



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:32 AM UTC

PDB ID : 1DJG / pdb_00001djg
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH LANTHANUM
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-09-25
Resolution : 2.60 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

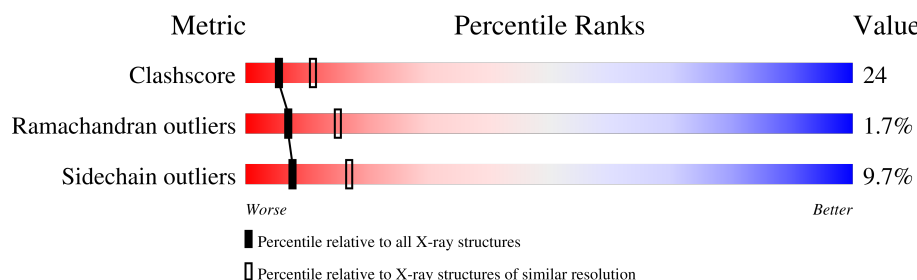
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	624	
1	B	624	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5	-	-	X	-

2 Entry composition [i](#)

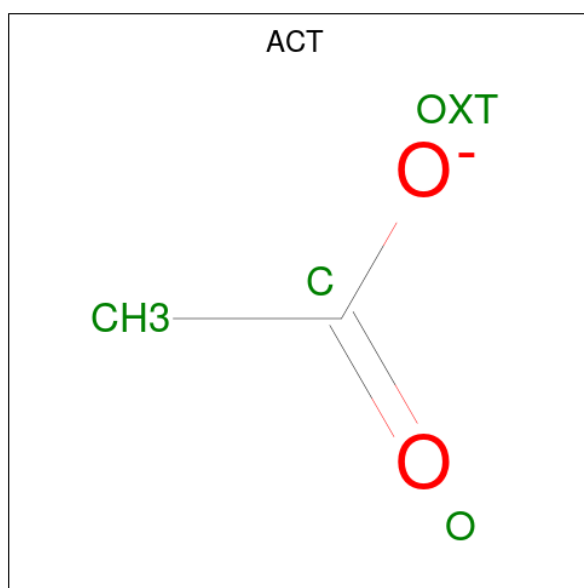
There are 4 unique types of molecules in this entry. The entry contains 9246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	86	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	101	0	0
			4465	2818	776	847	24			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is LANTHANUM (III) ION (CCD ID: LA) (formula: La).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	La 4	0	0
3	B	4	Total 4	La 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total 335	O 335	0	0
4	B	373	Total 373	O 373	0	0

L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L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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	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	397.92Å 397.92Å 397.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.5 (10.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.210 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: ACT, LA

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	1.11	8/4152 (0.2%)	1.17	24/5624 (0.4%)
1	B	1.13	16/4565 (0.4%)	1.19	30/6174 (0.5%)
All	All	1.12	24/8717 (0.3%)	1.18	54/11798 (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	A	0	1
1	B	1	0
All	All	1	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	LYS	C-O	-9.53	1.11	1.23
1	B	520	MET	SD-CE	-7.86	1.59	1.79
1	A	409	LEU	CG-CD1	-7.21	1.28	1.52
1	A	277	MET	SD-CE	7.05	1.97	1.79
1	B	409	LEU	CG-CD1	-6.80	1.30	1.52
1	B	409	LEU	CG-CD2	-6.27	1.31	1.52
1	A	409	LEU	CG-CD2	-5.97	1.32	1.52
1	B	588	VAL	CA-CB	-5.91	1.46	1.54
1	A	207	MET	SD-CE	5.74	1.94	1.79
1	B	715	PHE	CE1-CZ	-5.66	1.21	1.38
1	A	715	PHE	CE2-CZ	-5.65	1.21	1.38
1	B	730	TYR	CE2-CZ	-5.56	1.25	1.38
1	A	715	PHE	CG-CD1	-5.52	1.27	1.38
1	B	607	PHE	CE2-CZ	-5.35	1.22	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	715	PHE	CE2-CZ	-5.26	1.22	1.38
1	B	330	ILE	CA-CB	-5.26	1.48	1.54
1	B	730	TYR	CG-CD1	-5.25	1.28	1.39
1	A	607	PHE	CE2-CZ	-5.24	1.23	1.38
1	B	607	PHE	CE1-CZ	-5.17	1.23	1.38
1	B	358	TYR	CG-CD2	-5.14	1.28	1.39
1	B	721	ILE	CA-CB	5.08	1.58	1.54
1	B	528	ALA	CA-CB	-5.08	1.45	1.53
1	A	358	TYR	CE1-CZ	-5.02	1.26	1.38
1	B	715	PHE	CG-CD1	-5.00	1.28	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	CYS	N-CA-C	11.40	127.35	110.48
1	B	594	GLN	N-CA-C	-10.00	100.83	113.23
1	A	643	LYS	N-CA-C	-8.24	97.60	109.96
1	A	649	ASN	N-CA-C	8.24	123.11	112.89
1	A	208	LEU	N-CA-C	-7.85	102.67	111.07
1	A	594	GLN	N-CA-C	-7.76	103.26	112.89
1	A	509	SER	N-CA-C	7.61	126.63	109.81
1	A	645	ASN	N-CA-C	7.31	120.67	111.24
1	A	306	LEU	N-CA-C	-7.05	98.11	109.96
1	B	654	PRO	N-CA-C	6.93	122.07	111.19
1	A	675	ILE	N-CA-C	-6.90	98.50	108.36
1	B	306	LEU	N-CA-C	-6.74	98.64	109.96
1	A	202	GLU	N-CA-C	-6.54	104.07	111.07
1	B	393	CYS	N-CA-CB	6.49	120.15	110.29
1	A	654	PRO	N-CA-C	6.41	121.25	111.19
1	B	591	GLY	N-CA-C	-6.21	104.98	112.49
1	B	258	TYR	N-CA-C	6.20	121.78	113.72
1	B	393	CYS	CA-CB-SG	6.16	128.56	114.40
1	A	258	TYR	N-CA-C	6.05	121.58	113.72
1	A	409	LEU	CD1-CG-CD2	-6.04	97.50	110.80
1	B	486	LEU	N-CA-C	-6.00	105.72	113.16
1	B	180	TYR	N-CA-C	-5.91	103.53	112.04
1	B	177	ASP	N-CA-C	5.90	123.36	110.80
1	B	167	ASP	CB-CA-C	5.89	120.68	110.79
1	B	675	ILE	N-CA-C	-5.84	100.01	108.36
1	B	748	LEU	N-CA-C	-5.76	100.01	109.40
1	A	644	VAL	N-CA-C	5.75	121.31	109.34
1	A	210	GLN	N-CA-C	5.75	118.91	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	GLY	N-CA-C	-5.72	99.62	113.18
1	B	587	ASP	N-CA-C	-5.67	104.79	110.97
1	B	614	THR	N-CA-C	-5.65	105.97	112.92
1	B	645	ASN	N-CA-C	5.58	118.88	111.30
1	B	173	ASN	CB-CA-C	5.51	121.39	110.42
1	B	544	VAL	CB-CA-C	-5.44	104.89	112.02
1	A	591	GLY	N-CA-C	-5.42	105.84	112.77
1	A	412	ILE	CB-CA-C	-5.38	103.55	112.26
1	B	229	SER	N-CA-C	-5.38	102.09	110.42
1	B	711	SER	N-CA-C	5.37	115.38	108.34
1	B	324	SER	N-CA-C	-5.35	101.05	109.50
1	B	613	THR	CB-CA-C	-5.33	100.08	109.62
1	B	510	PRO	N-CA-C	5.33	125.95	112.10
1	B	226	GLU	N-CA-C	-5.29	106.68	113.02
1	B	498	TYR	N-CA-C	5.29	119.88	113.38
1	A	748	LEU	N-CA-C	-5.26	100.83	109.40
1	A	226	GLU	N-CA-C	-5.24	106.47	112.92
1	A	544	VAL	CB-CA-C	-5.23	105.00	112.22
1	B	546	CYS	N-CA-C	5.23	117.93	109.40
1	A	587	ASP	N-CA-C	-5.22	105.28	110.97
1	A	422	THR	N-CA-C	5.21	119.26	112.13
1	B	375	ASP	N-CA-C	5.13	117.77	111.82
1	A	573	GLN	N-CA-C	5.12	119.56	112.45
1	A	715	PHE	N-CA-C	-5.11	102.13	110.20
1	B	509	SER	N-CA-C	5.11	121.10	109.81
1	A	384	PRO	N-CA-C	5.05	119.14	111.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	393	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	691	GLU	Sidechain

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	4057	0	3972	180	0
1	B	4465	0	4375	221	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	335	0	0	11	0
4	B	373	0	0	18	0
All	All	9246	0	8353	390	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 24.

All (390) 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:161:ASN:H	1:B:164:GLU:HG3	1.18	1.07
1:A:613:THR:HG22	1:A:615:PHE:H	1.23	1.02
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.24	1.01
1:B:728:GLN:NE2	1:B:754:ILE:H	1.64	0.94
1:A:573:GLN:H	1:A:573:GLN:NE2	1.65	0.93
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.52	0.92
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.34	0.90
1:B:728:GLN:HE21	1:B:754:ILE:H	1.21	0.88
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.08	0.88
1:A:632:ARG:NH2	1:B:406:ARG:NH1	2.22	0.86
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.11	0.85
1:B:241:GLN:HE22	1:B:730:TYR:H	1.24	0.85
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.58	0.85
1:A:241:GLN:HE22	1:A:730:TYR:H	1.24	0.84
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:B:202:GLU:HB3	1:B:206:LYS:HE3	1.61	0.81
1:B:515:GLN:HB3	1:B:519:GLU:OE1	1.81	0.81
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.62	0.80
1:A:573:GLN:H	1:A:573:GLN:HE21	1.27	0.79
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.18	0.79
1:A:738:LYS:HG3	2:A:5:ACT:H3	1.63	0.79
1:B:159:LYS:O	4:B:1060:HOH:O	2.00	0.79
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HB3	1:B:206:LYS:CE	2.13	0.78
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.19	0.77
1:A:415:ASP:C	1:A:497:ILE:HD11	2.09	0.77
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.99	0.77
1:B:548:SER:H	1:B:573:GLN:NE2	1.81	0.77
1:B:573:GLN:NE2	1:B:573:GLN:H	1.83	0.76
1:B:438:LYS:HD2	1:B:520:MET:HE2	1.66	0.76
1:A:390:GLU:HG2	1:A:392:HIS:CE1	2.21	0.75
1:A:394:SER:O	1:A:398:GLN:HG3	1.87	0.75
1:B:605:PRO:HB2	1:B:607:PHE:CE1	2.22	0.75
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.21	0.74
1:A:613:THR:CG2	1:A:615:PHE:H	2.01	0.74
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.70	0.74
1:A:548:SER:H	1:A:573:GLN:NE2	1.86	0.74
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.69	0.74
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.22	0.73
1:A:252:LEU:HD23	1:A:256:GLU:OE2	1.89	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.70	0.73
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.71	0.73
1:B:161:ASN:N	1:B:164:GLU:HG3	2.01	0.72
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.25	0.71
1:B:166:LYS:HE2	4:B:1099:HOH:O	1.89	0.71
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.73	0.70
1:B:438:LYS:HD2	1:B:520:MET:CE	2.22	0.70
1:B:202:GLU:HB3	1:B:206:LYS:HZ1	1.56	0.69
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.21	0.69
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.75	0.69
1:B:683:ARG:HD2	4:B:1003:HOH:O	1.93	0.68
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.23	0.68
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.94	0.68
1:A:728:GLN:HE21	1:A:754:ILE:HB	1.57	0.68
1:B:728:GLN:HE21	1:B:754:ILE:N	1.92	0.68
1:B:755:GLN:HG2	4:B:1033:HOH:O	1.92	0.68
1:B:202:GLU:HB3	1:B:206:LYS:NZ	2.09	0.68
1:B:415:ASP:C	1:B:497:ILE:HD11	2.18	0.67
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.29	0.67
1:B:187:GLU:OE1	1:B:207:MET:HE1	1.95	0.67
1:B:654:PRO:HD2	1:B:675:ILE:O	1.96	0.67
1:B:607:PHE:HD1	1:B:607:PHE:H	1.43	0.66
1:B:293:ARG:NH1	4:B:1000:HOH:O	2.28	0.66
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:256:GLU:HG3	1.95	0.66
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.30	0.65
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.07	0.65
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.79	0.65
1:B:174:ILE:O	1:B:176:VAL:N	2.30	0.65
1:B:168:PHE:O	1:B:171:GLU:HB3	1.96	0.65
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.26	0.65
1:A:670:ARG:HD3	4:A:778:HOH:O	1.95	0.64
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.80	0.64
1:B:524:SER:HA	1:B:551:TYR:CE1	2.31	0.64
1:B:630:ARG:CD	1:B:755:GLN:HE21	2.11	0.64
1:A:728:GLN:NE2	1:A:754:ILE:HB	2.12	0.64
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.98	0.64
1:A:285:ASN:ND2	1:A:734:HIS:HD2	1.96	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.32	0.63
1:B:593:PHE:O	1:B:598:GLY:HA2	1.98	0.63
1:B:196:LEU:HB3	1:B:201:ILE:HG12	1.81	0.63
1:A:208:LEU:N	1:A:208:LEU:HD23	2.14	0.62
1:B:438:LYS:CD	1:B:520:MET:HE2	2.30	0.62
1:A:219:GLU:O	1:A:223:GLY:N	2.29	0.62
1:A:317:GLU:O	1:A:580:GLN:NE2	2.32	0.62
1:B:622:GLN:HG3	1:B:623:GLY:N	2.14	0.62
1:A:515:GLN:HB3	1:A:519:GLU:OE1	1.99	0.61
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.81	0.61
1:B:162:PHE:CE2	1:B:182:ARG:HG2	2.35	0.61
1:B:504:PHE:HD2	1:B:527:ARG:NH2	1.98	0.61
1:B:594:GLN:HA	1:B:594:GLN:HE21	1.66	0.61
1:A:622:GLN:OE1	1:B:445:LEU:HD12	2.00	0.61
1:A:607:PHE:CE1	1:A:608:LEU:HG	2.35	0.61
1:A:593:PHE:O	1:A:598:GLY:HA2	2.01	0.60
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.34	0.60
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.84	0.60
1:A:502:VAL:HG11	1:A:515:GLN:CD	2.26	0.60
1:A:504:PHE:HD2	1:A:527:ARG:NH2	1.98	0.60
1:B:391:ASN:N	4:B:766:HOH:O	2.27	0.60
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.83	0.59
1:B:184:ILE:HD12	1:B:207:MET:HE2	1.84	0.59
1:B:222:ALA:C	1:B:232:ARG:HH11	2.11	0.59
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.36	0.58
1:A:507:PHE:CD1	1:A:542:HIS:HB2	2.38	0.58
1:B:683:ARG:NH1	4:B:994:HOH:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:N	1:A:497:ILE:HD11	2.18	0.58
1:B:583:GLY:HA3	4:B:911:HOH:O	2.02	0.58
1:A:291:HIS:CD2	1:A:295:TYR:CZ	2.91	0.58
1:A:349:ASN:ND2	1:A:349:ASN:O	2.37	0.58
1:B:696:ASP:HB2	4:B:768:HOH:O	2.04	0.58
1:B:642:PRO:HD2	1:B:716:ILE:HG23	1.85	0.58
1:B:248:PRO:O	1:B:252:LEU:HG	2.05	0.57
1:B:418:LEU:HD12	1:B:426:PRO:HB3	1.86	0.57
1:A:390:GLU:HG2	1:A:392:HIS:HE1	1.68	0.57
1:B:183:LYS:HE3	4:B:906:HOH:O	2.03	0.57
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.40	0.57
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.38	0.57
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.05	0.57
1:B:711:SER:OG	1:B:712:LYS:N	2.32	0.57
1:B:183:LYS:O	1:B:187:GLU:HG3	2.05	0.56
1:A:417:PRO:HD3	1:A:497:ILE:HD13	1.86	0.56
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.69	0.56
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.35	0.56
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.06	0.56
1:A:632:ARG:HH22	1:B:406:ARG:NH1	2.02	0.56
1:B:346:ASP:OD2	1:B:394:SER:HB3	2.06	0.56
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.35	0.56
1:B:573:GLN:H	1:B:573:GLN:HE21	1.53	0.56
1:A:232:ARG:NH2	4:A:1066:HOH:O	2.38	0.56
1:B:595:ASP:OD1	1:B:596:ASN:N	2.38	0.55
1:B:634:ARG:CG	1:B:687:GLU:HB2	2.36	0.55
1:A:683:ARG:NH2	1:A:685:ASP:OD2	2.40	0.55
1:B:605:PRO:HB2	1:B:607:PHE:HE1	1.69	0.55
1:B:734:HIS:ND1	1:B:747:THR:HG22	2.22	0.55
1:A:734:HIS:ND1	1:A:747:THR:HG22	2.20	0.55
1:A:356:HIS:HD1	1:A:359:THR:HG21	1.71	0.55
1:B:161:ASN:OD1	1:B:164:GLU:HG2	2.06	0.55
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.07	0.55
1:B:394:SER:O	1:B:398:GLN:HG3	2.07	0.55
1:A:241:GLN:HE22	1:A:730:TYR:N	1.98	0.54
1:B:605:PRO:CB	1:B:607:PHE:HE1	2.20	0.54
1:B:632:ARG:HH22	1:B:755:GLN:NE2	2.06	0.54
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.73	0.54
1:B:205:TYR:O	1:B:208:LEU:HB3	2.08	0.54
1:B:197:GLU:O	1:B:201:ILE:HG13	2.08	0.54
1:B:379:LYS:HE2	4:B:891:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:CB	1:B:206:LYS:HE3	2.35	0.54
1:B:441:LYS:NZ	1:B:493:SER:O	2.41	0.54
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.88	0.53
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.33	0.53
1:A:738:LYS:HG3	2:A:5:ACT:CH3	2.35	0.53
1:B:426:PRO:HG2	1:B:431:LEU:CD1	2.34	0.53
1:A:595:ASP:OD1	1:A:596:ASN:N	2.38	0.53
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.38	0.53
1:A:626:TRP:CE3	1:B:445:LEU:HD21	2.43	0.53
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.08	0.53
1:B:681:ASN:HB2	4:B:922:HOH:O	2.07	0.53
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.34	0.53
1:B:738:LYS:HD2	4:B:1100:HOH:O	2.09	0.53
1:B:178:ASP:C	1:B:180:TYR:H	2.17	0.53
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.15	0.53
1:A:533:GLN:OE1	1:A:533:GLN:HA	2.08	0.53
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.21	0.52
1:B:206:LYS:O	1:B:210:GLN:HB3	2.09	0.52
1:A:240:GLN:OE1	1:A:240:GLN:HA	2.09	0.52
1:A:652:VAL:CG1	1:A:716:ILE:HD11	2.40	0.52
1:A:652:VAL:HG11	1:A:716:ILE:HD11	1.91	0.52
1:B:729:GLY:O	1:B:751:LYS:HA	2.09	0.52
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.78	0.52
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.18	0.52
1:A:345:TRP:CH2	1:A:392:HIS:CD2	2.98	0.52
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.38	0.52
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.37	0.52
1:B:630:ARG:HD2	1:B:755:GLN:NE2	2.25	0.52
1:B:638:GLY:O	1:B:681:ASN:HA	2.10	0.52
1:A:638:GLY:O	1:A:681:ASN:HA	2.10	0.51
1:B:177:ASP:O	1:B:178:ASP:HB2	2.10	0.51
1:B:345:TRP:CZ2	1:B:392:HIS:CD2	2.99	0.51
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.38	0.51
1:B:566:GLU:HB3	4:B:912:HOH:O	2.11	0.51
1:A:539:PHE:O	1:A:542:HIS:HB3	2.10	0.51
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.91	0.51
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.38	0.51
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.41	0.51
1:B:728:GLN:NE2	1:B:754:ILE:N	2.46	0.51
1:A:630:ARG:NH2	1:B:406:ARG:HH22	2.08	0.51
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:GLY:O	1:B:515:GLN:O	2.29	0.51
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.41	0.51
1:A:642:PRO:HD2	1:A:716:ILE:HG23	1.92	0.51
1:B:203:THR:N	1:B:206:LYS:HZ2	2.08	0.51
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.41	0.50
1:B:261:SER:O	1:B:265:LYS:HB2	2.11	0.50
1:B:582:PRO:HB3	1:B:738:LYS:HG2	1.92	0.50
1:A:651:ILE:HG21	1:A:677:ASN:C	2.37	0.50
1:B:267:GLN:O	1:B:269:GLN:HG3	2.12	0.50
1:B:405:LEU:O	1:B:409:LEU:HB2	2.10	0.50
1:B:630:ARG:HD3	1:B:755:GLN:HE21	1.77	0.50
1:B:202:GLU:O	1:B:206:LYS:HG2	2.12	0.50
1:B:504:PHE:CD2	1:B:527:ARG:NH2	2.79	0.50
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.11	0.50
1:B:178:ASP:CG	1:B:179:GLY:H	2.18	0.50
1:A:582:PRO:HB3	1:A:738:LYS:HG2	1.94	0.49
1:B:163:LYS:O	1:B:167:ASP:HB3	2.11	0.49
1:A:205:TYR:O	1:A:209:THR:OG1	2.27	0.49
1:A:551:TYR:CD1	1:A:551:TYR:N	2.80	0.49
1:A:356:HIS:ND1	1:A:359:THR:HG21	2.26	0.49
1:A:535:SER:O	1:A:537:ASN:N	2.45	0.49
1:B:253:SER:O	1:B:257:ARG:HB2	2.12	0.49
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.26	0.49
1:B:686:MET:HG3	1:B:687:GLU:N	2.26	0.49
1:B:202:GLU:CB	1:B:206:LYS:HZ1	2.21	0.49
1:A:659:GLU:OE1	1:A:661:HIS:HE1	1.95	0.49
1:A:613:THR:HG22	1:A:615:PHE:N	2.08	0.49
1:B:250:LEU:O	1:B:254:LEU:HG	2.12	0.49
1:A:622:GLN:HG3	1:A:623:GLY:N	2.27	0.49
1:A:652:VAL:HG11	1:A:716:ILE:CD1	2.43	0.49
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.42	0.49
1:B:390:GLU:HG2	1:B:392:HIS:NE2	2.27	0.49
1:B:607:PHE:CD1	1:B:607:PHE:N	2.78	0.49
1:A:253:SER:O	1:A:257:ARG:HB2	2.13	0.49
1:B:661:HIS:O	1:B:698:ALA:HA	2.13	0.49
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.43	0.49
1:A:607:PHE:CE2	1:A:625:TRP:CB	2.96	0.49
1:B:632:ARG:HH22	1:B:755:GLN:CD	2.20	0.48
1:A:304:HIS:O	1:A:604:LYS:HB2	2.13	0.48
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.95	0.48
1:B:730:TYR:CE1	1:B:751:LYS:CD	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LYS:NZ	1:A:493:SER:O	2.46	0.48
1:A:310:SER:HB3	1:A:337:CYS:SG	2.54	0.48
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.79	0.48
1:B:654:PRO:HG3	1:B:678:ASN:O	2.13	0.48
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.12	0.48
1:B:395:LEU:HB2	4:B:1120:HOH:O	2.13	0.48
1:A:345:TRP:CZ2	1:A:392:HIS:CG	3.01	0.48
1:A:242:ARG:HE	1:A:242:ARG:HB3	1.42	0.48
1:A:558:ASP:O	1:A:559:SER:HB2	2.12	0.48
1:B:607:PHE:HD1	1:B:607:PHE:N	2.10	0.48
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.78	0.48
1:A:755:GLN:HG2	1:A:756:ASP:N	2.28	0.47
1:B:313:THR:HB	1:B:329:TYR:CE1	2.48	0.47
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.44	0.47
1:A:676:THR:HG23	4:A:1077:HOH:O	2.15	0.47
1:B:416:GLN:N	1:B:497:ILE:HD11	2.29	0.47
1:A:525:GLU:O	1:A:529:LEU:HG	2.14	0.47
1:A:609:ARG:NH2	4:A:871:HOH:O	2.46	0.47
1:A:686:MET:HB2	4:A:885:HOH:O	2.13	0.47
1:B:571:GLY:HA2	1:B:604:LYS:HE3	1.97	0.47
1:A:669:SER:C	1:A:670:ARG:HG2	2.38	0.47
1:B:504:PHE:HD2	1:B:527:ARG:HH21	1.62	0.47
1:A:416:GLN:N	1:A:497:ILE:CD1	2.78	0.47
1:A:438:LYS:HE3	1:A:520:MET:HE2	1.96	0.47
1:A:654:PRO:HD2	1:A:675:ILE:O	2.14	0.47
1:A:756:ASP:N	1:A:756:ASP:OD1	2.47	0.47
1:B:548:SER:H	1:B:573:GLN:HE21	1.59	0.47
1:A:571:GLY:HA2	1:A:604:LYS:HE3	1.97	0.47
1:A:728:GLN:NE2	1:A:754:ILE:H	2.13	0.47
1:A:613:THR:HG21	1:A:615:PHE:HB3	1.96	0.47
1:B:345:TRP:CZ2	1:B:392:HIS:CG	3.03	0.47
1:A:502:VAL:CG1	1:A:503:HIS:N	2.78	0.46
1:B:205:TYR:O	1:B:209:THR:HG23	2.16	0.46
1:B:524:SER:CA	1:B:551:TYR:CE1	2.98	0.46
1:A:400:VAL:HG12	1:A:404:HIS:CD2	2.50	0.46
1:A:613:THR:CG2	1:A:615:PHE:HB3	2.46	0.46
1:B:277:MET:HE2	1:B:277:MET:HA	1.97	0.46
1:B:607:PHE:CE2	1:B:625:TRP:CB	2.96	0.46
1:B:416:GLN:N	1:B:497:ILE:CD1	2.79	0.46
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.31	0.46
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.30	0.45
1:A:557:THR:HA	4:A:958:HOH:O	2.16	0.45
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.50	0.45
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.98	0.45
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.17	0.45
1:A:509:SER:N	1:A:510:PRO:HD2	2.32	0.45
1:B:222:ALA:HB2	1:B:228:LEU:HD23	1.97	0.45
1:B:342:LEU:HD12	1:B:342:LEU:N	2.30	0.45
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.47	0.45
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.98	0.45
1:A:396:GLU:OE1	1:A:396:GLU:HA	2.15	0.45
1:A:412:ILE:O	1:A:412:ILE:HG22	2.16	0.45
1:B:304:HIS:O	1:B:604:LYS:HB2	2.16	0.45
1:B:605:PRO:HB2	1:B:607:PHE:CD1	2.52	0.45
1:B:735:LEU:O	1:B:743:HIS:HB2	2.16	0.45
1:B:164:GLU:HG2	1:B:164:GLU:H	1.57	0.45
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.63	0.45
1:A:405:LEU:HD13	1:A:437:LEU:HD11	1.97	0.45
1:A:507:PHE:CD1	1:A:542:HIS:CB	3.00	0.45
1:B:172:LEU:O	1:B:174:ILE:HG13	2.17	0.45
1:B:535:SER:O	1:B:537:ASN:N	2.49	0.45
1:A:686:MET:HG3	1:A:687:GLU:N	2.30	0.45
1:B:202:GLU:C	1:B:206:LYS:HZ2	2.25	0.45
1:B:436:LEU:N	1:B:436:LEU:HD23	2.32	0.45
1:B:573:GLN:H	1:B:573:GLN:CD	2.25	0.45
1:B:605:PRO:CB	1:B:607:PHE:CE1	2.94	0.45
1:A:573:GLN:NE2	1:A:573:GLN:N	2.48	0.44
1:B:191:SER:O	1:B:192:GLN:HB2	2.17	0.44
1:A:416:GLN:C	1:A:497:ILE:HD13	2.42	0.44
1:B:237:LEU:O	1:B:241:GLN:HB2	2.18	0.44
1:B:438:LYS:HE3	1:B:520:MET:HE2	1.99	0.44
1:A:438:LYS:HA	1:A:499:CYS:HB2	2.00	0.44
1:A:438:LYS:HE2	1:A:501:SER:OG	2.18	0.44
1:A:438:LYS:HD2	1:A:520:MET:HE2	1.99	0.44
1:A:607:PHE:CD1	1:A:608:LEU:HG	2.51	0.44
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.47	0.44
1:A:536:GLY:O	1:A:540:VAL:HG23	2.18	0.44
1:A:630:ARG:HD3	4:A:981:HOH:O	2.18	0.44
1:B:582:PRO:HA	4:B:780:HOH:O	2.18	0.44
1:B:558:ASP:O	1:B:559:SER:HB2	2.17	0.43
1:B:586:MET:HE3	1:B:586:MET:HB3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLU:HA	4:A:930:HOH:O	2.17	0.43
1:B:316:LEU:O	1:B:580:GLN:HG3	2.18	0.43
1:A:390:GLU:OE2	1:A:392:HIS:HE1	2.00	0.43
1:A:573:GLN:H	1:A:573:GLN:CD	2.20	0.43
1:A:654:PRO:HG3	1:A:678:ASN:O	2.18	0.43
1:B:161:ASN:HD21	1:B:164:GLU:CD	2.27	0.43
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.07	0.43
1:A:661:HIS:O	1:A:698:ALA:HA	2.19	0.43
1:A:291:HIS:CD2	1:A:295:TYR:CE1	3.07	0.43
1:A:300:GLN:HB3	1:A:301:PRO:HD2	2.01	0.43
1:B:412:ILE:O	1:B:412:ILE:HG22	2.18	0.43
1:A:212:ALA:O	1:A:215:ASP:HB2	2.19	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.82	0.43
1:B:162:PHE:CE2	1:B:182:ARG:CG	3.01	0.43
1:B:172:LEU:HB2	1:B:174:ILE:HG13	2.00	0.43
1:B:405:LEU:HD23	1:B:405:LEU:HA	1.87	0.43
1:B:438:LYS:HE2	1:B:501:SER:OG	2.19	0.43
1:B:502:VAL:CG1	1:B:503:HIS:N	2.80	0.43
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.90	0.42
1:A:411:PRO:O	1:A:434:LYS:NZ	2.52	0.42
1:A:406:ARG:HE	1:A:495:MET:HE3	1.83	0.42
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.54	0.42
1:B:199:GLU:O	1:B:202:GLU:N	2.49	0.42
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.35	0.42
1:A:300:GLN:O	1:A:305:TYR:HE1	2.03	0.42
1:A:436:LEU:N	1:A:436:LEU:HD23	2.34	0.42
1:B:563:SER:O	1:B:566:GLU:HG2	2.20	0.42
1:A:316:LEU:CD2	1:A:328:ALA:HB2	2.47	0.42
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.19	0.42
1:B:272:LYS:O	1:B:275:PHE:HB3	2.19	0.42
1:A:607:PHE:HE1	1:A:608:LEU:HG	1.83	0.42
1:A:588:VAL:HA	1:A:720:THR:HG21	2.02	0.42
1:A:743:HIS:HA	1:A:744:PRO:HD2	1.78	0.42
1:B:416:GLN:CA	1:B:497:ILE:CD1	2.97	0.42
1:B:701:ARG:HD3	1:B:701:ARG:HH11	1.70	0.42
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.45	0.42
1:A:651:ILE:HG22	1:A:677:ASN:HA	2.02	0.42
1:B:514:GLY:HA3	4:B:832:HOH:O	2.18	0.42
1:A:410:GLY:HA3	1:A:411:PRO:HD3	1.74	0.41
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.43	0.41
1:B:581:THR:HA	1:B:582:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ARG:CD	1:B:755:GLN:NE2	2.80	0.41
1:B:643:LYS:HD2	1:B:643:LYS:HA	1.65	0.41
1:B:388:SER:HA	1:B:438:LYS:HB3	2.02	0.41
1:A:338:ARG:HG3	1:A:601:TYR:CE1	2.56	0.41
1:A:351:GLU:HB2	4:A:973:HOH:O	2.21	0.41
1:A:622:GLN:HA	1:B:445:LEU:HD11	2.02	0.41
1:A:515:GLN:HE22	1:A:521:ALA:HB2	1.85	0.41
1:B:409:LEU:HA	1:B:409:LEU:HD12	1.88	0.41
1:B:610:ASP:C	1:B:612:ASN:N	2.79	0.41
1:B:211:ARG:HE	1:B:211:ARG:HB3	1.73	0.41
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.86	0.41
1:B:500:LYS:HE3	4:B:783:HOH:O	2.20	0.41
1:A:381:SER:HB2	1:A:599:CYS:HA	2.03	0.41
1:A:406:ARG:HE	1:A:495:MET:CE	2.34	0.41
1:A:600:GLY:HA2	4:A:779:HOH:O	2.20	0.41
1:B:196:LEU:O	1:B:201:ILE:HD11	2.21	0.41
1:B:329:TYR:OH	1:B:341:GLU:O	2.39	0.41
1:B:421:VAL:HG12	1:B:424:SER:O	2.21	0.41
1:B:442:LEU:HD21	1:B:488:LEU:HB3	2.03	0.41
1:B:525:GLU:O	1:B:529:LEU:HG	2.21	0.41
1:A:733:VAL:HB	1:A:748:LEU:HB2	2.04	0.40
1:B:300:GLN:O	1:B:427:SER:HA	2.22	0.40
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.57	0.40
1:B:216:ARG:HA	1:B:219:GLU:HG2	2.02	0.40
1:B:344:CYS:O	1:B:392:HIS:HB2	2.20	0.40
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.36	0.40
1:B:390:GLU:HG2	1:B:392:HIS:CD2	2.57	0.40
1:B:517:PHE:CD1	1:B:517:PHE:C	2.99	0.40
1:A:211:ARG:HG3	4:A:935:HOH:O	2.22	0.40
1:A:573:GLN:N	1:A:573:GLN:CD	2.79	0.40
1:B:202:GLU:C	1:B:206:LYS:NZ	2.79	0.40
1:A:383:TYR:CB	1:A:384:PRO:HD2	2.45	0.40
1:A:502:VAL:CG1	1:A:515:GLN:NE2	2.85	0.40
1:B:523:PHE:CD1	1:B:523:PHE:N	2.90	0.40
1:B:669:SER:C	1:B:670:ARG:HG2	2.47	0.40
1:A:517:PHE:CD1	1:A:517:PHE:C	2.99	0.40
1:A:522:SER:HA	1:A:549:ARG:O	2.21	0.40
1:B:310:SER:HB3	1:B:337:CYS:SG	2.62	0.40
1:B:551:TYR:C	1:B:551:TYR:CD1	2.97	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	509/624 (82%)	471 (92%)	31 (6%)	7 (1%)	9	19
1	B	557/624 (89%)	511 (92%)	35 (6%)	11 (2%)	6	12
All	All	1066/1248 (85%)	982 (92%)	66 (6%)	18 (2%)	7	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	B	175	GLN
1	B	176	VAL
1	B	177	ASP
1	B	510	PRO
1	B	515	GLN
1	B	649	ASN
1	A	511	GLY
1	A	513	SER
1	A	536	GLY
1	B	173	ASN
1	B	178	ASP
1	B	198	ASP
1	B	536	GLY
1	A	514	GLY
1	A	648	LYS
1	A	510	PRO
1	B	514	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	444/545 (82%)	407 (92%)	37 (8%)	10	23
1	B	492/545 (90%)	438 (89%)	54 (11%)	6	13
All	All	936/1090 (86%)	845 (90%)	91 (10%)	8	17

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	209	THR
1	A	216	ARG
1	A	238	GLN
1	A	242	ARG
1	A	252	LEU
1	A	257	ARG
1	A	277	MET
1	A	309	SER
1	A	350	GLN
1	A	406	ARG
1	A	419	ASP
1	A	432	LYS
1	A	436	LEU
1	A	440	LYS
1	A	508	SER
1	A	512	THR
1	A	526	SER
1	A	530	ARG
1	A	533	GLN
1	A	563	SER
1	A	573	GLN
1	A	577	LEU
1	A	594	GLN
1	A	621	THR
1	A	630	ARG
1	A	632	ARG
1	A	652	VAL
1	A	655	LYS
1	A	657	ILE
1	A	665	ARG
1	A	675	ILE
1	A	685	ASP

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Mol	Chain	Res	Type
1	A	709	SER
1	A	712	LYS
1	A	738	LYS
1	A	756	ASP
1	B	158	ASN
1	B	162	PHE
1	B	164	GLU
1	B	166	LYS
1	B	167	ASP
1	B	173	ASN
1	B	182	ARG
1	B	206	LYS
1	B	210	GLN
1	B	211	ARG
1	B	227	THR
1	B	228	LEU
1	B	231	GLU
1	B	242	ARG
1	B	309	SER
1	B	331	ARG
1	B	409	LEU
1	B	416	GLN
1	B	421	VAL
1	B	423	THR
1	B	432	LYS
1	B	440	LYS
1	B	484	ASP
1	B	488	LEU
1	B	502	VAL
1	B	509	SER
1	B	515	GLN
1	B	526	SER
1	B	533	GLN
1	B	573	GLN
1	B	577	LEU
1	B	594	GLN
1	B	607	PHE
1	B	613	THR
1	B	621	THR
1	B	643	LYS
1	B	646	LYS
1	B	647	ASN

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Mol	Chain	Res	Type
1	B	648	LYS
1	B	650	SER
1	B	651	ILE
1	B	652	VAL
1	B	655	LYS
1	B	657	ILE
1	B	665	ARG
1	B	675	ILE
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER
1	B	711	SER
1	B	738	LYS
1	B	753	SER
1	B	756	ASP

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	241	GLN
1	A	291	HIS
1	A	392	HIS
1	A	515	GLN
1	A	573	GLN
1	A	594	GLN
1	A	640	GLN
1	A	661	HIS
1	A	718	GLN
1	A	734	HIS
1	B	161	ASN
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	350	GLN
1	B	573	GLN
1	B	594	GLN
1	B	640	GLN
1	B	661	HIS
1	B	718	GLN
1	B	728	GLN
1	B	755	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	5	-	3,3,3	0.92	0	3,3,3	0.60	0
2	ACT	B	5	-	3,3,3	0.82	0	3,3,3	0.86	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.