



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 1FIE / pdb_00001fie
Title : RECOMBINANT HUMAN COAGULATION FACTOR XIII
Authors : Yee, V.C.; Teller, D.C.
Deposited on : 1996-08-24
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

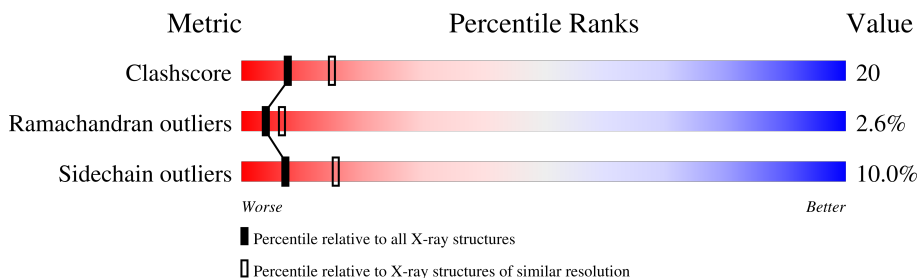
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11928 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	705	Total	C	N	O	S	0	0	0
			5651	3584	976	1064	27			
1	B	715	Total	C	N	O	S	0	0	0
			5720	3626	986	1081	27			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	270	Total	O	0	0
			270	270		
2	B	287	Total	O	0	0
			287	287		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.10Å 73.13Å 134.70Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	77.0 (10.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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	0.70	1/5784 (0.0%)	1.13	39/7848 (0.5%)
1	B	0.75	1/5853 (0.0%)	1.17	52/7941 (0.7%)
All	All	0.73	2/11637 (0.0%)	1.15	91/15789 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	MET	SD-CE	5.14	1.92	1.79
1	B	387	VAL	CA-CB	5.12	1.60	1.54

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	LYS	N-CA-C	10.14	122.03	110.97
1	A	638	GLY	N-CA-C	9.66	122.75	110.38
1	B	20	ASN	N-CA-C	-9.46	102.11	114.31
1	B	310	ARG	N-CA-C	8.97	122.97	109.25
1	A	365	THR	N-CA-C	-8.85	91.95	110.80
1	B	314	CYS	N-CA-C	8.84	121.88	111.71
1	A	310	ARG	N-CA-C	8.80	123.16	109.96
1	A	544	HIS	N-CA-C	-8.57	98.76	110.68
1	A	674	ARG	N-CA-C	-8.57	97.73	110.24
1	B	674	ARG	N-CA-C	-8.09	99.90	109.93
1	B	42	GLN	N-CA-C	-8.05	104.44	112.97
1	B	284	ALA	N-CA-C	7.80	119.47	110.97
1	A	501	GLY	N-CA-C	7.74	125.27	115.21
1	B	600	GLU	N-CA-C	7.68	123.97	111.37
1	B	217	VAL	N-CA-C	7.64	119.33	110.62
1	B	460	ILE	N-CA-C	7.56	125.06	109.34
1	A	507	ASN	N-CA-C	-7.37	100.11	110.50
1	B	528	VAL	N-CA-C	-7.33	99.26	109.45
1	B	280	ASP	N-CA-C	-7.19	100.43	110.35
1	A	204	TYR	N-CA-C	7.18	121.63	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ASP	N-CA-C	7.17	119.96	111.71
1	B	298	ILE	N-CA-C	7.14	117.93	110.72
1	B	425	GLN	N-CA-C	6.85	125.39	110.80
1	B	518	VAL	N-CA-C	-6.75	96.76	106.55
1	B	170	LEU	N-CA-C	-6.56	99.03	109.59
1	A	574	ASP	N-CA-C	-6.38	98.49	108.90
1	B	437	SER	N-CA-C	6.35	118.91	110.53
1	A	366	LYS	N-CA-C	6.35	121.17	113.17
1	A	425	GLN	N-CA-C	6.35	124.33	110.80
1	B	52	LEU	N-CA-C	-6.33	98.20	108.52
1	A	369	VAL	N-CA-C	-6.31	99.33	108.36
1	A	480	THR	N-CA-C	-6.31	105.40	113.23
1	A	559	PHE	N-CA-C	-6.30	101.45	110.59
1	B	137	ARG	N-CA-C	6.27	118.64	108.41
1	B	525	GLU	N-CA-C	-6.24	102.13	110.55
1	A	508	THR	N-CA-C	-6.20	105.44	112.87
1	B	510	GLY	N-CA-C	-6.19	105.07	113.37
1	B	436	ASN	N-CA-C	6.17	121.64	112.94
1	B	488	GLU	N-CA-C	6.09	121.43	111.37
1	A	58	ASP	N-CA-C	6.07	117.88	110.41
1	A	11	ARG	N-CA-C	6.04	117.87	111.28
1	A	194	TYR	N-CA-C	6.00	118.41	109.59
1	B	108	TYR	N-CA-C	5.98	119.35	109.79
1	B	44	PHE	N-CA-C	-5.96	98.11	110.80
1	B	544	HIS	N-CA-C	-5.93	99.96	109.39
1	A	657	LYS	N-CA-C	-5.91	105.16	113.20
1	A	436	ASN	N-CA-C	5.89	121.25	112.94
1	A	594	TYR	N-CA-C	5.89	120.49	113.12
1	A	619	LEU	N-CA-C	-5.85	100.65	109.95
1	B	188	CYS	N-CA-C	5.76	117.92	108.52
1	B	194	TYR	N-CA-C	5.75	118.57	110.23
1	A	234	ILE	N-CA-C	5.73	115.86	110.30
1	B	535	LEU	N-CA-C	-5.69	100.12	109.40
1	A	464	ILE	N-CA-C	-5.67	100.17	108.11
1	B	626	VAL	N-CA-C	-5.66	100.19	108.11
1	B	266	VAL	N-CA-C	5.65	115.85	110.42
1	B	431	VAL	N-CA-C	-5.60	103.93	111.44
1	A	528	VAL	N-CA-C	-5.57	100.10	108.12
1	B	547	TYR	N-CA-C	5.52	117.03	109.18
1	A	600	GLU	N-CA-C	5.50	122.52	110.80
1	A	432	PHE	N-CA-C	-5.48	105.20	111.07
1	B	165	THR	N-CA-C	-5.47	103.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	MET	N-CA-C	5.46	117.14	108.67
1	B	351	ASP	N-CA-C	5.44	117.83	109.07
1	A	229	GLN	N-CA-C	5.44	119.02	112.38
1	A	317	PHE	N-CA-C	-5.42	105.37	111.28
1	A	426	PHE	CB-CA-C	5.38	121.13	110.42
1	B	302	TYR	CA-C-N	5.35	127.76	120.54
1	B	302	TYR	C-N-CA	5.35	127.76	120.54
1	B	374	CYS	N-CA-C	5.31	117.89	109.24
1	B	480	THR	N-CA-C	-5.25	106.55	113.12
1	A	177	GLU	N-CA-C	5.25	119.17	112.87
1	B	718	TYR	N-CA-C	5.22	116.60	109.18
1	B	632	ILE	N-CA-C	-5.21	100.98	108.53
1	B	503	LYS	N-CA-C	5.21	117.59	109.52
1	A	339	PHE	N-CA-C	-5.20	99.72	110.80
1	A	696	ARG	CA-C-N	5.19	125.43	119.83
1	A	696	ARG	C-N-CA	5.19	125.43	119.83
1	B	58	ASP	N-CA-C	5.18	117.01	110.33
1	B	567	GLU	N-CA-C	-5.18	100.08	108.52
1	B	280	ASP	CA-C-N	-5.14	114.52	122.49
1	B	280	ASP	C-N-CA	-5.14	114.52	122.49
1	B	595	MET	N-CA-C	5.12	121.70	110.80
1	A	311	TYR	N-CA-C	5.08	121.61	110.80
1	A	673	THR	N-CA-C	5.03	116.89	108.99
1	B	344	ASN	N-CA-C	5.02	119.26	113.18
1	A	52	LEU	N-CA-C	-5.02	101.50	109.59
1	A	73	LYS	N-CA-C	-5.02	102.13	109.81
1	A	437	SER	N-CA-C	5.02	117.58	110.50
1	B	398	THR	CA-C-N	5.02	125.29	119.92
1	B	398	THR	C-N-CA	5.02	125.29	119.92

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	5651	0	5518	231	0
1	B	5720	0	5566	224	0
2	A	270	0	0	14	0
2	B	287	0	0	17	0
All	All	11928	0	11084	451	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 20.

All (451) 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:538:THR:HG22	1:B:584:LYS:HG3	1.37	1.06
1:B:528:VAL:HB	1:B:531:LYS:HD3	1.44	0.97
1:A:650:ILE:HB	1:A:691:TRP:HB3	1.50	0.90
1:B:40:ASN:C	1:B:41:LEU:CA	2.48	0.86
1:B:509:GLU:HB2	1:B:511:VAL:O	1.76	0.85
1:A:331:PRO:HB2	1:A:379:TRP:HB3	1.59	0.84
1:B:659:THR:HG22	1:B:685:PRO:HD3	1.60	0.84
1:A:549:ILE:HD12	1:A:612:ILE:HG12	1.60	0.82
1:B:565:LYS:HD2	1:B:599:LEU:HD21	1.61	0.81
1:A:517:ASN:HB3	1:A:542:ASN:HB2	1.62	0.81
1:A:337:ASN:HD21	1:A:461:GLY:HA2	1.45	0.81
1:A:667:LEU:HD11	1:A:705:LEU:HD22	1.62	0.81
1:B:650:ILE:HG21	1:B:665:VAL:HG11	1.63	0.79
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.48	0.79
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.66	0.78
1:B:540:ARG:HA	1:B:582:PHE:HD1	1.48	0.78
1:B:515:ARG:HB2	1:B:619:LEU:HD21	1.64	0.77
1:B:465:VAL:HG21	1:B:474:MET:SD	2.25	0.76
1:A:298:ILE:HG23	1:A:309:VAL:HG11	1.68	0.76
1:A:650:ILE:HD11	1:A:667:LEU:HD13	1.67	0.76
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.70	0.74
1:B:298:ILE:HG23	1:B:309:VAL:HG11	1.70	0.72
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.70	0.72
1:B:575:VAL:HG13	1:B:583:LYS:HD2	1.71	0.72
1:B:454:ASN:HA	2:B:967:HOH:O	1.89	0.72
1:A:636:VAL:HG12	1:A:648:VAL:HG22	1.70	0.72
1:A:143:ARG:HD2	2:A:735:HOH:O	1.89	0.71
1:A:484:GLN:HG2	1:A:487:GLN:HE21	1.55	0.71
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.54	0.70
1:A:531:LYS:O	1:A:591:ALA:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ILE:HG22	1:A:721:LEU:HD12	1.73	0.69
1:A:121:ILE:HG13	1:A:121:ILE:O	1.91	0.68
1:B:549:ILE:HG22	1:B:550:THR:H	1.58	0.68
1:B:411:PRO:O	1:B:426:PHE:HB2	1.94	0.67
1:B:581:SER:HB3	2:B:950:HOH:O	1.94	0.66
1:A:71:ASN:HB3	1:A:75:ILE:HD11	1.76	0.66
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.30	0.66
1:B:517:ASN:HB3	1:B:542:ASN:HB2	1.78	0.66
1:B:673:THR:OG1	1:B:676:MET:HE2	1.94	0.66
1:A:193:VAL:HG13	1:A:331:PRO:HD3	1.79	0.65
1:A:411:PRO:O	1:A:426:PHE:HB2	1.96	0.65
1:B:545:ASN:O	1:B:579:PRO:HA	1.96	0.65
1:B:612:ILE:O	1:B:612:ILE:HG22	1.95	0.65
1:B:121:ILE:HD13	1:B:134:ILE:HG13	1.78	0.65
1:A:268:ALA:HA	1:A:273:GLY:HA3	1.77	0.64
1:A:679:MET:HG2	1:A:680:PHE:N	2.11	0.64
1:A:484:GLN:HG2	1:A:487:GLN:NE2	2.12	0.64
1:A:540:ARG:HG2	1:A:582:PHE:CD2	2.31	0.64
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.63	0.64
1:A:134:ILE:HG13	1:A:142:VAL:HG21	1.79	0.64
1:B:91:PRO:HD3	1:B:140:ARG:HG2	1.79	0.64
1:A:600:GLU:HG3	1:A:715:ARG:HD2	1.79	0.63
1:B:214:TYR:HD2	2:B:831:HOH:O	1.81	0.63
1:A:446:LYS:O	1:B:164:TRP:HZ3	1.82	0.63
1:B:600:GLU:HA	2:B:956:HOH:O	1.99	0.62
1:A:134:ILE:HG13	1:A:142:VAL:CG2	2.28	0.62
1:A:439:LEU:O	1:A:455:VAL:HA	1.99	0.62
1:A:453:GLU:O	1:A:513:LYS:HG2	2.00	0.62
1:B:515:ARG:HH12	1:B:519:ASP:HA	1.64	0.62
1:B:528:VAL:HB	1:B:531:LYS:CD	2.25	0.62
1:A:189:GLU:HB3	2:A:891:HOH:O	1.99	0.61
1:B:318:ALA:O	1:B:322:ASN:HB2	1.99	0.61
1:B:659:THR:CG2	1:B:685:PRO:HD3	2.30	0.61
1:B:268:ALA:HA	1:B:273:GLY:HA3	1.82	0.61
1:A:665:VAL:HG22	1:A:680:PHE:HE1	1.65	0.61
1:B:270:ASP:HA	2:B:868:HOH:O	2.01	0.61
1:B:514:SER:O	1:B:515:ARG:HG2	2.00	0.61
1:B:549:ILE:HG22	1:B:550:THR:N	2.15	0.61
1:A:678:LYS:HB2	1:A:691:TRP:CZ2	2.35	0.61
1:A:484:GLN:HG3	1:A:487:GLN:HG3	1.82	0.61
1:B:703:ARG:HG3	1:B:725:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LYS:O	1:A:366:LYS:HE2	2.02	0.60
1:A:510:GLY:O	1:A:511:VAL:HB	2.01	0.60
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.37	0.60
1:A:51:His:HB2	1:A:85:GLN:HB3	1.83	0.60
1:A:640:GLN:O	1:A:726:GLN:HG2	2.02	0.60
1:B:518:VAL:HA	1:B:540:ARG:O	2.01	0.60
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.66	0.60
1:A:446:LYS:O	1:B:164:TRP:CZ3	2.55	0.59
1:A:649:THR:HA	1:A:691:TRP:O	2.02	0.59
1:B:515:ARG:NH1	1:B:519:ASP:HA	2.17	0.59
1:A:511:VAL:HG13	1:A:512:MET:N	2.17	0.59
1:B:538:THR:C	1:B:540:ARG:HH21	2.09	0.59
1:A:100:ARG:HE	1:A:164:TRP:HZ2	1.51	0.59
1:A:678:LYS:HB2	1:A:691:TRP:CE2	2.37	0.59
1:B:546:ARG:HG3	1:B:546:ARG:NH1	2.15	0.59
1:B:662:ASN:N	1:B:662:ASN:HD22	2.00	0.59
1:B:361:ASN:ND2	1:B:364:LEU:HD12	2.18	0.58
1:B:128:GLY:HA2	1:B:150:PRO:HD2	1.84	0.58
1:B:226:SER:CB	1:B:670:PRO:HD3	2.34	0.58
1:B:578:GLU:HB2	1:B:581:SER:OG	2.03	0.58
1:B:541:ASN:HB2	1:B:577:LEU:HD23	1.84	0.58
1:A:540:ARG:NE	1:A:582:PHE:HE2	2.01	0.58
1:B:128:GLY:HA2	1:B:150:PRO:CD	2.33	0.58
1:A:682:GLU:CD	1:A:684:ARG:HH12	2.12	0.57
1:B:540:ARG:HA	1:B:582:PHE:CD1	2.36	0.57
1:A:439:LEU:HB2	1:A:456:ASP:HB3	1.86	0.57
1:B:187:TRP:CH2	1:B:206:LEU:HD21	2.39	0.57
1:B:511:VAL:HG12	1:B:512:MET:N	2.20	0.57
1:A:44:PHE:O	1:A:45:LEU:HB2	2.04	0.57
1:A:656:LEU:HD12	1:A:660:LEU:HD21	1.86	0.57
1:B:31:LEU:HD23	1:B:168:GLY:HA3	1.86	0.57
1:A:513:LYS:HD3	1:A:618:VAL:H	1.70	0.56
1:A:513:LYS:HG3	1:A:618:VAL:O	2.05	0.56
1:B:92:TYR:O	1:B:94:PRO:HD3	2.04	0.56
1:B:511:VAL:HG12	1:B:512:MET:H	1.69	0.56
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.86	0.56
1:A:657:LYS:HD3	1:A:686:ASN:HD21	1.69	0.56
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.17	0.56
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.87	0.56
1:B:634:ILE:O	1:B:721:LEU:HD22	2.05	0.56
1:A:233:GLY:O	1:A:237:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:HD2	2:A:815:HOH:O	1.87	0.56
1:B:105:ILE:HD12	1:B:115:THR:HA	1.87	0.56
1:B:598:LEU:HD22	1:B:602:ALA:HA	1.86	0.56
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.56
1:B:392:TRP:HB2	2:B:976:HOH:O	2.04	0.56
1:B:678:LYS:HB2	1:B:691:TRP:CE2	2.40	0.56
1:B:670:PRO:O	1:B:703:ARG:NH1	2.38	0.56
1:A:507:ASN:C	1:A:509:GLU:N	2.62	0.56
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.39	0.56
1:A:709:MET:HB3	1:A:717:VAL:HB	1.86	0.56
1:A:578:GLU:HB2	1:A:581:SER:HB2	1.87	0.56
1:B:539:PHE:O	1:B:582:PHE:HA	2.06	0.56
1:A:116:TYR:CE2	1:A:118:PRO:HG3	2.41	0.55
1:A:658:GLU:C	1:A:685:PRO:HG3	2.32	0.55
1:A:507:ASN:C	1:A:509:GLU:H	2.14	0.55
1:B:540:ARG:HG3	1:B:582:PHE:CD1	2.42	0.55
1:A:121:ILE:HA	1:A:132:ALA:HB3	1.89	0.55
1:A:673:THR:OG1	1:A:676:MET:HE2	2.06	0.55
1:B:544:HIS:HD2	1:B:580:LEU:HD21	1.71	0.55
1:A:231:GLU:HB3	1:A:674:ARG:HH22	1.71	0.55
1:A:679:MET:HG2	1:A:680:PHE:H	1.71	0.55
1:B:153:ILE:HD13	1:B:249:LEU:O	2.07	0.55
1:B:616:ARG:H	1:B:616:ARG:HD3	1.72	0.55
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.89	0.54
1:A:347:ASN:ND2	1:A:503:LYS:HG3	2.21	0.54
1:B:81:SER:HA	1:B:146:ILE:O	2.06	0.54
1:A:268:ALA:HA	1:A:273:GLY:CA	2.38	0.54
1:A:276:VAL:O	1:A:311:TYR:HA	2.08	0.54
1:B:197:ASN:O	1:B:201:ARG:HG3	2.08	0.54
1:B:389:PHE:HE1	1:B:416:ALA:HA	1.72	0.54
1:B:282:ILE:HD12	1:B:282:ILE:H	1.72	0.54
1:A:93:ASP:OD2	1:A:95:ARG:HB3	2.08	0.54
1:A:247:MET:HA	2:A:778:HOH:O	2.07	0.54
1:A:697:PRO:HB3	1:A:725:ILE:HD13	1.90	0.54
1:B:302:TYR:HE1	2:B:869:HOH:O	1.89	0.54
1:B:606:PHE:O	1:B:622:GLN:HA	2.07	0.54
1:A:55:GLU:O	1:A:58:ASP:HB2	2.08	0.54
1:B:667:LEU:HB2	1:B:691:TRP:CZ3	2.43	0.53
1:B:683:ILE:HG12	1:B:689:VAL:HG11	1.89	0.53
1:B:557:ILE:HD13	1:B:597:GLN:HB3	1.91	0.53
1:A:515:ARG:HD3	1:A:518:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ILE:HG22	1:A:550:THR:H	1.73	0.53
1:A:507:ASN:HB3	1:A:509:GLU:OE1	2.08	0.53
1:A:557:ILE:HG13	1:A:597:GLN:HB2	1.91	0.53
1:B:227:TYR:CE2	1:B:326:ARG:NH1	2.76	0.53
1:B:662:ASN:HD21	1:B:681:ARG:HH21	1.56	0.53
1:A:217:VAL:HG22	1:A:338:TYR:HB3	1.91	0.53
1:B:276:VAL:O	1:B:311:TYR:HA	2.08	0.53
1:A:692:GLU:OE1	1:A:692:GLU:HA	2.09	0.52
1:B:356:GLU:HB2	1:B:446:LYS:NZ	2.23	0.52
1:B:544:HIS:CD2	1:B:580:LEU:HD21	2.45	0.52
1:A:600:GLU:HG3	1:A:715:ARG:CD	2.40	0.52
1:B:659:THR:HG22	1:B:684:ARG:HA	1.90	0.52
1:A:12:ARG:HD3	1:A:14:VAL:O	2.09	0.52
1:A:353:PHE:HB2	1:A:365:THR:OG1	2.09	0.52
1:B:515:ARG:HH22	1:B:520:MET:H	1.57	0.52
1:A:672:VAL:HG13	1:A:697:PRO:HG3	1.91	0.52
1:A:90:ARG:HH11	1:A:90:ARG:HG3	1.74	0.52
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.44	0.52
1:B:615:THR:O	1:B:617:ASP:N	2.43	0.52
1:A:231:GLU:HB3	1:A:674:ARG:NH2	2.25	0.51
1:A:153:ILE:HD11	1:A:250:SER:HA	1.93	0.51
1:B:662:ASN:HD22	1:B:662:ASN:H	1.55	0.51
1:A:44:PHE:O	1:A:45:LEU:CB	2.59	0.51
1:B:545:ASN:OD1	1:B:546:ARG:N	2.44	0.51
1:A:349:GLN:HG2	1:A:440:ILE:CG1	2.41	0.51
1:A:68:LYS:HB2	2:A:849:HOH:O	2.10	0.51
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.43	0.51
1:A:594:TYR:CD1	1:A:595:MET:N	2.79	0.51
1:A:511:VAL:HG22	1:A:512:MET:H	1.76	0.51
1:A:540:ARG:HG2	1:A:582:PHE:HD2	1.76	0.51
1:A:615:THR:HA	1:A:616:ARG:CZ	2.41	0.50
1:A:349:GLN:HG2	1:A:440:ILE:HG13	1.93	0.50
1:A:444:ALA:HB1	2:A:898:HOH:O	2.11	0.50
1:A:453:GLU:HB3	1:A:513:LYS:HD2	1.92	0.50
1:A:695:CYS:O	1:A:697:PRO:HD3	2.12	0.50
1:B:640:GLN:HB3	1:B:724:GLN:O	2.12	0.50
1:B:673:THR:HB	1:B:695:CYS:SG	2.50	0.50
1:B:709:MET:SD	1:B:710:SER:N	2.84	0.50
1:A:667:LEU:HD11	1:A:705:LEU:CD2	2.38	0.50
1:A:515:ARG:NH1	1:A:520:MET:H	2.10	0.50
1:A:642:VAL:HG13	1:A:697:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:CYS:HB3	1:B:427:ASP:HB2	1.92	0.50
1:A:635:LYS:O	1:A:648:VAL:HA	2.11	0.50
1:B:174:ARG:NH2	1:B:179:ASP:OD1	2.45	0.50
1:B:92:TYR:CE2	1:B:94:PRO:HG3	2.47	0.50
1:A:686:ASN:N	1:A:686:ASN:HD22	2.10	0.49
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.27	0.49
1:B:226:SER:HB2	1:B:670:PRO:HD3	1.94	0.49
1:A:90:ARG:NH2	1:A:97:ASP:OD1	2.46	0.49
1:A:88:PHE:HE2	1:A:142:VAL:HG12	1.78	0.49
1:A:223:ARG:NH2	2:A:768:HOH:O	2.46	0.49
1:A:338:TYR:O	1:A:339:PHE:HB2	2.12	0.49
1:A:515:ARG:CZ	1:A:619:LEU:HD22	2.42	0.49
1:B:511:VAL:HG12	1:B:513:LYS:H	1.78	0.49
1:B:727:ARG:HG3	1:B:727:ARG:HH11	1.78	0.49
1:A:26:LEU:HD11	1:A:104:VAL:HG11	1.95	0.49
1:A:527:ALA:HB2	1:A:533:PHE:CD1	2.48	0.49
1:A:656:LEU:HD12	1:A:660:LEU:CD2	2.42	0.49
1:B:56:ARG:HG3	2:B:929:HOH:O	2.13	0.49
1:A:100:ARG:CG	1:A:164:TRP:HE1	2.26	0.49
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.95	0.49
1:A:507:ASN:O	1:A:509:GLU:HG2	2.12	0.49
1:A:659:THR:N	1:A:685:PRO:HG3	2.28	0.49
1:B:15:PRO:HG2	1:B:108:TYR:CZ	2.48	0.49
1:A:615:THR:HA	1:A:616:ARG:NH1	2.27	0.48
1:B:104:VAL:HG12	1:B:116:TYR:HD1	1.77	0.48
1:A:629:ILE:CG2	1:A:630:PRO:HD2	2.42	0.48
1:B:214:TYR:HB2	1:B:372:TYR:CZ	2.48	0.48
1:B:452:VAL:O	1:B:452:VAL:HG23	2.13	0.48
1:B:697:PRO:HB2	1:B:725:ILE:HG21	1.95	0.48
1:A:126:GLN:HG3	1:A:129:LYS:HB3	1.95	0.48
1:A:192:ALA:HB1	1:A:381:THR:OG1	2.13	0.48
1:A:705:LEU:C	1:A:706:ILE:HG13	2.38	0.48
1:A:635:LYS:O	1:A:649:THR:N	2.45	0.48
1:B:221:LYS:HE2	1:B:626:VAL:CG2	2.43	0.48
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.48	0.48
1:A:656:LEU:C	1:A:658:GLU:H	2.22	0.48
1:B:281:ASN:OD1	1:B:600:GLU:HG3	2.14	0.48
1:A:217:VAL:HG23	2:A:783:HOH:O	2.12	0.48
1:A:465:VAL:HG21	1:A:474:MET:SD	2.54	0.48
1:A:55:GLU:HB2	1:A:58:ASP:OD2	2.13	0.48
1:A:68:LYS:HD3	1:A:230:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.45	0.48
1:A:549:ILE:HG22	1:A:550:THR:N	2.29	0.48
1:A:469:ILE:HD11	2:A:925:HOH:O	2.13	0.47
1:B:252:ARG:HD3	2:B:784:HOH:O	2.13	0.47
1:B:428:ALA:HB3	1:B:429:PRO:HD3	1.95	0.47
1:B:431:VAL:O	1:B:434:GLU:HB2	2.14	0.47
1:B:380:MET:HG3	1:B:381:THR:O	2.14	0.47
1:A:107:ARG:HG2	1:A:107:ARG:NH1	2.29	0.47
1:A:198:GLU:O	1:A:202:GLU:HG2	2.15	0.47
1:B:441:TYR:CD1	1:B:454:ASN:HB3	2.50	0.47
1:B:55:GLU:O	1:B:58:ASP:HB2	2.14	0.47
1:B:226:SER:HB3	1:B:670:PRO:HD3	1.97	0.47
1:A:220:ILE:HG21	1:A:474:MET:HE1	1.97	0.47
1:A:343:ASP:HA	1:A:400:GLN:HG3	1.97	0.47
1:A:439:LEU:HD12	1:A:459:HIS:HB3	1.96	0.47
1:A:605:HIS:HE1	1:A:622:GLN:HB3	1.79	0.47
1:B:519:ASP:HB3	1:B:540:ARG:NH1	2.28	0.47
1:B:544:HIS:HA	1:B:580:LEU:HD21	1.96	0.47
1:B:557:ILE:CD1	1:B:597:GLN:HB3	2.45	0.47
1:B:609:THR:HA	1:B:619:LEU:O	2.15	0.47
1:B:640:GLN:HB2	2:B:1013:HOH:O	2.14	0.47
1:A:351:ASP:HB2	2:A:806:HOH:O	2.15	0.47
1:A:498:LEU:HD12	1:A:502:ALA:O	2.15	0.47
1:B:515:ARG:HA	1:B:617:ASP:CB	2.44	0.47
1:B:614:GLU:CD	1:B:614:GLU:H	2.23	0.47
1:A:196:ASP:O	1:A:196:ASP:CG	2.58	0.46
1:A:235:LEU:O	1:A:235:LEU:HD22	2.15	0.46
1:B:524:VAL:HG22	1:B:535:LEU:HG	1.97	0.46
1:A:697:PRO:CB	1:A:725:ILE:HD13	2.45	0.46
1:B:396:ASP:O	1:B:408:ARG:HB2	2.15	0.46
1:B:644:SER:O	1:B:697:PRO:HD2	2.16	0.46
1:A:515:ARG:O	1:A:518:VAL:HB	2.16	0.46
1:A:666:HIS:O	1:A:707:ALA:HA	2.16	0.46
1:A:702:HIS:CE1	1:A:703:ARG:O	2.68	0.46
1:A:109:PRO:HA	1:A:115:THR:OG1	2.15	0.46
1:B:442:ILE:HG12	1:B:452:VAL:HG12	1.97	0.46
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.51	0.46
1:B:247:MET:O	1:B:248:ASP:C	2.58	0.46
1:B:342:HIS:HE1	2:B:752:HOH:O	1.98	0.46
1:B:507:ASN:OD1	1:B:508:THR:N	2.48	0.46
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG13	1:A:512:MET:H	1.81	0.46
1:A:650:ILE:HB	1:A:691:TRP:CB	2.35	0.46
1:B:130:TRP:HA	1:B:147:GLN:O	2.16	0.46
1:B:515:ARG:NE	1:B:619:LEU:HD22	2.31	0.46
1:B:657:LYS:HE3	2:B:867:HOH:O	2.15	0.46
1:B:227:TYR:CD2	1:B:326:ARG:NH1	2.84	0.46
1:A:685:PRO:O	1:A:686:ASN:HB2	2.15	0.46
1:B:559:PHE:HD2	2:B:829:HOH:O	1.97	0.46
1:B:684:ARG:HB2	1:B:687:SER:OG	2.16	0.46
1:A:636:VAL:HA	1:A:647:THR:O	2.17	0.45
1:A:641:VAL:HA	1:A:726:GLN:O	2.16	0.45
1:B:645:ASP:OD1	1:B:696:ARG:HG2	2.16	0.45
1:A:193:VAL:O	1:A:193:VAL:HG12	2.16	0.45
1:B:138:GLU:HG2	1:B:141:SER:HB2	1.98	0.45
1:B:643:GLY:O	1:B:696:ARG:NH2	2.50	0.45
1:B:616:ARG:CD	1:B:616:ARG:N	2.79	0.45
1:A:111:GLU:HB3	1:A:116:TYR:HD2	1.82	0.45
1:A:549:ILE:CD1	1:A:612:ILE:HG12	2.38	0.45
1:A:611:ARG:NH2	2:A:808:HOH:O	2.49	0.45
1:B:137:ARG:HD2	2:B:880:HOH:O	2.15	0.45
1:B:522:PHE:O	1:B:623:LYS:HE2	2.16	0.45
1:A:314:CYS:HB2	1:A:373:HIS:CE1	2.51	0.45
1:B:193:VAL:HG21	1:B:330:ILE:HG23	1.98	0.45
1:A:629:ILE:HG23	1:A:630:PRO:HD2	1.99	0.45
1:B:187:TRP:CZ2	1:B:206:LEU:HD21	2.52	0.45
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.99	0.45
1:B:629:ILE:HG21	1:B:717:VAL:HG22	1.99	0.45
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.99	0.45
1:B:508:THR:O	1:B:512:MET:HG3	2.17	0.45
1:A:353:PHE:HB2	1:A:364:LEU:O	2.16	0.45
1:B:113:LYS:HB3	1:B:250:SER:OG	2.16	0.45
1:A:305:SER:O	1:A:306:GLU:HB2	2.17	0.45
1:B:214:TYR:HB2	1:B:372:TYR:CE1	2.52	0.44
1:A:44:PHE:CD2	1:A:96:ARG:NH2	2.85	0.44
1:B:580:LEU:N	1:B:580:LEU:HD22	2.32	0.44
1:A:487:GLN:O	1:A:490:GLU:HB3	2.17	0.44
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.48	0.44
1:A:280:ASP:O	1:A:282:ILE:N	2.50	0.44
1:A:298:ILE:HG23	1:A:309:VAL:CG1	2.45	0.44
1:A:468:GLN:HA	1:A:475:MET:HE2	1.99	0.44
1:A:637:ARG:HH12	1:A:647:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:SER:O	1:B:580:LEU:HD22	2.18	0.44
1:B:642:VAL:C	1:B:644:SER:H	2.25	0.44
1:A:235:LEU:HA	1:A:327:CYS:SG	2.58	0.44
1:B:602:ALA:O	1:B:626:VAL:HA	2.18	0.44
1:A:54:LYS:O	1:A:61:LYS:HD2	2.18	0.44
1:A:117:ILE:HG21	1:A:130:TRP:CD2	2.53	0.44
1:A:516:SER:HB2	1:A:547:TYR:CZ	2.52	0.44
1:B:520:MET:HG2	1:B:521:ASP:N	2.32	0.44
1:B:541:ASN:O	1:B:580:LEU:HA	2.17	0.44
1:B:112:ASN:HB3	1:B:113:LYS:HD3	2.00	0.44
1:A:20:ASN:C	1:A:20:ASN:HD22	2.25	0.44
1:A:711:SER:C	1:A:713:SER:N	2.73	0.44
1:B:612:ILE:O	1:B:614:GLU:N	2.51	0.44
1:B:723:VAL:HG23	1:B:725:ILE:HG13	2.00	0.44
1:A:102:GLU:HB2	1:A:160:TYR:HB2	2.00	0.43
1:A:370:TRP:N	1:A:370:TRP:CD1	2.84	0.43
1:A:515:ARG:HG2	1:A:619:LEU:CD2	2.48	0.43
1:B:520:MET:HB3	1:B:520:MET:HE2	1.84	0.43
1:A:88:PHE:HE2	1:A:142:VAL:CG1	2.31	0.43
1:A:354:LEU:HD11	1:A:609:THR:HG21	2.00	0.43
1:A:370:TRP:O	1:A:371:ASN:C	2.61	0.43
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.99	0.43
1:B:635:LYS:HE3	1:B:635:LYS:HB2	1.68	0.43
1:A:402:ASN:HA	1:A:430:PHE:CE2	2.53	0.43
1:A:494:LEU:HD12	1:A:494:LEU:HA	1.85	0.43
1:B:512:MET:N	1:B:512:MET:HE3	2.34	0.43
1:A:553:LEU:HD13	1:A:554:SER:N	2.33	0.43
1:B:311:TYR:CD1	1:B:311:TYR:N	2.84	0.43
1:B:507:ASN:OD1	1:B:509:GLU:N	2.51	0.43
1:B:612:ILE:HD12	1:B:617:ASP:HB2	2.00	0.43
1:B:121:ILE:HA	1:B:132:ALA:O	2.18	0.43
1:B:282:ILE:HD12	1:B:282:ILE:N	2.32	0.43
1:A:515:ARG:HB3	1:A:518:VAL:O	2.19	0.43
1:B:223:ARG:HH12	1:B:225:TRP:HE3	1.65	0.43
1:B:400:GLN:NE2	1:B:430:PHE:HB3	2.33	0.43
1:B:653:THR:O	1:B:655:PRO:HD3	2.18	0.43
1:A:400:GLN:HG2	2:A:799:HOH:O	2.18	0.43
1:A:408:ARG:HD2	1:A:408:ARG:O	2.18	0.43
1:B:123:SER:O	1:B:133:LYS:HG3	2.19	0.43
1:B:408:ARG:HD2	1:B:408:ARG:C	2.43	0.43
1:B:636:VAL:HA	1:B:647:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:O	1:A:510:GLY:N	2.52	0.43
1:B:175:ASN:HB3	2:B:809:HOH:O	2.17	0.43
1:B:339:PHE:O	1:B:460:ILE:O	2.37	0.43
1:B:382:ARG:NH2	1:B:426:PHE:HD2	2.16	0.43
1:A:147:GLN:HG3	1:A:148:SER:N	2.33	0.43
1:A:602:ALA:HB1	1:A:627:LEU:HB2	2.00	0.43
1:A:665:VAL:CG2	1:A:680:PHE:HE1	2.30	0.43
1:B:69:TYR:O	1:B:71:ASN:N	2.50	0.42
1:B:538:THR:HG23	2:B:863:HOH:O	2.18	0.42
1:A:211:VAL:HG11	1:A:472:ASP:HB3	2.01	0.42
1:A:64:HIS:CE1	1:A:80:GLN:OE1	2.73	0.42
1:A:648:VAL:HG21	1:A:705:LEU:HD11	2.00	0.42
1:B:181:TYR:CE2	1:B:235:LEU:HD13	2.54	0.42
1:B:612:ILE:O	1:B:612:ILE:CG2	2.66	0.42
1:A:110:GLN:HE22	1:B:366:LYS:HB2	1.85	0.42
1:A:642:VAL:CG2	1:A:700:SER:HB3	2.50	0.42
1:A:713:SER:HB2	1:A:714:LEU:H	1.72	0.42
1:B:270:ASP:O	1:B:272:GLU:N	2.48	0.42
1:B:342:HIS:HA	1:B:434:GLU:OE2	2.19	0.42
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.48	0.42
1:A:193:VAL:O	1:A:193:VAL:CG1	2.67	0.42
1:A:476:ASP:C	1:A:478:THR:H	2.28	0.42
1:A:701:GLY:O	1:A:703:ARG:HG2	2.20	0.42
1:B:240:TYR:OH	1:B:244:ARG:NH1	2.52	0.42
1:B:678:LYS:HB2	1:B:691:TRP:CZ2	2.54	0.42
1:A:534:LYS:HD2	1:A:586:ALA:HB1	2.01	0.42
2:A:809:HOH:O	1:B:424:PHE:HA	2.19	0.42
1:B:529:LEU:HD12	1:B:656:LEU:CD2	2.49	0.42
1:B:552:TYR:N	1:B:609:THR:O	2.52	0.42
1:A:105:ILE:HG23	1:A:157:PHE:CD2	2.55	0.42
1:B:34:VAL:O	1:B:35:VAL:C	2.63	0.42
1:B:539:PHE:HB2	1:B:577:LEU:HD11	2.02	0.42
1:A:93:ASP:HA	1:A:94:PRO:HD3	1.85	0.42
1:A:364:LEU:C	1:A:364:LEU:HD23	2.44	0.42
1:A:514:SER:C	1:A:516:SER:H	2.28	0.42
1:A:704:LYS:HE3	1:A:704:LYS:HB2	1.89	0.42
1:B:54:LYS:O	1:B:61:LYS:HE3	2.20	0.42
1:A:136:MET:HE2	1:A:136:MET:HB3	1.97	0.41
1:A:247:MET:HE1	1:A:258:VAL:HG22	2.02	0.41
1:B:489:GLU:CD	1:B:489:GLU:H	2.27	0.41
1:A:280:ASP:C	1:A:282:ILE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:N	1:B:87:ASP:O	2.48	0.41
1:B:697:PRO:HB3	1:B:725:ILE:HD13	2.02	0.41
1:A:283:TYR:CZ	1:A:289:PRO:HD2	2.55	0.41
1:A:611:ARG:HD2	1:A:616:ARG:HA	2.02	0.41
1:A:615:THR:O	1:A:616:ARG:C	2.63	0.41
1:B:538:THR:O	1:B:540:ARG:NH2	2.53	0.41
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.50	0.41
1:A:484:GLN:CG	1:A:487:GLN:HG3	2.49	0.41
1:A:506:LEU:HD12	2:A:902:HOH:O	2.19	0.41
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.92	0.41
1:B:77:ARG:HB3	1:B:185:ASN:HB2	2.02	0.41
1:B:513:LYS:HE2	1:B:513:LYS:HB2	1.87	0.41
1:A:120:PRO:O	1:A:122:VAL:HG23	2.21	0.41
1:B:93:ASP:C	1:B:95:ARG:H	2.28	0.41
1:B:341:ALA:HB2	1:B:460:ILE:HD13	2.03	0.41
1:B:527:ALA:HB1	1:B:531:LYS:HB2	2.03	0.41
1:B:654:ASN:HB2	1:B:683:ILE:CG2	2.51	0.41
1:A:406:MET:HE1	1:B:11:ARG:HH21	1.86	0.41
1:B:172:THR:HB	2:B:876:HOH:O	2.21	0.41
1:B:398:THR:HA	1:B:399:PRO:HD3	1.80	0.41
1:B:515:ARG:CB	1:B:619:LEU:HD21	2.45	0.41
1:B:223:ARG:NH1	1:B:225:TRP:HE3	2.18	0.41
1:B:335:VAL:HG21	1:B:377:GLU:HG3	2.03	0.41
1:A:71:ASN:CB	1:A:75:ILE:HD11	2.48	0.41
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.56	0.41
1:A:646:MET:HE3	1:A:648:VAL:CG2	2.50	0.41
1:A:680:PHE:N	1:A:680:PHE:CD1	2.89	0.41
1:B:528:VAL:HG12	1:B:529:LEU:N	2.36	0.41
1:B:530:GLY:HA2	1:B:595:MET:SD	2.61	0.41
1:B:578:GLU:O	1:B:581:SER:HB2	2.21	0.41
1:A:74:LEU:HD23	1:A:180:THR:HG23	2.03	0.41
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.56	0.41
1:A:449:THR:HG22	1:A:450:HIS:N	2.36	0.41
1:B:186:PRO:O	1:B:194:TYR:HD1	2.04	0.41
1:B:221:LYS:HE2	1:B:626:VAL:HG23	2.01	0.41
1:B:277:GLY:HA2	1:B:312:GLY:O	2.20	0.41
1:B:515:ARG:HE	1:B:619:LEU:HD22	1.84	0.41
1:B:637:ARG:NH2	1:B:692:GLU:OE1	2.55	0.40
1:A:198:GLU:HA	1:A:201:ARG:NH1	2.37	0.40
1:A:537:ILE:O	1:A:584:LYS:HA	2.21	0.40
1:B:549:ILE:CG2	1:B:550:THR:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:MET:HE1	1:B:693:GLU:HG2	2.04	0.40
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.97	0.40
1:A:247:MET:HE2	1:A:252:ARG:HG2	2.03	0.40
1:A:404:ASP:O	1:A:407:TYR:HE2	2.05	0.40
1:A:535:LEU:HD23	1:A:535:LEU:C	2.46	0.40
1:B:410:GLY:HA2	1:B:411:PRO:C	2.46	0.40
1:A:90:ARG:HH22	1:A:97:ASP:CG	2.29	0.40
1:B:546:ARG:HB2	1:B:579:PRO:HG3	2.02	0.40
1:B:120:PRO:O	1:B:122:VAL:HG23	2.22	0.40
1:B:209:ILE:HG22	1:B:210:GLY:N	2.37	0.40
1:B:455:VAL:O	1:B:455:VAL:HG13	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	701/731 (96%)	617 (88%)	63 (9%)	21 (3%)	3 5
1	B	710/731 (97%)	626 (88%)	69 (10%)	15 (2%)	5 9
All	All	1411/1462 (96%)	1243 (88%)	132 (9%)	36 (3%)	4 7

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	511	VAL
1	B	426	PHE
1	B	613	ASN
1	B	616	ARG
1	A	268	ALA
1	A	273	GLY

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Mol	Chain	Res	Type
1	A	284	ALA
1	A	425	GLN
1	A	427	ASP
1	A	600	GLU
1	B	273	GLY
1	B	446	LYS
1	A	139	ASP
1	A	281	ASN
1	A	311	TYR
1	A	365	THR
1	A	426	PHE
1	B	270	ASP
1	A	446	LYS
1	A	470	GLY
1	B	252	ARG
1	B	271	ASP
1	B	470	GLY
1	B	612	ILE
1	B	614	GLU
1	A	60	ASN
1	A	94	PRO
1	B	512	MET
1	A	616	ARG
1	B	35	VAL
1	B	94	PRO
1	B	91	PRO
1	A	256	ILE
1	A	477	ILE
1	A	669	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	620/644 (96%)	560 (90%)	60 (10%)	8	17
1	B	626/644 (97%)	561 (90%)	65 (10%)	7	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1246/1288 (97%)	1121 (90%)	125 (10%)	7 15

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	81	SER
1	A	100	ARG
1	A	104	VAL
1	A	123	SER
1	A	127	SER
1	A	142	VAL
1	A	147	GLN
1	A	156	LYS
1	A	172	THR
1	A	173	SER
1	A	206	LEU
1	A	211	VAL
1	A	221	LYS
1	A	223	ARG
1	A	235	LEU
1	A	271	ASP
1	A	281	ASN
1	A	289	PRO
1	A	293	THR
1	A	310	ARG
1	A	314	CYS
1	A	320	VAL
1	A	336	THR
1	A	350	MET
1	A	354	LEU
1	A	363	LYS
1	A	368	SER
1	A	369	VAL
1	A	387	VAL
1	A	408	ARG
1	A	427	ASP
1	A	451	VAL
1	A	454	ASN

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Mol	Chain	Res	Type
1	A	479	ASP
1	A	489	GLU
1	A	498	LEU
1	A	513	LYS
1	A	516	SER
1	A	520	MET
1	A	553	LEU
1	A	556	ASN
1	A	572	THR
1	A	574	ASP
1	A	577	LEU
1	A	590	GLN
1	A	604	LEU
1	A	616	ARG
1	A	637	ARG
1	A	661	ARG
1	A	665	VAL
1	A	674	ARG
1	A	705	LEU
1	A	713	SER
1	A	716	HIS
1	A	721	LEU
1	A	722	ASP
1	B	29	VAL
1	B	30	GLU
1	B	47	VAL
1	B	58	ASP
1	B	76	VAL
1	B	91	PRO
1	B	98	LEU
1	B	104	VAL
1	B	105	ILE
1	B	112	ASN
1	B	115	THR
1	B	117	ILE
1	B	121	ILE
1	B	126	GLN
1	B	148	SER
1	B	167	TYR
1	B	171	ARG
1	B	172	THR
1	B	193	VAL

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	212	ILE
1	B	217	VAL
1	B	224	SER
1	B	235	LEU
1	B	295	SER
1	B	301	GLU
1	B	307	ASN
1	B	335	VAL
1	B	340	SER
1	B	350	MET
1	B	354	LEU
1	B	374	CYS
1	B	387	VAL
1	B	418	LYS
1	B	427	ASP
1	B	435	VAL
1	B	462	LYS
1	B	463	LEU
1	B	465	VAL
1	B	472	ASP
1	B	487	GLN
1	B	489	GLU
1	B	490	GLU
1	B	494	LEU
1	B	512	MET
1	B	526	ASN
1	B	540	ARG
1	B	546	ARG
1	B	553	LEU
1	B	554	SER
1	B	588	LEU
1	B	589	ILE
1	B	597	GLN
1	B	604	LEU
1	B	616	ARG
1	B	639	THR
1	B	640	GLN
1	B	650	ILE
1	B	662	ASN
1	B	681	ARG
1	B	692	GLU

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Mol	Chain	Res	Type
1	B	694	VAL
1	B	708	SER
1	B	713	SER
1	B	726	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	71	ASN
1	A	110	GLN
1	A	307	ASN
1	A	337	ASN
1	A	347	ASN
1	A	454	ASN
1	A	484	GLN
1	A	487	GLN
1	A	545	ASN
1	A	556	ASN
1	A	622	GLN
1	A	726	GLN
1	B	71	ASN
1	B	112	ASN
1	B	126	GLN
1	B	267	ASN
1	B	307	ASN
1	B	421	HIS
1	B	544	HIS
1	B	556	ASN
1	B	597	GLN
1	B	662	ASN
1	B	724	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.