Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGT
Title	:	THREE-DIMENSIONAL STRUCTURE OF A TRANSGLUTAMINASE: HUMAN BLOOD COAGULATION FACTOR XIII
Authors	:	Yee, V.C.; Pedersen, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on	:	1994-01-25
Resolution	:	2.65 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 (i)) were used in the production of this report:

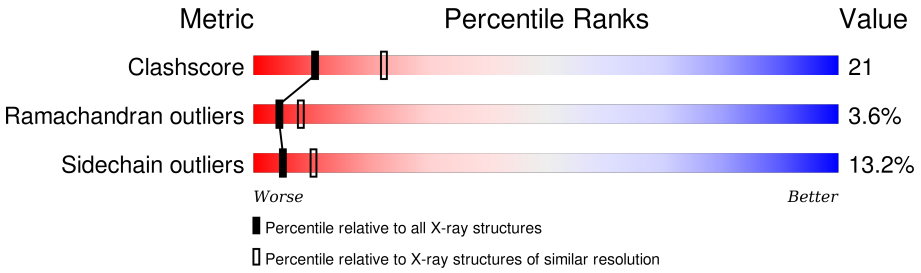
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.65 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))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	48% 40% 8%
1	B	731	53% 37% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11382 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 COAGULATION FACTOR XIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5700	3614	983	1076	27			
1	B	708	Total	C	N	O	S	0	0	0
			5682	3603	978	1074	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	CONFLICT	UNP P00488
B	651	GLU	GLN	CONFLICT	UNP P00488

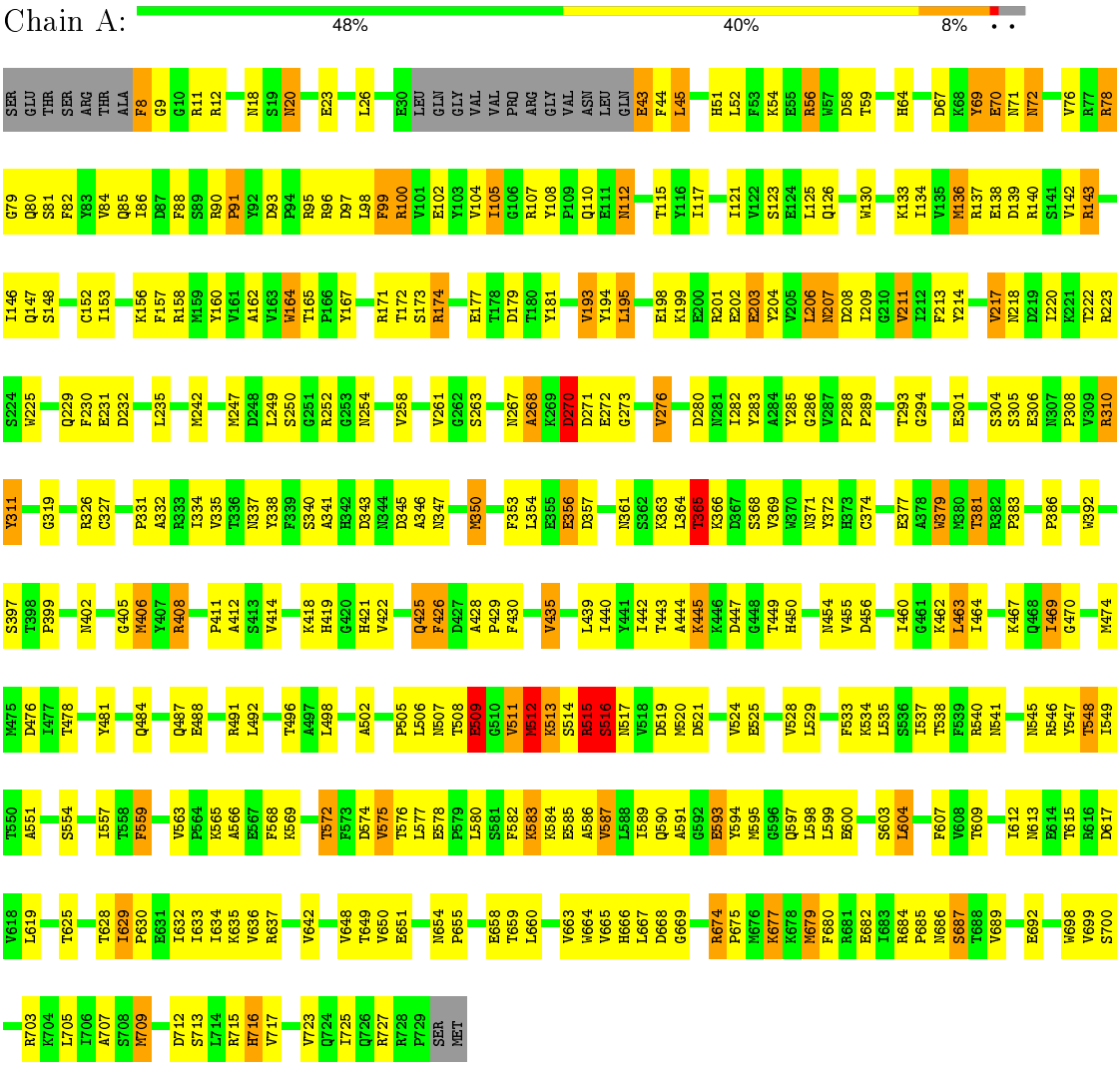
3 Residue-property plots (i)

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.

Note EDS was not executed.

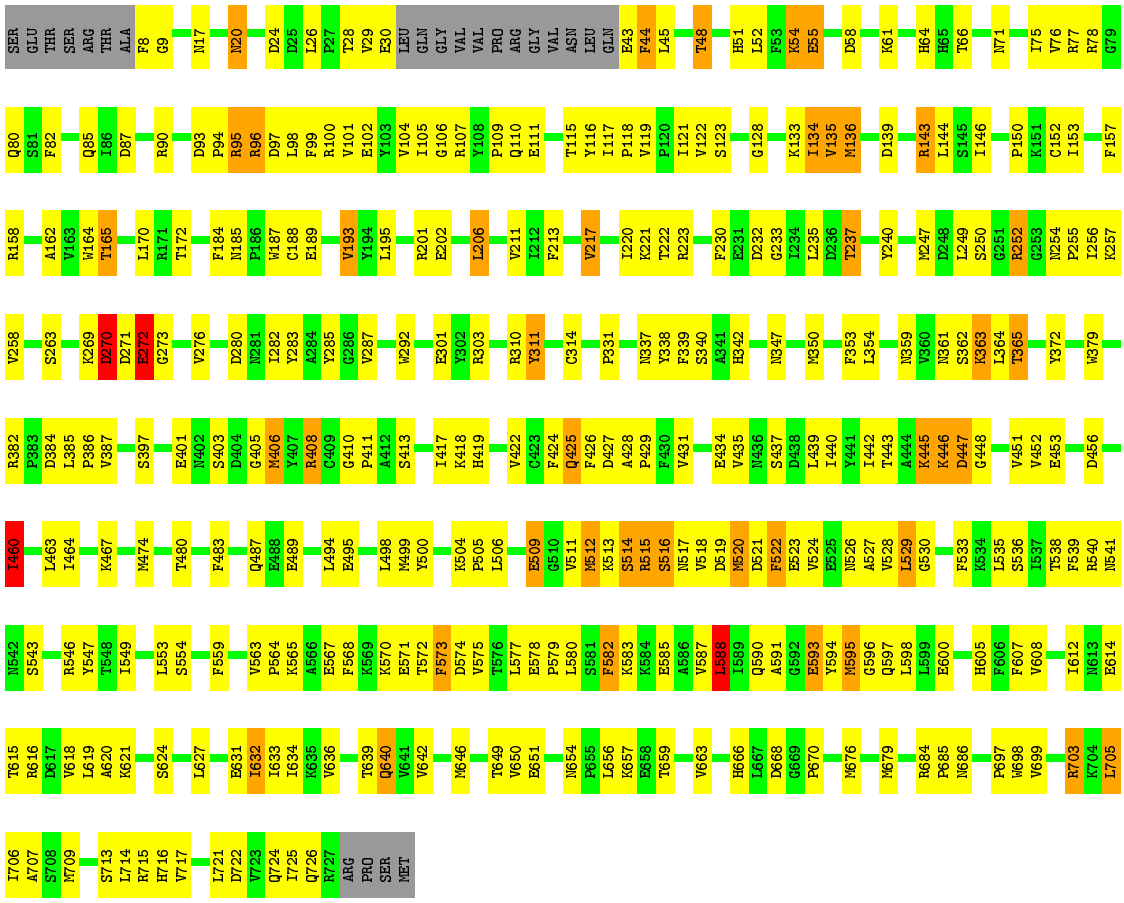
- Molecule 1: COAGULATION FACTOR XIII

Chain A:



- Molecule 1: COAGULATION FACTOR XIII

Chain B:


SER GLU THR SER ARG THR ALA F8 G9 N17 N20 D24 D25 L26 P27 T28 V29 E30 LEU GLN GLY VAL VAL PRO ARG GLY VAL ASN LEU GLN E43 F44 L45 T48 H51 L52 F53 K54 E55 D58 K61 H64 H65 T66 N71 I75 V76 R77 R78 G79
Q80 S81 F82 Q85 I86 D87 R90 D93 P94 R95 R96 D97 L98 F99 R100 V101 E102 Y103 V104 I105 G106 R107 Y108 P109 Q110 E111 T115 Y116 I117 P118 V119 P120 I121 V122 S123 G128 K133 I134 V135 M136 D139 R143 L144 S145 I146 P150 K151 C152 I153 F157
R158 A162 V163 W164 T165 L170 R171 T172 F184 N185 P186 W187 C188 E189 V193 Y194 L195 R201 E202 L206 V211 I212 F213 V217 I220 K221 T222 R223 F230 E231 D232 G233 I234 L235 D236 T237 Y240 M247 D248 L249 S250 G251 R252 G253 N254 P255 I256 K257
V258 S263 K269 D270 D271 E272 G273 V276 D280 N281 I282 Y283 A284 Y285 G286 V287 W292 E301 Y302 R303 R310 Y311 C314 P331 N337 Y338 F339 S340 A341 H342 N347 M350 F353 L354 N359 V360 M361 S362 K363 L364 T365 Y372 W379
R382 P383 D384 L385 P386 V387 S397 E401 N402 S403 D404 G405 M406 Y407 R408 C409 G410 P411 A412 S413 I417 K418 H419 V422 C423 F424 Q425 F426 D427 A428 P429 F430 V431 E434 V435 N436 S437 D438 L439 I440 Y441 I442 T443 A444 K445 K446 D447 G448 V451 V452 E453 D456
I460 L463 I464 K467 M474 T480 F483 Q487 E488 E489 L494 E495 L498 M499 Y500 K504 P505 L506 E509 G510 V511 M512 K513 S514 R515 S516 N517 V518 D519 M520 D521 F522 E523 V524 E525 N526 A527 V528 L529 G530 F533 K534 L535 S536 I537 T538 F539 R540 N541
N542 S543 R546 V547 T548 I549 L553 S554 F559 V563 P564 K565 A566 E567 F568 K569 K570 E571 T572 F573 D574 V575 T576 L577 E578 P579 L580 S581 F582 K583 K584 E585 A586 V587 I588 I589 Q590 A591 G592 E593 Y594 M595 G596 Q597 L598 L599 E600 H605 F606 F607 V608 I612 N613 E614
T615 R616 D617 V618 L619 A620 K621 S624 L627 E631 I632 I633 I634 K635 V636 T639 Q640 V641 V642 M646 T649 V650 E651 N654 P655 L656 K657 E658 T659 V663 H666 L667 D668 G669 P670 M676 M679 R684 P685 N686 P697 W698 V699 R703 K704 L705
I706 A707 S708 M709 S713 L714 R715 H716 V717 L721 D722 V723 Q724 I725 Q726 R727 ARG PRO SER MET

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.20Å 182.70Å 93.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	97.6 (10.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11382	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	1/5835 (0.0%)	0.90	9/7917 (0.1%)
1	B	0.69	3/5816 (0.1%)	0.92	11/7891 (0.1%)
All	All	0.67	4/11651 (0.0%)	0.91	20/15808 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	651	GLU	CD-OE2	8.44	1.34	1.25
1	A	651	GLU	CD-OE2	6.95	1.33	1.25
1	B	188	CYS	CB-SG	-6.20	1.71	1.82
1	B	152	CYS	CB-SG	-5.07	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	THR	N-CA-C	-9.94	84.15	111.00
1	B	460	ILE	N-CA-C	8.19	133.12	111.00
1	B	365	THR	N-CA-C	-7.38	91.07	111.00
1	B	425	GLN	N-CA-C	7.01	129.94	111.00
1	B	553	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	11	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	512	MET	N-CA-C	-5.66	95.72	111.00
1	B	574	ASP	N-CA-C	-5.66	95.72	111.00
1	A	425	GLN	N-CA-C	5.63	126.21	111.00
1	A	559	PHE	N-CA-C	-5.60	95.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	134	ILE	N-CA-C	-5.57	95.95	111.00
1	B	588	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	425	GLN	CA-C-N	-5.41	105.29	117.20
1	A	604	LEU	CA-CB-CG	5.40	127.71	115.30
1	B	425	GLN	CA-C-N	-5.20	105.75	117.20
1	B	632	ILE	N-CA-C	-5.18	97.00	111.00
1	A	9	GLY	N-CA-C	-5.13	100.27	113.10
1	A	310	ARG	N-CA-C	5.04	124.59	111.00
1	B	52	LEU	N-CA-C	-5.03	97.43	111.00
1	B	705	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	TYR	Sidechain

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	5700	0	5557	252	0
1	B	5682	0	5537	229	0
All	All	11382	0	11094	480	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 21.

All (480) 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:659:THR:HG22	1:B:685:PRO:HD3	1.43	0.98
1:A:538:THR:HG22	1:A:584:LYS:HG2	1.50	0.92
1:A:381:THR:HG23	1:A:383:PRO:HD3	1.51	0.91
1:A:100:ARG:HD2	1:A:164:TRP:HZ3	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.55	0.88
1:A:363:LYS:HG3	1:A:364:LEU:N	1.87	0.87
1:A:231:GLU:HB3	1:A:674:ARG:HH22	1.39	0.87
1:A:520:MET:HE2	1:A:619:LEU:HB3	1.57	0.85
1:A:363:LYS:HG3	1:A:364:LEU:H	1.40	0.85
1:A:356:GLU:HG2	1:A:445:LYS:NZ	1.92	0.84
1:A:56:ARG:HD2	1:A:67:ASP:O	1.80	0.81
1:B:43:GLU:HB2	1:B:165:THR:HG21	1.60	0.81
1:B:521:ASP:O	1:B:522:PHE:HB3	1.81	0.80
1:B:111:GLU:HB3	1:B:116:TYR:HD2	1.46	0.80
1:B:541:ASN:HB2	1:B:577:LEU:HD23	1.65	0.79
1:B:411:PRO:O	1:B:426:PHE:HB2	1.83	0.77
1:A:110:GLN:H	1:A:115:THR:HG23	1.49	0.76
1:A:211:VAL:HG13	1:A:467:LYS:HD2	1.66	0.75
1:A:516:SER:HB3	1:A:615:THR:HG21	1.67	0.75
1:A:217:VAL:HG22	1:A:338:TYR:HB3	1.69	0.75
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.69	0.74
1:B:233:GLY:O	1:B:237:THR:HG23	1.86	0.74
1:A:439:LEU:HB2	1:A:456:ASP:HB3	1.70	0.74
1:B:43:GLU:HA	1:B:165:THR:HB	1.67	0.74
1:A:559:PHE:HD1	1:A:563:VAL:O	1.71	0.74
1:B:520:MET:HA	1:B:538:THR:O	1.87	0.73
1:A:529:LEU:HD12	1:A:595:MET:HE1	1.71	0.73
1:A:549:ILE:HB	1:A:575:VAL:HG23	1.72	0.72
1:A:578:GLU:CD	1:A:578:GLU:H	1.93	0.71
1:A:492:LEU:O	1:A:496:THR:HG23	1.91	0.71
1:A:537:ILE:H	1:A:537:ILE:HD12	1.55	0.71
1:B:514:SER:O	1:B:515:ARG:HG2	1.90	0.71
1:A:285:TYR:O	1:A:310:ARG:HD3	1.91	0.71
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.25	0.71
1:B:51:HIS:HB2	1:B:85:GLN:HB3	1.71	0.71
1:A:242:MET:HB3	1:A:247:MET:HE3	1.73	0.70
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.74	0.70
1:B:211:VAL:HG22	1:B:467:LYS:HB2	1.75	0.69
1:A:650:VAL:HG11	1:A:665:VAL:HG11	1.73	0.68
1:A:110:GLN:N	1:A:115:THR:HG23	2.09	0.68
1:A:347:ASN:HD21	1:A:505:PRO:HG2	1.57	0.68
1:A:668:ASP:OD2	1:A:675:PRO:HB3	1.94	0.68
1:A:636:VAL:HG11	1:A:723:VAL:HG11	1.74	0.68
1:B:632:ILE:HG13	1:B:717:VAL:HG12	1.76	0.68
1:A:136:MET:HG3	1:A:143:ARG:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:HG2	1:A:445:LYS:HZ3	1.58	0.67
1:A:660:LEU:O	1:A:682:GLU:HA	1.95	0.67
1:B:363:LYS:HG2	1:B:364:LEU:N	2.08	0.67
1:A:529:LEU:HD22	1:A:529:LEU:H	1.59	0.66
1:A:440:ILE:HD13	1:A:455:VAL:HB	1.77	0.66
1:B:29:VAL:HG23	1:B:170:LEU:HD22	1.77	0.66
1:B:353:PHE:HB2	1:B:364:LEU:O	1.96	0.65
1:B:254:ASN:O	1:B:258:VAL:HG23	1.97	0.64
1:A:454:ASN:OD1	1:A:512:MET:SD	2.56	0.64
1:A:254:ASN:O	1:A:258:VAL:HG23	1.96	0.64
1:B:439:LEU:HB2	1:B:456:ASP:HB3	1.79	0.63
1:A:276:VAL:O	1:A:311:TYR:HA	1.98	0.63
1:A:648:VAL:O	1:A:692:GLU:HA	1.97	0.63
1:B:539:PHE:HB3	1:B:577:LEU:HD21	1.80	0.63
1:A:91:PRO:HD3	1:A:140:ARG:HG2	1.79	0.63
1:A:397:SER:HA	1:A:408:ARG:HB2	1.80	0.62
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.64	0.62
1:A:666:HIS:O	1:A:707:ALA:HA	1.98	0.62
1:A:709:MET:HB3	1:A:717:VAL:CG2	2.30	0.62
1:B:670:PRO:O	1:B:703:ARG:NH1	2.32	0.62
1:A:356:GLU:HG2	1:A:445:LYS:HZ2	1.60	0.62
1:A:535:LEU:HB2	1:A:587:VAL:HG13	1.80	0.62
1:B:43:GLU:HG3	1:B:170:LEU:HD11	1.81	0.62
1:B:582:PHE:N	1:B:582:PHE:HD1	1.99	0.61
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.64	0.61
1:A:411:PRO:O	1:A:426:PHE:HB2	2.00	0.61
1:B:594:TYR:CD1	1:B:595:MET:N	2.69	0.61
1:A:100:ARG:HD2	1:A:164:TRP:CZ3	2.26	0.61
1:A:100:ARG:HB3	1:A:100:ARG:HH11	1.65	0.61
1:A:193:VAL:HG13	1:A:331:PRO:HD3	1.81	0.61
1:A:419:HIS:O	1:B:387:VAL:HG11	2.00	0.60
1:B:445:LYS:NZ	1:B:445:LYS:HB3	2.16	0.60
1:B:66:THR:HG21	1:B:75:ILE:HG22	1.83	0.60
1:B:437:SER:HB2	1:B:460:ILE:HG12	1.83	0.60
1:A:435:VAL:CG2	1:A:464:ILE:HD11	2.32	0.60
1:A:529:LEU:HD21	1:A:629:ILE:HG23	1.83	0.60
1:A:379:TRP:HD1	1:A:392:TRP:CE2	2.20	0.60
1:A:443:THR:O	1:A:450:HIS:HA	2.02	0.60
1:A:213:PHE:CD2	1:A:222:THR:HG22	2.37	0.60
1:A:361:ASN:ND2	1:A:363:LYS:HG2	2.17	0.60
1:B:109:PRO:HB3	1:B:116:TYR:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ILE:HA	1:B:649:THR:O	2.02	0.60
1:B:185:ASN:OD1	1:B:187:TRP:HB2	2.01	0.60
1:B:405:GLY:O	1:B:406:MET:HB3	2.02	0.60
1:A:463:LEU:HD21	1:A:476:ASP:OD2	2.02	0.59
1:B:105:ILE:HG23	1:B:157:PHE:CD2	2.37	0.59
1:A:207:ASN:HD22	1:A:208:ASP:N	2.01	0.59
1:A:528:VAL:HG13	1:A:628:THR:O	2.02	0.59
1:B:512:MET:N	1:B:512:MET:SD	2.75	0.59
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.84	0.59
1:B:698:TRP:CD1	1:B:699:VAL:HG23	2.37	0.59
1:B:217:VAL:HG22	1:B:338:TYR:HB3	1.85	0.59
1:B:657:LYS:O	1:B:685:PRO:HB3	2.03	0.58
1:A:549:ILE:HB	1:A:575:VAL:CG2	2.32	0.58
1:A:679:MET:HG3	1:A:680:PHE:N	2.17	0.58
1:B:582:PHE:N	1:B:582:PHE:CD1	2.70	0.58
1:B:642:VAL:HG13	1:B:698:TRP:HA	1.85	0.58
1:B:518:VAL:HG21	1:B:612:ILE:HD12	1.85	0.58
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.86	0.58
1:B:64:HIS:CE1	1:B:76:VAL:HG22	2.40	0.57
1:B:122:VAL:HG12	1:B:123:SER:N	2.19	0.57
1:A:353:PHE:CD2	1:A:364:LEU:O	2.57	0.57
1:A:554:SER:HB3	1:A:607:PHE:HB2	1.87	0.57
1:A:231:GLU:HB3	1:A:674:ARG:NH2	2.16	0.57
1:A:654:ASN:ND2	1:A:660:LEU:HG	2.19	0.56
1:B:615:THR:O	1:B:616:ARG:HG2	2.04	0.56
1:B:43:GLU:O	1:B:44:PHE:HD1	1.87	0.56
1:A:537:ILE:O	1:A:584:LYS:HA	2.05	0.56
1:A:100:ARG:CD	1:A:164:TRP:HZ3	2.13	0.56
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.87	0.56
1:A:379:TRP:HD1	1:A:392:TRP:CD2	2.23	0.56
1:A:529:LEU:HD22	1:A:529:LEU:N	2.20	0.56
1:A:541:ASN:HB2	1:A:577:LEU:HD23	1.87	0.56
1:B:573:PHE:N	1:B:573:PHE:CD1	2.72	0.56
1:A:220:ILE:H	1:A:220:ILE:HD12	1.70	0.56
1:A:247:MET:HE2	1:A:261:VAL:HG11	1.88	0.56
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.39	0.56
1:A:577:LEU:HA	1:A:583:LYS:HE3	1.89	0.55
1:A:565:LYS:HD3	1:A:599:LEU:HD21	1.88	0.55
1:B:516:SER:HB2	1:B:547:TYR:CZ	2.41	0.55
1:A:263:SER:HB2	1:A:408:ARG:HG3	1.89	0.55
1:A:363:LYS:CG	1:A:364:LEU:N	2.66	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HA	1:A:366:LYS:HG2	1.88	0.55
1:B:382:ARG:NH1	1:B:384:ASP:OD2	2.39	0.55
1:A:78:ARG:HG2	1:A:152:CYS:HB3	1.88	0.55
1:B:598:LEU:HD11	1:B:627:LEU:HD12	1.89	0.55
1:A:207:ASN:ND2	1:A:209:ILE:H	2.05	0.55
1:B:247:MET:CE	1:B:257:LYS:HG2	2.37	0.55
1:A:551:ALA:O	1:A:572:THR:HA	2.06	0.55
1:A:43:GLU:N	1:A:165:THR:HG1	2.04	0.55
1:A:488:GLU:CD	1:A:491:ARG:HH12	2.10	0.54
1:B:363:LYS:CG	1:B:364:LEU:N	2.70	0.54
1:B:303:ARG:NH1	1:B:303:ARG:HG2	2.21	0.54
1:A:156:LYS:HE2	1:A:181:TYR:CZ	2.41	0.54
1:B:657:LYS:C	1:B:685:PRO:HB3	2.28	0.54
1:B:659:THR:HG22	1:B:685:PRO:CD	2.29	0.54
1:B:541:ASN:HB2	1:B:577:LEU:HB3	1.89	0.54
1:B:554:SER:HB3	1:B:567:GLU:OE2	2.07	0.54
1:B:43:GLU:HG2	1:B:43:GLU:O	2.06	0.54
1:A:642:VAL:CG2	1:A:700:SER:HB3	2.38	0.54
1:A:107:ARG:HG2	1:A:108:TYR:CE2	2.43	0.54
1:A:663:VAL:O	1:A:679:MET:HA	2.08	0.53
1:B:516:SER:OG	1:B:612:ILE:HG21	2.07	0.53
1:B:109:PRO:CB	1:B:116:TYR:HB2	2.39	0.53
1:B:153:ILE:HD11	1:B:250:SER:HA	1.90	0.53
1:A:591:ALA:O	1:A:595:MET:HB2	2.08	0.53
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.44	0.53
1:B:51:HIS:CD2	1:B:85:GLN:HE21	2.27	0.53
1:A:363:LYS:CG	1:A:364:LEU:H	2.19	0.53
1:B:530:GLY:HA2	1:B:595:MET:SD	2.49	0.53
1:B:263:SER:OG	1:B:408:ARG:HD3	2.08	0.53
1:A:629:ILE:H	1:A:629:ILE:HD12	1.74	0.53
1:A:435:VAL:HG21	1:A:464:ILE:HD11	1.91	0.53
1:A:52:LEU:HD23	1:A:84:VAL:HG22	1.90	0.53
1:A:455:VAL:HG13	1:A:512:MET:HG2	1.91	0.52
1:A:454:ASN:HA	1:A:512:MET:SD	2.49	0.52
1:B:100:ARG:HB2	1:B:119:VAL:O	2.09	0.52
1:B:524:VAL:HG22	1:B:535:LEU:HG	1.92	0.52
1:A:455:VAL:HG11	1:A:508:THR:HG21	1.91	0.52
1:A:229:GLN:HB2	1:A:327:CYS:HB2	1.90	0.52
1:A:529:LEU:CD2	1:A:529:LEU:H	2.23	0.52
1:A:203:GLU:HG3	1:A:469:ILE:HA	1.91	0.52
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG22	1:B:445:LYS:HG3	1.92	0.52
1:A:484:GLN:O	1:A:487:GLN:HG2	2.09	0.52
1:A:524:VAL:HG12	1:A:525:GLU:O	2.10	0.52
1:A:345:ASP:O	1:A:346:ALA:HB3	2.10	0.52
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.91	0.51
1:B:573:PHE:N	1:B:573:PHE:HD1	2.08	0.51
1:A:674:ARG:HE	1:A:674:ARG:HA	1.75	0.51
1:B:515:ARG:HG3	1:B:518:VAL:O	2.11	0.51
1:B:105:ILE:CD1	1:B:115:THR:HG22	2.41	0.51
1:B:77:ARG:HB3	1:B:185:ASN:HB2	1.92	0.51
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.45	0.51
1:A:578:GLU:N	1:A:578:GLU:CD	2.64	0.51
1:A:455:VAL:HG13	1:A:512:MET:CG	2.41	0.51
1:A:213:PHE:CE2	1:A:474:MET:HB2	2.46	0.51
1:A:418:LYS:HA	1:A:481:TYR:O	2.11	0.51
1:B:410:GLY:C	1:B:426:PHE:HB3	2.32	0.50
1:A:513:LYS:O	1:A:515:ARG:HD2	2.11	0.50
1:B:428:ALA:N	1:B:429:PRO:HD2	2.26	0.50
1:A:270:ASP:O	1:A:271:ASP:HB2	2.10	0.50
1:A:45:LEU:HD22	1:A:45:LEU:O	2.11	0.50
1:B:418:LYS:HD2	1:B:480:THR:O	2.11	0.50
1:A:537:ILE:HD12	1:A:537:ILE:N	2.23	0.50
1:A:509:GLU:OE1	1:A:511:VAL:HG12	2.11	0.50
1:A:338:TYR:O	1:A:371:ASN:O	2.29	0.50
1:B:520:MET:O	1:B:520:MET:HG3	2.11	0.50
1:B:337:ASN:O	1:B:372:TYR:HA	2.12	0.50
1:B:568:PHE:HD2	1:B:593:GLU:HG2	1.75	0.50
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.93	0.50
1:A:81:SER:HA	1:A:146:ILE:O	2.12	0.50
1:A:525:GLU:HG3	1:A:533:PHE:HB2	1.94	0.50
1:A:64:HIS:CE1	1:A:76:VAL:HG22	2.47	0.50
1:A:548:THR:HB	1:A:613:ASN:HD22	1.76	0.50
1:A:633:ILE:HG22	1:A:635:LYS:HD3	1.94	0.50
1:B:363:LYS:HE3	1:B:364:LEU:CB	2.42	0.50
1:A:557:ILE:CD1	1:A:597:GLN:HG3	2.42	0.50
1:B:256:ILE:N	1:B:256:ILE:HD12	2.27	0.50
1:A:136:MET:HG3	1:A:143:ARG:CB	2.42	0.50
1:B:283:TYR:HE2	1:B:600:GLU:OE1	1.94	0.50
1:A:659:THR:HG22	1:A:682:GLU:HB2	1.93	0.50
1:B:714:LEU:HG	1:B:715:ARG:N	2.27	0.50
1:B:559:PHE:HD1	1:B:563:VAL:O	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:O	1:B:55:GLU:O	2.30	0.50
1:A:634:ILE:HA	1:A:649:THR:O	2.12	0.49
1:B:119:VAL:HG11	1:B:146:ILE:HG23	1.94	0.49
1:B:24:ASP:O	1:B:158:ARG:NH2	2.45	0.49
1:B:516:SER:HB2	1:B:547:TYR:CE2	2.47	0.49
1:B:445:LYS:HZ3	1:B:445:LYS:HB3	1.77	0.49
1:A:521:ASP:HB2	1:A:540:ARG:HH22	1.78	0.49
1:A:445:LYS:HB3	1:A:447:ASP:OD1	2.12	0.49
1:B:541:ASN:HB2	1:B:577:LEU:CD2	2.40	0.49
1:A:220:ILE:N	1:A:220:ILE:HD12	2.26	0.49
1:B:513:LYS:HE3	1:B:618:VAL:H	1.77	0.49
1:B:529:LEU:HD13	1:B:656:LEU:HD21	1.93	0.49
1:A:93:ASP:O	1:A:97:ASP:HB2	2.12	0.49
1:A:595:MET:CE	1:A:598:LEU:HD12	2.43	0.49
1:B:440:ILE:HG22	1:B:442:ILE:HG13	1.95	0.49
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.93	0.49
1:A:594:TYR:CD1	1:A:595:MET:N	2.81	0.49
1:B:594:TYR:O	1:B:596:GLY:N	2.46	0.49
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.47	0.49
1:A:381:THR:CG2	1:A:383:PRO:HD3	2.34	0.49
1:B:521:ASP:HB2	1:B:540:ARG:HH21	1.77	0.48
1:B:237:THR:HA	1:B:240:TYR:HB3	1.95	0.48
1:A:283:TYR:HE2	1:A:600:GLU:OE1	1.96	0.48
1:B:270:ASP:O	1:B:271:ASP:HB2	2.13	0.48
1:A:498:LEU:HD23	1:A:502:ALA:O	2.12	0.48
1:B:93:ASP:O	1:B:97:ASP:HB2	2.13	0.48
1:B:587:VAL:HG12	1:B:588:LEU:H	1.78	0.48
1:A:469:ILE:CG2	1:A:470:GLY:N	2.75	0.48
1:B:419:HIS:HD2	1:B:483:PHE:HZ	1.60	0.48
1:B:522:PHE:CD1	1:B:535:LEU:HD21	2.48	0.48
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.48	0.48
1:B:220:ILE:HG21	1:B:474:MET:CE	2.42	0.48
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.46	0.48
1:B:418:LYS:HB2	1:B:480:THR:O	2.13	0.48
1:A:442:ILE:CG2	1:A:450:HIS:HB3	2.44	0.48
1:A:541:ASN:HB2	1:A:577:LEU:HB3	1.96	0.48
1:A:165:THR:HG22	1:A:167:TYR:H	1.79	0.48
1:B:133:LYS:O	1:B:144:LEU:HA	2.13	0.48
1:A:568:PHE:O	1:A:593:GLU:HG3	2.14	0.48
1:B:61:LYS:NZ	1:B:71:ASN:O	2.47	0.48
1:A:123:SER:O	1:A:133:LYS:NZ	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLY:O	1:A:406:MET:HB3	2.14	0.47
1:A:204:TYR:O	1:A:326:ARG:HG2	2.14	0.47
1:A:449:THR:HG22	1:A:450:HIS:N	2.30	0.47
1:B:405:GLY:O	1:B:406:MET:CB	2.63	0.47
1:B:573:PHE:HZ	1:B:587:VAL:HG22	1.78	0.47
1:B:285:TYR:CB	1:B:310:ARG:HH11	2.28	0.47
1:B:654:ASN:O	1:B:686:ASN:HA	2.14	0.47
1:B:95:ARG:NH2	1:B:96:ARG:HB2	2.30	0.47
1:B:549:ILE:HD12	1:B:577:LEU:HD13	1.96	0.47
1:A:217:VAL:O	1:A:220:ILE:HD11	2.15	0.47
1:B:51:HIS:HD2	1:B:85:GLN:HE21	1.62	0.47
1:A:664:TRP:CE2	1:A:679:MET:HE3	2.49	0.47
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.44	0.47
1:B:705:LEU:HA	1:B:705:LEU:HD23	1.74	0.47
1:B:546:ARG:HE	1:B:578:GLU:HG3	1.78	0.47
1:B:64:HIS:CE1	1:B:80:GLN:HB3	2.50	0.47
1:A:267:ASN:ND2	1:A:399:PRO:HG2	2.30	0.47
1:A:630:PRO:HG3	1:A:655:PRO:HB3	1.96	0.47
1:B:570:LYS:O	1:B:570:LYS:HG2	2.14	0.47
1:A:280:ASP:O	1:A:282:ILE:HD12	2.15	0.46
1:B:193:VAL:HG13	1:B:193:VAL:O	2.16	0.46
1:A:98:LEU:HD12	1:A:121:ILE:HD11	1.97	0.46
1:A:206:LEU:O	1:A:230:PHE:HE2	1.98	0.46
1:A:548:THR:HA	1:A:575:VAL:O	2.15	0.46
1:A:207:ASN:C	1:A:207:ASN:HD22	2.19	0.46
1:B:122:VAL:CG1	1:B:123:SER:N	2.77	0.46
1:B:247:MET:HE3	1:B:257:LYS:HG2	1.98	0.46
1:B:95:ARG:CZ	1:B:96:ARG:HB2	2.46	0.46
1:A:153:ILE:HD12	1:A:153:ILE:N	2.30	0.46
1:B:506:LEU:HA	1:B:506:LEU:HD23	1.71	0.46
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.96	0.46
1:B:422:VAL:HG23	1:B:500:TYR:HB2	1.95	0.46
1:B:78:ARG:HG3	1:B:150:PRO:HA	1.98	0.46
1:B:213:PHE:CZ	1:B:474:MET:HA	2.51	0.46
1:B:528:VAL:HG12	1:B:529:LEU:N	2.30	0.46
1:B:546:ARG:HE	1:B:578:GLU:CG	2.28	0.46
1:A:95:ARG:HE	1:A:95:ARG:HB2	1.63	0.46
1:B:111:GLU:HB3	1:B:116:TYR:CD2	2.38	0.46
1:B:549:ILE:CD1	1:B:577:LEU:HD13	2.46	0.46
1:A:350:MET:HB3	1:A:439:LEU:HD23	1.97	0.46
1:A:549:ILE:HG23	1:A:612:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG21	1:A:82:PHE:CD1	2.51	0.46
1:B:347:ASN:HD21	1:B:505:PRO:HG3	1.81	0.46
1:B:547:TYR:HD1	1:B:614:GLU:CG	2.29	0.46
1:B:98:LEU:HD23	1:B:164:TRP:HB2	1.98	0.46
1:A:165:THR:HG22	1:A:167:TYR:N	2.30	0.46
1:B:554:SER:HB2	1:B:607:PHE:HB2	1.96	0.46
1:A:700:SER:HA	1:A:725:ILE:HB	1.98	0.46
1:B:220:ILE:HG21	1:B:474:MET:HE2	1.98	0.46
1:B:359:ASN:HD21	1:B:570:LYS:HE3	1.81	0.46
1:B:632:ILE:CG2	1:B:650:VAL:HG13	2.46	0.46
1:A:86:ILE:HD12	1:A:86:ILE:N	2.30	0.46
1:B:539:PHE:CB	1:B:577:LEU:HD21	2.45	0.46
1:B:202:GLU:HA	1:B:206:LEU:HB2	1.97	0.45
1:A:515:ARG:HB3	1:A:617:ASP:HB3	1.98	0.45
1:B:578:GLU:O	1:B:579:PRO:C	2.53	0.45
1:A:23:GLU:HG2	1:A:158:ARG:HD2	1.98	0.45
1:A:26:LEU:HD12	1:A:160:TYR:CE2	2.51	0.45
1:A:463:LEU:HD23	1:A:478:THR:OG1	2.16	0.45
1:A:537:ILE:HD12	1:A:585:GLU:O	2.16	0.45
1:A:546:ARG:HD3	1:A:578:GLU:HA	1.98	0.45
1:B:51:HIS:N	1:B:85:GLN:O	2.48	0.45
1:A:105:ILE:HG12	1:A:157:PHE:CE2	2.52	0.45
1:A:549:ILE:O	1:A:574:ASP:HA	2.17	0.45
1:B:51:HIS:HD2	1:B:85:GLN:NE2	2.14	0.45
1:B:666:HIS:O	1:B:707:ALA:HA	2.17	0.45
1:A:428:ALA:N	1:A:429:PRO:HD2	2.32	0.45
1:A:64:HIS:CE1	1:A:80:GLN:OE1	2.70	0.45
1:A:56:ARG:NH2	1:A:70:GLU:OE2	2.49	0.45
1:B:515:ARG:O	1:B:518:VAL:HG23	2.17	0.45
1:B:528:VAL:CG1	1:B:529:LEU:N	2.80	0.45
1:B:133:LYS:HE3	1:B:133:LYS:HB3	1.78	0.45
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.79	0.45
1:A:112:ASN:HD22	1:A:112:ASN:N	2.13	0.45
1:B:546:ARG:HH21	1:B:578:GLU:HG2	1.82	0.45
1:B:663:VAL:O	1:B:679:MET:HA	2.17	0.45
1:B:43:GLU:HB2	1:B:165:THR:CG2	2.39	0.45
1:A:665:VAL:O	1:A:677:LYS:HA	2.17	0.45
1:B:453:GLU:O	1:B:512:MET:HB2	2.17	0.45
1:B:605:HIS:HE1	1:B:607:PHE:CZ	2.35	0.45
1:A:332:ALA:HA	1:A:377:GLU:O	2.17	0.45
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HD11	1:B:115:THR:HG22	2.00	0.44
1:A:663:VAL:HB	1:A:680:PHE:HB2	1.99	0.44
1:B:634:ILE:HD13	1:B:650:VAL:HG22	1.99	0.44
1:B:636:VAL:HG11	1:B:646:MET:HE3	1.98	0.44
1:A:331:PRO:HB2	1:A:379:TRP:HB2	2.00	0.44
1:B:640:GLN:O	1:B:726:GLN:OE1	2.35	0.44
1:A:529:LEU:HD12	1:A:598:LEU:CD1	2.48	0.44
1:B:460:ILE:HA	1:B:460:ILE:HD12	1.68	0.44
1:B:511:VAL:HG22	1:B:512:MET:H	1.83	0.44
1:B:276:VAL:O	1:B:311:TYR:HA	2.18	0.44
1:B:515:ARG:HH12	1:B:519:ASP:CG	2.21	0.44
1:A:379:TRP:CD1	1:A:392:TRP:CE2	3.04	0.44
1:B:443:THR:HB	1:B:451:VAL:HG13	1.98	0.44
1:A:337:ASN:O	1:A:372:TYR:HA	2.18	0.44
1:A:674:ARG:HG3	1:A:675:PRO:HD2	1.99	0.44
1:A:547:TYR:O	1:A:576:THR:HA	2.17	0.44
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.74	0.44
1:A:99:PHE:HA	1:A:162:ALA:O	2.18	0.44
1:A:577:LEU:HG	1:A:583:LYS:HE3	1.99	0.44
1:A:565:LYS:O	1:A:566:ALA:HB2	2.18	0.44
1:A:402:ASN:HA	1:A:430:PHE:CE1	2.52	0.44
1:B:636:VAL:HG11	1:B:646:MET:CE	2.47	0.44
1:B:107:ARG:NH1	1:B:107:ARG:HG3	2.31	0.44
1:A:107:ARG:HG2	1:A:108:TYR:CD2	2.53	0.44
1:A:249:LEU:HA	1:A:252:ARG:HG3	2.00	0.44
1:A:506:LEU:HA	1:A:506:LEU:HD23	1.83	0.43
1:A:405:GLY:O	1:A:406:MET:CB	2.65	0.43
1:B:541:ASN:O	1:B:580:LEU:HA	2.18	0.43
1:A:157:PHE:CD1	1:A:157:PHE:N	2.87	0.43
1:B:195:LEU:O	1:B:201:ARG:NE	2.51	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.17	0.43
1:B:527:ALA:HB2	1:B:533:PHE:CB	2.38	0.43
1:B:547:TYR:HD1	1:B:614:GLU:HG2	1.82	0.43
1:A:247:MET:HE2	1:A:261:VAL:CG1	2.48	0.43
1:B:385:LEU:CD2	1:B:424:PHE:HB3	2.47	0.43
1:A:444:ALA:HA	1:A:450:HIS:ND1	2.33	0.43
1:B:620:ALA:O	1:B:621:LYS:HG2	2.18	0.43
1:B:520:MET:CE	1:B:608:VAL:HG12	2.49	0.43
1:B:17:ASN:OD1	1:B:106:GLY:HA3	2.18	0.43
1:B:446:LYS:C	1:B:448:GLY:H	2.20	0.43
1:A:69:TYR:O	1:A:71:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:VAL:HG12	1:B:588:LEU:N	2.33	0.43
1:A:26:LEU:HD12	1:A:160:TYR:CD2	2.54	0.43
1:A:268:ALA:HB2	1:A:308:PRO:HB3	2.01	0.43
1:B:82:PHE:CD1	1:B:82:PHE:N	2.86	0.43
1:A:353:PHE:HB2	1:A:365:THR:OG1	2.18	0.43
1:B:543:SER:O	1:B:580:LEU:HD12	2.19	0.43
1:A:513:LYS:NZ	1:A:516:SER:H	2.15	0.43
1:A:194:TYR:HE1	1:A:201:ARG:HH21	1.66	0.43
1:A:684:ARG:HA	1:A:684:ARG:HD3	1.73	0.43
1:A:703:ARG:HA	1:A:703:ARG:NE	2.33	0.43
1:B:666:HIS:HA	1:B:676:MET:O	2.18	0.43
1:A:535:LEU:O	1:A:586:ALA:HA	2.18	0.43
1:B:220:ILE:HD13	1:B:474:MET:HE1	2.00	0.43
1:A:283:TYR:CD2	1:A:288:PRO:HB3	2.53	0.43
1:A:20:ASN:C	1:A:20:ASN:HD22	2.22	0.43
1:A:286:GLY:HA3	1:A:310:ARG:HB3	2.00	0.43
1:B:573:PHE:HZ	1:B:587:VAL:CG2	2.32	0.43
1:B:447:ASP:N	1:B:447:ASP:OD1	2.52	0.43
1:B:135:VAL:HG12	1:B:143:ARG:O	2.19	0.43
1:B:153:ILE:HD13	1:B:249:LEU:O	2.19	0.42
1:A:335:VAL:O	1:A:374:CYS:HA	2.19	0.42
1:A:535:LEU:N	1:A:535:LEU:HD12	2.35	0.42
1:B:213:PHE:CE2	1:B:474:MET:HB3	2.54	0.42
1:A:534:LYS:HB2	1:A:587:VAL:O	2.19	0.42
1:A:582:PHE:O	1:A:583:LYS:HE2	2.19	0.42
1:A:519:ASP:HB2	1:A:540:ARG:CG	2.49	0.42
1:A:72:ASN:N	1:A:72:ASN:OD1	2.52	0.42
1:B:633:ILE:HA	1:B:633:ILE:HD13	1.90	0.42
1:A:455:VAL:HG11	1:A:508:THR:CG2	2.49	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.74	0.42
1:B:206:LEU:HD12	1:B:230:PHE:HZ	1.84	0.42
1:B:361:ASN:OD1	1:B:362:SER:N	2.53	0.42
1:A:134:ILE:H	1:A:134:ILE:HD12	1.85	0.42
1:B:363:LYS:HE3	1:B:364:LEU:HB3	2.00	0.42
1:A:43:GLU:OE1	1:A:43:GLU:HA	2.19	0.42
1:A:88:PHE:HE2	1:A:142:VAL:CG2	2.33	0.42
1:B:489:GLU:H	1:B:489:GLU:HG2	1.60	0.42
1:B:99:PHE:HB2	1:B:162:ALA:O	2.19	0.42
1:A:535:LEU:CD1	1:A:589:ILE:HD11	2.50	0.42
1:A:90:ARG:HA	1:A:91:PRO:HD2	1.77	0.42
1:B:605:HIS:HD2	1:B:624:SER:OG	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:LEU:N	1:B:580:LEU:HD12	2.35	0.42
1:B:598:LEU:HD11	1:B:627:LEU:CD1	2.50	0.42
1:B:256:ILE:H	1:B:256:ILE:CD1	2.32	0.42
1:B:578:GLU:HB3	1:B:579:PRO:HD2	2.00	0.42
1:A:414:VAL:O	1:A:414:VAL:HG12	2.19	0.42
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.48	0.42
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.77	0.42
1:B:48:THR:N	1:B:87:ASP:O	2.50	0.42
1:B:413:SER:O	1:B:417:ILE:HG12	2.19	0.42
1:A:629:ILE:H	1:A:629:ILE:CD1	2.32	0.42
1:A:419:HIS:HB3	1:A:421:HIS:CD2	2.54	0.42
1:B:668:ASP:HB3	1:B:706:ILE:HB	2.01	0.42
1:B:280:ASP:O	1:B:282:ILE:N	2.53	0.42
1:B:43:GLU:O	1:B:44:PHE:CD1	2.71	0.41
1:B:575:VAL:HG22	1:B:585:GLU:OE2	2.20	0.41
1:B:353:PHE:HE2	1:B:364:LEU:HD22	1.85	0.41
1:B:530:GLY:O	1:B:591:ALA:CB	2.68	0.41
1:A:45:LEU:HD22	1:A:88:PHE:HB3	2.02	0.41
1:B:269:LYS:O	1:B:272:GLU:HB2	2.19	0.41
1:A:8:PHE:CD1	1:A:8:PHE:N	2.88	0.41
1:A:568:PHE:HB2	1:A:593:GLU:OE1	2.20	0.41
1:A:206:LEU:HD12	1:A:230:PHE:HZ	1.85	0.41
1:B:347:ASN:ND2	1:B:505:PRO:HG3	2.35	0.41
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.55	0.41
1:A:633:ILE:CG2	1:A:635:LYS:HD3	2.50	0.41
1:B:20:ASN:ND2	1:B:20:ASN:O	2.43	0.41
1:A:513:LYS:NZ	1:A:514:SER:O	2.40	0.41
1:B:401:GLU:HA	1:B:406:MET:H	1.84	0.41
1:B:247:MET:HE2	1:B:257:LYS:HG2	2.03	0.41
1:B:153:ILE:HG23	1:B:252:ARG:HB2	2.03	0.41
1:A:102:GLU:CD	1:A:171:ARG:HH21	2.24	0.41
1:A:268:ALA:HA	1:A:272:GLU:O	2.20	0.41
1:B:684:ARG:HD3	1:B:684:ARG:HA	1.95	0.41
1:B:101:VAL:HG12	1:B:102:GLU:N	2.36	0.41
1:B:634:ILE:HD11	1:B:707:ALA:CB	2.51	0.41
1:B:93:ASP:HA	1:B:94:PRO:HD2	1.73	0.41
1:A:134:ILE:N	1:A:134:ILE:HD12	2.35	0.41
1:A:685:PRO:C	1:A:687:SER:H	2.24	0.41
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.56	0.41
1:A:105:ILE:HG12	1:A:157:PHE:CD2	2.56	0.41
1:A:199:LYS:HA	1:A:202:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HD2	1:A:90:ARG:HH11	1.73	0.41
1:A:412:ALA:HB2	1:A:426:PHE:O	2.21	0.41
1:B:446:LYS:HD3	1:B:446:LYS:HA	1.67	0.41
1:A:319:GLY:HA2	1:A:334:ILE:HD11	2.02	0.41
1:A:353:PHE:HD2	1:A:364:LEU:O	2.02	0.41
1:A:516:SER:O	1:A:517:ASN:HB2	2.21	0.41
1:A:559:PHE:CD1	1:A:563:VAL:O	2.63	0.40
1:B:338:TYR:O	1:B:339:PHE:HB2	2.21	0.40
1:A:715:ARG:O	1:A:716:HIS:CB	2.69	0.40
1:B:117:ILE:HA	1:B:118:PRO:HD2	1.92	0.40
1:B:513:LYS:HB3	1:B:514:SER:H	1.70	0.40
1:A:268:ALA:HA	1:A:273:GLY:HA3	2.03	0.40
1:B:134:ILE:HD12	1:B:134:ILE:H	1.87	0.40
1:B:64:HIS:HE1	1:B:80:GLN:HB3	1.87	0.40
1:A:283:TYR:CE2	1:A:600:GLU:OE1	2.75	0.40
1:A:86:ILE:HD12	1:A:86:ILE:H	1.86	0.40
1:A:172:THR:HG22	1:A:173:SER:H	1.86	0.40
1:B:184:PHE:CE2	1:B:255:PRO:HG3	2.56	0.40
1:A:305:SER:O	1:A:306:GLU:HB2	2.21	0.40
1:B:515:ARG:CB	1:B:619:LEU:HD21	2.50	0.40
1:B:515:ARG:HB2	1:B:619:LEU:HD21	2.03	0.40
1:B:71:ASN:HB3	1:B:75:ILE:HD11	2.03	0.40
1:A:541:ASN:ND2	1:A:545:ASN:O	2.54	0.40
1:B:563:VAL:HA	1:B:564:PRO:HD3	1.93	0.40
1:B:55:GLU:OE1	1:B:55:GLU:HA	2.21	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	706/731 (97%)	633 (90%)	49 (7%)	24 (3%)	5 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	4 7
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	4 8

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	91	PRO
1	A	139	ASP
1	A	426	PHE
1	A	509	GLU
1	B	54	LYS
1	B	55	GLU
1	B	270	ASP
1	B	272	GLU
1	B	365	THR
1	B	509	GLU
1	B	522	PHE
1	A	69	TYR
1	A	217	VAL
1	A	512	MET
1	A	513	LYS
1	A	515	ARG
1	A	580	LEU
1	B	45	LEU
1	B	128	GLY
1	B	273	GLY
1	B	460	ILE
1	B	595	MET
1	B	716	HIS
1	A	78	ARG
1	A	138	GLU
1	A	406	MET
1	A	516	SER
1	B	136	MET
1	B	139	ASP
1	B	189	GLU
1	B	252	ARG
1	B	514	SER
1	B	631	GLU
1	A	268	ALA
1	A	270	ASP

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Mol	Chain	Res	Type
1	A	70	GLU
1	A	311	TYR
1	A	425	GLN
1	A	687	SER
1	B	232	ASP
1	B	311	TYR
1	B	406	MET
1	B	425	GLN
1	B	447	ASP
1	A	686	ASN
1	A	716	HIS
1	B	445	LYS
1	B	697	PRO
1	A	669	GLY
1	B	9	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	626/644 (97%)	536 (86%)	90 (14%)	4 8
1	B	624/644 (97%)	549 (88%)	75 (12%)	6 13
All	All	1250/1288 (97%)	1085 (87%)	165 (13%)	5 10

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	12	ARG
1	A	18	ASN
1	A	20	ASN
1	A	43	GLU
1	A	45	LEU
1	A	54	LYS
1	A	56	ARG

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Mol	Chain	Res	Type
1	A	58	ASP
1	A	59	THR
1	A	72	ASN
1	A	96	ARG
1	A	99	PHE
1	A	100	ARG
1	A	104	VAL
1	A	105	ILE
1	A	112	ASN
1	A	126	GLN
1	A	136	MET
1	A	137	ARG
1	A	143	ARG
1	A	147	GLN
1	A	164	TRP
1	A	174	ARG
1	A	177	GLU
1	A	193	VAL
1	A	195	LEU
1	A	203	GLU
1	A	206	LEU
1	A	207	ASN
1	A	211	VAL
1	A	218	ASN
1	A	223	ARG
1	A	232	ASP
1	A	235	LEU
1	A	250	SER
1	A	270	ASP
1	A	276	VAL
1	A	293	THR
1	A	301	GLU
1	A	304	SER
1	A	340	SER
1	A	343	ASP
1	A	350	MET
1	A	354	LEU
1	A	356	GLU
1	A	357	ASP
1	A	365	THR
1	A	368	SER
1	A	369	VAL

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Mol	Chain	Res	Type
1	A	379	TRP
1	A	381	THR
1	A	386	PRO
1	A	408	ARG
1	A	422	VAL
1	A	435	VAL
1	A	445	LYS
1	A	462	LYS
1	A	463	LEU
1	A	469	ILE
1	A	507	ASN
1	A	509	GLU
1	A	511	VAL
1	A	515	ARG
1	A	516	SER
1	A	548	THR
1	A	569	LYS
1	A	572	THR
1	A	575	VAL
1	A	583	LYS
1	A	587	VAL
1	A	590	GLN
1	A	593	GLU
1	A	603	SER
1	A	604	LEU
1	A	609	THR
1	A	625	THR
1	A	629	ILE
1	A	632	ILE
1	A	637	ARG
1	A	658	GLU
1	A	667	LEU
1	A	674	ARG
1	A	677	LYS
1	A	679	MET
1	A	689	VAL
1	A	709	MET
1	A	712	ASP
1	A	713	SER
1	A	727	ARG
1	B	8	PHE
1	B	20	ASN

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Mol	Chain	Res	Type
1	B	28	THR
1	B	30	GLU
1	B	44	PHE
1	B	48	THR
1	B	58	ASP
1	B	95	ARG
1	B	96	ARG
1	B	110	GLN
1	B	121	ILE
1	B	135	VAL
1	B	136	MET
1	B	143	ARG
1	B	165	THR
1	B	172	THR
1	B	193	VAL
1	B	206	LEU
1	B	217	VAL
1	B	221	LYS
1	B	223	ARG
1	B	235	LEU
1	B	237	THR
1	B	270	ASP
1	B	272	GLU
1	B	301	GLU
1	B	314	CYS
1	B	340	SER
1	B	350	MET
1	B	354	LEU
1	B	363	LYS
1	B	386	PRO
1	B	397	SER
1	B	403	SER
1	B	408	ARG
1	B	427	ASP
1	B	431	VAL
1	B	446	LYS
1	B	452	VAL
1	B	460	ILE
1	B	463	LEU
1	B	487	GLN
1	B	494	LEU
1	B	495	GLU

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Mol	Chain	Res	Type
1	B	498	LEU
1	B	499	MET
1	B	504	LYS
1	B	509	GLU
1	B	512	MET
1	B	515	ARG
1	B	516	SER
1	B	517	ASN
1	B	520	MET
1	B	523	GLU
1	B	526	ASN
1	B	529	LEU
1	B	536	SER
1	B	565	LYS
1	B	571	GLU
1	B	572	THR
1	B	573	PHE
1	B	582	PHE
1	B	583	LYS
1	B	588	LEU
1	B	590	GLN
1	B	593	GLU
1	B	597	GLN
1	B	639	THR
1	B	640	GLN
1	B	703	ARG
1	B	713	SER
1	B	721	LEU
1	B	722	ASP
1	B	724	GLN
1	B	725	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	126	GLN
1	A	207	ASN
1	A	218	ASN
1	A	267	ASN
1	A	322	ASN
1	A	347	ASN

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Mol	Chain	Res	Type
1	A	459	HIS
1	A	526	ASN
1	A	545	ASN
1	A	590	GLN
1	A	622	GLN
1	B	51	HIS
1	B	322	ASN
1	B	337	ASN
1	B	419	HIS
1	B	517	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

There are no ligands in this entry.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.