



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 09:57 PM EST

PDB ID : 1GGT  
Title : THREE-DIMENSIONAL STRUCTURE OF A TRANSGLUTAMINASE:  
HUMAN BLOOD COAGULATION FACTOR XIII  
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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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

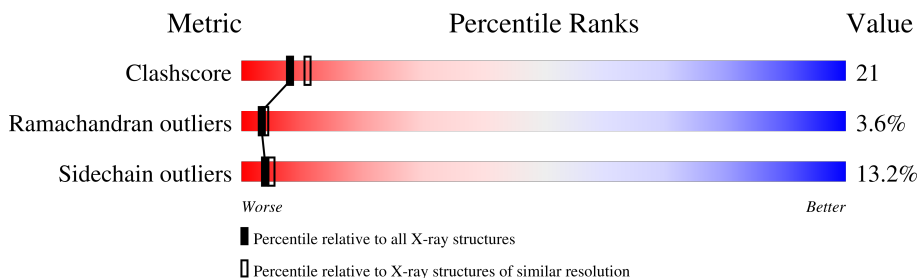
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

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

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
			Total	C	N	O	S			
1	A	710	5700	3614	983	1076	27	0	0	0
1	B	708	5682	3603	978	1074	27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

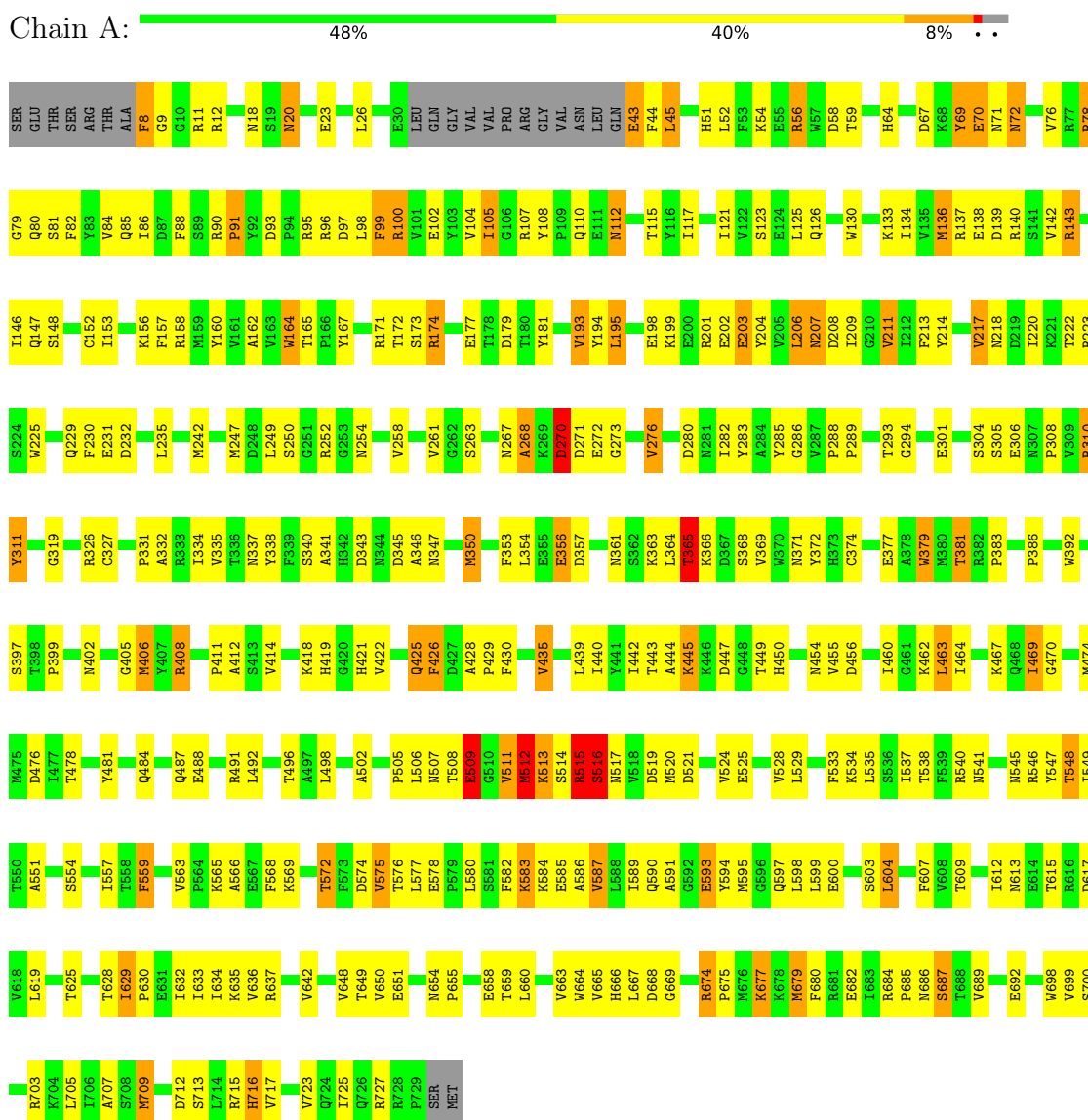
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



- Molecule 1: COAGULATION FACTOR XIII





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	11382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	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(°)	Ideal(°)
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(°)	Ideal(°)
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

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:100:ARG:HD2	1:A:164:TRP:HZ3	1.34	0.91
1:A:381:THR:HG23	1:A:383:PRO:HD3	1.51	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:231:GLU:HB3	1:A:674:ARG:HH22	1.39	0.87
1:A:363:LYS:HG3	1:A:364:LEU:N	1.87	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:636:VAL:HG11	1:A:723:VAL:HG11	1.74	0.68
1:A:668:ASP:OD2	1:A:675:PRO:HB3	1.94	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:A:91:PRO:HD3	1:A:140:ARG:HG2	1.79	0.63
1:B:539:PHE:HB3	1:B:577:LEU:HD21	1.80	0.63
1:A:397:SER:HA	1:A:408:ARG:HB2	1.80	0.62
1:A:666:HIS:O	1:A:707:ALA:HA	1.98	0.62
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.64	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:303:ARG:HG2	1:B:303:ARG:HH11	1.64	0.61
1:B:582:PHE:N	1:B:582:PHE:HD1	1.99	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:66:THR:HG21	1:B:75:ILE:HG22	1.83	0.60
1:B:445:LYS:NZ	1:B:445:LYS:HB3	2.16	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: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:529:LEU:HD21	1:A:629:ILE:HG23	1.83	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: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:B:634:ILE:HA	1:B:649:THR:O	2.02	0.60
1:A:463:LEU:HD21	1:A:476:ASP:OD2	2.02	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:105:ILE:HG23	1:B:157:PHE:CD2	2.37	0.59
1:B:512:MET:SD	1:B:512:MET:N	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: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:657:LYS:O	1:B:685:PRO:HB3	2.03	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:100:ARG:CD	1:A:164:TRP:HZ3	2.13	0.56
1:A:537:ILE:O	1:A:584:LYS:HA	2.05	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:CD1	1:B:573:PHE:N	2.72	0.56
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.39	0.56
1:A:220:ILE:HD12	1:A:220:ILE:H	1.70	0.56
1:A:247:MET:HE2	1:A:261:VAL:HG11	1.88	0.56
1:A:565:LYS:HD3	1:A:599:LEU:HD21	1.88	0.55
1:A:577:LEU:HA	1:A:583:LYS:HE3	1.89	0.55
1:A:263:SER:HB2	1:A:408:ARG:HG3	1.89	0.55
1:B:516:SER:HB2	1:B:547:TYR:CZ	2.41	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:43:GLU:N	1:A:165:THR:HG1	2.04	0.55
1:A:551:ALA:O	1:A:572:THR:HA	2.06	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:A:156:LYS:HE2	1:A:181:TYR:CZ	2.41	0.54
1:B:303:ARG:HG2	1:B:303:ARG:NH1	2.21	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: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:A:642:VAL:CG2	1:A:700:SER:HB3	2.38	0.54
1:B:43:GLU:O	1:B:43:GLU:HG2	2.06	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:263:SER:OG	1:B:408:ARG:HD3	2.08	0.53
1:B:530:GLY:HA2	1:B:595:MET:SD	2.49	0.53
1:A:52:LEU:HD23	1:A:84:VAL:HG22	1.90	0.53
1:A:435:VAL:HG21	1:A:464:ILE:HD11	1.91	0.53
1:A:629:ILE:HD12	1:A:629:ILE:H	1.74	0.53
1:A:454:ASN:HA	1:A:512:MET:SD	2.49	0.52
1:A:455:VAL:HG13	1:A:512:MET:HG2	1.91	0.52
1:B:100:ARG:HB2	1:B:119:VAL:O	2.09	0.52
1:A:455:VAL:HG11	1:A:508:THR:HG21	1.91	0.52
1:B:524:VAL:HG22	1:B:535:LEU:HG	1.92	0.52
1:A:229:GLN:HB2	1:A:327:CYS:HB2	1.90	0.52
1:A:203:GLU:HG3	1:A:469:ILE:HA	1.91	0.52
1:A:529:LEU:H	1:A:529:LEU:CD2	2.23	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:573:PHE:N	1:B:573:PHE:HD1	2.08	0.51
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.91	0.51
1:A:674:ARG:HE	1:A:674:ARG:HA	1.75	0.51
1:B:105:ILE:CD1	1:B:115:THR:HG22	2.41	0.51
1:B:515:ARG:HG3	1:B:518:VAL:O	2.11	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: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:A:455:VAL:HG13	1:A:512:MET:CG	2.41	0.51
1:A:578:GLU:CD	1:A:578:GLU:N	2.64	0.51
1:A:45:LEU:HD22	1:A:45:LEU:O	2.11	0.50
1:A:270:ASP:O	1:A:271:ASP:HB2	2.10	0.50
1:A:513:LYS:O	1:A:515:ARG:HD2	2.11	0.50
1:B:410:GLY:C	1:B:426:PHE:HB3	2.32	0.50
1:B:418:LYS:HD2	1:B:480:THR:O	2.11	0.50
1:B:428:ALA:N	1:B:429:PRO:HD2	2.26	0.50
1:A:509:GLU:OE1	1:A:511:VAL:HG12	2.11	0.50
1:A:537:ILE:HD12	1:A:537:ILE:N	2.23	0.50
1:A:338:TYR:O	1:A:371:ASN:O	2.29	0.50
1:B:337:ASN:O	1:B:372:TYR:HA	2.12	0.50
1:B:520:MET:O	1:B:520:MET:HG3	2.11	0.50
1:B:568:PHE:HD2	1:B:593:GLU:HG2	1.75	0.50
1:A:81:SER:HA	1:A:146:ILE:O	2.12	0.50
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.93	0.50
1:A:64:HIS:CE1	1:A:76:VAL:HG22	2.47	0.50
1:A:525:GLU:HG3	1:A:533:PHE:HB2	1.94	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:A:557:ILE:CD1	1:A:597:GLN:HG3	2.42	0.50
1:B:256:ILE:HD12	1:B:256:ILE:N	2.27	0.50
1:B:363:LYS:HE3	1:B:364:LEU:CB	2.42	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:54:LYS:O	1:B:55:GLU:O	2.30	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:714:LEU:HG	1:B:715:ARG:N	2.27	0.50
1:A:634:ILE:HA	1:A:649:THR:O	2.12	0.49
1:B:24:ASP:O	1:B:158:ARG:NH2	2.45	0.49
1:B:119:VAL:HG11	1:B:146:ILE:HG23	1.94	0.49
1:A:521:ASP:HB2	1:A:540:ARG:HH22	1.78	0.49
1:B:445:LYS:HB3	1:B:445:LYS:HZ3	1.77	0.49
1:B:516:SER:HB2	1:B:547:TYR:CE2	2.47	0.49
1:A:445:LYS:HB3	1:A:447:ASP:OD1	2.12	0.49
1:A:93:ASP:O	1:A:97:ASP:HB2	2.12	0.49
1:A:220:ILE:HD12	1:A:220:ILE:N	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:B:541:ASN:HB2	1:B:577:LEU:CD2	2.40	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:402:ASN:HA	1:A:430:PHE:CZ	2.47	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:381:THR:CG2	1:A:383:PRO:HD3	2.34	0.49
1:A:283:TYR:HE2	1:A:600:GLU:OE1	1.96	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:237:THR:HA	1:B:240:TYR:HB3	1.95	0.48
1:B:270:ASP:O	1:B:271:ASP:HB2	2.13	0.48
1:B:521:ASP:HB2	1:B:540:ARG:HH21	1.77	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:587:VAL:HG12	1:B:588:LEU:H	1.78	0.48
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.48	0.48
1:B:522:PHE:CD1	1:B:535:LEU:HD21	2.48	0.48
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.46	0.48
1:B:220:ILE:HG21	1:B:474:MET:CE	2.42	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:165:THR:HG22	1:A:167:TYR:H	1.79	0.48
1:A:541:ASN:HB2	1:A:577:LEU:HB3	1.96	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:204:TYR:O	1:A:326:ARG:HG2	2.14	0.47
1:A:405:GLY:O	1:A:406:MET:HB3	2.14	0.47
1:A:449:THR:HG22	1:A:450:HIS:N	2.30	0.47
1:B:285:TYR:CB	1:B:310:ARG:HH11	2.28	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:95:ARG:NH2	1:B:96:ARG:HB2	2.30	0.47
1:B:654:ASN:O	1:B:686:ASN:HA	2.14	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:A:664:TRP:CE2	1:A:679:MET:HE3	2.49	0.47
1:B:51:HIS:HD2	1:B:85:GLN:HE21	1.62	0.47
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.44	0.47
1:B:546:ARG:HE	1:B:578:GLU:HG3	1.78	0.47
1:B:705:LEU:HD23	1:B:705:LEU:HA	1.74	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:64:HIS:CE1	1:B:80:GLN:HB3	2.50	0.47
1:B:570:LYS:O	1:B:570:LYS:HG2	2.14	0.47
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: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:153:ILE:N	1:A:153:ILE:HD12	2.30	0.46
1:A:207:ASN:HD22	1:A:207:ASN:C	2.19	0.46
1:A:548:THR:HA	1:A:575:VAL:O	2.15	0.46
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.96	0.46
1:B:95:ARG:CZ	1:B:96:ARG:HB2	2.46	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:422:VAL:HG23	1:B:500:TYR:HB2	1.95	0.46
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.71	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:A:95:ARG:HE	1:A:95:ARG:HB2	1.63	0.46
1:B:546:ARG:HE	1:B:578:GLU:CG	2.28	0.46
1:A:76:VAL:HG21	1:A:82:PHE:CD1	2.51	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
1:B:111:GLU:HB3	1:B:116:TYR:CD2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASN:HD21	1:B:505:PRO:HG3	1.81	0.46
1:B:549:ILE:CD1	1:B:577:LEU:HD13	2.46	0.46
1:B:98:LEU:HD23	1:B:164:TRP:HB2	1.98	0.46
1:B:547:TYR:HD1	1:B:614:GLU:CG	2.29	0.46
1:A:165:THR:HG22	1:A:167:TYR:N	2.30	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:554:SER:HB2	1:B:607:PHE:HB2	1.96	0.46
1:A:86:ILE:N	1:A:86:ILE:HD12	2.30	0.46
1:B:632:ILE:CG2	1:B:650:VAL:HG13	2.46	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: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: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:463:LEU:HD23	1:A:478:THR:OG1	2.16	0.45
1:A:105:ILE:HG12	1:A:157:PHE:CE2	2.52	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:428:ALA:N	1:A:429:PRO:HD2	2.32	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: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:A:112:ASN:N	1:A:112:ASN:HD22	2.13	0.45
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.79	0.45
1:B:133:LYS:HB3	1:B:133:LYS:HE3	1.78	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: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:A:225:TRP:CE2	1:A:294:GLY:HA2	2.52	0.45
1:A:332:ALA:HA	1:A:377:GLU:O	2.17	0.45
1:A:665:VAL:O	1:A:677:LYS:HA	2.17	0.45
1:B:43:GLU:HB2	1:B:165:THR:CG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:VAL:HB	1:A:680:PHE:HB2	1.99	0.44
1:B:105:ILE:HD11	1:B:115:THR:HG22	2.00	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:276:VAL:O	1:B:311:TYR:HA	2.18	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:A:337:ASN:O	1:A:372:TYR:HA	2.18	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:B:515:ARG:HH12	1:B:519:ASP:CG	2.21	0.44
1:A:99:PHE:HA	1:A:162:ALA:O	2.18	0.44
1:A:547:TYR:O	1:A:576:THR:HA	2.17	0.44
1:A:674:ARG:HG3	1:A:675:PRO:HD2	1.99	0.44
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.74	0.44
1:A:402:ASN:HA	1:A:430:PHE:CE1	2.52	0.44
1:A:565:LYS:O	1:A:566:ALA:HB2	2.18	0.44
1:A:577:LEU:HG	1:A:583:LYS:HE3	1.99	0.44
1:B:107:ARG:NH1	1:B:107:ARG:HG3	2.31	0.44
1:B:636:VAL:HG11	1:B:646:MET:CE	2.47	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:HD23	1:A:506:LEU:HA	1.83	0.43
1:A:405:GLY:O	1:A:406:MET:CB	2.65	0.43
1:A:157:PHE:CD1	1:A:157:PHE:N	2.87	0.43
1:B:541:ASN:O	1:B:580:LEU:HA	2.18	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.17	0.43
1:B:195:LEU:O	1:B:201:ARG:NE	2.51	0.43
1:A:247:MET:HE2	1:A:261:VAL:CG1	2.48	0.43
1:A:444:ALA:HA	1:A:450:HIS:ND1	2.33	0.43
1:B:385:LEU:CD2	1:B:424:PHE:HB3	2.47	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:B:620:ALA:O	1:B:621:LYS:HG2	2.18	0.43
1:A:69:TYR:O	1:A:71:ASN:N	2.52	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:B:520:MET:CE	1:B:608:VAL:HG12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:587:VAL:HG12	1:B:588:LEU:N	2.33	0.43
1:A:194:TYR:HE1	1:A:201:ARG:HH21	1.66	0.43
1:A:353:PHE:HB2	1:A:365:THR:OG1	2.18	0.43
1:A:513:LYS:NZ	1:A:516:SER:H	2.15	0.43
1:A:684:ARG:HD3	1:A:684:ARG:HA	1.73	0.43
1:A:703:ARG:HA	1:A:703:ARG:NE	2.33	0.43
1:B:543:SER:O	1:B:580:LEU:HD12	2.19	0.43
1:A:20:ASN:HD22	1:A:20:ASN:C	2.22	0.43
1:A:283:TYR:CD2	1:A:288:PRO:HB3	2.53	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:B:666:HIS:HA	1:B:676:MET:O	2.18	0.43
1:A:286:GLY:HA3	1:A:310:ARG:HB3	2.00	0.43
1:B:135:VAL:HG12	1:B:143:ARG:O	2.19	0.43
1:B:447:ASP:OD1	1:B:447:ASP:N	2.52	0.43
1:B:573:PHE:HZ	1:B:587:VAL:CG2	2.32	0.43
1:A:335:VAL:O	1:A:374:CYS:HA	2.19	0.42
1:B:153:ILE:HD13	1:B:249:LEU:O	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:72:ASN:OD1	1:A:72:ASN:N	2.52	0.42
1:A:519:ASP:HB2	1:A:540:ARG:CG	2.49	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:B:633:ILE:HD13	1:B:633:ILE:HA	1.90	0.42
1:A:134:ILE:HD12	1:A:134:ILE:H	1.85	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.74	0.42
1:A:455:VAL:HG11	1:A:508:THR:CG2	2.49	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: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:99:PHE:HB2	1:B:162:ALA:O	2.19	0.42
1:B:363:LYS:HE3	1:B:364:LEU:HB3	2.00	0.42
1:B:489:GLU:H	1:B:489:GLU:HG2	1.60	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:A:414:VAL:O	1:A:414:VAL:HG12	2.19	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:B:580:LEU:HD12	1:B:580:LEU:N	2.35	0.42
1:B:598:LEU:HD11	1:B:627:LEU:CD1	2.50	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:342:HIS:ND1	1:B:434:GLU:OE2	2.48	0.42
1:B:413:SER:O	1:B:417:ILE:HG12	2.19	0.42
1:A:419:HIS:HB3	1:A:421:HIS:CD2	2.54	0.42
1:A:629:ILE:H	1:A:629:ILE:CD1	2.32	0.42
1:B:280:ASP:O	1:B:282:ILE:N	2.53	0.42
1:B:668:ASP:HB3	1:B:706:ILE:HB	2.01	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:A:8:PHE:N	1:A:8:PHE:CD1	2.88	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: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:206:LEU:HD12	1:A:230:PHE:HZ	1.85	0.41
1:A:568:PHE:HB2	1:A:593:GLU:OE1	2.20	0.41
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.55	0.41
1:B:347:ASN:ND2	1:B:505:PRO:HG3	2.35	0.41
1:A:633:ILE:CG2	1:A:635:LYS:HD3	2.50	0.41
1:B:20:ASN:O	1:B:20:ASN:ND2	2.43	0.41
1:A:102:GLU:CD	1:A:171:ARG:HH21	2.24	0.41
1:A:513:LYS:NZ	1:A:514:SER:O	2.40	0.41
1:B:153:ILE:HG23	1:B:252:ARG:HB2	2.03	0.41
1:B:247:MET:HE2	1:B:257:LYS:HG2	2.03	0.41
1:B:401:GLU:HA	1:B:406:MET:H	1.84	0.41
1:A:268:ALA:HA	1:A:272:GLU:O	2.20	0.41
1:B:101:VAL:HG12	1:B:102:GLU:N	2.36	0.41
1:B:684:ARG:HD3	1:B:684:ARG:HA	1.95	0.41
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.56	0.41
1:A:134:ILE:HD12	1:A:134:ILE:N	2.35	0.41
1:A:685:PRO:C	1:A:687:SER:H	2.24	0.41
1:B:93:ASP:HA	1:B:94:PRO:HD2	1.73	0.41
1:B:634:ILE:HD11	1:B:707:ALA:CB	2.51	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:HH11	1:A:90:ARG:HD2	1.73	0.41
1:A:319:GLY:HA2	1:A:334:ILE:HD11	2.02	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: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: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:338:TYR:O	1:B:339:PHE:HB2	2.21	0.40
1:A:268:ALA:HA	1:A:273:GLY:HA3	2.03	0.40
1:B:134:ILE:H	1:B:134:ILE:HD12	1.87	0.40
1:B:513:LYS:HB3	1:B:514:SER:H	1.70	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:A:283:TYR:CE2	1:A:600:GLU:OE1	2.75	0.40
1:A:305:SER:O	1:A:306:GLU:HB2	2.21	0.40
1:B:64:HIS:HE1	1:B:80:GLN:HB3	1.87	0.40
1:B:184:PHE:CE2	1:B:255:PRO:HG3	2.56	0.40
1:B:71:ASN:HB3	1:B:75:ILE:HD11	2.03	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:A:541:ASN:ND2	1:A:545:ASN:O	2.54	0.40
1:B:55:GLU:OE1	1:B:55:GLU:HA	2.21	0.40
1:B:563:VAL:HA	1:B:564:PRO:HD3	1.93	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%)	<b>3</b> <b>4</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	3	3
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	3	4

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 [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	626/644 (97%)	536 (86%)	90 (14%)	<b>3</b> <b>3</b>
1	B	624/644 (97%)	549 (88%)	75 (12%)	<b>5</b> <b>7</b>
All	All	1250/1288 (97%)	1085 (87%)	165 (13%)	<b>4</b> <b>5</b>

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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 [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.