



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1GGY / pdb_00001ggy
Title : HUMAN FACTOR XIII WITH YTTERBIUM BOUND IN THE ION SITE
Authors : Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on : 1998-07-23
Resolution : 2.50 Å(reported)

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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

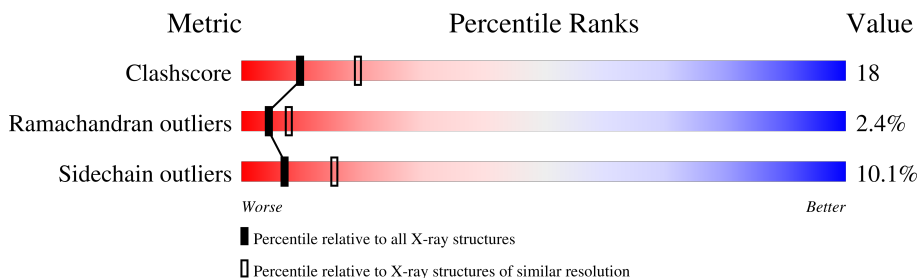
1 Overall quality at a glance

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 3 unique types of molecules in this entry. The entry contains 11569 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 PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	702	Total	C	N	O	S	0	0	0
			5637	3577	968	1066	26			
1	B	705	Total	C	N	O	S	0	0	0
			5659	3589	973	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Yb	0	0
			5	5		
2	B	3	Total	Yb	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	126	Total	O	0	0
			126	126		

L714	R715	H716	V717	L721	D722	V723	T724	T725	Q726	R727	ARG	PRO	SER	MET	F539	R540	N541	N542	S543	H544	N545	T548	T549	T550	T551	A551	Y552	L553	L554	S554	A555	R556	R557	F558	K559	T558	T559	Q560	R561	V562	M563	K564	K565	A566	E567	F568	K569	F570	F571	L572	V573	T574	V575	T576	L577	E578	P579	L580	S581	F582	K583	K584	L585	L586	Q587	L588	Q589	A590	Y591	Y592	Q593	L594	L595	L596	L597	L598	L599	E600	L601	L602	H603	L604	H605	F606	F607	V608	T609	A610	R611	R612	R613	R614	R615	A620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	L652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	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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	101.06Å 72.39Å 135.99Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	75.9 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11569	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YB

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	0.69	0/5770	1.10	38/7830 (0.5%)
1	B	0.67	0/5792	1.11	43/7859 (0.5%)
All	All	0.68	0/11562	1.10	81/15689 (0.5%)

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

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

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	117	ILE	CA-C-N	10.80	130.21	118.97
1	B	117	ILE	C-N-CA	10.80	130.21	118.97
1	A	52	LEU	N-CA-C	-8.24	97.64	110.42
1	A	269	LYS	N-CA-C	-7.58	96.20	108.41
1	B	382	ARG	CA-C-N	7.37	127.07	119.56
1	B	382	ARG	C-N-CA	7.37	127.07	119.56
1	B	674	ARG	N-CA-C	-7.36	100.83	110.39
1	A	488	GLU	N-CA-C	7.27	119.83	111.11
1	B	295	SER	N-CA-C	7.20	119.21	111.36
1	B	559	PHE	N-CA-C	-7.10	101.37	110.53
1	B	504	LYS	CA-C-N	7.00	128.59	119.84
1	B	504	LYS	C-N-CA	7.00	128.59	119.84
1	B	296	VAL	N-CA-C	6.88	117.58	110.36
1	B	83	TYR	N-CA-C	6.87	120.65	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASN	N-CA-C	6.79	120.72	109.46
1	A	175	ASN	CA-C-N	6.67	126.93	119.32
1	A	175	ASN	C-N-CA	6.67	126.93	119.32
1	A	504	LYS	CA-C-N	6.59	126.83	119.32
1	A	504	LYS	C-N-CA	6.59	126.83	119.32
1	A	205	VAL	CB-CA-C	-6.59	105.19	111.05
1	B	198	GLU	N-CA-C	6.58	119.29	111.33
1	B	558	THR	N-CA-C	6.49	118.81	109.14
1	A	518	VAL	N-CA-C	-6.46	97.00	107.28
1	A	629	ILE	N-CA-C	-6.42	103.11	108.63
1	B	269	LYS	N-CA-C	-6.40	100.18	109.59
1	B	194	TYR	N-CA-C	6.29	119.39	109.96
1	B	565	LYS	N-CA-C	-6.20	106.36	114.04
1	A	339	PHE	N-CA-C	-6.18	103.68	110.91
1	A	597	GLN	N-CA-C	6.17	121.31	111.81
1	A	329	GLY	CA-C-N	-6.16	118.15	122.59
1	A	329	GLY	C-N-CA	-6.16	118.15	122.59
1	B	532	ASP	N-CA-C	-6.15	100.54	110.32
1	B	217	VAL	N-CA-C	6.11	122.06	109.34
1	A	657	LYS	N-CA-C	-6.08	106.11	112.93
1	A	170	LEU	N-CA-C	-6.01	99.91	109.59
1	B	149	SER	N-CA-C	-6.01	102.58	110.39
1	A	559	PHE	N-CA-C	-5.96	102.12	110.35
1	A	436	ASN	N-CA-C	5.91	121.83	113.02
1	B	323	THR	N-CA-C	-5.82	104.84	111.07
1	B	134	ILE	N-CA-C	-5.81	101.17	108.84
1	A	58	ASP	N-CA-C	5.80	118.01	110.53
1	B	280	ASP	N-CA-C	5.78	120.19	113.20
1	B	307	ASN	CA-C-N	5.76	126.05	119.83
1	B	307	ASN	C-N-CA	5.76	126.05	119.83
1	B	170	LEU	N-CA-C	-5.73	99.08	108.76
1	A	408	ARG	N-CA-C	-5.72	102.97	110.53
1	A	633	ILE	N-CA-C	5.63	116.42	108.36
1	B	314	CYS	N-CA-C	5.63	122.80	110.80
1	B	428	ALA	N-CA-C	5.59	120.35	112.75
1	A	612	ILE	CB-CA-C	-5.56	105.91	111.80
1	A	663	VAL	N-CA-C	5.56	116.73	108.23
1	B	118	PRO	N-CA-C	5.53	121.38	113.47
1	B	542	ASN	N-CA-C	5.51	119.17	112.23
1	B	501	GLY	N-CA-C	5.49	124.40	114.46
1	A	205	VAL	N-CA-C	5.48	115.95	111.62
1	B	517	ASN	N-CA-C	5.47	118.88	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	GLY	N-CA-C	5.45	126.09	113.18
1	A	419	HIS	N-CA-C	5.43	120.06	113.38
1	B	206	LEU	N-CA-C	5.41	119.14	112.54
1	B	274	VAL	N-CA-C	5.40	116.06	110.82
1	A	565	LYS	N-CA-C	-5.40	104.81	111.40
1	B	567	GLU	N-CA-C	-5.39	99.72	108.41
1	A	587	VAL	N-CA-C	-5.37	102.05	109.46
1	B	502	ALA	N-CA-C	-5.36	100.50	109.24
1	A	296	VAL	N-CA-C	5.35	120.47	109.34
1	A	402	ASN	N-CA-C	-5.32	102.03	109.69
1	B	227	TYR	N-CA-C	-5.28	105.19	111.69
1	A	285	TYR	N-CA-C	5.24	118.74	111.71
1	B	175	ASN	CA-C-N	5.24	124.90	119.56
1	B	175	ASN	C-N-CA	5.24	124.90	119.56
1	A	442	ILE	CB-CA-C	-5.23	102.89	110.63
1	B	58	ASP	N-CA-C	5.20	117.04	110.33
1	A	674	ARG	N-CA-C	-5.20	102.60	110.39
1	A	505	PRO	N-CA-C	5.17	121.46	113.75
1	B	116	TYR	N-CA-C	-5.14	99.92	108.34
1	B	597	GLN	N-CA-C	5.06	116.38	110.41
1	A	501	GLY	N-CA-C	5.06	121.72	114.64
1	A	140	ARG	N-CA-C	5.05	118.56	111.74
1	A	111	GLU	N-CA-C	-5.04	105.92	111.71
1	A	291	ALA	N-CA-C	5.04	116.58	111.14
1	B	72	ASN	N-CA-C	5.03	119.49	112.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5637	0	5489	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5659	0	5508	195	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	139	0	0	7	0
3	B	126	0	0	8	0
All	All	11569	0	10997	395	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 18.

All (395) 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:575:VAL:HG13	1:B:583:LYS:HD3	1.43	1.01
1:B:220:ILE:HD13	1:B:474:MET:HE1	1.41	0.99
1:B:356:GLU:HG3	1:B:446:LYS:HD2	1.48	0.96
1:A:331:PRO:HG2	1:A:379:TRP:HB3	1.46	0.96
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.49	0.93
1:A:356:GLU:HG3	1:A:446:LYS:HG2	1.52	0.92
1:A:437:SER:HB2	1:A:460:ILE:HD12	1.55	0.87
1:B:659:THR:HG22	1:B:684:ARG:HA	1.60	0.84
1:B:44:PHE:O	1:B:45:LEU:HB2	1.78	0.83
1:A:651:GLU:HB3	1:A:690:GLN:HG3	1.60	0.81
1:B:548:THR:HB	1:B:613:ASN:HD21	1.44	0.81
1:A:95:ARG:HG2	1:A:96:ARG:HG3	1.63	0.80
1:A:8:PHE:O	1:B:563:VAL:HG11	1.85	0.77
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.64	0.76
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.68	0.75
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.50	0.75
1:A:100:ARG:HG2	1:A:164:TRP:NE1	2.01	0.75
1:B:281:ASN:OD1	1:B:600:GLU:HG3	1.88	0.73
1:B:709:MET:HE1	1:B:714:LEU:HG	1.68	0.73
1:A:635:LYS:HG3	1:A:649:THR:HB	1.69	0.73
1:A:64:HIS:HE1	1:A:80:GLN:HB3	1.53	0.73
1:B:345:ASP:O	1:B:503:LYS:HE2	1.88	0.73
1:A:350:MET:HE2	1:A:369:VAL:HG12	1.70	0.72
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.71	0.72
1:A:443:THR:HB	1:A:451:VAL:HG13	1.70	0.72
1:A:483:PHE:HB3	1:A:487:GLN:HE21	1.55	0.72
1:A:44:PHE:HD2	1:A:90:ARG:HE	1.39	0.71
1:A:527:ALA:HB2	1:A:533:PHE:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ILE:HB	1:A:575:VAL:HB	1.73	0.71
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.25	0.71
1:A:29:VAL:HG22	1:A:31:LEU:HD22	1.73	0.70
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.54	0.69
1:B:678:LYS:HD3	1:B:679:MET:H	1.57	0.69
1:A:337:ASN:HD21	1:A:461:GLY:HA2	1.57	0.69
1:A:467:LYS:HE2	1:A:472:ASP:HA	1.73	0.69
1:A:399:PRO:HB2	1:A:406:MET:HE3	1.75	0.69
1:A:198:GLU:O	1:A:202:GLU:HG3	1.92	0.68
1:A:559:PHE:HZ	1:B:8:PHE:CD1	2.11	0.68
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.74	0.68
1:B:290:SER:OG	1:B:716:HIS:HD2	1.76	0.68
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.76	0.68
1:B:541:ASN:HB2	1:B:577:LEU:HB3	1.75	0.67
1:A:44:PHE:O	1:A:45:LEU:HB2	1.94	0.67
1:B:126:GLN:HG3	1:B:127:SER:N	2.09	0.67
1:A:636:VAL:HG12	1:A:648:VAL:HA	1.77	0.66
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.30	0.66
1:A:90:ARG:HH11	1:A:90:ARG:HG3	1.60	0.66
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.77	0.66
1:B:172:THR:HB	3:B:3044:HOH:O	1.95	0.66
1:B:642:VAL:HG21	1:B:700:SER:HB3	1.77	0.66
1:A:557:ILE:HG21	1:A:597:GLN:O	1.96	0.66
1:B:565:LYS:HE2	1:B:597:GLN:HB2	1.79	0.65
1:A:235:LEU:HA	1:A:327:CYS:SG	2.37	0.65
1:A:157:PHE:CD1	1:A:182:ILE:HD12	2.31	0.65
1:B:78:ARG:HG2	1:B:183:LEU:O	1.97	0.65
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.33	0.64
1:B:522:PHE:O	1:B:623:LYS:HE3	1.98	0.63
1:B:280:ASP:OD2	1:B:282:ILE:HB	1.99	0.63
1:A:465:VAL:HG13	1:A:474:MET:HG3	1.79	0.63
1:B:638:GLY:HA3	1:B:646:MET:HA	1.81	0.63
1:A:237:THR:HG22	1:A:303:ARG:HD2	1.81	0.62
1:A:524:VAL:HG22	1:A:535:LEU:HG	1.80	0.62
1:B:528:VAL:HB	1:B:531:LYS:HG2	1.79	0.62
1:A:465:VAL:CG1	1:A:474:MET:HG3	2.30	0.62
1:B:557:ILE:HG21	1:B:597:GLN:O	1.99	0.62
1:B:52:LEU:O	1:B:54:LYS:HG3	2.00	0.62
1:A:263:SER:OG	1:A:408:ARG:HD3	1.98	0.62
1:A:135:VAL:HG12	1:A:143:ARG:O	1.99	0.62
1:B:136:MET:HE3	1:B:138:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:MET:HE1	1:B:608:VAL:HG12	1.82	0.61
1:B:127:SER:O	1:B:129:LYS:HG3	2.01	0.61
1:A:356:GLU:HB2	1:A:446:LYS:HE2	1.83	0.61
1:B:350:MET:HA	1:B:350:MET:HE3	1.83	0.61
1:B:678:LYS:HD3	1:B:679:MET:N	2.16	0.60
1:B:535:LEU:HD11	1:B:606:PHE:CD1	2.37	0.60
1:A:652:PHE:CE2	1:A:709:MET:HE2	2.37	0.59
1:A:139:ASP:O	1:A:140:ARG:HG2	2.02	0.59
1:A:247:MET:HE3	1:A:257:LYS:HG2	1.83	0.59
1:A:280:ASP:O	1:A:282:ILE:N	2.36	0.59
1:B:105:ILE:HD11	1:B:157:PHE:CE2	2.38	0.59
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.84	0.59
1:B:673:THR:OG1	1:B:676:MET:HE2	2.03	0.59
1:A:254:ASN:O	1:A:258:VAL:HG23	2.03	0.58
1:B:335:VAL:HG13	1:B:477:ILE:HD11	1.85	0.57
1:B:468:GLN:HG2	1:B:473:GLY:O	2.04	0.57
1:A:547:TYR:HB3	1:A:612:ILE:HG23	1.87	0.57
1:B:193:VAL:HG13	1:B:193:VAL:O	2.04	0.57
1:B:349:GLN:HE21	1:B:504:LYS:HG3	1.69	0.57
1:B:558:THR:HG22	1:B:564:PRO:HA	1.86	0.57
1:A:90:ARG:HG3	1:A:90:ARG:NH1	2.18	0.57
1:B:656:LEU:HA	3:B:6075:HOH:O	2.04	0.56
1:B:247:MET:HE3	1:B:257:LYS:HG2	1.86	0.56
1:A:112:ASN:HB2	3:A:3003:HOH:O	2.05	0.56
1:A:24:ASP:O	1:A:158:ARG:NH2	2.38	0.56
1:A:237:THR:HG22	1:A:303:ARG:CD	2.35	0.56
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.87	0.56
1:B:611:ARG:HD2	1:B:616:ARG:NH1	2.20	0.56
1:A:117:ILE:HG21	1:A:130:TRP:CD2	2.41	0.55
1:B:684:ARG:HB3	1:B:685:PRO:HD2	1.87	0.55
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.41	0.55
1:B:105:ILE:CD1	1:B:115:THR:HA	2.35	0.55
1:B:356:GLU:HB2	1:B:446:LYS:NZ	2.21	0.55
1:B:52:LEU:HD21	1:B:159:MET:SD	2.46	0.55
1:B:401:GLU:HA	1:B:406:MET:H	1.72	0.55
1:B:575:VAL:HG12	1:B:577:LEU:HD12	1.89	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:A:163:VAL:HB	1:A:170:LEU:HB2	1.89	0.54
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.71	0.54
1:B:273:GLY:O	1:B:308:PRO:HG3	2.07	0.54
1:B:549:ILE:HG22	1:B:550:THR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:PHE:HB3	1:A:577:LEU:HD11	1.90	0.54
1:B:297:ASP:O	1:B:301:GLU:HB2	2.07	0.54
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.89	0.54
1:B:105:ILE:HD12	1:B:115:THR:HA	1.88	0.54
1:B:485:GLU:HA	1:B:490:GLU:HG2	1.90	0.53
1:B:634:ILE:HG22	1:B:721:LEU:HD12	1.90	0.53
1:A:70:GLU:HB3	3:A:6058:HOH:O	2.07	0.53
1:A:565:LYS:HB2	1:A:599:LEU:HD11	1.90	0.53
1:B:126:GLN:HG3	1:B:127:SER:H	1.71	0.53
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.23	0.53
1:B:545:ASN:C	1:B:579:PRO:HG3	2.33	0.53
1:B:634:ILE:HD11	1:B:707:ALA:HB2	1.90	0.53
1:B:52:LEU:HD11	1:B:178:THR:HA	1.90	0.53
1:B:136:MET:HG2	1:B:137:ARG:N	2.24	0.53
1:B:223:ARG:NH2	3:B:6078:HOH:O	2.42	0.53
1:B:555:ALA:HB3	1:B:569:LYS:HB3	1.90	0.53
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.45	0.52
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.91	0.52
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.92	0.52
1:B:52:LEU:O	1:B:54:LYS:N	2.42	0.52
1:B:458:THR:O	1:B:462:LYS:HE3	2.09	0.52
1:B:535:LEU:HD12	1:B:589:ILE:HD11	1.92	0.52
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.40	0.52
1:B:217:VAL:HG22	1:B:338:TYR:HB3	1.92	0.51
1:A:14:VAL:HG21	1:A:110:GLN:NE2	2.26	0.51
1:A:551:ALA:HB3	1:A:573:PHE:HB2	1.92	0.51
1:A:629:ILE:HG21	1:A:717:VAL:HG22	1.92	0.51
1:B:575:VAL:CG1	1:B:583:LYS:HD3	2.30	0.51
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:NH2	2.26	0.51
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.11	0.51
1:B:103:TYR:HA	1:B:158:ARG:O	2.11	0.50
1:B:220:ILE:HG21	1:B:474:MET:CE	2.41	0.50
1:B:540:ARG:HA	1:B:582:PHE:HA	1.93	0.50
1:B:101:VAL:O	1:B:118:PRO:O	2.30	0.50
1:B:554:SER:HB3	1:B:607:PHE:HB2	1.92	0.50
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.41	0.50
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.92	0.50
1:A:224:SER:HB2	3:A:3058:HOH:O	2.11	0.50
1:B:715:ARG:HG2	1:B:716:HIS:N	2.25	0.50
1:B:402:ASN:HA	1:B:430:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:O	1:A:60:ASN:HB2	2.12	0.50
1:A:103:TYR:OH	1:A:159:MET:HE2	2.11	0.50
1:A:247:MET:HA	3:B:3004:HOH:O	2.11	0.50
1:B:211:VAL:HG23	1:B:467:LYS:HB2	1.93	0.50
1:B:255:PRO:HD2	3:B:3022:HOH:O	2.12	0.50
1:B:53:PHE:O	1:B:60:ASN:HB2	2.11	0.50
1:B:260:ARG:NH1	1:B:408:ARG:CZ	2.74	0.50
1:A:165:THR:HB	1:A:166:PRO:HD2	1.93	0.49
1:B:211:VAL:CG2	1:B:467:LYS:HB2	2.42	0.49
1:B:609:THR:HG22	1:B:620:ALA:CB	2.41	0.49
1:A:237:THR:O	1:A:240:TYR:HB3	2.12	0.49
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.47	0.49
1:A:12:ARG:NH2	1:B:406:MET:HE1	2.27	0.49
1:B:640:GLN:O	1:B:725:ILE:HA	2.12	0.49
1:A:260:ARG:HH11	1:A:410:GLY:HA3	1.78	0.49
1:B:443:THR:O	1:B:450:HIS:HA	2.12	0.49
1:B:672:VAL:HG11	1:B:705:LEU:HD21	1.92	0.49
1:B:260:ARG:HH12	1:B:408:ARG:CZ	2.24	0.49
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.44	0.49
1:A:364:LEU:O	1:A:366:LYS:HG2	2.13	0.49
1:A:684:ARG:H	1:A:684:ARG:HD2	1.77	0.49
1:B:54:LYS:O	1:B:55:GLU:O	2.30	0.49
1:B:200:GLU:HG2	1:B:469:ILE:HD11	1.93	0.49
1:A:548:THR:HB	1:A:613:ASN:HB2	1.94	0.49
1:A:641:VAL:HG12	1:A:642:VAL:O	2.13	0.49
1:A:700:SER:HA	1:A:725:ILE:HB	1.93	0.49
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.28	0.49
1:A:164:TRP:CD1	1:A:164:TRP:N	2.81	0.49
1:A:437:SER:HB2	1:A:460:ILE:CD1	2.36	0.49
1:B:211:VAL:HG22	1:B:467:LYS:CD	2.34	0.49
1:A:629:ILE:CG2	1:A:717:VAL:HG22	2.43	0.48
1:B:112:ASN:C	1:B:113:LYS:HG2	2.38	0.48
1:B:541:ASN:HB3	1:B:578:GLU:O	2.14	0.48
1:A:632:ILE:HG13	1:A:717:VAL:HG12	1.95	0.48
1:A:654:ASN:HB2	1:A:683:ILE:CG2	2.43	0.48
1:A:66:THR:HG21	1:A:75:ILE:HG22	1.96	0.48
1:A:220:ILE:HG21	1:A:474:MET:HE2	1.96	0.48
1:B:185:ASN:ND2	1:B:188:CYS:HB2	2.28	0.48
1:A:517:ASN:HA	3:A:5040:HOH:O	2.13	0.48
1:A:93:ASP:O	1:A:97:ASP:HB2	2.14	0.48
1:B:705:LEU:O	1:B:706:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:O	1:A:460:ILE:HG23	2.14	0.47
1:A:186:PRO:HA	1:A:194:TYR:HA	1.96	0.47
1:A:220:ILE:HG21	1:A:474:MET:CE	2.44	0.47
1:B:539:PHE:CD1	1:B:539:PHE:N	2.82	0.47
1:A:498:LEU:HD13	1:A:498:LEU:HA	1.75	0.47
1:B:153:ILE:HG23	1:B:252:ARG:HB2	1.96	0.47
1:A:100:ARG:HB2	1:A:119:VAL:O	2.14	0.47
1:A:107:ARG:C	1:A:109:PRO:HD3	2.39	0.47
1:B:345:ASP:O	1:B:346:ALA:HB3	2.14	0.47
1:B:402:ASN:HA	1:B:430:PHE:CZ	2.50	0.47
1:B:709:MET:HE3	1:B:717:VAL:HB	1.95	0.47
1:B:192:ALA:O	1:B:381:THR:HG23	2.13	0.47
1:B:356:GLU:HB2	1:B:446:LYS:HZ2	1.78	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.15	0.47
1:A:516:SER:O	1:A:517:ASN:HB2	2.15	0.47
1:A:128:GLY:HA2	1:A:150:PRO:HD2	1.97	0.47
1:A:549:ILE:HG13	1:A:612:ILE:HD13	1.96	0.47
1:A:567:GLU:OE2	1:A:570:LYS:HD3	2.14	0.47
1:A:642:VAL:HA	1:A:697:PRO:O	2.14	0.47
1:A:117:ILE:HD12	1:A:117:ILE:N	2.29	0.47
1:A:197:ASN:O	1:A:201:ARG:HG3	2.15	0.47
1:A:549:ILE:HG13	1:A:612:ILE:CD1	2.45	0.47
1:A:598:LEU:HD11	1:A:627:LEU:HD12	1.96	0.47
1:B:55:GLU:HB2	1:B:58:ASP:HB2	1.97	0.47
1:B:342:HIS:O	1:B:343:ASP:HB2	2.15	0.47
1:B:64:HIS:CG	1:B:76:VAL:HG22	2.50	0.47
1:B:124:GLU:HB2	3:B:5056:HOH:O	2.14	0.47
1:B:705:LEU:C	1:B:706:ILE:HG13	2.40	0.47
1:A:52:LEU:HD23	1:A:84:VAL:HG12	1.97	0.46
1:B:56:ARG:NH1	1:B:67:ASP:O	2.43	0.46
1:B:102:GLU:HB2	1:B:160:TYR:HB2	1.97	0.46
1:B:349:GLN:NE2	1:B:504:LYS:HG3	2.30	0.46
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.45	0.46
1:B:533:PHE:CE2	1:B:589:ILE:HG13	2.50	0.46
1:A:385:LEU:HB3	1:A:386:PRO:HD2	1.96	0.46
1:A:654:ASN:HB2	1:A:683:ILE:HG21	1.97	0.46
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.31	0.46
1:B:348:LEU:HA	1:B:437:SER:HB2	1.97	0.46
1:B:535:LEU:HD11	1:B:606:PHE:CE1	2.50	0.46
1:B:220:ILE:HG21	1:B:474:MET:HE3	1.95	0.46
1:B:237:THR:O	1:B:240:TYR:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:MET:HG3	1:B:381:THR:O	2.14	0.46
1:B:549:ILE:HG21	1:B:610:ALA:HB1	1.96	0.46
1:A:297:ASP:O	1:A:301:GLU:HB2	2.15	0.46
1:A:558:THR:C	1:A:599:LEU:HD12	2.41	0.46
1:B:240:TYR:OH	1:B:306:GLU:HG2	2.15	0.46
1:B:701:GLY:N	1:B:725:ILE:O	2.47	0.46
1:B:703:ARG:NE	1:B:703:ARG:HA	2.30	0.46
1:A:423:CYS:HB3	1:A:500:TYR:CD1	2.51	0.46
1:A:602:ALA:HB1	1:A:627:LEU:HB2	1.97	0.46
1:A:138:GLU:O	1:A:140:ARG:N	2.49	0.46
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.64	0.46
1:A:658:GLU:C	1:A:685:PRO:HG3	2.41	0.46
1:B:44:PHE:N	1:B:44:PHE:CD1	2.84	0.46
1:A:661:ARG:NH2	1:A:681:ARG:O	2.49	0.45
1:A:558:THR:HG22	1:A:564:PRO:HA	1.98	0.45
1:B:333:ARG:HG2	1:B:392:TRP:CZ3	2.51	0.45
1:A:100:ARG:HE	1:A:100:ARG:HB3	1.63	0.45
1:A:107:ARG:O	1:A:107:ARG:HG2	2.15	0.45
1:A:590:GLN:HB3	1:A:593:GLU:HG3	1.98	0.45
1:A:29:VAL:HG13	1:A:29:VAL:O	2.16	0.45
1:A:580:LEU:N	1:A:580:LEU:HD12	2.32	0.45
1:A:43:GLU:HA	1:A:165:THR:CG2	2.47	0.45
1:B:542:ASN:O	1:B:580:LEU:HD23	2.15	0.45
1:B:419:HIS:HB2	1:B:421:HIS:HD2	1.82	0.45
1:A:280:ASP:O	1:A:280:ASP:CG	2.60	0.45
1:B:623:LYS:HD3	3:B:6029:HOH:O	2.15	0.45
1:A:54:LYS:O	1:A:55:GLU:C	2.60	0.45
1:B:674:ARG:HH11	1:B:674:ARG:HG2	1.82	0.45
1:A:76:VAL:O	1:A:182:ILE:HA	2.17	0.45
1:A:352:ILE:HG21	1:A:441:TYR:CE1	2.52	0.45
1:B:54:LYS:HG2	1:B:74:LEU:HB2	1.98	0.45
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.46	0.45
1:B:575:VAL:HG12	1:B:577:LEU:CD1	2.47	0.45
1:A:483:PHE:CE2	1:A:489:GLU:HB2	2.52	0.44
1:B:174:ARG:NH2	1:B:179:ASP:OD1	2.50	0.44
1:A:337:ASN:ND2	1:A:464:ILE:HG12	2.32	0.44
1:A:573:PHE:HZ	1:A:587:VAL:CG2	2.30	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CD1	2.51	0.44
1:B:532:ASP:OD2	1:B:590:GLN:HA	2.17	0.44
1:A:98:LEU:CD2	1:A:164:TRP:HB2	2.46	0.44
1:B:498:LEU:HD12	1:B:498:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:O	1:A:179:ASP:C	2.61	0.44
1:B:635:LYS:HG3	1:B:649:THR:HB	1.99	0.44
1:A:674:ARG:HD2	1:A:674:ARG:HA	1.82	0.44
1:B:538:THR:HG22	1:B:584:LYS:HG3	2.00	0.44
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.99	0.44
1:A:602:ALA:O	1:A:626:VAL:HA	2.18	0.44
1:B:153:ILE:HG22	1:B:154:VAL:N	2.32	0.44
1:B:674:ARG:HG3	1:B:675:PRO:HD2	1.99	0.44
1:A:43:GLU:HA	1:A:165:THR:HG21	2.00	0.44
1:A:280:ASP:C	1:A:282:ILE:H	2.25	0.44
1:A:401:GLU:HA	1:A:406:MET:H	1.83	0.44
1:A:552:TYR:CD1	1:A:572:THR:HB	2.53	0.44
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.53	0.44
1:B:337:ASN:O	1:B:372:TYR:HA	2.17	0.44
1:A:154:VAL:HG21	1:A:184:PHE:CD2	2.53	0.43
1:A:528:VAL:HG12	1:A:529:LEU:N	2.33	0.43
1:B:235:LEU:HA	1:B:327:CYS:SG	2.58	0.43
1:A:350:MET:HE3	1:A:350:MET:HB3	1.81	0.43
1:A:639:THR:OG1	1:A:644:SER:HB3	2.18	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.18	0.43
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.49	0.43
1:A:354:LEU:HD22	1:A:441:TYR:HB3	1.99	0.43
1:A:546:ARG:HA	1:A:577:LEU:O	2.18	0.43
1:A:559:PHE:CD2	1:B:10:GLY:HA2	2.53	0.43
1:B:193:VAL:HG22	1:B:331:PRO:HD2	2.00	0.43
1:B:275:LEU:HA	1:B:309:VAL:O	2.19	0.43
1:B:559:PHE:CD1	1:B:599:LEU:HD13	2.54	0.43
1:A:44:PHE:HD2	1:A:90:ARG:NE	2.13	0.43
1:A:337:ASN:OD1	1:A:340:SER:HB2	2.18	0.43
1:A:678:LYS:HD3	1:A:680:PHE:CZ	2.53	0.43
1:A:355:GLU:N	1:A:359:ASN:O	2.52	0.43
1:B:229:GLN:HB2	1:B:327:CYS:HB2	2.01	0.43
1:B:333:ARG:HG2	1:B:392:TRP:CH2	2.54	0.43
1:A:12:ARG:HH22	1:B:406:MET:HE1	1.82	0.43
1:A:587:VAL:HG12	1:A:588:LEU:N	2.34	0.43
1:B:348:LEU:C	1:B:349:GLN:HG3	2.44	0.43
1:B:637:ARG:NH2	1:B:647:THR:HG21	2.33	0.43
1:B:703:ARG:HB2	1:B:723:VAL:HG23	2.00	0.43
1:A:189:GLU:HA	1:A:194:TYR:CG	2.54	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.91	0.43
1:A:337:ASN:ND2	1:A:461:GLY:HA2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:O	1:A:475:MET:N	2.52	0.43
1:A:666:HIS:O	1:A:707:ALA:HA	2.19	0.43
1:B:126:GLN:HG2	1:B:129:LYS:HD3	2.01	0.43
1:A:43:GLU:HA	1:A:165:THR:HB	2.01	0.42
1:A:559:PHE:HD1	1:A:563:VAL:O	2.02	0.42
1:B:703:ARG:HA	1:B:703:ARG:HE	1.83	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.74	0.42
1:A:709:MET:CE	1:A:717:VAL:HG21	2.49	0.42
1:B:166:PRO:HG2	1:B:167:TYR:CZ	2.53	0.42
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.52	0.42
1:A:559:PHE:HZ	1:B:8:PHE:CE1	2.36	0.42
1:B:143:ARG:HB2	1:B:143:ARG:HH11	1.83	0.42
1:A:684:ARG:HD2	1:A:684:ARG:N	2.35	0.42
1:B:558:THR:C	1:B:599:LEU:HD12	2.44	0.42
1:A:399:PRO:HA	1:A:407:TYR:O	2.20	0.42
1:A:331:PRO:CG	1:A:379:TRP:HB3	2.34	0.42
1:A:543:SER:O	1:A:580:LEU:HD12	2.20	0.42
1:B:674:ARG:O	1:B:676:MET:HG3	2.20	0.42
1:A:88:PHE:HE2	1:A:142:VAL:CG2	2.32	0.42
1:A:193:VAL:HG13	1:A:331:PRO:HD2	2.01	0.42
1:A:281:ASN:ND2	1:A:715:ARG:NH1	2.67	0.42
1:A:445:LYS:HB2	1:A:449:THR:HB	2.00	0.42
1:A:449:THR:HG22	1:A:450:HIS:N	2.35	0.42
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.75	0.42
1:B:126:GLN:HA	1:B:126:GLN:HE21	1.84	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.87	0.42
1:A:44:PHE:O	1:A:45:LEU:CB	2.66	0.42
1:A:267:ASN:C	1:A:267:ASN:ND2	2.78	0.42
1:A:642:VAL:C	1:A:644:SER:H	2.28	0.42
1:A:654:ASN:O	1:A:686:ASN:HA	2.20	0.42
1:B:715:ARG:CG	1:B:716:HIS:N	2.82	0.42
1:A:424:PHE:HA	3:A:4006:HOH:O	2.20	0.42
1:A:64:HIS:CD2	1:A:76:VAL:HG12	2.55	0.42
1:B:158:ARG:HG2	1:B:174:ARG:CZ	2.50	0.42
1:B:401:GLU:HA	1:B:406:MET:N	2.35	0.42
1:A:220:ILE:HD13	1:A:474:MET:HE1	2.02	0.41
1:B:363:LYS:O	1:B:366:LYS:HE2	2.20	0.41
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.53	0.41
1:A:264:ALA:HA	1:A:408:ARG:HG2	2.02	0.41
1:A:280:ASP:C	1:A:282:ILE:N	2.77	0.41
1:A:469:ILE:HD11	3:A:3080:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ARG:HG3	1:A:675:PRO:HD2	2.03	0.41
1:A:726:GLN:HE21	1:A:726:GLN:HA	1.85	0.41
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.83	0.41
1:A:118:PRO:O	1:A:120:PRO:HD3	2.20	0.41
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.51	0.41
1:A:557:ILE:HG13	1:A:568:PHE:CD1	2.56	0.41
1:A:590:GLN:O	1:A:591:ALA:C	2.64	0.41
1:B:12:ARG:CB	1:B:12:ARG:HH11	2.32	0.41
1:B:555:ALA:HB1	1:B:568:PHE:CZ	2.55	0.41
1:A:267:ASN:C	1:A:267:ASN:HD22	2.29	0.41
1:A:337:ASN:HD22	1:A:464:ILE:HG12	1.86	0.41
1:B:605:HIS:HD2	1:B:624:SER:OG	2.03	0.41
1:A:504:LYS:HE2	1:A:504:LYS:HB3	1.96	0.41
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.56	0.41
1:A:656:LEU:HD12	1:A:660:LEU:HD21	2.03	0.41
1:B:42:GLN:OE1	1:B:44:PHE:HE1	2.04	0.41
1:B:335:VAL:HG21	1:B:377:GLU:HG3	2.03	0.41
1:B:600:GLU:OE2	1:B:715:ARG:HD2	2.21	0.41
1:A:93:ASP:C	1:A:95:ARG:H	2.29	0.41
1:A:223:ARG:NH2	3:A:5021:HOH:O	2.53	0.41
1:B:425:GLN:HA	1:B:426:PHE:HA	1.79	0.41
1:B:697:PRO:CB	1:B:725:ILE:HD13	2.51	0.41
1:A:217:VAL:HG11	1:A:339:PHE:CE2	2.56	0.41
1:A:226:SER:HB3	1:A:294:GLY:HA3	2.01	0.41
1:A:337:ASN:O	1:A:372:TYR:HA	2.21	0.41
1:B:307:ASN:HA	1:B:308:PRO:HD3	1.93	0.40
1:A:442:ILE:HG12	1:A:452:VAL:HG12	2.03	0.40
1:A:563:VAL:HA	1:A:564:PRO:HD3	1.85	0.40
1:B:121:ILE:H	1:B:121:ILE:HD13	1.86	0.40
1:B:519:ASP:HB2	3:B:4008:HOH:O	2.19	0.40
1:A:372:TYR:CD1	1:A:372:TYR:C	3.00	0.40
1:B:45:LEU:HD22	1:B:97:ASP:HB3	2.02	0.40
1:B:137:ARG:HH11	1:B:137:ARG:HG3	1.86	0.40
1:B:105:ILE:HG13	1:B:157:PHE:CD2	2.57	0.40
1:B:184:PHE:HD2	1:B:328:LEU:O	2.05	0.40
1:B:486:GLY:O	1:B:487:GLN:HG3	2.22	0.40
1:B:92:TYR:HD2	1:B:137:ARG:HD3	1.85	0.40
1:B:551:ALA:HA	1:B:610:ALA:HA	2.03	0.40
1:B:582:PHE:CD1	1:B:582:PHE:C	3.00	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	696/731 (95%)	617 (89%)	60 (9%)	19 (3%)	4	6
1	B	699/731 (96%)	620 (89%)	65 (9%)	14 (2%)	6	10
All	All	1395/1462 (95%)	1237 (89%)	125 (9%)	33 (2%)	4	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	139	ASP
1	B	45	LEU
1	B	55	GLU
1	B	600	GLU
1	A	54	LYS
1	A	55	GLU
1	A	56	ARG
1	A	270	ASP
1	A	273	GLY
1	A	281	ASN
1	A	296	VAL
1	A	410	GLY
1	B	53	PHE
1	B	219	ASP
1	B	284	ALA
1	B	314	CYS
1	B	406	MET
1	A	595	MET
1	A	600	GLU
1	B	54	LYS
1	B	268	ALA
1	A	217	VAL
1	A	284	ALA
1	A	365	THR

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Mol	Chain	Res	Type
1	A	716	HIS
1	B	581	SER
1	B	613	ASN
1	A	60	ASN
1	A	386	PRO
1	B	172	THR
1	B	470	GLY
1	A	470	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	619/644 (96%)	562 (91%)	57 (9%)	8	19
1	B	621/644 (96%)	553 (89%)	68 (11%)	6	13
All	All	1240/1288 (96%)	1115 (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	31	LEU
1	A	43	GLU
1	A	44	PHE
1	A	46	ASN
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	72	ASN
1	A	76	VAL
1	A	96	ARG
1	A	104	VAL
1	A	143	ARG
1	A	165	THR
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	206	LEU
1	A	211	VAL
1	A	220	ILE
1	A	223	ARG
1	A	224	SER
1	A	259	SER
1	A	267	ASN
1	A	271	ASP
1	A	281	ASN
1	A	293	THR
1	A	301	GLU
1	A	323	THR
1	A	340	SER
1	A	354	LEU
1	A	355	GLU
1	A	357	ASP
1	A	364	LEU
1	A	369	VAL
1	A	386	PRO
1	A	425	GLN
1	A	431	VAL
1	A	451	VAL
1	A	463	LEU
1	A	484	GLN
1	A	489	GLU
1	A	498	LEU
1	A	508	THR
1	A	520	MET
1	A	526	ASN
1	A	538	THR
1	A	553	LEU
1	A	556	ASN
1	A	572	THR
1	A	574	ASP
1	A	604	LEU
1	A	607	PHE
1	A	609	THR
1	A	616	ARG
1	A	640	GLN
1	A	661	ARG
1	A	674	ARG
1	A	721	LEU

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Mol	Chain	Res	Type
1	B	12	ARG
1	B	25	ASP
1	B	43	GLU
1	B	47	VAL
1	B	52	LEU
1	B	56	ARG
1	B	58	ASP
1	B	59	THR
1	B	70	GLU
1	B	76	VAL
1	B	78	ARG
1	B	98	LEU
1	B	104	VAL
1	B	105	ILE
1	B	119	VAL
1	B	121	ILE
1	B	123	SER
1	B	126	GLN
1	B	135	VAL
1	B	139	ASP
1	B	140	ARG
1	B	142	VAL
1	B	143	ARG
1	B	148	SER
1	B	172	THR
1	B	174	ARG
1	B	193	VAL
1	B	196	ASP
1	B	202	GLU
1	B	206	LEU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	301	GLU
1	B	303	ARG
1	B	340	SER
1	B	359	ASN
1	B	363	LYS
1	B	369	VAL
1	B	415	GLN
1	B	431	VAL
1	B	435	VAL

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Mol	Chain	Res	Type
1	B	452	VAL
1	B	463	LEU
1	B	490	GLU
1	B	492	LEU
1	B	498	LEU
1	B	519	ASP
1	B	520	MET
1	B	525	GLU
1	B	526	ASN
1	B	529	LEU
1	B	535	LEU
1	B	540	ARG
1	B	544	HIS
1	B	553	LEU
1	B	576	THR
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	613	ASN
1	B	639	THR
1	B	640	GLN
1	B	674	ARG
1	B	678	LYS
1	B	679	MET
1	B	713	SER
1	B	721	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	64	HIS
1	A	71	ASN
1	A	85	GLN
1	A	267	ASN
1	A	337	ASN
1	A	373	HIS
1	A	436	ASN
1	A	484	GLN
1	A	487	GLN
1	A	526	ASN
1	A	601	GLN

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Mol	Chain	Res	Type
1	A	726	GLN
1	B	72	ASN
1	B	112	ASN
1	B	126	GLN
1	B	267	ASN
1	B	421	HIS
1	B	605	HIS
1	B	613	ASN
1	B	686	ASN
1	B	716	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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.