3	C	23	0	0	2	0
3	D	20	0	0	5	0
All	All	21740	0	20791	1125	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 27.

All (1125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:PRO:HA	1:B:669:VAL:CG2	1.65	1.26
1:D:347:MET:CE	1:D:374:LEU:HD13	1.69	1.20
1:D:347:MET:HE1	1:D:374:LEU:CD1	1.72	1.19
1:D:347:MET:CE	1:D:374:LEU:CD1	2.24	1.15
1:B:208:ILE:CD1	1:B:259:PHE:HB2	1.76	1.15
1:D:607:THR:HG22	1:D:608:GLN:HG3	1.20	1.13
1:A:157:ILE:HG13	1:A:381:PRO:HG2	1.14	1.13
1:A:481:GLN:NE2	1:A:481:GLN:H	1.49	1.10
1:B:617:ARG:HH11	1:B:617:ARG:HG2	0.98	1.10
1:B:37:LYS:HD2	1:B:77:TYR:CD2	1.86	1.10
1:D:481:GLN:H	1:D:481:GLN:NE2	1.48	1.10
1:B:67:MET:HA	1:B:67:MET:CE	1.82	1.09
1:B:630:PRO:HA	1:B:669:VAL:HG23	1.27	1.07
1:A:617:ARG:CG	1:A:617:ARG:HH11	1.66	1.07
1:D:630:PRO:HA	1:D:669:VAL:HG12	1.37	1.06
1:A:617:ARG:NH1	1:A:617:ARG:HG3	1.51	1.06
1:B:67:MET:HA	1:B:67:MET:HE2	1.09	1.05
1:D:642:ILE:HB	1:D:653:PHE:CE2	1.92	1.03
1:C:642:ILE:HD13	1:C:653:PHE:CZ	1.92	1.03
1:B:633:TYR:CD1	1:B:638:GLU:HA	1.94	1.01
1:C:307:LYS:HE3	1:C:310:PHE:CZ	1.95	1.01
1:D:630:PRO:HA	1:D:669:VAL:CG1	1.91	1.00
1:C:629:THR:HG22	3:C:1:HOH:O	1.59	1.00
1:B:202:SER:OG	1:B:204:LYS:HG3	1.62	0.99
1:A:78:GLU:HG3	1:A:151:LYS:HA	1.45	0.98
1:A:179:THR:HG22	1:A:180:GLU:O	1.63	0.98
1:B:630:PRO:CA	1:B:669:VAL:CG2	2.41	0.98
1:D:99:PHE:CE2	1:D:131:GLU:HG3	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:NH1	1:B:217:ALA:HB2	1.79	0.97
1:A:654:ASP:HB2	1:A:655:ASN:ND2	1.79	0.97
1:B:41:ALA:H	1:B:50:GLN:HE22	1.11	0.97
1:B:689:ASN:ND2	1:B:692:ILE:HG13	1.79	0.97
1:A:692:ILE:CG2	1:A:692:ILE:O	2.13	0.97
1:A:41:ALA:H	1:A:50:GLN:HE22	1.13	0.96
1:B:67:MET:CA	1:B:67:MET:HE2	1.96	0.96
1:A:661:GLY:HA3	3:A:737:HOH:O	1.63	0.96
1:C:187:THR:CG2	1:C:187:THR:O	2.12	0.96
1:B:659:ALA:N	1:B:663:ASN:HD21	1.64	0.95
1:D:684:TYR:CD2	1:D:685:SER:N	2.33	0.95
1:D:662:LYS:C	1:D:663:ASN:HD22	1.67	0.95
1:A:498:LYS:H	1:B:250:GLN:HE22	1.04	0.95
1:D:662:LYS:HE2	1:D:681:GLU:OE2	1.67	0.95
1:B:617:ARG:CG	1:B:617:ARG:HH11	1.80	0.94
1:B:595:LYS:HG2	1:B:603:VAL:HG21	1.45	0.94
1:C:662:LYS:HE3	1:C:681:GLU:OE2	1.67	0.94
1:B:659:ALA:H	1:B:663:ASN:ND2	1.65	0.94
1:B:356:PHE:CE2	1:B:365:LEU:HD21	2.02	0.94
1:B:633:TYR:HD1	1:B:638:GLU:HA	1.30	0.93
1:B:633:TYR:HE1	1:B:638:GLU:HB2	1.31	0.93
1:B:179:THR:HG21	1:B:183:ASN:HB3	1.49	0.93
1:B:630:PRO:CA	1:B:669:VAL:HG23	1.97	0.93
1:B:659:ALA:H	1:B:663:ASN:HD21	0.95	0.93
1:D:111:VAL:HG23	1:D:118:ALA:HB3	1.51	0.92
1:A:179:THR:CG2	1:A:180:GLU:N	2.33	0.92
1:B:181:GLN:HA	1:B:181:GLN:HE21	1.35	0.92
1:A:133:GLY:HA2	1:A:136:LEU:HD23	1.47	0.92
1:D:607:THR:HG22	1:D:608:GLN:CG	1.98	0.92
1:D:510:LEU:HD21	1:D:588:LYS:HG2	1.51	0.92
1:D:347:MET:HE3	1:D:374:LEU:HD22	1.50	0.91
1:B:208:ILE:HD13	1:B:259:PHE:HB2	1.50	0.91
1:B:179:THR:HG22	1:B:180:GLU:N	1.86	0.91
1:C:583:ASP:O	1:C:584:ARG:HB2	1.71	0.91
1:A:481:GLN:HE21	1:A:481:GLN:H	1.12	0.90
1:B:684:TYR:OH	1:B:687:GLU:HG2	1.71	0.90
1:A:629:THR:HG22	1:A:651:TYR:HE2	1.33	0.90
1:A:633:TYR:HD2	1:A:638:GLU:HA	1.33	0.90
1:A:470:ASN:OD1	1:A:503:GLU:HB2	1.70	0.90
1:B:395:GLN:HG2	1:B:437:LEU:CD1	2.02	0.90
1:B:664:ILE:HG22	1:B:681:GLU:HG3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:TYR:CE1	1:D:638:GLU:HB2	2.07	0.89
1:D:565:MET:CE	1:D:565:MET:HA	2.02	0.89
1:A:654:ASP:HB2	1:A:655:ASN:HD22	1.33	0.89
1:B:41:ALA:N	1:B:50:GLN:HE22	1.71	0.89
1:D:478:LYS:HB3	1:D:482:ASP:OD2	1.73	0.89
1:B:680:ILE:HD12	1:B:682:TRP:NE1	1.87	0.89
1:D:557:ASN:HD22	1:D:558:MET:N	1.71	0.88
1:B:512:HIS:CD2	1:B:527:PHE:CE1	2.60	0.88
1:D:632:VAL:CG2	1:D:653:PHE:CE1	2.57	0.88
1:A:179:THR:HG22	1:A:180:GLU:N	1.88	0.87
1:B:680:ILE:HD12	1:B:682:TRP:HE1	1.38	0.87
1:A:507:ASP:OD1	1:A:577:LYS:HE2	1.75	0.87
1:D:557:ASN:HD22	1:D:558:MET:H	1.22	0.86
1:B:181:GLN:HA	1:B:181:GLN:NE2	1.88	0.86
1:D:632:VAL:HG21	1:D:653:PHE:HE1	1.41	0.86
1:D:347:MET:HE1	1:D:374:LEU:HD13	0.88	0.86
1:A:629:THR:HG22	1:A:651:TYR:CE2	2.11	0.86
1:B:97:ARG:HH11	1:B:217:ALA:HB2	1.38	0.86
1:B:617:ARG:NH1	1:B:617:ARG:HG2	1.80	0.86
1:A:692:ILE:O	1:A:692:ILE:HG22	1.75	0.85
1:D:684:TYR:HD2	1:D:685:SER:N	1.73	0.85
1:A:477:GLU:HG2	1:A:478:LYS:HD3	1.55	0.85
1:D:632:VAL:HG21	1:D:653:PHE:CE1	2.12	0.85
1:C:356:PHE:CE2	1:C:365:LEU:HD21	2.11	0.85
1:D:635:ASN:HD21	1:D:663:ASN:HA	1.41	0.84
1:A:481:GLN:NE2	1:A:481:GLN:N	2.26	0.84
1:A:181:GLN:HA	1:A:181:GLN:HE21	1.42	0.84
1:B:456:MET:CE	1:B:467:GLN:HG2	2.07	0.84
1:D:481:GLN:H	1:D:481:GLN:HE21	1.22	0.83
1:B:487:VAL:O	1:B:491:GLU:HG2	1.78	0.83
1:C:307:LYS:HE3	1:C:310:PHE:HZ	1.37	0.83
1:B:34:GLN:HE21	1:B:57:THR:HG22	1.42	0.83
1:D:560:ASP:O	1:D:582:PHE:CD1	2.33	0.82
1:B:621:VAL:HG21	1:B:665:LEU:HD13	1.62	0.82
1:B:609:ARG:HG2	1:B:609:ARG:HH21	1.44	0.82
1:B:41:ALA:H	1:B:50:GLN:NE2	1.77	0.82
1:C:608:GLN:OE1	1:C:614:ARG:NH2	2.11	0.82
1:A:157:ILE:CG1	1:A:381:PRO:HG2	2.04	0.82
1:C:659:ALA:H	1:C:663:ASN:HD21	1.27	0.82
1:C:78:GLU:HG3	1:C:151:LYS:HA	1.62	0.82
1:A:489:GLN:HA	1:A:489:GLN:NE2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:O	1:A:285:ASP:HB2	1.78	0.81
1:D:377:TRP:HZ3	1:D:500:MET:CE	1.94	0.81
1:D:632:VAL:CG2	1:D:653:PHE:HE1	1.93	0.81
1:A:633:TYR:HD2	1:A:638:GLU:CA	1.94	0.80
1:A:489:GLN:HA	1:A:489:GLN:HE21	1.46	0.80
1:D:347:MET:HE2	1:D:374:LEU:HD11	1.64	0.80
1:B:621:VAL:HG21	1:B:665:LEU:CD1	2.12	0.80
1:C:187:THR:O	1:C:187:THR:HG22	1.80	0.80
1:B:383:VAL:HG12	1:B:418:ASN:HB3	1.62	0.80
1:D:131:GLU:HG2	3:D:723:HOH:O	1.81	0.80
1:A:451:ASN:ND2	1:A:453:TYR:H	1.80	0.80
1:B:181:GLN:CA	1:B:181:GLN:HE21	1.93	0.79
1:D:347:MET:HE2	1:D:374:LEU:CD1	2.11	0.79
1:D:471:ARG:HG3	1:D:471:ARG:HH11	1.46	0.79
1:D:618:THR:O	1:D:618:THR:HG23	1.82	0.79
1:B:494:TYR:HB3	1:B:497:GLN:HG3	1.64	0.79
1:A:510:LEU:HD11	1:A:588:LYS:HG2	1.63	0.79
1:B:267:TRP:CZ2	1:B:373:GLY:HA2	2.17	0.79
1:C:29:PHE:CZ	1:C:85:LYS:HE2	2.17	0.79
1:C:484:LYS:HB3	1:C:485:PRO:CD	2.13	0.79
1:C:595:LYS:HG2	1:C:603:VAL:HG21	1.64	0.78
1:D:400:GLU:O	1:D:404:GLN:HG3	1.83	0.78
1:B:205:SER:OG	1:B:260:LYS:HE3	1.83	0.78
1:B:475:TRP:CH2	1:B:507:ASP:HB2	2.19	0.78
1:D:664:ILE:HG13	1:D:679:GLU:OE1	1.82	0.78
1:B:456:MET:HE3	1:B:469:MET:HE1	1.65	0.78
1:A:41:ALA:N	1:A:50:GLN:HE22	1.80	0.78
1:C:448:VAL:HG23	1:C:466:ILE:HB	1.66	0.78
1:D:94:GLU:HA	1:D:94:GLU:OE1	1.84	0.78
1:B:296:LEU:HA	3:B:725:HOH:O	1.85	0.77
1:A:498:LYS:N	1:B:250:GLN:HE22	1.80	0.77
1:D:481:GLN:NE2	1:D:481:GLN:N	2.30	0.77
1:B:67:MET:CA	1:B:67:MET:CE	2.51	0.77
1:D:577:LYS:HE2	3:D:718:HOH:O	1.84	0.77
1:D:399:ARG:HG3	1:D:399:ARG:O	1.83	0.77
1:D:684:TYR:C	1:D:684:TYR:CD2	2.57	0.77
1:D:111:VAL:CG2	1:D:118:ALA:HB3	2.14	0.77
1:D:684:TYR:HD2	1:D:684:TYR:C	1.88	0.77
1:B:179:THR:CG2	1:B:183:ASN:HB3	2.14	0.76
1:A:41:ALA:H	1:A:50:GLN:NE2	1.82	0.76
1:D:347:MET:HE3	1:D:374:LEU:CD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:VAL:HG21	1:A:653:PHE:CE1	2.21	0.76
1:A:179:THR:CG2	1:A:180:GLU:O	2.33	0.76
1:B:680:ILE:CD1	1:B:682:TRP:HE1	1.99	0.76
1:A:633:TYR:CD2	1:A:638:GLU:HA	2.20	0.76
1:D:30:ASN:HB3	1:D:60:ILE:HB	1.65	0.76
1:B:456:MET:HE1	1:B:467:GLN:HG2	1.65	0.76
1:D:663:ASN:N	1:D:663:ASN:HD22	1.82	0.76
1:B:208:ILE:HD11	1:B:259:PHE:HB2	1.67	0.75
1:A:634:LEU:HD22	1:A:656:VAL:CG1	2.15	0.75
1:D:635:ASN:HA	1:D:664:ILE:HG22	1.69	0.75
1:A:477:GLU:HG2	1:A:478:LYS:CD	2.17	0.75
1:B:82:TYR:CE1	1:B:147:LYS:HG2	2.21	0.75
1:A:475:TRP:CZ3	1:A:521:LEU:HD22	2.21	0.75
1:D:632:VAL:HG23	1:D:653:PHE:CE1	2.21	0.74
1:B:654:ASP:N	1:B:654:ASP:OD2	2.20	0.74
1:C:642:ILE:HD13	1:C:653:PHE:CE1	2.21	0.74
1:A:43:ASP:OD2	1:A:45:MET:HB3	1.87	0.74
1:D:322:THR:HG22	1:D:355:ARG:HB3	1.68	0.74
1:D:182:ASN:ND2	1:D:216:ASN:HB2	2.02	0.74
1:D:561:PHE:HA	1:D:582:PHE:CE1	2.22	0.74
1:B:512:HIS:CD2	1:B:527:PHE:CD1	2.75	0.74
1:C:494:TYR:HB3	1:C:497:GLN:HG3	1.69	0.74
1:B:179:THR:HG21	1:B:183:ASN:CB	2.17	0.73
1:C:337:GLU:H	1:C:337:GLU:CD	1.91	0.73
1:D:565:MET:HE2	1:D:565:MET:HA	1.70	0.73
1:D:43:ASP:HB2	1:D:46:ARG:HH12	1.54	0.73
1:C:187:THR:HG23	1:C:187:THR:O	1.88	0.73
1:A:46:ARG:O	1:A:50:GLN:HG3	1.88	0.73
1:A:663:ASN:C	1:A:664:ILE:HD12	2.09	0.73
1:B:179:THR:HG21	1:B:183:ASN:HD22	1.54	0.73
1:B:157:ILE:HD12	1:B:381:PRO:HD2	1.69	0.73
1:D:347:MET:CE	1:D:374:LEU:HD11	2.18	0.72
1:D:634:LEU:HB3	1:D:639:LEU:HD21	1.71	0.72
1:A:296:LEU:HD12	1:A:297:GLY:N	2.04	0.72
1:D:377:TRP:CZ3	1:D:500:MET:CE	2.72	0.72
1:C:46:ARG:HB2	1:C:46:ARG:CZ	2.19	0.72
1:B:680:ILE:CD1	1:B:682:TRP:NE1	2.52	0.72
1:B:208:ILE:HD11	1:B:230:ILE:HD11	1.72	0.72
1:A:132:ILE:O	1:A:136:LEU:HD22	1.89	0.72
1:D:82:TYR:CE1	1:D:147:LYS:HG2	2.24	0.72
1:C:377:TRP:CD1	1:C:377:TRP:C	2.63	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:GLU:OE1	1:B:616:LYS:HB2	1.88	0.72
1:B:633:TYR:CD1	1:B:638:GLU:CA	2.71	0.72
1:B:208:ILE:HD11	1:B:259:PHE:CD2	2.25	0.71
1:C:521:LEU:HG	1:C:522:ASN:N	2.04	0.71
1:C:579:LEU:O	1:C:588:LYS:HG3	1.90	0.71
1:B:395:GLN:HG2	1:B:437:LEU:HD12	1.71	0.71
1:D:616:LYS:HA	1:D:687:GLU:OE2	1.91	0.71
1:A:617:ARG:HH11	1:A:617:ARG:HG3	0.71	0.71
1:D:565:MET:HE3	1:D:565:MET:HA	1.73	0.71
1:B:268:GLN:O	1:B:268:GLN:HG3	1.89	0.70
1:A:132:ILE:HG13	1:A:136:LEU:HD21	1.73	0.70
1:D:322:THR:O	1:D:557:ASN:ND2	2.23	0.70
1:B:609:ARG:CG	1:B:609:ARG:HH21	2.04	0.70
1:B:179:THR:CG2	1:B:180:GLU:N	2.55	0.70
1:B:633:TYR:HD1	1:B:638:GLU:CA	2.04	0.70
1:B:456:MET:HE3	1:B:456:MET:HA	1.72	0.70
1:C:90:PRO:HB2	1:C:92:ASP:HB2	1.73	0.70
1:D:472:TYR:CE1	1:D:577:LYS:HE3	2.27	0.70
1:A:481:GLN:HE21	1:A:481:GLN:N	1.88	0.70
1:D:630:PRO:CA	1:D:669:VAL:CG1	2.69	0.70
1:D:619:THR:HB	1:D:658:LEU:HD11	1.73	0.70
1:A:172:ARG:HA	3:A:716:HOH:O	1.91	0.69
1:D:347:MET:CE	1:D:374:LEU:CD2	2.70	0.69
1:A:530:GLU:OE2	1:A:610:ARG:NH2	2.23	0.69
1:B:662:LYS:HA	1:B:683:ASN:HB3	1.73	0.69
1:C:78:GLU:CG	1:C:151:LYS:HA	2.21	0.69
1:C:83:TYR:CE2	1:C:170:ILE:HG13	2.26	0.69
1:D:182:ASN:ND2	1:D:216:ASN:CB	2.55	0.69
1:D:668:VAL:HG13	1:D:675:GLU:OE2	1.91	0.69
1:B:626:ASN:HA	1:B:649:VAL:HG12	1.75	0.69
1:D:627:ILE:HG13	1:D:669:VAL:HG21	1.75	0.69
1:A:179:THR:HG21	1:A:183:ASN:HD22	1.58	0.69
1:D:634:LEU:CB	1:D:639:LEU:HD21	2.23	0.69
1:A:474:GLY:HA2	1:A:478:LYS:O	1.93	0.68
1:A:604:LEU:HD22	1:A:669:VAL:HG12	1.74	0.68
1:B:377:TRP:HZ3	1:B:500:MET:CE	2.06	0.68
1:A:692:ILE:HG23	1:A:692:ILE:O	1.92	0.68
1:B:521:LEU:HD23	1:B:522:ASN:C	2.13	0.68
1:C:322:THR:HG22	1:C:355:ARG:HB3	1.74	0.68
1:C:557:ASN:O	1:C:578:GLY:HA2	1.92	0.68
1:C:388:GLY:HA2	1:C:426:TYR:CZ	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:TYR:CE1	1:B:638:GLU:HB2	2.22	0.68
1:A:689:ASN:OD1	1:A:692:ILE:HB	1.94	0.68
1:C:266:LEU:HD23	1:C:298:VAL:CG2	2.22	0.68
1:D:337:GLU:N	1:D:337:GLU:OE2	2.26	0.68
1:D:471:ARG:NH1	1:D:471:ARG:HG3	2.03	0.68
1:D:43:ASP:CB	1:D:46:ARG:NH1	2.57	0.68
1:B:377:TRP:CD1	1:B:377:TRP:C	2.65	0.68
1:D:642:ILE:HB	1:D:653:PHE:HE2	1.56	0.68
1:B:417:HIS:CD2	1:B:417:HIS:C	2.67	0.68
1:C:494:TYR:HB3	1:C:497:GLN:CG	2.24	0.68
1:C:180:GLU:HG3	1:C:289:ILE:HB	1.75	0.68
1:D:182:ASN:HD21	1:D:216:ASN:CB	2.06	0.67
1:B:395:GLN:HG2	1:B:437:LEU:HD13	1.76	0.67
1:C:84:ARG:HD2	1:C:143:GLU:OE2	1.93	0.67
1:A:632:VAL:CG2	1:A:653:PHE:CE1	2.77	0.67
1:C:659:ALA:N	1:C:663:ASN:HD21	1.93	0.67
1:A:383:VAL:HG12	1:A:418:ASN:HB3	1.76	0.67
1:D:377:TRP:CD1	1:D:377:TRP:C	2.66	0.67
1:D:43:ASP:OD2	1:D:45:MET:HB3	1.93	0.67
1:A:512:HIS:CD2	1:A:527:PHE:HA	2.30	0.67
1:C:477:GLU:HG2	1:C:478:LYS:HG3	1.75	0.67
1:C:327:TRP:CZ2	1:C:584:ARG:HG2	2.29	0.67
1:A:527:PHE:O	1:A:529:PRO:HD3	1.95	0.67
1:B:187:THR:O	1:B:187:THR:HG23	1.93	0.67
1:B:456:MET:HE3	1:B:469:MET:CE	2.23	0.67
1:B:108:CYS:SG	1:B:122:LYS:HG2	2.35	0.67
1:C:299:ARG:NH2	1:C:409:PRO:HA	2.09	0.67
1:D:617:ARG:O	1:D:658:LEU:HD12	1.95	0.67
1:D:635:ASN:ND2	1:D:663:ASN:HA	2.10	0.67
1:D:634:LEU:HD12	1:D:634:LEU:C	2.15	0.67
1:A:187:THR:CG2	1:A:187:THR:O	2.43	0.67
1:A:575:ASN:OD1	1:A:577:LYS:HG3	1.94	0.66
1:C:422:GLN:OE1	1:C:423:PRO:HA	1.94	0.66
1:C:641:GLY:O	1:C:642:ILE:C	2.32	0.66
1:D:662:LYS:C	1:D:663:ASN:ND2	2.47	0.66
1:B:633:TYR:HE1	1:B:638:GLU:CB	2.07	0.66
1:D:634:LEU:HD12	1:D:635:ASN:N	2.11	0.66
1:A:516:TYR:OH	1:A:616:LYS:HD3	1.95	0.66
1:D:560:ASP:O	1:D:582:PHE:HD1	1.76	0.66
1:B:322:THR:HG22	1:B:355:ARG:HB3	1.77	0.66
1:A:484:LYS:HB3	1:A:485:PRO:CD	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:HD22	1:B:182:ASN:N	1.93	0.66
1:B:506:ALA:O	1:B:533:GLN:NE2	2.26	0.66
1:B:609:ARG:NH2	1:B:609:ARG:HB3	2.11	0.66
1:B:668:VAL:O	1:B:669:VAL:HG23	1.95	0.66
1:B:78:GLU:OE1	1:B:161:GLN:NE2	2.29	0.66
1:B:642:ILE:HG23	1:B:642:ILE:O	1.95	0.66
1:A:478:LYS:HB3	1:A:482:ASP:OD2	1.95	0.65
1:B:114:ASN:ND2	1:B:143:GLU:H	1.93	0.65
1:A:353:THR:HA	1:A:375:ILE:O	1.97	0.65
1:A:203:LYS:O	1:A:264:PRO:HD2	1.97	0.65
1:B:184:ILE:HD13	1:B:292:VAL:HG13	1.79	0.65
1:B:634:LEU:HD22	1:B:656:VAL:CG1	2.26	0.65
1:D:619:THR:HG23	1:D:620:ALA:N	2.10	0.65
1:A:618:THR:HA	1:A:656:VAL:O	1.97	0.65
1:D:105:VAL:O	1:D:124:GLY:HA2	1.97	0.65
1:A:663:ASN:O	1:A:664:ILE:HD12	1.97	0.65
1:B:377:TRP:C	1:B:377:TRP:HD1	2.00	0.65
1:A:555:LEU:C	1:A:555:LEU:HD12	2.18	0.64
1:B:357:ALA:HB1	1:B:358:HIS:ND1	2.13	0.64
1:B:630:PRO:HA	1:B:669:VAL:HG22	1.72	0.64
1:A:451:ASN:HD22	1:A:453:TYR:H	1.43	0.64
1:A:475:TRP:CZ3	1:A:521:LEU:CD2	2.80	0.64
1:D:557:ASN:ND2	1:D:558:MET:H	1.94	0.64
1:B:93:LEU:O	1:B:96:LYS:HB2	1.98	0.64
1:B:583:ASP:O	1:B:584:ARG:HB2	1.98	0.64
1:A:133:GLY:HA2	1:A:136:LEU:CD2	2.24	0.64
1:C:629:THR:CG2	3:C:1:HOH:O	2.31	0.64
1:A:689:ASN:O	1:A:689:ASN:OD1	2.16	0.64
1:B:58:VAL:HG21	1:B:62:HIS:CD2	2.33	0.64
1:B:283:MET:HG2	1:B:288:VAL:HG22	1.80	0.64
1:C:327:TRP:CH2	1:C:584:ARG:HG2	2.33	0.63
1:B:563:VAL:HG21	1:B:575:ASN:HB2	1.79	0.63
1:B:477:GLU:HG3	1:B:478:LYS:CG	2.27	0.63
1:D:680:ILE:HD12	1:D:682:TRP:NE1	2.13	0.63
1:D:470:ASN:OD1	1:D:503:GLU:HB2	1.98	0.63
1:D:182:ASN:HD21	1:D:216:ASN:CG	2.01	0.63
1:D:377:TRP:HD1	1:D:377:TRP:C	2.02	0.63
1:C:671:THR:HG23	1:C:672:LYS:N	2.12	0.63
1:D:353:THR:HA	1:D:375:ILE:O	1.99	0.63
1:B:631:LYS:O	1:B:667:ALA:HA	1.99	0.63
1:B:182:ASN:ND2	1:B:182:ASN:N	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TRP:HZ3	1:C:500:MET:CE	2.10	0.62
1:D:665:LEU:O	1:D:679:GLU:HA	1.99	0.62
1:D:163:LEU:HD22	1:D:384:ASN:HB2	1.80	0.62
1:B:422:GLN:OE1	1:B:422:GLN:HA	1.99	0.62
1:C:377:TRP:HD1	1:C:377:TRP:C	2.02	0.62
1:D:481:GLN:HE21	1:D:481:GLN:N	1.96	0.62
1:D:475:TRP:CH2	1:D:507:ASP:HB2	2.34	0.62
1:A:626:ASN:HA	1:A:649:VAL:HG12	1.81	0.62
1:A:618:THR:HG22	1:A:657:SER:OG	1.99	0.62
1:B:182:ASN:HD22	1:B:182:ASN:H	1.47	0.62
1:A:642:ILE:HG23	1:A:642:ILE:O	1.97	0.62
1:B:82:TYR:CE1	1:B:147:LYS:CG	2.83	0.62
1:B:617:ARG:CG	1:B:617:ARG:NH1	2.50	0.62
1:B:595:LYS:HG2	1:B:603:VAL:CG2	2.24	0.62
1:A:632:VAL:HG21	1:A:653:PHE:HE1	1.63	0.62
1:B:374:LEU:O	1:B:410:SER:HB2	2.00	0.62
1:B:337:GLU:CD	1:B:337:GLU:H	2.03	0.62
1:D:233:GLN:NE2	1:D:274:TYR:CD1	2.68	0.62
1:C:633:TYR:CE1	1:C:638:GLU:HB2	2.35	0.62
1:B:567:THR:O	1:B:567:THR:CG2	2.47	0.61
1:B:567:THR:O	1:B:567:THR:HG23	1.99	0.61
1:D:207:ASP:OD2	1:D:260:LYS:HG2	2.01	0.61
1:A:668:VAL:HG11	1:A:675:GLU:OE2	1.99	0.61
1:D:186:VAL:O	1:D:186:VAL:HG23	2.00	0.61
1:B:658:LEU:CD2	1:B:663:ASN:ND2	2.64	0.61
1:A:633:TYR:CD2	1:A:638:GLU:CA	2.80	0.61
1:C:502:THR:O	1:C:503:GLU:HG3	2.00	0.61
1:B:299:ARG:O	1:B:299:ARG:HD2	2.00	0.61
1:B:630:PRO:CA	1:B:669:VAL:HG21	2.28	0.61
1:B:634:LEU:HD13	1:B:665:LEU:HD21	1.81	0.61
1:B:456:MET:HE2	1:B:467:GLN:HG2	1.79	0.61
1:A:512:HIS:HB2	1:A:529:PRO:HA	1.82	0.61
3:A:728:HOH:O	1:B:252:THR:HG22	2.01	0.61
1:D:614:ARG:HD3	1:D:682:TRP:CG	2.36	0.61
1:A:451:ASN:HD22	1:A:453:TYR:N	1.98	0.61
1:D:527:PHE:CE2	1:D:529:PRO:HG3	2.35	0.61
1:A:557:ASN:O	1:A:578:GLY:HA2	1.99	0.61
1:B:484:LYS:H	1:B:485:PRO:HD2	1.65	0.61
1:A:399:ARG:HH21	1:B:399:ARG:NH2	1.98	0.61
1:D:642:ILE:HD12	1:D:653:PHE:CZ	2.36	0.61
1:B:309:PHE:CE1	1:B:318:MET:HE3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:HG21	1:B:183:ASN:ND2	2.15	0.61
1:C:90:PRO:HG2	1:C:92:ASP:HB3	1.83	0.61
1:B:377:TRP:HZ3	1:B:500:MET:HE3	1.64	0.60
1:C:625:SER:O	1:C:649:VAL:HG22	2.01	0.60
1:D:607:THR:CG2	1:D:608:GLN:HG3	2.13	0.60
1:D:609:ARG:HB2	1:D:680:ILE:HG22	1.84	0.60
1:A:512:HIS:HD2	1:A:528:TYR:N	1.99	0.60
1:B:633:TYR:CE1	1:B:638:GLU:HA	2.34	0.60
1:D:43:ASP:HB3	1:D:46:ARG:NH1	2.16	0.60
1:B:299:ARG:C	1:B:299:ARG:HD2	2.21	0.60
1:B:346:ILE:O	1:B:349:VAL:HG12	2.02	0.60
1:B:37:LYS:HD2	1:B:77:TYR:CE2	2.34	0.60
1:D:182:ASN:HD22	1:D:247:LEU:HD23	1.67	0.60
1:C:516:TYR:CZ	1:C:616:LYS:HE2	2.37	0.60
1:B:689:ASN:HD21	1:B:692:ILE:HG13	1.60	0.60
1:D:78:GLU:HG3	1:D:151:LYS:HA	1.84	0.60
1:B:512:HIS:CG	1:B:527:PHE:CE1	2.90	0.60
1:B:113:VAL:HG11	1:B:132:ILE:HB	1.83	0.60
1:C:523:TRP:CZ3	1:C:568:ARG:NH2	2.69	0.60
1:A:498:LYS:H	1:B:250:GLN:NE2	1.87	0.60
1:A:284:ALA:O	1:A:285:ASP:CB	2.48	0.60
1:B:367:SER:O	1:B:370:ASP:HB2	2.02	0.60
1:D:574:ARG:HG2	1:D:576:MET:HG3	1.84	0.59
1:D:642:ILE:CB	1:D:653:PHE:CE2	2.79	0.59
1:D:614:ARG:HD3	1:D:682:TRP:HB3	1.83	0.59
1:B:377:TRP:CZ3	1:B:500:MET:CE	2.85	0.59
1:A:595:LYS:HG2	1:A:603:VAL:HG21	1.84	0.59
1:B:30:ASN:HB3	1:B:60:ILE:HB	1.84	0.59
1:B:202:SER:HG	1:B:204:LYS:HG3	1.67	0.59
1:A:448:VAL:HG22	1:A:449:SER:N	2.17	0.59
1:B:494:TYR:HB3	1:B:497:GLN:CG	2.32	0.59
1:C:323:ARG:HD3	1:C:324:HIS:O	2.02	0.59
1:D:180:GLU:HG3	1:D:289:ILE:HB	1.84	0.59
1:D:299:ARG:HD2	1:D:299:ARG:C	2.23	0.59
1:C:642:ILE:HD11	1:C:651:TYR:HB3	1.83	0.59
1:A:179:THR:HG21	1:A:183:ASN:ND2	2.16	0.59
1:D:664:ILE:O	1:D:664:ILE:CG2	2.50	0.59
1:B:418:ASN:ND2	1:B:419:GLU:HG3	2.17	0.59
1:A:448:VAL:HG23	1:A:466:ILE:O	2.02	0.59
1:B:282:LEU:CD2	1:B:289:ILE:HD11	2.32	0.59
1:C:563:VAL:HG21	1:C:575:ASN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ILE:CG1	1:D:679:GLU:OE1	2.50	0.59
1:C:484:LYS:HB3	1:C:485:PRO:HD2	1.85	0.59
1:D:182:ASN:ND2	1:D:247:LEU:HD23	2.18	0.59
1:A:82:TYR:CE1	1:A:147:LYS:HG2	2.38	0.59
1:C:571:VAL:CG2	1:C:574:ARG:HB3	2.33	0.59
1:C:377:TRP:CZ3	1:C:500:MET:HE1	2.38	0.59
1:C:671:THR:CG2	1:C:672:LYS:N	2.65	0.59
1:B:668:VAL:HA	1:B:676:TYR:O	2.03	0.58
1:B:617:ARG:NE	1:B:658:LEU:O	2.32	0.58
1:B:512:HIS:CD2	1:B:527:PHE:HE1	2.15	0.58
1:B:187:THR:O	1:B:187:THR:CG2	2.51	0.58
1:C:525:LYS:CD	1:C:694:SER:HB2	2.33	0.58
1:A:71:VAL:O	1:A:71:VAL:HG12	2.02	0.58
1:A:630:PRO:HD2	1:A:642:ILE:HD11	1.85	0.58
1:D:583:ASP:O	1:D:584:ARG:HB2	2.03	0.58
1:A:114:ASN:ND2	1:A:143:GLU:H	2.02	0.58
1:A:515:GLU:OE1	1:A:619:THR:OG1	2.20	0.58
1:B:34:GLN:NE2	1:B:57:THR:HG22	2.15	0.58
1:B:658:LEU:HD22	1:B:663:ASN:ND2	2.18	0.58
1:B:630:PRO:CB	1:B:669:VAL:CG2	2.82	0.58
1:D:634:LEU:HB3	1:D:639:LEU:CD2	2.33	0.58
1:D:43:ASP:HB2	1:D:46:ARG:NH1	2.16	0.58
1:B:477:GLU:HG3	1:B:478:LYS:HG2	1.84	0.58
1:A:346:ILE:O	1:A:349:VAL:HG12	2.04	0.58
1:D:632:VAL:HG23	1:D:653:PHE:CZ	2.38	0.58
1:D:406:PHE:HE1	1:D:442:ASP:HB2	1.68	0.57
1:B:609:ARG:NH2	1:B:609:ARG:CG	2.66	0.57
1:D:484:LYS:HB3	1:D:485:PRO:CD	2.33	0.57
1:D:514:THR:HA	1:D:615:GLU:OE2	2.03	0.57
1:C:492:LYS:NZ	1:C:492:LYS:CB	2.66	0.57
1:B:621:VAL:CG2	1:B:665:LEU:CD1	2.80	0.57
1:B:567:THR:OG1	1:B:572:PRO:HA	2.03	0.57
1:A:58:VAL:HG13	1:A:59:GLU:N	2.19	0.57
1:A:179:THR:HG23	1:A:180:GLU:N	2.18	0.57
1:B:478:LYS:HB3	1:B:482:ASP:OD2	2.05	0.57
1:A:555:LEU:O	1:A:555:LEU:HD12	2.05	0.57
1:A:471:ARG:HD2	1:A:486:TRP:CZ2	2.39	0.57
1:B:609:ARG:CZ	1:B:609:ARG:HB3	2.35	0.57
1:C:595:LYS:HG2	1:C:603:VAL:CG2	2.35	0.57
1:D:645:GLY:HA3	1:D:650:HIS:ND1	2.19	0.57
1:B:662:LYS:HA	1:B:683:ASN:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ASN:C	1:C:522:ASN:HD22	2.08	0.57
1:B:176:LEU:HD23	1:B:177:ILE:N	2.20	0.57
1:C:455:HIS:CD2	1:C:455:HIS:H	2.22	0.57
1:C:58:VAL:CG1	1:C:59:GLU:N	2.67	0.57
1:B:97:ARG:HD3	1:B:180:GLU:O	2.05	0.57
1:B:642:ILE:CG2	1:B:642:ILE:O	2.53	0.57
1:A:388:GLY:HA2	1:A:426:TYR:CZ	2.40	0.57
1:A:229:THR:CG2	1:A:231:TYR:CE2	2.88	0.57
1:A:489:GLN:CA	1:A:489:GLN:HE21	2.11	0.56
1:A:677:THR:O	1:A:677:THR:HG22	2.03	0.56
1:A:72:GLN:NE2	1:A:75:SER:O	2.38	0.56
1:B:179:THR:HG22	1:B:180:GLU:H	1.65	0.56
1:D:182:ASN:HD21	1:D:216:ASN:HB2	1.68	0.56
1:B:422:GLN:OE1	1:B:423:PRO:HA	2.05	0.56
1:D:78:GLU:CG	1:D:151:LYS:HA	2.35	0.56
1:A:377:TRP:CD1	1:A:377:TRP:C	2.78	0.56
1:B:303:ILE:CG2	1:B:498:LYS:HD3	2.35	0.56
1:A:216:ASN:HB2	1:A:247:LEU:HG	1.87	0.56
1:D:356:PHE:CE2	1:D:365:LEU:HD21	2.41	0.56
1:C:126:SER:HB3	1:C:360:GLN:OE1	2.06	0.56
1:D:647:THR:C	1:D:649:VAL:H	2.08	0.56
1:A:632:VAL:HG23	1:A:653:PHE:CZ	2.39	0.56
1:B:456:MET:CE	1:B:469:MET:CE	2.83	0.56
1:C:478:LYS:HB3	1:C:482:ASP:OD2	2.05	0.56
1:A:557:ASN:HD22	1:A:559:PHE:H	1.54	0.56
1:B:560:ASP:OD1	1:B:576:MET:HA	2.06	0.56
1:D:668:VAL:CG1	1:D:675:GLU:OE2	2.54	0.56
1:B:114:ASN:HD21	1:B:143:GLU:H	1.51	0.56
1:B:407:ASN:O	1:B:409:PRO:HD3	2.06	0.56
1:C:481:GLN:HE22	1:C:519:ASP:HB3	1.71	0.56
1:C:437:LEU:HD23	1:C:437:LEU:C	2.26	0.56
1:C:22:LEU:HA	1:C:291:GLU:OE2	2.04	0.56
1:C:388:GLY:HA2	1:C:426:TYR:CE1	2.41	0.56
1:B:630:PRO:CB	1:B:669:VAL:HG23	2.36	0.56
1:B:512:HIS:HD2	1:B:527:PHE:HE1	1.52	0.56
1:D:303:ILE:O	1:D:498:LYS:NZ	2.39	0.56
1:A:179:THR:HG23	1:A:180:GLU:H	1.69	0.55
1:B:677:THR:O	1:B:677:THR:CG2	2.54	0.55
1:B:633:TYR:CE1	1:B:638:GLU:CA	2.89	0.55
1:A:538:GLU:HA	1:A:593:TRP:CZ2	2.42	0.55
1:A:516:TYR:CZ	1:A:616:LYS:HD3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:LYS:O	1:C:527:PHE:N	2.32	0.55
1:C:89:PHE:O	1:C:139:GLY:N	2.37	0.55
1:D:137:LYS:O	1:D:140:ALA:HB3	2.06	0.55
1:B:303:ILE:HG21	1:B:498:LYS:HD3	1.88	0.55
1:A:642:ILE:HB	1:A:653:PHE:CE2	2.42	0.55
1:D:527:PHE:O	1:D:529:PRO:HD3	2.05	0.55
1:A:179:THR:CG2	1:A:180:GLU:H	2.19	0.55
1:B:356:PHE:CZ	1:B:365:LEU:HD21	2.42	0.55
1:D:503:GLU:HG2	1:D:556:TRP:HB2	1.89	0.55
1:C:319:TYR:HB3	1:C:598:TRP:CE2	2.41	0.55
1:C:205:SER:HA	1:C:261:LEU:O	2.06	0.55
1:D:647:THR:O	1:D:649:VAL:N	2.40	0.55
1:C:205:SER:HA	1:C:264:PRO:HD3	1.89	0.55
1:B:241:HIS:ND1	1:B:241:HIS:C	2.60	0.55
1:D:325:GLN:HG2	1:D:359:TYR:CE1	2.42	0.55
1:A:460:VAL:O	1:A:460:VAL:CG1	2.55	0.55
1:D:512:HIS:CE1	1:D:527:PHE:HA	2.42	0.54
1:C:492:LYS:NZ	1:C:492:LYS:HB3	2.22	0.54
1:A:179:THR:CG2	1:A:183:ASN:HB3	2.37	0.54
1:C:266:LEU:CD2	1:C:298:VAL:CG2	2.85	0.54
1:B:100:LEU:HG	1:B:132:ILE:HD13	1.89	0.54
1:C:484:LYS:HB3	1:C:485:PRO:HD3	1.88	0.54
1:A:538:GLU:HA	1:A:593:TRP:CE2	2.42	0.54
1:D:484:LYS:HG3	1:D:543:ILE:HD12	1.88	0.54
1:A:633:TYR:CE2	1:A:638:GLU:HG3	2.43	0.54
1:B:521:LEU:HD23	1:B:521:LEU:C	2.28	0.54
1:A:492:LYS:HB3	1:A:492:LYS:HZ2	1.72	0.54
1:C:90:PRO:C	1:C:92:ASP:N	2.61	0.54
1:C:90:PRO:HB2	1:C:92:ASP:CB	2.36	0.54
1:A:356:PHE:CE2	1:A:365:LEU:HD21	2.41	0.54
1:C:442:ASP:OD2	1:C:445:ARG:HD2	2.07	0.54
1:B:580:ILE:HG22	1:B:581:THR:N	2.22	0.54
1:A:521:LEU:O	1:A:522:ASN:C	2.45	0.54
1:D:78:GLU:O	1:D:78:GLU:HG2	2.08	0.54
1:A:417:HIS:CD2	1:A:417:HIS:C	2.80	0.54
1:A:458:HIS:ND1	1:A:459:PRO:HD2	2.22	0.54
1:B:219:LEU:N	1:B:219:LEU:HD13	2.23	0.54
1:B:377:TRP:CZ3	1:B:500:MET:HE1	2.42	0.54
1:C:299:ARG:HH21	1:C:409:PRO:HA	1.71	0.54
1:C:626:ASN:HB3	1:C:627:ILE:HG23	1.89	0.54
1:C:502:THR:O	1:C:503:GLU:CG	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:TRP:HZ3	1:D:500:MET:HE2	1.70	0.54
1:A:69:MET:HG2	1:A:564:PRO:HG2	1.89	0.54
1:D:614:ARG:NH1	1:D:682:TRP:CE2	2.77	0.53
1:C:516:TYR:OH	1:C:616:LYS:HE2	2.07	0.53
1:A:392:GLU:OE2	1:B:122:LYS:CE	2.56	0.53
1:B:484:LYS:N	1:B:485:PRO:HD2	2.23	0.53
1:A:69:MET:HG2	1:A:564:PRO:CG	2.38	0.53
1:B:309:PHE:CD1	1:B:318:MET:HE2	2.44	0.53
1:C:157:ILE:HD13	1:C:394:ALA:HA	1.89	0.53
1:D:162:ASN:ND2	1:D:565:MET:HG2	2.23	0.53
1:A:663:ASN:C	1:A:664:ILE:CD1	2.76	0.53
1:C:649:VAL:CG1	1:C:649:VAL:O	2.56	0.53
1:C:216:ASN:HB2	1:C:247:LEU:HG	1.91	0.53
1:B:630:PRO:HB3	1:B:669:VAL:HG21	1.89	0.53
1:B:626:ASN:O	1:B:627:ILE:HG23	2.08	0.53
1:B:393:ASN:OD1	1:B:397:GLN:NE2	2.41	0.53
1:B:368:ARG:O	1:B:372:LEU:HG	2.09	0.53
1:A:654:ASP:CB	1:A:655:ASN:HD22	2.15	0.53
1:C:234:GLU:H	1:C:234:GLU:CD	2.12	0.53
1:A:560:ASP:OD1	1:A:576:MET:HA	2.09	0.53
1:D:484:LYS:N	1:D:485:PRO:HD2	2.24	0.53
1:A:162:ASN:HD22	1:A:565:MET:HG2	1.73	0.53
1:B:481:GLN:H	1:B:481:GLN:NE2	2.06	0.53
1:D:417:HIS:CD2	1:D:417:HIS:C	2.82	0.53
1:B:456:MET:HE1	1:B:469:MET:HE2	1.90	0.53
1:A:187:THR:HG23	1:A:187:THR:O	2.08	0.53
1:A:393:ASN:HA	1:B:392:GLU:OE1	2.09	0.53
1:C:203:LYS:O	1:C:263:ASN:HA	2.08	0.53
1:A:181:GLN:HA	1:A:181:GLN:NE2	2.19	0.52
1:A:634:LEU:HD22	1:A:656:VAL:HG11	1.88	0.52
1:C:97:ARG:NH2	1:C:215:ASP:OD2	2.38	0.52
1:B:188:ASP:O	1:B:189:CYS:HB2	2.08	0.52
1:A:91:HIS:CE1	1:A:139:GLY:HA3	2.43	0.52
1:C:91:HIS:CE1	1:C:139:GLY:HA3	2.44	0.52
1:B:196:ILE:HD13	1:B:278:VAL:HG21	1.91	0.52
1:B:34:GLN:HG2	1:B:57:THR:HG22	1.90	0.52
1:C:484:LYS:CB	1:C:485:PRO:CD	2.85	0.52
1:B:406:PHE:O	1:B:445:ARG:NH1	2.37	0.52
1:B:116:LYS:HE2	1:B:135:ALA:HB1	1.90	0.52
1:B:671:THR:O	1:B:672:LYS:C	2.48	0.52
1:B:639:LEU:HD13	1:B:656:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:CG	1:A:617:ARG:NH1	2.38	0.52
1:D:60:ILE:CG2	1:D:61:PRO:HA	2.39	0.52
1:C:196:ILE:HG12	1:C:210:VAL:HG22	1.91	0.52
1:D:672:LYS:O	1:D:674:LYS:N	2.42	0.52
1:A:296:LEU:HD12	1:A:296:LEU:C	2.29	0.52
1:C:71:VAL:O	1:C:71:VAL:HG13	2.09	0.52
1:C:565:MET:HB3	1:C:566:TRP:CD1	2.43	0.52
1:B:181:GLN:CA	1:B:181:GLN:NE2	2.58	0.52
1:B:419:GLU:OE1	1:B:470:ASN:ND2	2.36	0.52
1:D:327:TRP:CZ2	1:D:584:ARG:HG2	2.44	0.52
1:D:633:TYR:CD1	1:D:638:GLU:HB2	2.45	0.52
1:A:664:ILE:CD1	1:A:664:ILE:N	2.73	0.52
1:B:579:LEU:O	1:B:588:LYS:HG3	2.10	0.52
1:B:417:HIS:C	1:B:417:HIS:HD2	2.13	0.52
1:A:383:VAL:O	1:A:384:ASN:CB	2.58	0.52
1:D:99:PHE:CZ	1:D:131:GLU:HG3	2.44	0.52
1:A:392:GLU:OE1	1:B:393:ASN:HA	2.09	0.52
1:C:578:GLY:O	1:C:588:LYS:HD2	2.09	0.52
1:C:589:ASP:OD2	1:C:607:THR:HB	2.10	0.51
1:A:512:HIS:HD2	1:A:528:TYR:H	1.58	0.51
1:D:320:GLY:HA2	1:D:353:THR:HG23	1.93	0.51
1:B:604:LEU:HA	1:B:624:TYR:O	2.10	0.51
1:B:639:LEU:HD13	1:B:656:VAL:HG21	1.91	0.51
1:B:655:ASN:OD1	1:B:655:ASN:N	2.44	0.51
1:C:299:ARG:O	1:C:299:ARG:HD2	2.10	0.51
1:B:517:LEU:HD11	1:B:531:THR:HB	1.92	0.51
1:D:413:VAL:HG21	1:D:448:VAL:HB	1.92	0.51
1:D:367:SER:OG	1:D:408:HIS:HE1	1.93	0.51
1:A:190:ALA:HB3	1:A:404:GLN:NE2	2.25	0.51
1:A:179:THR:HG22	1:A:180:GLU:C	2.28	0.51
1:B:475:TRP:CZ2	1:B:507:ASP:HB2	2.46	0.51
1:C:525:LYS:HG2	1:C:526:PRO:CD	2.41	0.51
1:C:525:LYS:HD3	1:C:694:SER:HB2	1.92	0.51
1:C:93:LEU:HB2	1:C:138:LEU:CD2	2.39	0.51
1:D:618:THR:O	1:D:618:THR:CG2	2.52	0.51
1:A:382:CYS:C	1:A:383:VAL:HG13	2.30	0.51
1:D:377:TRP:CZ3	1:D:500:MET:HE1	2.44	0.51
1:D:208:ILE:HD13	1:D:208:ILE:N	2.24	0.51
1:B:664:ILE:HD12	1:B:664:ILE:C	2.31	0.51
1:D:430:LEU:O	1:D:434:LEU:HG	2.11	0.51
1:C:603:VAL:HB	1:C:626:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:CD	1:A:610:ARG:HH21	2.12	0.51
1:B:179:THR:CG2	1:B:180:GLU:H	2.22	0.51
1:A:475:TRP:CH2	1:A:507:ASP:HB2	2.46	0.51
1:B:161:GLN:HB2	1:B:565:MET:HE1	1.93	0.51
1:D:666:LYS:HG3	1:D:679:GLU:HB2	1.93	0.51
1:A:642:ILE:O	1:A:642:ILE:CG2	2.58	0.51
1:B:267:TRP:HZ2	1:B:373:GLY:HA2	1.75	0.51
1:D:545:LYS:HG3	1:D:545:LYS:O	2.10	0.51
1:D:638:GLU:HG2	1:D:639:LEU:O	2.11	0.51
1:D:319:TYR:HB3	1:D:598:TRP:CE2	2.46	0.51
1:B:208:ILE:HD11	1:B:259:PHE:HD2	1.75	0.50
1:A:517:LEU:HD11	1:A:531:THR:HB	1.92	0.50
1:A:183:ASN:HB2	1:A:290:ASP:OD2	2.11	0.50
1:B:370:ASP:CG	1:B:409:PRO:HD2	2.31	0.50
1:D:484:LYS:HB3	1:D:485:PRO:HD3	1.93	0.50
1:B:501:LEU:O	1:B:553:SER:HA	2.11	0.50
1:C:303:ILE:HG23	1:C:551:ILE:HG12	1.93	0.50
1:B:630:PRO:HB3	1:B:669:VAL:CG2	2.42	0.50
1:A:630:PRO:HD2	1:A:642:ILE:CD1	2.41	0.50
1:B:34:GLN:HE21	1:B:57:THR:CG2	2.19	0.50
1:A:451:ASN:ND2	1:A:453:TYR:N	2.54	0.50
1:B:405:SER:HB2	1:B:414:TRP:HH2	1.76	0.50
1:D:663:ASN:N	1:D:663:ASN:ND2	2.55	0.50
1:B:477:GLU:HG3	1:B:478:LYS:HG3	1.92	0.50
1:B:98:VAL:HG13	1:B:133:GLY:HA2	1.93	0.50
1:B:323:ARG:HD3	1:B:324:HIS:O	2.12	0.50
1:A:416:LEU:HD21	1:A:435:HIS:HA	1.93	0.50
1:A:392:GLU:OE2	1:B:122:LYS:HE3	2.11	0.50
1:C:299:ARG:C	1:C:299:ARG:HD2	2.32	0.50
1:A:484:LYS:HB3	1:A:485:PRO:HD2	1.93	0.50
1:B:484:LYS:HG2	1:B:485:PRO:HD3	1.94	0.50
1:C:631:LYS:HG2	1:C:638:GLU:OE2	2.11	0.50
1:B:634:LEU:HD22	1:B:656:VAL:HG13	1.94	0.50
1:D:662:LYS:O	1:D:663:ASN:ND2	2.44	0.50
1:B:61:PRO:HD2	1:B:335:LYS:NZ	2.26	0.50
1:C:398:LEU:O	1:C:402:ILE:HG13	2.11	0.50
1:D:627:ILE:CD1	1:D:676:TYR:CD2	2.94	0.50
1:A:637:GLN:O	1:A:638:GLU:C	2.50	0.50
1:B:89:PHE:CD2	1:B:136:LEU:HD22	2.47	0.50
1:B:216:ASN:HB2	1:B:247:LEU:HG	1.94	0.50
1:A:629:THR:HA	1:A:651:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:THR:O	1:B:673:GLY:N	2.45	0.50
1:A:357:ALA:HB1	1:A:358:HIS:ND1	2.27	0.50
1:C:233:GLN:HB3	1:C:234:GLU:OE2	2.11	0.49
1:A:512:HIS:HD2	1:A:527:PHE:HA	1.76	0.49
1:B:473:PHE:HB3	1:B:479:LYS:O	2.11	0.49
1:A:633:TYR:HE2	1:A:638:GLU:HG3	1.77	0.49
1:B:456:MET:CE	1:B:469:MET:HE2	2.42	0.49
1:D:512:HIS:ND1	1:D:528:TYR:N	2.57	0.49
1:C:489:GLN:HA	1:C:492:LYS:HE3	1.93	0.49
1:D:595:LYS:HG2	1:D:603:VAL:HG21	1.94	0.49
1:A:78:GLU:HG2	1:A:78:GLU:O	2.12	0.49
1:D:377:TRP:CE3	1:D:500:MET:HE1	2.48	0.49
1:A:538:GLU:OE2	1:A:624:TYR:OH	2.13	0.49
1:C:266:LEU:CD2	1:C:298:VAL:HG23	2.43	0.49
1:C:318:MET:HE3	1:C:375:ILE:HD12	1.94	0.49
1:B:665:LEU:O	1:B:679:GLU:HA	2.13	0.49
1:D:563:VAL:O	1:D:573:ALA:HA	2.12	0.49
1:C:198:GLN:OE1	1:C:298:VAL:HA	2.13	0.49
1:A:512:HIS:CD2	1:A:528:TYR:H	2.31	0.49
1:C:671:THR:CG2	1:C:672:LYS:H	2.25	0.49
1:D:406:PHE:CE1	1:D:442:ASP:HB2	2.48	0.49
1:A:391:THR:OG1	1:A:430:LEU:HD13	2.12	0.49
1:D:565:MET:O	1:D:566:TRP:CD2	2.65	0.49
1:D:530:GLU:OE2	1:D:610:ARG:NH2	2.45	0.49
1:B:233:GLN:HB3	1:B:274:TYR:CE1	2.48	0.49
1:A:436:ASP:C	1:A:436:ASP:OD1	2.50	0.49
1:B:632:VAL:CB	1:B:653:PHE:CE1	2.96	0.49
1:D:403:ARG:NE	1:D:441:GLU:OE2	2.39	0.49
1:B:266:LEU:HD23	1:B:298:VAL:HG22	1.95	0.49
1:C:97:ARG:CZ	1:C:217:ALA:HB2	2.43	0.49
1:B:294:GLN:HB3	1:B:295:PRO:HD2	1.95	0.49
1:C:155:ASP:OD1	1:C:155:ASP:N	2.45	0.49
1:D:626:ASN:OD1	1:D:627:ILE:HG23	2.13	0.48
1:B:512:HIS:HB3	1:B:527:PHE:CE1	2.48	0.48
1:B:157:ILE:CD1	1:B:381:PRO:HD2	2.38	0.48
1:B:282:LEU:HD23	1:B:289:ILE:HD11	1.95	0.48
1:C:565:MET:HA	1:C:565:MET:CE	2.43	0.48
1:D:91:HIS:CE1	1:D:139:GLY:HA3	2.48	0.48
1:C:555:LEU:HD12	1:C:555:LEU:C	2.33	0.48
1:D:347:MET:CE	1:D:374:LEU:CG	2.89	0.48
1:B:97:ARG:HH21	1:B:99:PHE:HZ	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:MET:HB3	1:C:566:TRP:NE1	2.28	0.48
1:B:35:PHE:CG	1:B:36:LYS:N	2.81	0.48
1:B:357:ALA:HB1	1:B:358:HIS:CG	2.48	0.48
1:A:383:VAL:CG1	1:A:418:ASN:HB3	2.43	0.48
1:B:508:ALA:HB2	1:B:533:GLN:HB2	1.95	0.48
1:B:309:PHE:CE1	1:B:318:MET:CE	2.96	0.48
1:A:67:MET:O	1:A:71:VAL:HG23	2.13	0.48
1:C:238:VAL:HG13	1:C:238:VAL:O	2.13	0.48
1:B:116:LYS:CE	1:B:135:ALA:HB1	2.44	0.48
3:A:735:HOH:O	1:B:462:LEU:HA	2.13	0.48
1:B:630:PRO:CB	1:B:669:VAL:HG21	2.44	0.48
1:D:565:MET:HB2	3:D:727:HOH:O	2.12	0.48
1:C:475:TRP:CH2	1:C:507:ASP:HB2	2.49	0.48
1:A:121:HIS:HE1	1:A:123:GLY:O	1.96	0.48
1:A:468:GLY:HA3	1:A:502:THR:CG2	2.44	0.48
1:A:319:TYR:HB3	1:A:598:TRP:CE2	2.48	0.48
1:C:61:PRO:HB3	1:C:171:TYR:O	2.14	0.48
1:A:448:VAL:HG22	1:A:449:SER:H	1.79	0.48
1:B:37:LYS:CG	1:B:77:TYR:CE2	2.96	0.48
1:D:664:ILE:HG23	1:D:664:ILE:O	2.12	0.48
1:C:58:VAL:HG13	1:C:59:GLU:N	2.29	0.48
1:A:128:PHE:HA	1:A:190:ALA:HB2	1.95	0.48
1:B:658:LEU:HD23	1:B:663:ASN:ND2	2.29	0.48
1:D:265:HIS:HB3	1:D:274:TYR:CD2	2.49	0.48
1:D:530:GLU:OE1	1:D:610:ARG:NH2	2.46	0.48
1:A:101:ARG:NH2	1:A:190:ALA:O	2.32	0.48
1:A:632:VAL:CG2	1:A:653:PHE:CZ	2.97	0.48
1:A:377:TRP:HD1	1:A:377:TRP:C	2.16	0.48
1:A:357:ALA:HB1	1:A:358:HIS:CG	2.49	0.48
1:A:468:GLY:HA3	1:A:502:THR:HG21	1.95	0.48
1:B:403:ARG:NE	1:B:441:GLU:OE2	2.40	0.48
1:B:22:LEU:HD12	1:B:291:GLU:OE1	2.14	0.48
1:D:574:ARG:CG	1:D:576:MET:HG3	2.43	0.48
1:A:565:MET:HB3	1:A:566:TRP:CD1	2.48	0.48
1:B:22:LEU:HA	1:B:291:GLU:CD	2.34	0.48
1:D:377:TRP:CZ3	1:D:500:MET:HE2	2.47	0.47
1:D:529:PRO:O	1:D:530:GLU:C	2.50	0.47
1:B:484:LYS:CB	1:B:485:PRO:CD	2.92	0.47
1:D:299:ARG:HD2	1:D:299:ARG:O	2.13	0.47
1:D:479:LYS:HD3	1:D:519:ASP:HB2	1.95	0.47
1:A:162:ASN:ND2	1:A:565:MET:HG2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:SER:O	1:D:352:THR:OG1	2.29	0.47
1:C:662:LYS:HE3	1:C:681:GLU:CD	2.35	0.47
1:B:166:VAL:O	1:B:167:TYR:C	2.52	0.47
1:B:633:TYR:CE1	1:B:638:GLU:CB	2.90	0.47
1:C:266:LEU:HD23	1:C:298:VAL:HG22	1.95	0.47
1:A:527:PHE:O	1:A:529:PRO:CD	2.62	0.47
1:A:229:THR:HG21	1:A:231:TYR:CE2	2.48	0.47
1:C:35:PHE:CG	1:C:36:LYS:N	2.82	0.47
1:A:330:LEU:N	1:A:330:LEU:CD1	2.77	0.47
1:A:258:THR:O	1:A:258:THR:HG22	2.14	0.47
1:A:78:GLU:CG	1:A:151:LYS:HA	2.31	0.47
1:B:654:ASP:HA	1:B:655:ASN:HA	1.56	0.47
1:B:241:HIS:ND1	1:B:242:SER:N	2.63	0.47
1:A:106:GLY:HA2	1:A:107:ALA:HA	1.65	0.47
1:D:455:HIS:H	1:D:455:HIS:CD2	2.33	0.47
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.72	0.47
1:D:684:TYR:OH	1:D:687:GLU:HG2	2.15	0.47
1:C:90:PRO:C	1:C:92:ASP:H	2.17	0.47
1:D:137:LYS:HB2	1:D:137:LYS:HE2	1.64	0.47
1:A:70:GLN:OE1	1:A:329:GLY:N	2.29	0.47
1:D:634:LEU:HB2	1:D:639:LEU:HD21	1.97	0.47
1:B:22:LEU:HG	1:B:291:GLU:OE2	2.15	0.47
1:A:330:LEU:N	1:A:330:LEU:HD13	2.30	0.47
1:D:605:TYR:O	1:D:624:TYR:N	2.36	0.47
1:A:84:ARG:HG3	1:A:145:ILE:HG12	1.96	0.47
1:D:641:GLY:O	1:D:642:ILE:C	2.52	0.47
1:B:181:GLN:HB3	1:B:182:ASN:ND2	2.30	0.47
1:B:626:ASN:O	1:B:627:ILE:CG2	2.63	0.47
1:D:513:GLN:HE22	1:D:530:GLU:HB3	1.79	0.47
1:C:417:HIS:C	1:C:417:HIS:CD2	2.88	0.47
1:B:689:ASN:ND2	1:B:692:ILE:CG1	2.65	0.46
1:D:614:ARG:CD	1:D:682:TRP:HB3	2.45	0.46
1:D:614:ARG:HD3	1:D:682:TRP:CB	2.45	0.46
1:C:259:PHE:CD2	1:C:259:PHE:N	2.83	0.46
1:A:179:THR:HG23	1:A:183:ASN:HB3	1.96	0.46
1:D:182:ASN:ND2	1:D:216:ASN:HA	2.30	0.46
1:B:58:VAL:CG2	1:B:62:HIS:CD2	2.97	0.46
1:B:106:GLY:HA2	1:B:107:ALA:HA	1.65	0.46
1:D:100:LEU:O	1:D:129:ALA:HA	2.16	0.46
1:B:621:VAL:HG12	1:B:653:PHE:HD1	1.80	0.46
1:B:658:LEU:HA	1:B:663:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:LEU:HD23	1:B:665:LEU:HA	1.57	0.46
1:B:609:ARG:NH2	1:B:609:ARG:CB	2.77	0.46
1:B:299:ARG:HA	1:B:312:ASN:OD1	2.15	0.46
1:A:229:THR:HG21	1:A:231:TYR:CZ	2.50	0.46
1:D:92:ASP:OD1	1:D:92:ASP:N	2.49	0.46
1:A:341:PHE:CD2	1:A:341:PHE:C	2.89	0.46
1:D:513:GLN:HE22	1:D:530:GLU:CB	2.28	0.46
1:B:297:GLY:H	1:B:409:PRO:HG3	1.80	0.46
1:B:303:ILE:HG23	1:B:551:ILE:HG12	1.97	0.46
1:A:207:ASP:OD2	1:A:260:LYS:HE3	2.16	0.46
1:A:133:GLY:CA	1:A:136:LEU:HD23	2.32	0.46
1:B:474:GLY:HA2	1:B:478:LYS:O	2.16	0.46
1:B:311:LEU:O	1:B:312:ASN:C	2.54	0.46
1:B:512:HIS:HB3	1:B:527:PHE:CZ	2.50	0.46
1:C:666:LYS:HD2	1:C:679:GLU:OE1	2.16	0.46
1:A:301:TYR:CD2	1:A:412:TYR:HB2	2.51	0.46
1:B:617:ARG:HD3	1:B:617:ARG:O	2.15	0.46
1:D:672:LYS:O	1:D:673:GLY:C	2.54	0.46
1:D:214:LEU:O	1:D:252:THR:HG23	2.16	0.46
1:D:341:PHE:C	1:D:341:PHE:CD2	2.89	0.46
1:B:208:ILE:CD1	1:B:230:ILE:HD11	2.43	0.46
1:C:642:ILE:CD1	1:C:653:PHE:CE1	2.95	0.46
1:A:460:VAL:O	1:A:460:VAL:HG13	2.16	0.46
1:C:250:GLN:HB3	1:D:464:ALA:O	2.15	0.46
1:D:99:PHE:HB2	1:D:177:ILE:HB	1.97	0.46
1:D:661:GLY:N	1:D:684:TYR:O	2.48	0.46
1:D:60:ILE:HG22	1:D:61:PRO:HA	1.97	0.46
1:D:320:GLY:HA2	1:D:353:THR:CG2	2.45	0.46
1:B:94:GLU:HG3	1:B:95:GLY:N	2.31	0.46
1:C:358:HIS:O	1:C:381:PRO:HA	2.16	0.46
1:B:639:LEU:CD1	1:B:656:VAL:HG21	2.45	0.45
1:C:86:THR:HA	1:C:142:ASN:O	2.16	0.45
1:D:501:LEU:O	1:D:553:SER:HA	2.15	0.45
1:C:176:LEU:HA	1:C:176:LEU:HD12	1.74	0.45
1:A:509:ASN:O	1:A:510:LEU:C	2.55	0.45
1:C:522:ASN:ND2	1:C:522:ASN:C	2.69	0.45
1:A:512:HIS:CB	1:A:529:PRO:HA	2.46	0.45
1:A:203:LYS:HB3	1:A:203:LYS:HE3	1.63	0.45
1:A:399:ARG:HH21	1:B:399:ARG:HH22	1.64	0.45
1:C:132:ILE:HD12	1:C:136:LEU:HD21	1.97	0.45
1:B:483:ILE:HG12	1:B:483:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:CG2	1:B:118:ALA:HB3	2.45	0.45
1:A:477:GLU:CG	1:A:478:LYS:CD	2.92	0.45
1:A:399:ARG:NH2	1:B:399:ARG:NH2	2.65	0.45
1:C:230:ILE:O	1:C:238:VAL:HG12	2.16	0.45
1:A:395:GLN:HE21	1:A:433:SER:HB2	1.81	0.45
1:D:614:ARG:HG2	1:D:683:ASN:O	2.15	0.45
1:D:399:ARG:HB2	1:D:399:ARG:HE	1.60	0.45
1:A:467:GLN:O	1:A:499:LEU:HA	2.17	0.45
1:B:458:HIS:CG	1:B:459:PRO:HD2	2.51	0.45
1:C:181:GLN:CA	1:C:181:GLN:HE21	2.29	0.45
1:B:595:LYS:O	1:B:599:SER:CB	2.65	0.45
1:B:563:VAL:CG2	1:B:575:ASN:HB2	2.44	0.45
1:A:229:THR:HG22	1:A:231:TYR:CE2	2.50	0.45
1:B:580:ILE:CG2	1:B:581:THR:N	2.80	0.45
1:D:89:PHE:O	1:D:139:GLY:N	2.50	0.45
1:D:474:GLY:HA2	1:D:479:LYS:HA	1.99	0.45
1:B:203:LYS:O	1:B:263:ASN:HA	2.15	0.45
1:B:325:GLN:HG2	1:B:359:TYR:CE1	2.52	0.45
1:D:630:PRO:CA	1:D:669:VAL:HG12	2.25	0.45
1:B:619:THR:HG21	1:B:682:TRP:HZ3	1.81	0.45
1:A:618:THR:CG2	1:A:657:SER:OG	2.65	0.45
1:B:225:THR:HA	1:B:243:ARG:O	2.17	0.45
1:A:645:GLY:HA3	1:A:650:HIS:ND1	2.31	0.45
1:B:208:ILE:HD11	1:B:259:PHE:CB	2.41	0.45
1:B:512:HIS:CG	1:B:527:PHE:CD1	3.05	0.45
1:D:446:TYR:HA	1:D:465:ASP:OD2	2.16	0.45
1:A:157:ILE:HD11	1:A:381:PRO:HD2	1.98	0.45
1:A:461:ASN:HB3	1:A:467:GLN:OE1	2.17	0.45
1:C:267:TRP:CZ2	1:C:373:GLY:HA2	2.52	0.45
1:A:543:ILE:HD13	1:A:543:ILE:N	2.32	0.45
1:B:662:LYS:HG2	1:B:663:ASN:N	2.31	0.45
1:B:637:GLN:O	1:B:638:GLU:C	2.54	0.45
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.75	0.45
1:D:94:GLU:CA	1:D:94:GLU:OE1	2.61	0.45
1:B:335:LYS:HB3	1:B:337:GLU:OE2	2.17	0.45
1:B:580:ILE:HG22	1:B:581:THR:H	1.82	0.45
1:B:516:TYR:O	1:B:517:LEU:HD23	2.17	0.45
1:C:501:LEU:O	1:C:553:SER:HA	2.17	0.45
1:C:125:TYR:CG	1:C:359:TYR:HB2	2.52	0.45
1:A:416:LEU:CD1	1:A:416:LEU:N	2.79	0.45
1:B:372:LEU:N	1:B:372:LEU:HD23	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLY:HA2	1:D:107:ALA:HA	1.59	0.44
1:A:327:TRP:CZ2	1:A:584:ARG:HG2	2.52	0.44
1:D:627:ILE:HG13	1:D:669:VAL:CG2	2.43	0.44
1:B:456:MET:CE	1:B:456:MET:HA	2.43	0.44
1:D:528:TYR:CD2	1:D:569:GLY:HA3	2.52	0.44
1:A:105:VAL:O	1:A:124:GLY:HA2	2.16	0.44
1:A:617:ARG:NH1	1:A:658:LEU:O	2.50	0.44
1:C:299:ARG:HH21	1:C:409:PRO:C	2.21	0.44
1:C:408:HIS:HA	1:C:409:PRO:HD2	1.86	0.44
1:A:517:LEU:HD21	1:A:531:THR:OG1	2.17	0.44
1:A:497:GLN:HA	1:B:250:GLN:NE2	2.32	0.44
1:D:323:ARG:HA	1:D:557:ASN:HD21	1.82	0.44
1:B:358:HIS:O	1:B:381:PRO:HA	2.17	0.44
1:D:319:TYR:HB3	1:D:598:TRP:CD2	2.53	0.44
1:C:689:ASN:OD1	1:C:691:GLU:N	2.49	0.44
1:C:106:GLY:HA2	1:C:107:ALA:HA	1.55	0.44
1:D:512:HIS:O	1:D:529:PRO:HA	2.16	0.44
1:C:437:LEU:O	1:C:437:LEU:HD23	2.18	0.44
1:C:120:THR:HG23	1:C:121:HIS:N	2.31	0.44
1:B:88:PHE:CD2	1:B:140:ALA:O	2.71	0.44
1:A:337:GLU:CD	1:A:337:GLU:H	2.20	0.44
1:C:601:GLU:HG2	1:C:601:GLU:H	1.58	0.44
1:B:121:HIS:CD2	1:B:128:PHE:HB3	2.52	0.44
1:C:484:LYS:O	1:C:488:GLU:HG3	2.17	0.44
1:C:46:ARG:NH1	1:C:46:ARG:HB2	2.33	0.44
1:C:353:THR:HA	1:C:375:ILE:O	2.18	0.44
1:D:505:GLY:HA2	1:D:537:HIS:CE1	2.52	0.44
1:C:557:ASN:OD1	1:C:558:MET:N	2.50	0.44
1:B:580:ILE:CG2	1:B:581:THR:H	2.31	0.44
1:C:232:THR:O	1:C:233:GLN:C	2.56	0.44
1:D:155:ASP:HA	1:D:389:TYR:O	2.18	0.44
1:D:306:GLY:HA2	1:D:549:TYR:HA	1.99	0.44
1:C:508:ALA:HB2	1:C:533:GLN:HB2	1.99	0.44
1:B:667:ALA:O	1:B:677:THR:HA	2.18	0.44
1:A:179:THR:CG2	1:A:183:ASN:HD22	2.28	0.44
1:B:111:VAL:HG23	1:B:118:ALA:HB3	1.99	0.44
1:A:645:GLY:HA3	1:A:650:HIS:CG	2.53	0.44
1:C:374:LEU:O	1:C:410:SER:HB2	2.18	0.44
1:C:416:LEU:HD23	1:C:416:LEU:N	2.32	0.44
1:A:470:ASN:CG	1:A:503:GLU:HB2	2.35	0.43
1:B:512:HIS:CB	1:B:527:PHE:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:CD2	1:A:605:TYR:CE1	3.06	0.43
1:A:413:VAL:HG22	1:A:414:TRP:N	2.32	0.43
1:D:320:GLY:HA2	1:D:353:THR:O	2.18	0.43
1:B:72:GLN:HA	1:B:572:PRO:HB2	2.00	0.43
1:D:448:VAL:HG23	1:D:466:ILE:HB	2.00	0.43
1:D:109:ALA:HA	1:D:147:LYS:O	2.18	0.43
1:B:641:GLY:O	1:B:642:ILE:C	2.55	0.43
1:B:184:ILE:HD13	1:B:292:VAL:CG1	2.47	0.43
1:C:613:ASP:O	1:C:690:ARG:NH2	2.48	0.43
1:C:692:ILE:HG22	1:C:692:ILE:O	2.19	0.43
1:A:188:ASP:OD1	1:A:403:ARG:NH1	2.50	0.43
1:B:634:LEU:O	1:B:635:ASN:HB2	2.17	0.43
1:B:603:VAL:O	1:B:625:SER:HA	2.18	0.43
1:C:337:GLU:N	1:C:337:GLU:CD	2.65	0.43
1:D:593:TRP:HE3	1:D:624:TYR:CE2	2.36	0.43
1:C:181:GLN:NE2	1:C:181:GLN:HA	2.33	0.43
1:A:60:ILE:CG2	1:A:61:PRO:HA	2.49	0.43
1:C:199:LYS:HB3	1:C:207:ASP:HB2	2.00	0.43
1:A:179:THR:HG21	1:A:183:ASN:HB3	2.00	0.43
1:C:377:TRP:HD1	1:C:377:TRP:O	2.01	0.43
1:D:205:SER:HA	1:D:261:LEU:O	2.18	0.43
1:D:571:VAL:HG23	1:D:572:PRO:HD2	2.00	0.43
1:D:300:LYS:HE3	2:D:803:CL:CL	2.56	0.43
1:D:614:ARG:CG	1:D:682:TRP:HB3	2.48	0.43
1:C:649:VAL:HG13	1:C:649:VAL:O	2.18	0.43
1:C:525:LYS:CD	1:C:694:SER:CB	2.96	0.43
1:B:102:PHE:O	1:B:127:ALA:HA	2.19	0.43
1:A:104:GLY:HA3	1:A:172:ARG:HD2	1.99	0.43
1:B:510:LEU:HD22	1:B:530:GLU:OE1	2.18	0.43
1:A:320:GLY:CA	1:A:353:THR:HG23	2.47	0.43
1:C:563:VAL:CG2	1:C:575:ASN:HB2	2.46	0.43
1:A:619:THR:HG23	1:A:620:ALA:O	2.17	0.43
1:D:208:ILE:HG12	1:D:261:LEU:HD22	2.00	0.43
1:A:36:LYS:HB2	1:A:55:TRP:CD2	2.54	0.43
1:D:84:ARG:HD2	1:D:143:GLU:OE2	2.19	0.43
1:C:214:LEU:HD12	1:C:255:TYR:CE2	2.53	0.43
1:B:265:HIS:NE2	1:B:272:ASP:OD2	2.33	0.43
1:B:620:ALA:HA	1:B:653:PHE:O	2.19	0.43
1:D:111:VAL:HG23	1:D:111:VAL:O	2.17	0.43
1:B:309:PHE:CD1	1:B:318:MET:CE	3.02	0.43
1:A:82:TYR:CE1	1:A:147:LYS:CG	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TYR:HB3	1:C:360:GLN:O	2.19	0.43
1:C:667:ALA:O	1:C:677:THR:HA	2.17	0.43
1:D:211:LYS:HB2	1:D:256:LEU:CD2	2.48	0.43
1:C:244:SER:O	1:C:245:PHE:HB3	2.18	0.43
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.77	0.43
1:D:294:GLN:HB3	1:D:295:PRO:HD2	2.00	0.43
1:D:65:ASN:HB3	1:D:69:MET:HB2	2.01	0.43
1:D:619:THR:HG21	1:D:682:TRP:HZ3	1.84	0.43
1:D:609:ARG:CB	1:D:680:ILE:CG2	2.97	0.43
1:B:614:ARG:HG2	1:B:682:TRP:HB3	2.01	0.43
1:B:133:GLY:HA2	1:B:136:LEU:HD12	2.00	0.43
1:B:320:GLY:HA2	1:B:353:THR:O	2.19	0.43
1:A:439:LYS:NZ	1:A:465:ASP:OD2	2.37	0.43
1:B:395:GLN:O	1:B:396:SER:C	2.56	0.42
1:C:487:VAL:HG13	1:C:488:GLU:N	2.34	0.42
1:A:383:VAL:HG23	1:A:383:VAL:O	2.19	0.42
1:C:539:TYR:O	1:C:542:SER:OG	2.25	0.42
1:B:189:CYS:O	1:B:190:ALA:HB3	2.19	0.42
1:B:471:ARG:HB2	1:B:501:LEU:HD11	2.01	0.42
1:A:121:HIS:CE1	1:A:123:GLY:O	2.72	0.42
1:D:153:ARG:HB2	1:D:155:ASP:OD1	2.18	0.42
1:D:56:GLU:HG2	1:D:58:VAL:HG23	2.01	0.42
1:B:664:ILE:HD12	1:B:665:LEU:N	2.34	0.42
1:D:684:TYR:CD2	1:D:685:SER:CA	3.01	0.42
1:A:103:GLU:HB2	1:A:172:ARG:HB3	2.01	0.42
1:B:468:GLY:HA2	1:B:500:MET:O	2.19	0.42
1:D:475:TRP:CZ3	1:D:521:LEU:HD22	2.54	0.42
1:D:90:PRO:HB2	1:D:92:ASP:OD1	2.18	0.42
1:D:330:LEU:HA	1:D:330:LEU:HD12	1.64	0.42
1:A:93:LEU:O	1:A:96:LYS:HB2	2.18	0.42
1:A:642:ILE:HD12	1:A:653:PHE:CZ	2.54	0.42
1:D:565:MET:CB	3:D:727:HOH:O	2.66	0.42
1:D:560:ASP:HB2	1:D:582:PHE:HB2	2.00	0.42
1:A:383:VAL:O	1:A:384:ASN:HB3	2.19	0.42
1:A:187:THR:HG22	1:A:187:THR:O	2.20	0.42
1:D:167:TYR:OH	1:D:326:ASP:OD2	2.31	0.42
1:C:545:LYS:HG3	1:C:545:LYS:O	2.17	0.42
1:C:603:VAL:CB	1:C:626:ASN:HD22	2.32	0.42
1:C:377:TRP:CD1	1:C:377:TRP:O	2.72	0.42
1:A:382:CYS:C	1:A:383:VAL:CG1	2.88	0.42
1:D:647:THR:C	1:D:649:VAL:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:CG2	1:C:121:HIS:N	2.79	0.42
1:B:631:LYS:HB2	1:B:668:VAL:HG13	2.02	0.42
1:B:634:LEU:HD11	1:B:663:ASN:HB3	2.01	0.42
1:D:662:LYS:HG3	1:D:663:ASN:N	2.34	0.42
1:C:484:LYS:O	1:C:487:VAL:HG12	2.19	0.42
1:A:392:GLU:OE2	1:B:122:LYS:HE2	2.20	0.42
1:C:525:LYS:HG2	1:C:526:PRO:HD2	2.02	0.42
1:B:270:ARG:NH2	1:B:347:MET:HE3	2.35	0.42
1:A:633:TYR:HD2	1:A:638:GLU:N	2.18	0.42
1:D:471:ARG:HA	1:D:471:ARG:NE	2.34	0.42
1:B:205:SER:HB2	1:B:261:LEU:O	2.20	0.42
1:A:377:TRP:CH2	1:A:448:VAL:HG11	2.55	0.42
1:B:574:ARG:HG3	1:B:576:MET:HG3	2.01	0.42
1:B:387:THR:N	1:B:390:GLU:OE2	2.40	0.42
1:D:216:ASN:HB3	1:D:248:SER:O	2.20	0.42
1:B:60:ILE:N	1:B:60:ILE:HD13	2.33	0.42
1:B:152:ALA:HB1	1:B:159:VAL:O	2.20	0.42
1:B:658:LEU:CA	1:B:663:ASN:HD21	2.33	0.42
1:A:40:PHE:HA	1:A:50:GLN:HE22	1.84	0.42
1:D:612:ALA:O	1:D:683:ASN:HB2	2.20	0.42
1:A:509:ASN:O	1:A:511:ALA:N	2.52	0.42
1:B:388:GLY:HA2	1:B:426:TYR:CZ	2.54	0.42
1:B:557:ASN:O	1:B:578:GLY:HA2	2.19	0.42
1:C:299:ARG:HH21	1:C:409:PRO:CA	2.32	0.42
1:B:61:PRO:HD2	1:B:335:LYS:HZ3	1.83	0.42
1:D:325:GLN:HB2	3:D:714:HOH:O	2.18	0.42
1:B:203:LYS:O	1:B:264:PRO:HD2	2.19	0.42
1:B:125:TYR:CG	1:B:359:TYR:HB2	2.55	0.42
1:A:654:ASP:HA	1:A:655:ASN:HA	1.81	0.42
1:B:689:ASN:CG	1:B:692:ILE:HG13	2.35	0.42
1:D:684:TYR:HD2	1:D:685:SER:CA	2.32	0.42
1:B:182:ASN:HA	1:B:215:ASP:O	2.19	0.42
1:B:157:ILE:HG13	1:B:397:GLN:NE2	2.35	0.42
1:B:243:ARG:HG2	1:B:244:SER:N	2.35	0.42
1:B:304:VAL:O	1:B:305:ALA:C	2.57	0.42
1:A:353:THR:HG23	1:A:554:TYR:CE1	2.54	0.41
1:A:280:CYS:O	1:A:291:GLU:HA	2.20	0.41
1:B:71:VAL:HG12	1:B:71:VAL:O	2.20	0.41
1:D:357:ALA:HB1	1:D:358:HIS:CG	2.55	0.41
1:B:229:THR:CG2	1:B:230:ILE:N	2.83	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:HB2	1:B:116:LYS:HE3	1.61	0.41
1:C:447:THR:O	1:C:465:ASP:HB2	2.20	0.41
1:D:63:THR:HG23	1:D:63:THR:O	2.19	0.41
1:C:642:ILE:CD1	1:C:653:PHE:CZ	2.84	0.41
1:B:205:SER:HG	1:B:260:LYS:HE3	1.81	0.41
1:C:525:LYS:HD2	1:C:694:SER:CB	2.50	0.41
1:D:261:LEU:HA	1:D:261:LEU:HD12	1.78	0.41
1:A:403:ARG:NE	1:A:441:GLU:OE2	2.48	0.41
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.82	0.41
1:D:617:ARG:HA	1:D:684:TYR:CE1	2.56	0.41
1:B:82:TYR:CZ	1:B:147:LYS:HG2	2.55	0.41
1:D:384:ASN:C	1:D:385:ARG:HG2	2.41	0.41
1:A:357:ALA:HA	1:A:358:HIS:HA	1.86	0.41
1:C:618:THR:HA	1:C:656:VAL:O	2.20	0.41
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.90	0.41
1:D:591:TYR:CD1	1:D:591:TYR:C	2.93	0.41
1:B:633:TYR:CD1	1:B:638:GLU:N	2.88	0.41
1:D:186:VAL:CG2	1:D:186:VAL:O	2.67	0.41
1:D:439:LYS:NZ	1:D:465:ASP:OD2	2.44	0.41
1:A:583:ASP:O	1:A:584:ARG:HB2	2.20	0.41
1:A:606:LEU:HD12	1:A:678:ASP:O	2.20	0.41
1:D:460:VAL:HG13	1:D:460:VAL:O	2.21	0.41
1:B:635:ASN:OD1	1:B:663:ASN:HA	2.20	0.41
1:A:47:ALA:HA	1:A:50:GLN:HE21	1.85	0.41
1:C:475:TRP:CZ2	1:C:507:ASP:HB2	2.55	0.41
1:A:527:PHE:C	1:A:529:PRO:HD3	2.41	0.41
1:A:484:LYS:CB	1:A:485:PRO:CD	2.93	0.41
1:C:492:LYS:HB3	1:C:492:LYS:HZ1	1.84	0.41
1:D:303:ILE:CG2	1:D:498:LYS:HZ2	2.33	0.41
1:C:447:THR:H	1:C:465:ASP:HB2	1.86	0.41
1:A:179:THR:HG22	1:A:180:GLU:CA	2.51	0.41
1:D:557:ASN:ND2	1:D:558:MET:N	2.52	0.41
1:B:533:GLN:O	1:B:536:THR:HB	2.20	0.41
1:A:668:VAL:CG1	1:A:675:GLU:OE2	2.68	0.41
1:C:232:THR:O	1:C:235:GLY:N	2.49	0.41
1:B:634:LEU:HD22	1:B:656:VAL:HG11	1.99	0.41
1:D:355:ARG:HG3	1:D:377:TRP:CD2	2.55	0.41
1:C:475:TRP:CZ3	1:C:521:LEU:HD22	2.55	0.41
1:A:320:GLY:HA2	1:A:353:THR:HG23	2.02	0.41
1:C:516:TYR:CZ	1:C:616:LYS:CE	3.02	0.41
1:B:579:LEU:HA	1:B:579:LEU:HD12	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLN:HA	1:C:181:GLN:HE21	1.85	0.41
1:B:415:GLY:HA2	1:B:448:VAL:HG13	2.03	0.41
1:B:538:GLU:HA	1:B:593:TRP:CZ2	2.56	0.41
1:B:658:LEU:HA	1:B:663:ASN:HD21	1.85	0.41
1:B:37:LYS:CD	1:B:77:TYR:CE2	3.02	0.41
1:D:630:PRO:HA	1:D:669:VAL:HG13	1.89	0.41
1:D:619:THR:HG23	1:D:620:ALA:O	2.21	0.41
1:B:357:ALA:HB1	1:B:358:HIS:CE1	2.56	0.41
1:B:357:ALA:HA	1:B:358:HIS:HA	1.82	0.41
1:B:508:ALA:HB1	1:B:530:GLU:HA	2.03	0.41
1:B:575:ASN:OD1	1:B:577:LYS:HG3	2.21	0.41
1:A:346:ILE:HG23	1:A:351:ALA:HB3	2.02	0.41
1:C:481:GLN:HA	1:C:539:TYR:CE1	2.56	0.41
1:A:514:THR:O	1:A:531:THR:HG21	2.20	0.41
1:A:513:GLN:O	1:A:514:THR:HB	2.20	0.41
1:D:122:LYS:HB2	1:D:122:LYS:HE3	1.84	0.41
1:D:59:GLU:O	1:D:62:HIS:HB2	2.21	0.41
1:D:60:ILE:HA	1:D:61:PRO:C	2.42	0.41
1:B:482:ASP:C	1:B:484:LYS:H	2.24	0.41
1:D:574:ARG:HG2	1:D:576:MET:CG	2.51	0.41
1:D:413:VAL:HG22	1:D:414:TRP:N	2.36	0.41
1:C:668:VAL:HA	1:C:676:TYR:O	2.21	0.41
1:C:583:ASP:O	1:C:584:ARG:CB	2.49	0.40
1:B:394:ALA:O	1:B:395:GLN:C	2.59	0.40
1:D:377:TRP:HD1	1:D:378:ALA:N	2.19	0.40
1:A:521:LEU:HG	1:A:522:ASN:O	2.21	0.40
1:A:634:LEU:CD2	1:A:656:VAL:CG1	2.94	0.40
1:D:356:PHE:HB3	1:D:361:GLN:NE2	2.35	0.40
1:D:325:GLN:HG2	1:D:359:TYR:HE1	1.84	0.40
1:C:247:LEU:HD12	1:C:248:SER:N	2.36	0.40
1:C:306:GLY:HA2	1:C:549:TYR:HA	2.03	0.40
1:B:71:VAL:CG1	1:B:71:VAL:O	2.69	0.40
1:B:570:GLY:C	1:B:571:VAL:HG12	2.42	0.40
1:A:533:GLN:O	1:A:534:THR:C	2.60	0.40
1:A:65:ASN:HA	1:A:68:ASP:OD1	2.21	0.40
1:D:307:LYS:HB3	1:D:307:LYS:HE3	1.81	0.40
1:A:481:GLN:HA	1:A:539:TYR:CE1	2.56	0.40
1:C:497:GLN:H	1:C:497:GLN:HG2	1.75	0.40
1:B:417:HIS:CD2	1:B:417:HIS:O	2.74	0.40
1:D:353:THR:HG23	1:D:554:TYR:CE1	2.56	0.40
1:C:125:TYR:O	1:C:360:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CD1	1:B:219:LEU:N	2.83	0.40
1:C:555:LEU:O	1:C:555:LEU:HD12	2.21	0.40
1:C:284:ALA:O	1:C:285:ASP:HB2	2.21	0.40
1:D:458:HIS:CG	1:D:459:PRO:HD2	2.57	0.40
1:A:665:LEU:O	1:A:679:GLU:HA	2.22	0.40
1:A:317:SER:O	1:A:318:MET:HE3	2.22	0.40
1:D:411:ILE:HG21	1:D:414:TRP:CH2	2.57	0.40
1:D:408:HIS:HA	1:D:409:PRO:HD2	1.93	0.40
1:C:549:TYR:O	1:C:551:ILE:HD12	2.22	0.40
1:B:408:HIS:HB2	1:B:411:ILE:HD12	2.02	0.40
1:B:327:TRP:CZ3	1:B:338:HIS:HD2	2.40	0.40
1:A:37:LYS:HG2	1:A:38:GLY:O	2.21	0.40
1:A:100:LEU:O	1:A:129:ALA:HA	2.21	0.40
1:C:490:LEU:HA	1:C:490:LEU:HD12	1.90	0.40
1:D:76:PHE:CE2	1:D:564:PRO:HB2	2.57	0.40
1:A:629:THR:HA	1:A:630:PRO:HD3	1.95	0.40
1:C:377:TRP:CH2	1:C:448:VAL:HG11	2.56	0.40
1:B:283:MET:HG2	1:B:288:VAL:HA	2.04	0.40
1:A:448:VAL:CG2	1:A:449:SER:N	2.83	0.40
1:D:302:GLU:HG2	1:D:303:ILE:N	2.37	0.40
1:D:303:ILE:HB	1:D:498:LYS:HZ2	1.86	0.40
1:D:538:GLU:HA	1:D:593:TRP:CZ2	2.57	0.40
1:A:614:ARG:NH2	1:A:682:TRP:CE2	2.89	0.40
1:D:518:GLY:O	1:D:535:LYS:NZ	2.54	0.40
1:D:666:LYS:HA	1:D:678:ASP:O	2.22	0.40
1:A:303:ILE:CG2	1:A:498:LYS:HD3	2.52	0.40
1:C:607:THR:O	1:C:608:GLN:HB2	2.22	0.40
1:D:82:TYR:CZ	1:D:147:LYS:HG2	2.57	0.40
1:A:604:LEU:HA	1:A:624:TYR:O	2.22	0.40
1:C:84:ARG:CD	1:C:143:GLU:OE2	2.66	0.40
1:D:357:ALA:HA	1:D:358:HIS:HA	1.85	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	670/692 (97%)	617 (92%)	50 (8%)	3 (0%)	39 69
1	B	670/692 (97%)	613 (92%)	51 (8%)	6 (1%)	21 49
1	C	671/692 (97%)	626 (93%)	44 (7%)	1 (0%)	56 83
1	D	664/692 (96%)	620 (93%)	40 (6%)	4 (1%)	30 59
All	All	2675/2768 (97%)	2476 (93%)	185 (7%)	14 (0%)	34 63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	C	238	VAL
1	A	692	ILE
1	B	627	ILE
1	B	638	GLU
1	B	672	LYS
1	B	685	SER
1	D	648	ASP
1	D	673	GLY
1	B	636	GLY
1	B	689	ASN
1	D	133	GLY
1	A	528	TYR
1	D	642	ILE

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	570/591 (96%)	524 (92%)	46 (8%)	15 33
1	B	564/591 (95%)	493 (87%)	71 (13%)	5 13
1	C	571/591 (97%)	530 (93%)	41 (7%)	18 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	564/591 (95%)	518 (92%)	46 (8%)	14 32
All	All	2269/2364 (96%)	2065 (91%)	204 (9%)	12 27

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	58	VAL
1	A	78	GLU
1	A	86	THR
1	A	96	LYS
1	A	111	VAL
1	A	120	THR
1	A	130	CYS
1	A	138	LEU
1	A	147	LYS
1	A	163	LEU
1	A	181	GLN
1	A	187	THR
1	A	197	THR
1	A	199	LYS
1	A	243	ARG
1	A	258	THR
1	A	260	LYS
1	A	261	LEU
1	A	277	LYS
1	A	285	ASP
1	A	291	GLU
1	A	299	ARG
1	A	314	GLU
1	A	330	LEU
1	A	337	GLU
1	A	374	LEU
1	A	377	TRP
1	A	399	ARG
1	A	416	LEU
1	A	417	HIS
1	A	451	ASN
1	A	481	GLN
1	A	499	LEU
1	A	600	GLU
1	A	609	ARG

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Mol	Chain	Res	Type
1	A	617	ARG
1	A	619	THR
1	A	643	ARG
1	A	658	LEU
1	A	664	ILE
1	A	666	LYS
1	A	674	LYS
1	A	677	THR
1	A	683	ASN
1	A	692	ILE
1	B	22	LEU
1	B	31	THR
1	B	42	THR
1	B	43	ASP
1	B	49	SER
1	B	52	ASP
1	B	67	MET
1	B	86	THR
1	B	93	LEU
1	B	94	GLU
1	B	98	VAL
1	B	111	VAL
1	B	113	VAL
1	B	130	CYS
1	B	147	LYS
1	B	151	LYS
1	B	153	ARG
1	B	163	LEU
1	B	181	GLN
1	B	182	ASN
1	B	186	VAL
1	B	187	THR
1	B	194	VAL
1	B	199	LYS
1	B	204	LYS
1	B	207	ASP
1	B	208	ILE
1	B	219	LEU
1	B	241	HIS
1	B	242	SER
1	B	252	THR
1	B	257	SER

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Mol	Chain	Res	Type
1	B	261	LEU
1	B	292	VAL
1	B	293	VAL
1	B	298	VAL
1	B	299	ARG
1	B	307	LYS
1	B	330	LEU
1	B	335	LYS
1	B	337	GLU
1	B	362	SER
1	B	374	LEU
1	B	377	TRP
1	B	390	GLU
1	B	416	LEU
1	B	417	HIS
1	B	419	GLU
1	B	436	ASP
1	B	456	MET
1	B	481	GLN
1	B	484	LYS
1	B	499	LEU
1	B	567	THR
1	B	571	VAL
1	B	579	LEU
1	B	586	THR
1	B	601	GLU
1	B	609	ARG
1	B	614	ARG
1	B	617	ARG
1	B	621	VAL
1	B	629	THR
1	B	637	GLN
1	B	654	ASP
1	B	655	ASN
1	B	657	SER
1	B	664	ILE
1	B	677	THR
1	B	685	SER
1	B	690	ARG
1	C	31	THR
1	C	42	THR
1	C	56	GLU

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Mol	Chain	Res	Type
1	C	57	THR
1	C	63	THR
1	C	71	VAL
1	C	72	GLN
1	C	86	THR
1	C	120	THR
1	C	130	CYS
1	C	163	LEU
1	C	181	GLN
1	C	186	VAL
1	C	187	THR
1	C	211	LYS
1	C	238	VAL
1	C	252	THR
1	C	259	PHE
1	C	261	LEU
1	C	277	LYS
1	C	298	VAL
1	C	299	ARG
1	C	314	GLU
1	C	337	GLU
1	C	374	LEU
1	C	377	TRP
1	C	390	GLU
1	C	417	HIS
1	C	483	ILE
1	C	492	LYS
1	C	522	ASN
1	C	565	MET
1	C	571	VAL
1	C	601	GLU
1	C	609	ARG
1	C	629	THR
1	C	649	VAL
1	C	664	ILE
1	C	670	SER
1	C	688	LYS
1	C	694	SER
1	D	31	THR
1	D	57	THR
1	D	58	VAL
1	D	75	SER

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Mol	Chain	Res	Type
1	D	86	THR
1	D	130	CYS
1	D	137	LYS
1	D	147	LYS
1	D	153	ARG
1	D	163	LEU
1	D	181	GLN
1	D	204	LYS
1	D	211	LYS
1	D	260	LYS
1	D	261	LEU
1	D	293	VAL
1	D	299	ARG
1	D	314	GLU
1	D	330	LEU
1	D	337	GLU
1	D	349	VAL
1	D	374	LEU
1	D	377	TRP
1	D	390	GLU
1	D	399	ARG
1	D	416	LEU
1	D	471	ARG
1	D	481	GLN
1	D	490	LEU
1	D	514	THR
1	D	557	ASN
1	D	565	MET
1	D	571	VAL
1	D	579	LEU
1	D	590	SER
1	D	601	GLU
1	D	606	LEU
1	D	609	ARG
1	D	613	ASP
1	D	619	THR
1	D	625	SER
1	D	634	LEU
1	D	663	ASN
1	D	666	LYS
1	D	681	GLU
1	D	684	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	72	GLN
1	A	91	HIS
1	A	114	ASN
1	A	121	HIS
1	A	162	ASN
1	A	181	GLN
1	A	336	ASN
1	A	395	GLN
1	A	451	ASN
1	A	481	GLN
1	A	489	GLN
1	A	512	HIS
1	A	547	HIS
1	A	557	ASN
1	A	637	GLN
1	A	655	ASN
1	B	34	GLN
1	B	50	GLN
1	B	114	ASN
1	B	121	HIS
1	B	162	ASN
1	B	181	GLN
1	B	182	ASN
1	B	250	GLN
1	B	253	GLN
1	B	336	ASN
1	B	393	ASN
1	B	397	GLN
1	B	455	HIS
1	B	481	GLN
1	B	489	GLN
1	B	637	GLN
1	B	663	ASN
1	C	91	HIS
1	C	162	ASN
1	C	181	GLN
1	C	228	ASN
1	C	336	ASN
1	C	455	HIS
1	C	481	GLN

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Mol	Chain	Res	Type
1	C	522	ASN
1	C	626	ASN
1	C	663	ASN
1	D	91	HIS
1	D	162	ASN
1	D	182	ASN
1	D	233	GLN
1	D	263	ASN
1	D	336	ASN
1	D	455	HIS
1	D	481	GLN
1	D	513	GLN
1	D	557	ASN
1	D	635	ASN
1	D	644	ASN
1	D	655	ASN
1	D	663	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	672/692 (97%)	-0.14	9 (1%) 79 79	23, 36, 61, 81	0
1	B	672/692 (97%)	-0.00	14 (2%) 67 68	22, 40, 62, 87	0
1	C	673/692 (97%)	-0.25	3 (0%) 93 94	22, 36, 53, 72	0
1	D	666/692 (96%)	-0.08	13 (1%) 68 69	21, 36, 61, 77	0
All	All	2683/2768 (96%)	-0.12	39 (1%) 76 76	21, 37, 60, 87	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	612	ALA	4.2
1	D	661	GLY	3.7
1	B	692	ILE	3.6
1	B	516	TYR	3.3
1	D	686	GLY	3.2
1	B	656	VAL	3.2
1	D	566	TRP	3.1
1	C	671	THR	3.1
1	B	688	LYS	3.0
1	A	692	ILE	3.0
1	A	687	GLU	2.9
1	B	659	ALA	2.8
1	B	691	GLU	2.8
1	B	682	TRP	2.7
1	B	22	LEU	2.6
1	D	664	ILE	2.5
1	B	689	ASN	2.5
1	D	663	ASN	2.4
1	B	570	GLY	2.4
1	A	691	GLU	2.4
1	C	59	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	665	LEU	2.4
1	B	658	LEU	2.4
1	C	524	GLY	2.4
1	D	679	GLU	2.4
1	B	662	LYS	2.3
1	B	686	GLY	2.3
1	D	568	ARG	2.3
1	B	683	ASN	2.2
1	D	619	THR	2.2
1	A	674	LYS	2.2
1	D	22	LEU	2.2
1	A	568	ARG	2.2
1	A	523	TRP	2.1
1	D	680	ILE	2.1
1	A	656	VAL	2.1
1	A	673	GLY	2.1
1	A	682	TRP	2.1
1	D	524	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	A	802	1/1	0.96	0.29	-	50,50,50,50	0
2	CL	A	801	1/1	0.97	0.24	-	39,39,39,39	0
2	CL	A	807	1/1	0.85	0.29	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	C	805	1/1	0.96	0.34	-	59,59,59,59	0
2	CL	D	803	1/1	0.89	0.25	-	56,56,56,56	0
2	CL	D	804	1/1	0.84	0.15	-	74,74,74,74	0
2	CL	D	806	1/1	0.98	0.21	-	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.