



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:25 PM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

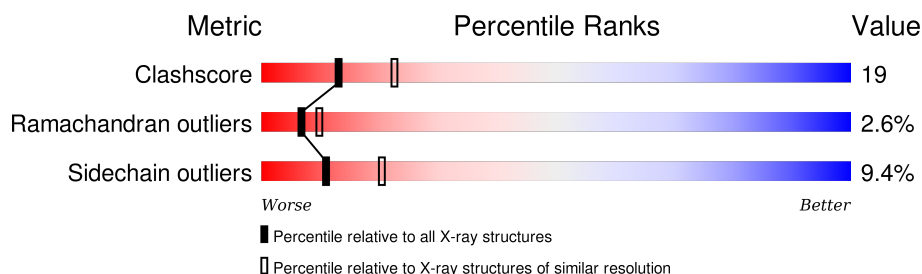
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	 56% 35% 5% .
1	B	731	 58% 36% . .

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.

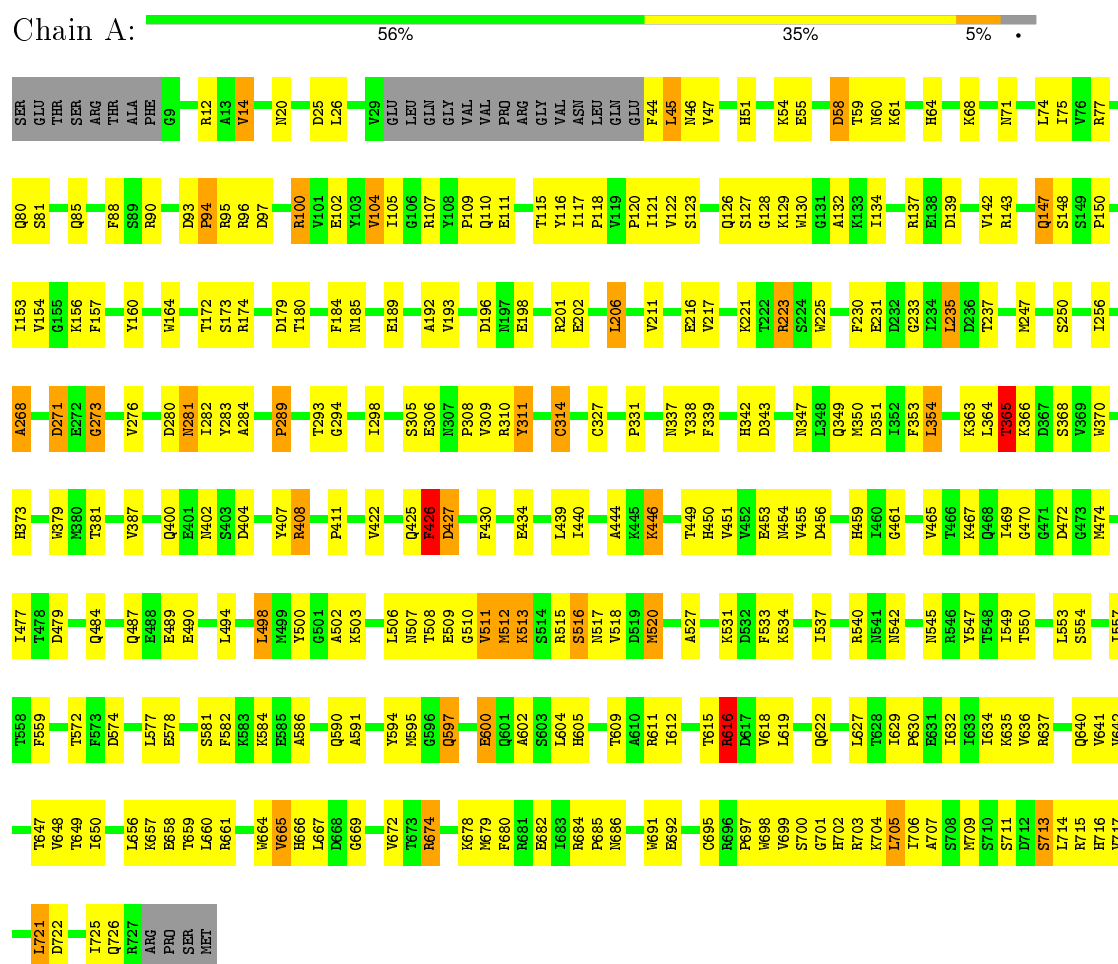
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	270	Total	O	0	0
			270	270		
2	B	287	Total	O	0	0
			287	287		

3 Residue-property plots [i](#)

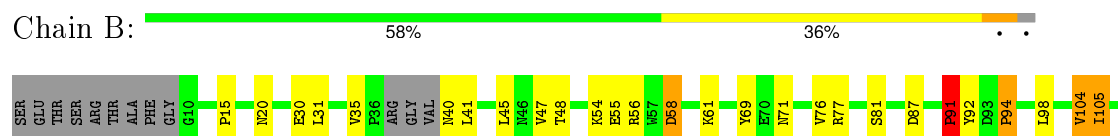
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: COAGULATION FACTOR XIII



• Molecule 1: COAGULATION FACTOR XIII



V665	H666	L667	P670	T673	K678	R681	E682	I683	R684	P685	M686	S687	T688	V689	Q690	M691	E692	E693	V694	C695	R696	P697	R703	S708	M709	S710	S713	V717	L721	D722	Q724	I725	Q726	R727	ARG	PRO	SER	MET														
G596	Q597	L598	E599	E600	Q601	A602	S603	L604	H605	F606	T609	A610	R611	M612	N613	E614	T615	R616	D617	V618	L619	Q622	K623	V626	I629	I632	I633	I634	K635	V636	R637	G638	T639	Q640	G643	S644	D645	K646	T647	I650	T653	N654	P655	L656	K657	E658	T659	L660	R661	N662		
D519	M520	D521	F522	E523	V524	E525	H526	A527	V528	L529	G530	K531	E532	F533	K534	L535	T538	F539	R540	N541	N542	S543	H544	N545	R546	I549	T550	A551	T552	L553	S554	I557	T558	F559	I560	K565	V575	T576	L577	E578	P579	L580	S581	F582	K583	K584	L588	I589	O590	A591	Y594	N595
K418	F424	Q425	F426	D427	A428	P429	V430	V431	E434	V435	Y441	I442	K446	V452	E453	N454	V455	I460	L463	I464	V465	T466	K467	G470	G471	D472	G473	M474	E485	G486	Q487	E488	E489	E490	K491	L494	N507	T508	E509	G510	V511	M512	K513	S514	R515	S516	N517	V518				
G312	A318	N322	L206	R326	I209	G210	I221	V211	Y214	V335	F339	S340	A341	H342	L354	E355	E356	N361	L364	T365	K366	W370	N371	Y372	H373	C374	E377	A378	K379	K380	T381	R382	F389	W392	D396	S397	T398	P399	Q400	M406	Y407	R408	C409	G410	P411	A416	I417					
M197	R201	L206	I209	G210	V211	Y214	V217	K221	T222	R223	S224	W225	Y227	L235	Y240	R244	M247	D248	L249	S250	G251	R252	A268	K269	D270	D271	E272	G273	V276	G277	N281	I282	S285	I298	Y302	N307	F308	V309	R310	Y311	N185	P186	W187	V193	Y194							
Y108	M112	K113	G114	T115	Y116	P120	I121	V122	S123	Q126	S127	G128	K129	W130	G131	A132	K133	I134	R137	E138	D139	R140	S141	I146	Q147	S148	S149	P150	I153	R158	W164	Y167	G168	R171	T172	S173	R174	N175	D179	T180	Y181	N185	P186	W187	V193	Y194						

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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:667:LEU:HD11	1:A:705:LEU:HD22	1.62	0.81
1:A:337:ASN:HD21	1:A:461:GLY:HA2	1.45	0.81
1:B:650:ILE:HG21	1:B:665:VAL:HG11	1.63	0.79
1:B:223:ARG:HH11	1:B:223:ARG:HG3	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:650:ILE:HD11	1:A:667:LEU:HD13	1.67	0.76
1:A:298:ILE:HG23	1:A:309:VAL:HG11	1.68	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:HG3	1:B:546:ARG:HH11	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:B:515:ARG:HH12	1:B:519:ASP:HA	1.64	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: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:B:518:VAL:HA	1:B:540:ARG:O	2.01	0.60
1:A:640:GLN:O	1:A:726:GLN:HG2	2.02	0.60
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.83	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: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:A:100:ARG:HE	1:A:164:TRP:HZ2	1.51	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:B:511:VAL:HG12	1:B:512:MET:N	2.20	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: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:B:511:VAL:HG12	1:B:512:MET:H	1.69	0.56
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:223:ARG:HG3	1:B:223:ARG:NH1	2.17	0.56
1:A:657:LYS:HD3	1:A:686:ASN:HD21	1.69	0.56
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.87	0.56
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.86	0.56
1:B:634:ILE:O	1:B:721:LEU:HD22	2.05	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:A:233:GLY:O	1:A:237:THR:HG23	2.04	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: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:B:539:PHE:O	1:B:582:PHE:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLU:HB2	1:A:581:SER:HB2	1.87	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: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:231:GLU:HB3	1:A:674:ARG:HH22	1.71	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: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:A:247:MET:HA	2:A:778:HOH:O	2.07	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:A:682:GLU:CD	1:A:684:ARG:HH12	2.12	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:549:ILE:HG22	1:A:550:THR:H	1.73	0.53
1:A:515:ARG:HD3	1:A:518:VAL:O	2.08	0.53
1:A:557:ILE:HG13	1:A:597:GLN:HB2	1.91	0.53
1:A:507:ASN:HB3	1:A:509:GLU:OE1	2.08	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:B:276:VAL:O	1:B:311:TYR:HA	2.08	0.53
1:A:217:VAL:HG22	1:A:338:TYR:HB3	1.91	0.53
1:B:356:GLU:HB2	1:B:446:LYS:NZ	2.23	0.52
1:A:692:GLU:OE1	1:A:692:GLU:HA	2.09	0.52
1:B:544:HIS:CD2	1:B:580:LEU:HD21	2.45	0.52
1:B:659:THR:HG22	1:B:684:ARG:HA	1.90	0.52
1:A:600:GLU:HG3	1:A:715:ARG:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HH22	1:B:520:MET:H	1.57	0.52
1:A:353:PHE:HB2	1:A:365:THR:OG1	2.09	0.52
1:A:12:ARG:HD3	1:A:14:VAL:O	2.09	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:B:615:THR:O	1:B:617:ASP:N	2.43	0.52
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.44	0.52
1:A:231:GLU:HB3	1:A:674:ARG:NH2	2.25	0.51
1:B:662:ASN:H	1:B:662:ASN:HD22	1.55	0.51
1:A:153:ILE:HD11	1:A:250:SER:HA	1.93	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:594:TYR:CD1	1:A:595:MET:N	2.79	0.51
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.43	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: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:A:507:ASN:C	1:A:509:GLU:H	2.14	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: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:642:VAL:HG13	1:A:697:PRO:O	2.11	0.50
1:A:515:ARG:NH1	1:A:520:MET:H	2.10	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:HD22	1:A:686:ASN:N	2.10	0.49
1:B:226:SER:HB2	1:B:670:PRO:HD3	1.94	0.49
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.27	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:B:511:VAL:HG12	1:B:513:LYS:H	1.78	0.49
1:A:515:ARG:CZ	1:A:619:LEU:HD22	2.42	0.49
1:A:338:TYR:O	1:A:339:PHE:HB2	2.12	0.49
1:B:727:ARG:HG3	1:B:727:ARG:HH11	1.78	0.49
1:A:656:LEU:HD12	1:A:660:LEU:CD2	2.42	0.49
1:A:527:ALA:HB2	1:A:533:PHE:CD1	2.48	0.49
1:A:26:LEU:HD11	1:A:104:VAL:HG11	1.95	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:659:THR:N	1:A:685:PRO:HG3	2.28	0.49
1:A:507:ASN:O	1:A:509:GLU:HG2	2.12	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:B:214:TYR:HB2	1:B:372:TYR:CZ	2.48	0.48
1:B:697:PRO:HB2	1:B:725:ILE:HG21	1.95	0.48
1:A:629:ILE:CG2	1:A:630:PRO:HD2	2.42	0.48
1:B:452:VAL:HG23	1:B:452:VAL:O	2.13	0.48
1:B:370:TRP:HZ3	1:B:560:TYR:HH	1.60	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:B:281:ASN:OD1	1:B:600:GLU:HG3	2.14	0.48
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.48	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:549:ILE:HG22	1:A:550:THR:N	2.29	0.48
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.45	0.48
1:B:252:ARG:HD3	2:B:784:HOH:O	2.13	0.47
1:A:469:ILE:HD11	2:A:925:HOH:O	2.13	0.47
1:B:431:VAL:O	1:B:434:GLU:HB2	2.14	0.47
1:B:428:ALA:HB3	1:B:429:PRO:HD3	1.95	0.47
1:B:380:MET:HG3	1:B:381:THR:O	2.14	0.47
1:B:441:TYR:CD1	1:B:454:ASN:HB3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:SER:HB3	1:B:670:PRO:HD3	1.97	0.47
1:B:55:GLU:O	1:B:58:ASP:HB2	2.14	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:609:THR:HA	1:B:619:LEU:O	2.15	0.47
1:A:439:LEU:HD12	1:A:459:HIS:HB3	1.96	0.47
1:B:557:ILE:CD1	1:B:597:GLN:HB3	2.45	0.47
1:A:343:ASP:HA	1:A:400:GLN:HG3	1.97	0.47
1:A:605:HIS:HE1	1:A:622:GLN:HB3	1.79	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:524:VAL:HG22	1:B:535:LEU:HG	1.97	0.46
1:A:235:LEU:HD22	1:A:235:LEU:O	2.15	0.46
1:A:697:PRO:CB	1:A:725:ILE:HD13	2.45	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:B:396:ASP:O	1:B:408:ARG:HB2	2.15	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:B:442:ILE:HG12	1:B:452:VAL:HG12	1.97	0.46
1:A:109:PRO:HA	1:A:115:THR:OG1	2.15	0.46
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.51	0.46
1:B:507:ASN:OD1	1:B:508:THR:N	2.48	0.46
1:B:342:HIS:HE1	2:B:752:HOH:O	1.98	0.46
1:B:515:ARG:NE	1:B:619:LEU:HD22	2.31	0.46
1:A:650:ILE:HB	1:A:691:TRP:CB	2.35	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:B:657:LYS:HE3	2:B:867:HOH:O	2.15	0.46
1:B:130:TRP:HA	1:B:147:GLN:O	2.16	0.46
1:B:227:TYR:CD2	1:B:326:ARG:NH1	2.84	0.46
1:B:684:ARG:HB2	1:B:687:SER:OG	2.16	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: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: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:643:GLY:O	1:B:696:ARG:NH2	2.50	0.45
1:B:138:GLU:HG2	1:B:141:SER:HB2	1.98	0.45
1:B:616:ARG:N	1:B:616:ARG:CD	2.79	0.45
1:A:549:ILE:CD1	1:A:612:ILE:HG12	2.38	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:B:522:PHE:O	1:B:623:LYS:HE2	2.16	0.45
1:B:137:ARG:HD2	2:B:880:HOH:O	2.15	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:B:187:TRP:CZ2	1:B:206:LEU:HD21	2.52	0.45
1:A:629:ILE:HG23	1:A:630:PRO:HD2	1.99	0.45
1:B:629:ILE:HG21	1:B:717:VAL:HG22	1.99	0.45
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.99	0.45
1:B:508:THR:O	1:B:512:MET:HG3	2.17	0.45
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.99	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:B:580:LEU:HD22	1:B:580:LEU:N	2.32	0.44
1:A:44:PHE:CD2	1:A:96:ARG:NH2	2.85	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:B:543:SER:O	1:B:580:LEU:HD22	2.18	0.44
1:A:637:ARG:HH12	1:A:647:THR:HG21	1.82	0.44
1:A:298:ILE:HG23	1:A:309:VAL:CG1	2.45	0.44
1:A:280:ASP:O	1:A:282:ILE:N	2.50	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:235:LEU:HA	1:A:327:CYS:SG	2.58	0.44
1:A:54:LYS:O	1:A:61:LYS:HD2	2.18	0.44
1:B:541:ASN:O	1:B:580:LEU:HA	2.17	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: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:515:ARG:HG2	1:A:619:LEU:CD2	2.48	0.43
1:A:370:TRP:N	1:A:370:TRP:CD1	2.84	0.43
1:A:102:GLU:HB2	1:A:160:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:B:635:LYS:HB2	1.68	0.43
1:A:354:LEU:HD11	1:A:609:THR:HG21	2.00	0.43
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.99	0.43
1:A:656:LEU:C	1:A:658:GLU:H	2.22	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:612:ILE:HD12	1:B:617:ASP:HB2	2.00	0.43
1:B:507:ASN:OD1	1:B:509:GLU:N	2.51	0.43
1:B:311:TYR:N	1:B:311:TYR:CD1	2.84	0.43
1:A:553:LEU:HD13	1:A:554:SER:N	2.33	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:B:223:ARG:HH12	1:B:225:TRP:HE3	1.65	0.43
1:A:515:ARG:HB3	1:A:518:VAL:O	2.19	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:B:636:VAL:HA	1:B:647:THR: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:382:ARG:NH2	1:B:426:PHE:HD2	2.16	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:A:665:VAL:CG2	1:A:680:PHE:HE1	2.30	0.43
1:A:602:ALA:HB1	1:A:627:LEU:HB2	2.00	0.43
1:A:147:GLN:HG3	1:A:148:SER:N	2.33	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:B:612:ILE:CG2	1:B:612:ILE:O	2.66	0.42
1:A:648:VAL:HG21	1:A:705:LEU:HD11	2.00	0.42
1:A:64:HIS:CE1	1:A:80:GLN:OE1	2.73	0.42
1:B:181:TYR:CE2	1:B:235:LEU:HD13	2.54	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:A:110:GLN:HE22	1:B:366:LYS:HB2	1.85	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:435:VAL:CG2	1:B:464:ILE:HD11	2.48	0.42
1:B:342:HIS:HA	1:B:434:GLU:OE2	2.19	0.42
1:A:193:VAL:O	1:A:193:VAL:CG1	2.67	0.42
1:B:678:LYS:HB2	1:B:691:TRP:CZ2	2.54	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:529:LEU:HD12	1:B:656:LEU:CD2	2.49	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: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:B:539:PHE:HB2	1:B:577:LEU:HD11	2.02	0.42
1:A:196:ASP:CG	1:A:196:ASP:O	2.58	0.42
1:A:105:ILE:HG23	1:A:157:PHE:CD2	2.55	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:A:704:LYS:HB2	1:A:704:LYS:HE3	1.89	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:B:538:THR:O	1:B:540:ARG:NH2	2.53	0.41
1:A:611:ARG:HD2	1:A:616:ARG:HA	2.02	0.41
1:A:283:TYR:CZ	1:A:289:PRO:HD2	2.55	0.41
1:B:513:LYS:HE2	1:B:513:LYS:HB2	1.87	0.41
1:A:484:GLN:CG	1:A:487:GLN:HG3	2.49	0.41
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.50	0.41
1:B:45:LEU:HA	1:B:45:LEU:HD12	1.92	0.41
1:B:77:ARG:HB3	1:B:185:ASN:HB2	2.02	0.41
1:A:506:LEU:HD12	2:A:902:HOH:O	2.19	0.41
1:B:247:MET:O	1:B:248:ASP:C	2.58	0.41
1:A:120:PRO:O	1:A:122:VAL:HG23	2.21	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:341:ALA:HB2	1:B:460:ILE:HD13	2.03	0.41
1:B:515:ARG:CB	1:B:619:LEU:HD21	2.45	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:223:ARG:NH1	1:B:225:TRP:HE3	2.18	0.41
1:A:711:SER:C	1:A:713:SER:N	2.73	0.41
1:B:335:VAL:HG21	1:B:377:GLU:HG3	2.03	0.41
1:B:528:VAL:HG12	1:B:529:LEU:N	2.36	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:B:578:GLU:O	1:B:581:SER:HB2	2.21	0.41
1:A:71:ASN:CB	1:A:75:ILE:HD11	2.48	0.41
1:A:680:PHE:CD1	1:A:680:PHE:N	2.89	0.41
1:B:530:GLY:HA2	1:B:595:MET:SD	2.61	0.41
1:B:515:ARG:HE	1:B:619:LEU:HD22	1.84	0.41
1:B:221:LYS:HE2	1:B:626:VAL:HG23	2.01	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:277:GLY:HA2	1:B:312:GLY:O	2.20	0.41
1:B:186:PRO:O	1:B:194:TYR:HD1	2.04	0.41
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.56	0.41
1:B:637:ARG:NH2	1:B:692:GLU:OE1	2.55	0.40
1:B:549:ILE:CG2	1:B:550:THR:N	2.84	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: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:455:VAL:HG13	1:B:455:VAL:O	2.21	0.40
1:B:209:ILE:HG22	1:B:210:GLY:N	2.37	0.40
1:B:120:PRO:O	1:B:122:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	5	7
1	B	710/731 (97%)	626 (88%)	69 (10%)	15 (2%)	9	14
All	All	1411/1462 (96%)	1243 (88%)	132 (9%)	36 (3%)	7	10

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 [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	620/644 (96%)	561 (90%)	59 (10%)	11	20
1	B	626/644 (97%)	568 (91%)	58 (9%)	11	21
All	All	1246/1288 (97%)	1129 (91%)	117 (9%)	11	20

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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