



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:24 am BST

PDB ID : 1FIE
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (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) : 2.11

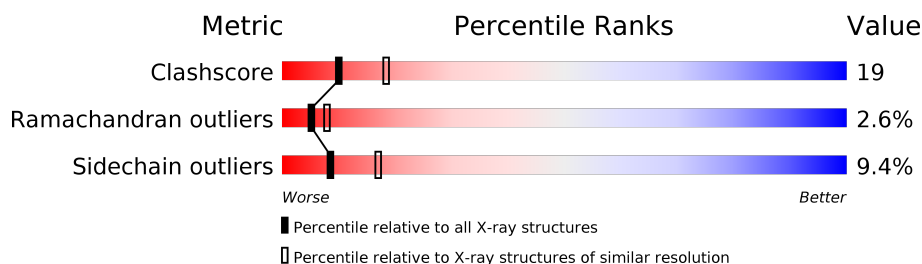
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on 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		

V665	G596	D519	K418	G312	M197	Y108
R666	Q597	M520	F424	A318	R201	N112
L667	L598	D521	Q425	A318	R201	K113
P670	L599	F522	F426	N322	L206	G114
T673	E600	E523	D427	R326	I209	T115
	G601	E524	A428	I330	G210	Y116
	A602	E525	P429	P331	V211	
R678	S603	M526	F430	V335	Y214	
	L604	A527	V431	F339	V217	P120
R681	H605	V528	E434	S340	K221	I121
E682	F606	L529	V435	A341	R223	V122
I683	T609	G530	E434	R342	S224	S123
R684	A610	K531	V435	L354	W225	
P685	E611	E532	Y441	E355	Y227	Q126
S686	L612	F533	I442	E356	L235	S127
T687	N613	K534	K446	N361	Y240	G128
V688	E614	L535	V455	L364	R244	W130
G689	T615	T538	L460	E377	M247	G131
Q690	R616	F539	V463	A378	D248	A132
W691	D617	R540	E463	W379	L249	K133
E692	V618	M541	N454	W380	S250	I134
E693	L619	N542	V455	T381	G251	
V694		S543	L460	R382	R252	P150
C695	Q622	H544	L463	F389	V276	I153
R696	K623	M545	L464	W392	G277	R137
P697	V626	R546	V465	D396	N281	E138
R703	I629	I549	L466	T398	I282	D139
S708	L632	T550	T466	P399	S295	R140
W709	I633	A551	K467	Q400	I298	S141
S710	L634	Y552	G471	M406	Y302	
S713	I635	L553	D472	Y407	Y302	
	K635	S554	G473	R408	N307	P186
V717	V636	I557	M474	K513	F308	W187
	R637	T558	E488	K514	V309	
	G638	F559	E489	S515	R310	V193
L721	T639	Y560	E490	S516	Y311	Y194
D722	Q640	K565	R491	N517		
V723	G643	V575	L494	V518		
Q724	S644	L577	N507			
I725	D645	E578	T508			
Q726	R646	P579	E509			
R727	T647	L580	G510			
ARG	I650	S581	V511			
PRO	T653	F582	E509			
SER	M654	K583	G510			
MET	L656	K584	V511			
	K657	L588	R512			
	E658	I589	K513			
	T659	Q590	S514			
	L660	A591	R515			
	R661	Y594	S516			
	N662	M595	V518			

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 [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	0.58	0/5784	0.83	2/7848 (0.0%)
1	B	0.61	0/5853	0.84	3/7941 (0.0%)
All	All	0.60	0/11637	0.83	5/15789 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-7.06	91.95	111.00
1	A	426	PHE	CB-CA-C	5.36	121.13	110.40
1	B	425	GLN	N-CA-C	5.33	125.39	111.00
1	B	518	VAL	N-CA-C	-5.28	96.76	111.00
1	B	460	ILE	N-CA-C	5.21	125.06	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5518	214	0
1	B	5720	0	5566	216	0
2	A	270	0	0	14	0
2	B	287	0	0	17	0
All	All	11928	0	11084	427	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 19.

All (427) 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: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:40:ASN:C	1:B:41:LEU:CA	2.48	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
1:A:634:ILE:HG22	1:A:721:LEU:HD12	1.73	0.69
1:A:121:ILE:O	1:A:121:ILE:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASN:HB3	1:B:542:ASN:HB2	1.78	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:HG22	1:B:612:ILE:O	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:HH11	1:A:107:ARG:HG2	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
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:649:THR:HA	1:A:691:TRP:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:O	1:B:164:TRP:CZ3	2.55	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: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:578:GLU:HB2	1:B:581:SER:OG	2.03	0.58
1:B:226:SER:CB	1:B:670:PRO:HD3	2.34	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: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:511:VAL:HG12	1:B:512:MET:H	1.69	0.56
1:B:92:TYR:O	1:B:94:PRO:HD3	2.04	0.56
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.86	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:A:657:LYS:HD3	1:A:686:ASN:HD21	1.69	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
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:392:TRP:HB2	2:B:976:HOH:O	2.04	0.56
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:538:THR:C	1:B:540:ARG:HH21	2.09	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:H	1:B:282:ILE:HD12	1.72	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:A:93:ASP:OD2	1:A:95:ARG:HB3	2.08	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:A:682:GLU:CD	1:A:684:ARG:HH12	2.12	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:507:ASN:C	1:A:509:GLU:N	2.62	0.52
1:A:90:ARG:HG3	1:A:90:ARG:HH11	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:H	1:B:662:ASN:HD22	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:658:GLU:C	1:A:685:PRO:HG3	2.32	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:507:ASN:C	1:A:509:GLU:H	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:727:ARG:HG3	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:370:TRP:HZ3	1:B:560:TYR:HH	1.60	0.48
1:B:452:VAL:HG23	1:B:452:VAL:O	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: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: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
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:NH1	1:A:107:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:235:LEU:HD22	1:A:235:LEU:O	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:B:662:ASN:ND2	1:B:662:ASN:N	2.63	0.46
1:A:515:ARG:O	1:A:518:VAL:HB	2.16	0.46
1:A:702:HIS:CE1	1:A:703:ARG:O	2.68	0.46
1:A:666:HIS:O	1:A:707:ALA:HA	2.16	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: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
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:641:VAL:HA	1:A:726:GLN:O	2.16	0.45
1:A:636:VAL:HA	1:A:647:THR:O	2.17	0.45
1:B:645:ASP:OD1	1:B:696:ARG:HG2	2.16	0.45
1:A:193:VAL:HG12	1:A:193:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:616:ARG:CD	2.79	0.45
1:A:111:GLU:HB3	1:A:116:TYR:HD2	1.82	0.45
1:A:611:ARG:NH2	2:A:808:HOH:O	2.49	0.45
1:A:549:ILE:CD1	1:A:612:ILE:HG12	2.38	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:HD22	1:B:580:LEU:N	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:637:ARG:HH12	1:A:647:THR:HG21	1.82	0.44
1:B:543:SER:O	1:B:580:LEU:HD22	2.18	0.44
1:A:235:LEU:HA	1:A:327:CYS:SG	2.58	0.44
1:B:520:MET:HG2	1:B:521:ASP:N	2.32	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.99	0.43
1:A:354:LEU:HD11	1:A:609:THR:HG21	2.00	0.43
1:A:705:LEU:C	1:A:706:ILE:HG13	2.38	0.43
1:A:88:PHE:HE2	1:A:142:VAL:CG1	2.31	0.43
1:B:635:LYS:HB2	1:B:635:LYS:HE3	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:A:656:LEU:C	1:A:658:GLU:H	2.22	0.43
1:A:553:LEU:HD13	1:A:554:SER:N	2.33	0.43
1:B:311:TYR:N	1:B:311:TYR:CD1	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:N	1:B:282:ILE:HD12	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:636:VAL:HA	1:B:647:THR:O	2.18	0.43
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:538:THR:HG23	2:B:863:HOH:O	2.18	0.42
1:B:69:TYR:O	1:B:71:ASN:N	2.50	0.42
1:A:211:VAL:HG11	1:A:472:ASP:HB3	2.01	0.42
1:B:356:GLU:HB2	1:B:446:LYS:HZ3	1.83	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:CG2	1:B:612:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG1	1:A:193:VAL:O	2.67	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:B:614:GLU:H	1:B:614:GLU:CD	2.23	0.42
1:A:105:ILE:HG23	1:A:157:PHE:CD2	2.55	0.42
1:A:196:ASP:CG	1:A:196:ASP:O	2.58	0.42
1:B:539:PHE:HB2	1:B:577:LEU:HD11	2.02	0.42
1:A:704:LYS:HE3	1:A:704:LYS:HB2	1.89	0.42
1:A:93:ASP:HA	1:A:94:PRO:HD3	1.85	0.42
1:B:54:LYS:O	1:B:61:LYS:HE3	2.20	0.42
1:B:697:PRO:HB3	1:B:725:ILE:HD13	2.02	0.41
1:B:48:THR:N	1:B:87:ASP:O	2.48	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: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:77:ARG:HB3	1:B:185:ASN:HB2	2.02	0.41
1:B:45:LEU:HA	1:B:45:LEU:HD12	1.92	0.41
1:B:513:LYS:HB2	1:B:513:LYS:HE2	1.87	0.41
1:A:120:PRO:O	1:A:122:VAL:HG23	2.21	0.41
1:B:247:MET:O	1:B:248:ASP:C	2.58	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: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:A:711:SER:C	1:A:713:SER:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PHE:CD1	1:A:680:PHE:N	2.89	0.41
1:B:528:VAL:HG12	1:B:529:LEU:N	2.36	0.41
1:B:578:GLU:O	1:B:581:SER:HB2	2.21	0.41
1:B:530:GLY:HA2	1:B:595:MET:SD	2.61	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:A:74:LEU:HD23	1:A:180:THR:HG23	2.03	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
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.97	0.40
1:A:404:ASP:O	1:A:407:TYR:HE2	2.05	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%)	4	6
1	B	710/731 (97%)	626 (88%)	69 (10%)	15 (2%)	7	11
All	All	1411/1462 (96%)	1243 (88%)	132 (9%)	36 (3%)	5	8

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
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%)	561 (90%)	59 (10%)	8	17
1	B	626/644 (97%)	568 (91%)	58 (9%)	9	17
All	All	1246/1288 (97%)	1129 (91%)	117 (9%)	8	17

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	20	ASN
1	A	25	ASP
1	A	46	ASN
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	137	ARG
1	A	147	GLN
1	A	156	LYS
1	A	172	THR
1	A	173	SER
1	A	206	LEU
1	A	216	GLU
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	350	MET
1	A	354	LEU
1	A	368	SER
1	A	387	VAL
1	A	408	ARG

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Mol	Chain	Res	Type
1	A	427	ASP
1	A	451	VAL
1	A	454	ASN
1	A	479	ASP
1	A	489	GLU
1	A	498	LEU
1	A	512	MET
1	A	513	LYS
1	A	516	SER
1	A	520	MET
1	A	545	ASN
1	A	572	THR
1	A	574	ASP
1	A	577	LEU
1	A	590	GLN
1	A	597	GLN
1	A	604	LEU
1	A	616	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	20	ASN
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	121	ILE
1	B	126	GLN
1	B	148	SER
1	B	167	TYR
1	B	171	ARG

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Mol	Chain	Res	Type
1	B	172	THR
1	B	174	ARG
1	B	193	VAL
1	B	217	VAL
1	B	224	SER
1	B	235	LEU
1	B	295	SER
1	B	307	ASN
1	B	340	SER
1	B	354	LEU
1	B	374	CYS
1	B	406	MET
1	B	408	ARG
1	B	418	LYS
1	B	427	ASP
1	B	435	VAL
1	B	463	LEU
1	B	465	VAL
1	B	472	ASP
1	B	485	GLU
1	B	487	GLN
1	B	489	GLU
1	B	490	GLU
1	B	491	ARG
1	B	494	LEU
1	B	512	MET
1	B	526	ASN
1	B	540	ARG
1	B	546	ARG
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	661	ARG
1	B	681	ARG
1	B	694	VAL
1	B	708	SER
1	B	713	SER
1	B	726	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	110	GLN
1	A	267	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	18	ASN
1	B	110	GLN
1	B	126	GLN
1	B	307	ASN
1	B	544	HIS
1	B	613	ASN
1	B	662	ASN
1	B	686	ASN
1	B	724	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 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.