



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:21 AM GMT

PDB ID : 2GLS
Title : REFINED ATOMIC MODEL OF GLUTAMINE SYNTHETASE AT 3.5
ANGSTROMS RESOLUTION
Authors : Eisenberg, D.; Almasy, R.J.; Yamashita, M.M.
Deposited on : 1989-05-19
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

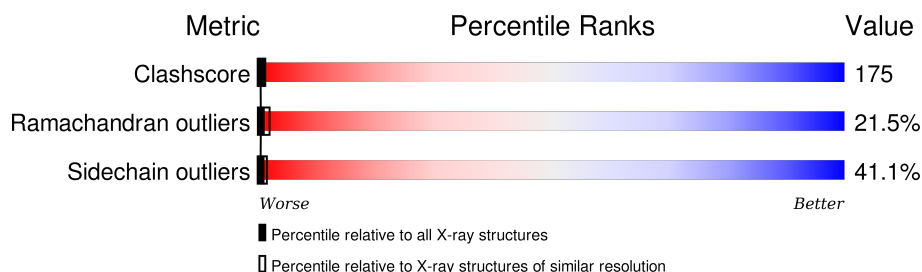
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)






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	469	
1	B	469	
1	C	469	
1	D	469	
1	E	469	
1	F	469	
1	G	469	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	469	
1	I	469	
1	J	469	
1	K	469	
1	L	469	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43692 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	B	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	C	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	D	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	E	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	F	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	G	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	H	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	I	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	J	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	K	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			
1	L	468	Total	C	N	O	S	0	0	0
			3636	2301	624	691	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Mn 2	0	0
2	K	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	H	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0
2	I	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	3	Total 3	O 3	0	0
3	C	3	Total 3	O 3	0	0
3	D	3	Total 3	O 3	0	0
3	E	3	Total 3	O 3	0	0
3	F	3	Total 3	O 3	0	0
3	G	3	Total 3	O 3	0	0
3	H	3	Total 3	O 3	0	0
3	I	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

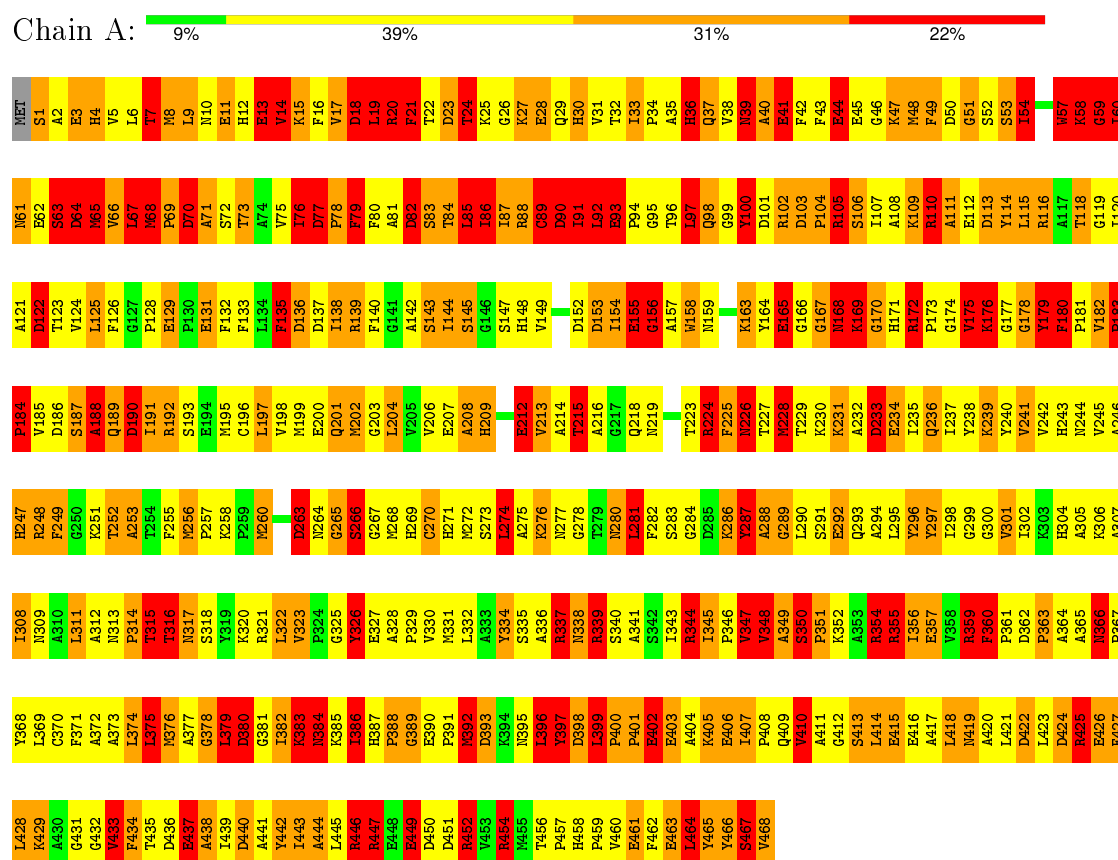
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	3	Total 3	O 3	0	0
3	K	3	Total 3	O 3	0	0
3	L	3	Total 3	O 3	0	0

3 Residue-property plots

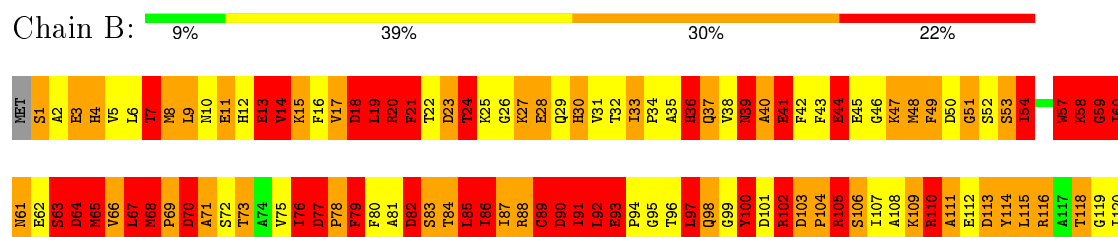
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

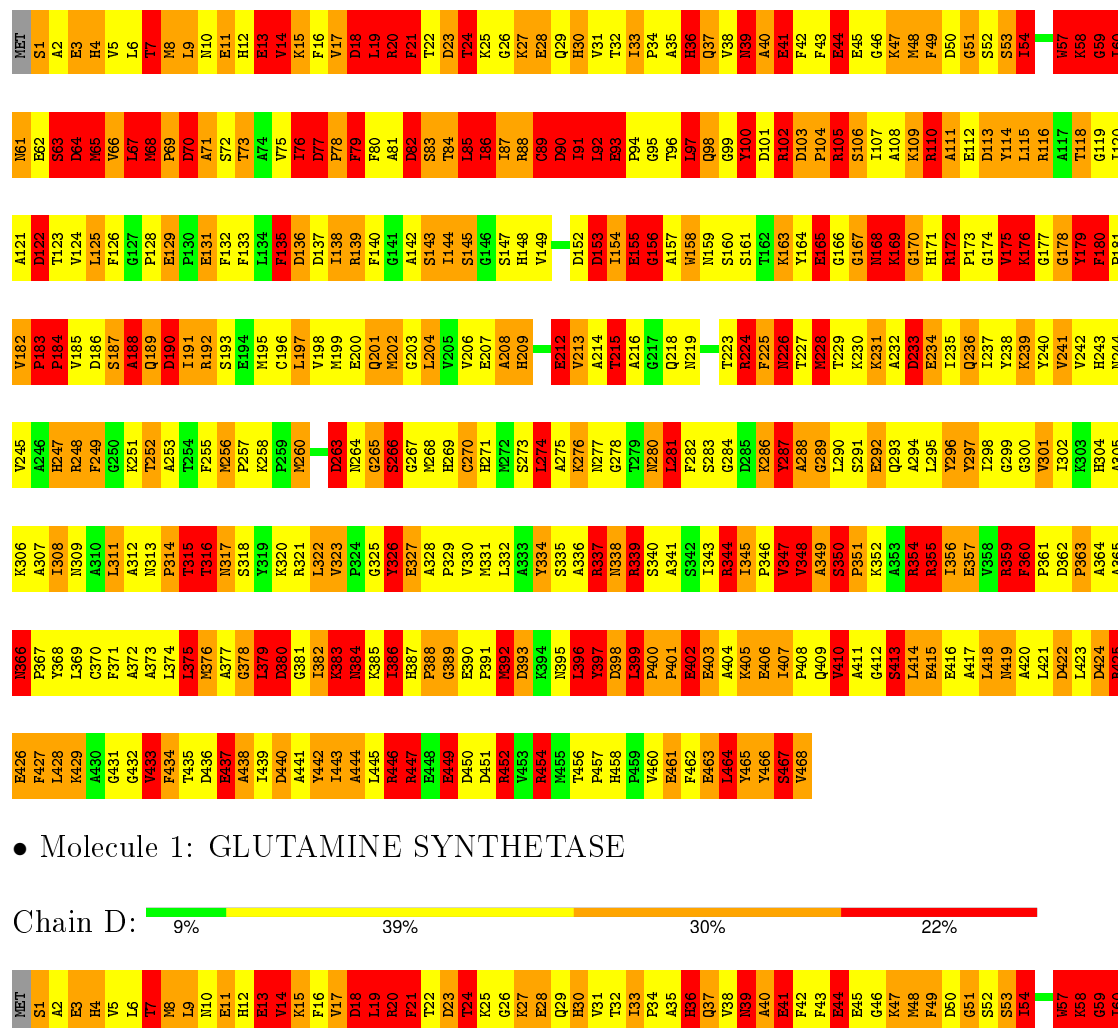
Note EDS was not executed.

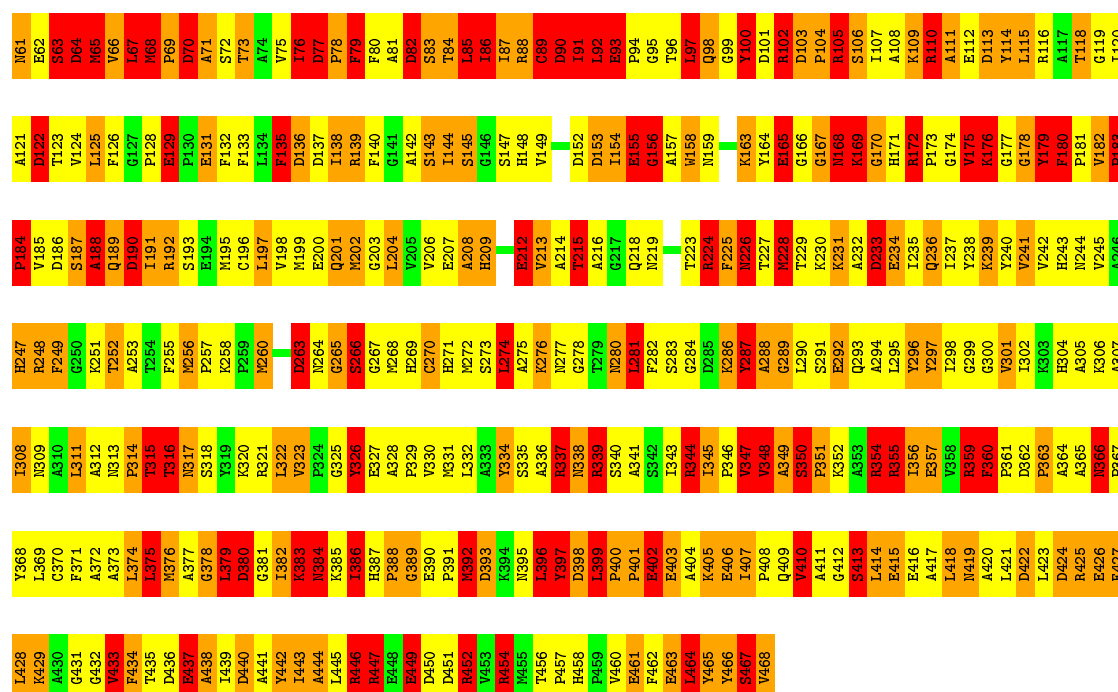
• Molecule 1: GLUTAMINE SYNTHETASE



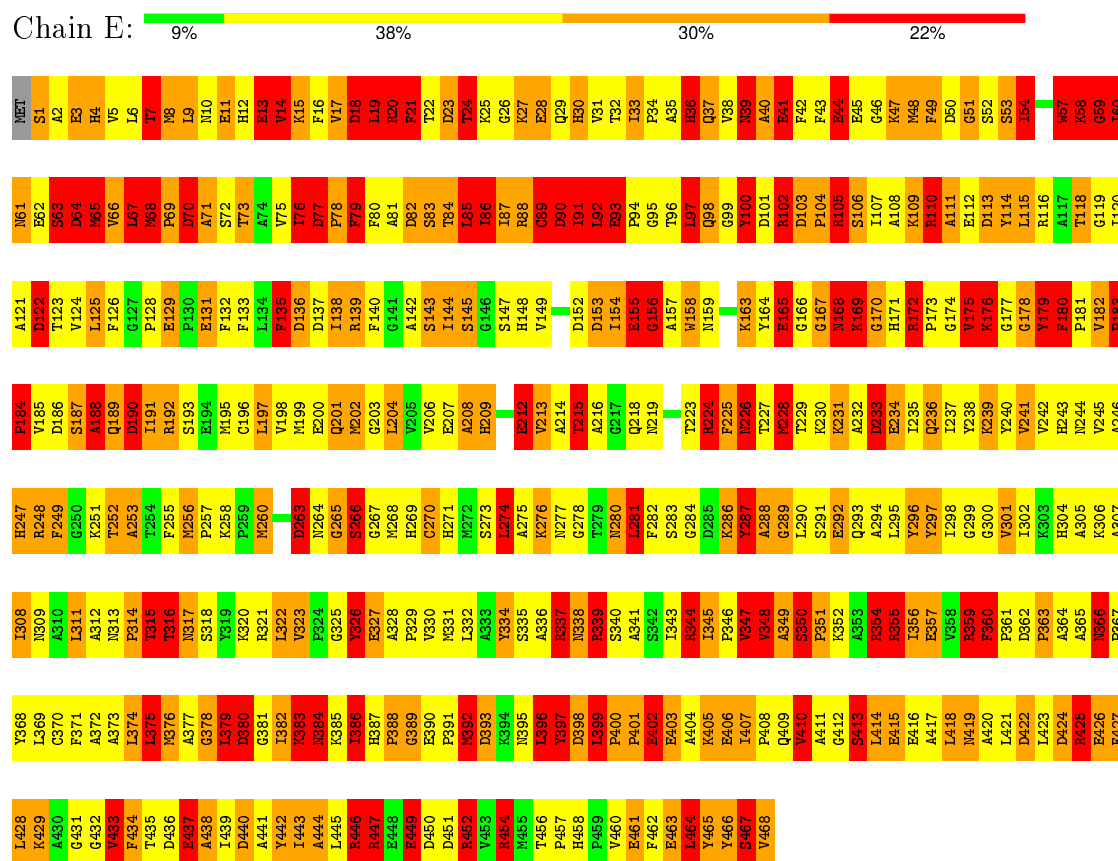
• Molecule 1: GLUTAMINE SYNTHETASE







• Molecule 1: GLUTAMINE SYNTHETASE





L428	Y368	T308	H247	P184	A121	M61
L429	L369	L309	R248	H185	D122	B62
A430	C370	A310	F249	D186	T123	S63
G431	F371	L311	G250	S187	V124	D64
G432	A372	A312	K251	A188	L125	M65
V433	A373	K313	T252	Q189	F126	V66
F434	L374	F314	A253	D190	G127	L67
L435	L375	T315	T254	R191	P128	M68
B436	K376	K316	F255	R192	K129	P69
B437	A377	K317	M256	S193	P130	D70
A438	G378	F318	P257	F194	E131	A71
L439	L379	L319	K258	M195	F132	S72
D440	D380	K320	P259	C196	F133	T73
A441	G381	R321	M260			
L442	L382	L322				
L443	K383	P323	D263	D197	L134	A74
A444	K384	V324	M264	M199	F135	V75
L445	K385	G325	K265	E200	D136	I76
R446	L386	Y326	G266	Q201	L138	P78
R447	R387	F327	S267	M202	R139	F79
E448	P388	A328	M268	G203	F140	F80
E449	G389	P329	E269	L204	G141	A81
A450	E390	V330	C370	V205	A142	D82
D451	P391	K331	H271	V206	S143	S83
R452	K392	L332	P272	E207	L144	T84
F453	K393	F333	S273	A208	G146	L85
R454	K394	K334	L274	H209	I147	I86
M455	K395	S335	A275		S147	I87
T456	L396	A336	K276		H148	R88
P457	Y397	R337	N277	V213	V149	G89
H458	D398	K338	G278	A214		D90
P459	L399	R339	T279	T215	D152	I91
V460	P400	S340	N280	A216	D153	L92
E461	P401	A341	L281	G217	L154	E93
F462	E402	S342	F282	Q218	E155	P94
E463	B403	L343	S283	M219	G156	G95
L464	A404	R344			A157	T96
V465	K405	L345	D284	T223	M158	L97
V466	B406	P346	K286	R224	N159	G98
S467	L407	V347	Y287	F225		G99
	P408	K348	A288	T227	K163	Y100
	Q409	L349	G289	K228	V164	A40
	V410	S350	G290		E165	R102
	A411	P351	L290	T229	G166	D103
	G412	K352	S291	K230	G167	P104
	S413	K353	E292	K231	N168	R105
	L414	L354	Q293	A232	K169	S106
	E415	R355	A294	D233	G170	I107
	E416	L356	T296	E234	H171	A108
	A417	F357	Y297	T235	R172	K109
	L418	K358	L298	Q236	P173	R110
	M419	R359	G299	K238	G174	A111
	K420	F360	G300	Y239	V175	E112
	L421	P361	V301		K176	D113
	D422	D362	L302	Y240	G177	Y114
	L423	P363	K303	V241	F178	L115
	D424	A364	H304	T242	Y179	R116
	R425	A365	A305	E244	F180	T118
	E426	K366	K306	V245	P181	G119
	F427	P367	A207	D246	T182	T120

• Molecule 1: GLUTAMINE SYNTHETASE

Chain H: 

MT	S1	A2	E3	H4	V5	L6	I7	M8	P9	D0	L9	N10	E11	H12	E13	V14	K15	F16	V17	D18	L19	R20	F21	D22	T23	T84	D85	T24	K25	G26	K27	C88	D29	R30	I91	L92	V31	T32	P34	G95	T96	A35	H36	Q37	V38	Y100	D101	R102	E41	F42	P104	R105	E44	E45	G46	K47	N48	F49	D50	E51	S52	Y114	S53	L115	E154	E57	K58	G59	T118	G119	V182	I120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
N61	E62	S63	D64	H65	V66	L67	M68	P69	D70	L79	A71	N80	E81	H82	E83	V84	K85	F86	V87	D88	L89	R90	F91	D92	T93	T94	L85	T86	K87	G88	H89	C90	D91	R92	I93	L94	V95	T96	A97	H98	Q99	V100	D101	R102	E103	F104	R105	E106	G107	K108	N109	F110	D111	E112	S113	Y114	S115	E116	A117	K118	G119	V120	I121																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A121	D122	T123	L124	E125	F126	G127	P128	E129	L130	N131	E132	H133	E134	V135	K136	F137	V138	D139	L140	R141	F142	D143	T144	E145	H146	K147	G148	C149	D150	E151	G152	H153	F154	V155	K156	F157	V158	N159	K160	D161	E162	F163	G164	R165	S166	T167	K168	N169	F170	D171	E172	S173	Y174	S175	L176	E177	K178	G179	V180	I181	T182	G183																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
P184	V185	D186	S187	L188	E189	F190	I191	R192	N193	E194	H195	E196	V197	K198	F199	D200	L201	R202	F203	D204	T205	E206	H207	K208	G209	C210	D211	E212	G213	H214	F215	V216	K217	F218	N219	T220	A221	H222	Q223	V224	D225	E226	F227	K228	N229	F230	G231	R232	S233	T234	K235	L236	Y237	S238	Y239	D240	E241	S242	Y243	S244	L245	E246																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
H247	R248	F249	G250	K251	T252	A253	T254	P255	M256	L257	N258	E259	H260	D261	K262	G263	F264	V265	D266	L267	R268	F269	D270	T271	E272	H273	K274	G275	H276	C277	D278	I279	N280	E281	F282	G283	H284	Q285	V286	D287	E288	F289	G290	S291	R292	Q293	A294	L295	K296	Y297	L298	G299	V300	D301	E302	S303	Y304	S305	L306	E307	K308	G309	V310	I311	T312	P313	G314	R315	S316	T317	K318	N319	F320	D321	E322	G323	H324	C325	D326	E327	F328	V329	N330	E331	H332	K333	G334	F335	V336	D337	L338	R339	F340	T341	E342	H343	K344	G345	C346	D347	I348	N349	E350	F351	G352	R353	S354	T355	K356	L357	Y358	S359	Y360	D361	E362	S363	Y364	S365	L366	E367	K368	G369	V370	I371	T372	P373	G374	R375	S376	T377	K378	N379	F380	D381	E382	G383	H384	C385	D386	E387	F388	V389	N390	E391	H392	K393	G394	F395	V396	D397	L398	R399	F400	T401	E402	S403	T404	K405	L406	Y407	S408	Y409	D410	E411	S412	Y413	S414	L415	E416	F417	K418	N419	F420	D421	E422	G423	H424	C425	D426	E427	F428	V429	N430	E431	H432	K433	G434	F435	V436	D437	L438	R439	F440	T441	E442	H443	K444	G445	C446	D447	I448	N449	E450	F451	G452	R453	S454	T455	K456	L457	Y458	S459	Y460	D461	E462	S463	Y464	S465	L466	E467	K468	G469	V470	I471	T472	P473	G474	R475	S476	T477	K478	N479	F480	D481	E482	G483	H484	C485	D486	E487	F488	V489	N490	E491	H492	K493	G494	F495	V496	D497	L498	R499	F500	T501	E502	S503	T504	K505	L506	Y507	S508	Y509	D510	E511	S512	Y513	S514	L515	E516	F517	K518	N519	F520	D521	E522	G523	H524	C525	D526	E527	F528	V529	N530	E531	H532	K533	G534	F535	V536	D537	L538	R539	F540	T541	E542	H543	K544	G545	C546	D547	I548	N549	E550	F551	G552	R553	S554	T555	K556	L557	Y558	S559	Y560	D561	E562	S563	Y564	S565	L566	E567	K568	G569	V570	I571	T572	P573	G574	R575	S576	T577	K578	N579	F580	D581	E582	G583	H584	C585	D586	E587	F588	V589	N590	E591	H592	K593	G594	F595	V596	D597	L598	R599	F600	T601	E602	S603	T604	K605	L606	Y607	S608	Y609	D610	E611	S612	Y613	S614	L615	E616	F617	K618	N619	F620	D621	E622	G623	H624	C625	D626	E627	F628	V629	N630	E631	H632	K633	G634	F635	V636	D637	L638	R639	F640	T641	E642	H643	K644	G645	C646	D647	I648	N649	E650	F651	G652	R653	S654	T655	K656	L657	Y658	S659	Y660	D661	E662	S663	Y664	S665	L666	E667	K668	G669	V670	I671	T672	P673	G674	R675	S676	T677	K678	N679	F680	D681	E682	G683	H684	C685	D686	E687	F688	V689	N690	E691	H692	K693	G694	F695	V696	D697	L698	R699	F700	T701	E702	S703	T704	K705	L706	Y707	S708	Y709	D710	E711	S712	Y713	S714	L715	E716	F717	K718	N719	F720	D721	E722	G723	H724	C725	D726	E727	F728	V729	N730	E731	H732	K733	G734	F735	V736	D737	L738	R739	F740	T741	E742	H743	K744	G745	C746	D747	I748	N749	E750	F751	G752	R753	S754	T755	K756	L757	Y758	S759	Y760	D761	E762	S763	Y764	S765	L766	E767	K768	G769	V770	I771	T772	P773	G774	R775	S776	T777	K778	N779	F780	D781	E782	G783	H784	C785	D786	E787	F788	V789	N790	E791	H792	K793	G794	F795	V796	D797	L798	R799	F800	T801	E802	S803	T804	K805	L806	Y807	S808	Y809	D810	E811	S812	Y813	S814	L815	E816	F817	K818	N819	F820	D821	E822	G823	H824	C825	D826	E827	F828	V829	N830	E831	H832	K833	G834	F835	V836	D837	L838	R839	F840	T841	E842	H843	K844	G845	C846	D847	I848	N849	E850	F851	G852	R853	S854	T855	K856	L857	Y858	S859	Y860	D861	E862	S863	Y864	S865	L866	E867	K868	G869	V870	I871	T872	P873	G874	R875	S876	T877	K878	N879	F880	D881	E882	G883	H884	C885	D886	E887	F888	V889	N890	E891	H892	K893	G894	F895	V896	D897	L898	R899	F900	T901	E902	S903	T904	K905	L906	Y907	S908	Y909	D910	E911	S912	Y913	S914	L915	E916	F917	K918	N919	F920	D921	E922	G923	H924	C925	D926	E927	F928	V929	N930	E931	H932	K933	G934	F935	V936	D937	L938	R939	F940	T941	E942	H943	K944	G945	C946	D947	I948	N949	E950	F951	G952	R953	S954	T955	K956	L957	Y958	S959	Y960	D961	E962	S963	Y964	S965	L966	E967	K968	G969	V970	I971	T972	P973	G974	R975	S976	T977	K978	N979	F980	D981	E982	G983	H984	C985	D986	E987	F988	V989	N990	E991	H992	K993	G994	F995	V996	D997	L998	R999	F1000	T1001	E1002	S1003	T1004	K1005	L1006	Y1007	S1008	Y1009	D1010	E1011	S1012	Y1013	S1014	L1015	E1016	F1017	K1018	N1019	F1020	D1021	E1022	G1023	H1024	C1025	D1026	E1027	F1028	V1029	N1030	E1031	H1032	K1033	G1034	F1035	V1036	D1037	L1038	R1039	F1040	T1041	E1042	H1043	K1044	G1045	C1046	D1047	I1048	N1049	E1050	F1051	G1052	R1053	S1054	T1055	K1056	L1057	Y1058	S1059	Y1060	D1061	E1062	S1063	Y1064	S1065	L1066	E1067	K1068	G1069	V1070	I1071	T1072	P1073	G1074	R1075	S1076	T1077	K1078	N1079	F1080	D1081	E1082	G1083	H1084	C1085	D1086	E1087	F1088	V1089	N1090	E1091	H1092	K1093	G1094	F1095	V1096	D1097	L1098	R1099	F1100	T1101	E1102	S1103	T1104	K1105	L1106	Y1107	S1108	Y1109	D1110	E1111	S1112	Y1113	S1114	L1115	E1116	F1117	K1118	N1119	F1120	D1121	E1122	G1123	H1124	C1125	D1126	E1127	F1128	V1129	N1130	E1131	H1132	K1133	G1134	F1135	V1136	D1137	L1138	R1139	F1140	T1141	E1142	H1143	K1144	G1145	C1146	D1147	I1148	N1149	E1150	F1151	G1152	R1153	S1154	T1155	K1156	L1157	Y1158	S1159	Y1160	D1161	E1162	S1163	Y1164	S1165	L1166	E1167	K1168	G1169	V1170	I1171	T1172	P1173	G1174	R1175	S1176	T1177	K1178	N1179	F1180	D1181	E1182	G1183	H1184	C1185	D1186	E1187	F1188	V1189	N1190	E1191	H1192	K1193	G1194	F1195	V1196	D1197	L1198	R1199	F1200	T1201	E1202	S1203	T1204	K1205	L1206	Y1207	S1208	Y1209	D1210	E1211	S1212	Y1213	S1214	L1215	E1216	F1217	K1218	N1219	F1220	D1221	E1222	G1223	H1224	C1225	D1226	E1227	F1228	V1229	N1230	E1231	H1232	K1233	G1234	F1235	V1236	D1237	L1238	R1239	F1240	T1241	E1242	H1243	K1244	G1245	C1246	D1247	I1248	N1249	E1250	F1251	G1252	R1253	S1254	T1255	K1256	L1257	Y1258	S1259	Y1260	D1261	E1262	S1263	Y1264	S1265	L1266	E1267	K1268	G1269	V1270	I1271	T1272	P1273	G1274	R1275	S1276	T1277	K1278	N1279	F1280	D1281	E1282	G1283	H1284	C1285	D1286	E1287	F1288	V1289	N1290	E1291	H1292	K1293	G1294	F1295	V1296	D1297	L1298	R1299	F1300	T1301	E1302	S1303	T1304	K1305	L1306	Y1307	S1308	Y1309	D1310	E1311	S1312	Y1313	S1314	L1315	E1316	F1317	K1318	N1319	F1320	D1321	E1322	G1323	H1324	C1325	D1326	E1327	F1328	V1329	N1330	E1331	H1332	K1333	G1334	F1335	V1336	D1337	L1338	R1339	F1340	T1341	E1342	H1343	K1344	G1345	C1346	D1347	I1348	N1349	E1350	F1351	G1352	R1353	S1354	T1355	K1356	L1357	Y1358	S1359	Y1360	D1361	E1362	S1363	Y1364	S1365	L1366	E1367	K1368	G1369	V1370	I1371	T1372	P1373	G1374	R1375	S1376	T1377	K1378	N1379	F1380	D1381	E1382	G1383	H1384	C1385	D1386	E1387	F1388	V1389	N1390	E1391	H1392	K1393	G1394	F1395	V1396	D1397	L1398	R1399	F1400	T1401	E1402	S1403	T1404	K1405	L1406	Y1407	S1408	Y1409	D1410	E1411	S1412	Y1413	S1414	L1415	E1416	F1417	K1418	N1419	F1420	D1421	E1422	G1423	H1424	C1425	D1426	E1427	F1428	V1429	N1430	E1431	H1432	K1433	G1434	F1435	V1436	D1437	L1438	R1439	F1440	T1441	E1442	H1443

L428	K429
A430	G431
G432	V433
F434	T435
D436	E437
A438	N439
D440	A441
Y442	K443
A444	L445
R446	R447
E448	E449
D450	D451
R452	V453
R454	T455
T456	P457
H458	P459
V460	E461
F462	E463
L464	Y465
Y466	S467
V468	

• Molecule 1: GLUTAMINE SYNTHETASE

Chain J: 10% 38% 30% 22%

L428	K429	A430	G431	G432	V433	F434	T435	D436	E437	A438	L439	D440	A441	Y442	K443	A444	L445	R446	R447	E448	E449	D450	D451	R452	V453	R454	T455	T456	P457	H458	P459	V460	E461	E462	E463	L464	Y465	Y466	S467	V468																					
Y368	L369	C370	F371	A372	A373	L374	M375	K376	G377	G378	L379	D380	G381	L382	K383	N384	K385	L386	H387	P388	G389	E390	P391	R392	D393	R394	N395	L396	R397	D398	L399	P400	P401	E402	E403	A404	K405	E406	L407	P408	Q409	V410	A411	G412	S413	L414	E415	E416	A417	L418	M419	A420	L421	D422	L423	D424	R425	E426	F427		
I308	A309	L310	L311	A312	R313	P314	T315	R316	N317	S318	V319	R320	R321	L322	V323	P324	G325	V326	E327	A328	P329	V330	R331	L332	L333	A334	Y335	S336	A337	R338	L339	P340	A341	S342	R343	L344	R345	P346	V347	A348	A349	S350	P351	K352	A353	L354	R355	L356	F357	V358	R359	A360	P361	D362	P363	A364	A365	R366	F367		
H247	R248	F249	G250	K251	T252	A253	T254	P255	M256	P257	K258	M260	D263	N264	G265	S266	G267	M268	H269	C270	H271	A272	S273	L274	A275	K276	N277	A278	T279	N280	L281	F282	S283	G284	D285	K286	Y287	A288	G289	L290	S291	E292	Q293	A294	L295	Y296	Y297	I298	G299	V300	I301	I302	V241	V242	H243	N244	A246				
P184	D185	V186	S187	A188	D189	I191	E192	S193	E194	M195	C196	L197	V198	M199	E200	Q201	N202	G203	L204	V205	V206	H207	A208	H209	E212	V213	A214	T215	A216	G217	Q218	N219	T223	R224	F225	R226	T227	R228	G229	E230	A232	D233	E234	T235	Q236	I237	I238	K239	V301	I302	V241	V242	H243	N244	A246						
A121	D122	T123	D124	L125	F126	G127	P128	E129	F130	E131	F132	F133	L134	F135	D136	D137	I138	R139	F140	G141	D142	S143	T144	S145	G146	H147	H148	V149	D152	D153	I154	E155	G156	A157	H158	N159	K163	Y164	E165	R166	G167	R168	E169	G170	A171	H172	P173	G174	V175	K176	D177	G178	Y179	F180	P181	G182	P183				
M61	E62	S63	D64	V65	V66	L67	M68	P69	D70	A71	S72	T73	E74	V75	I76	D77	F78	F79	F80	A81	D82	S83	T84	L85	T86	I87	R88	C89	D90	I91	L92	E93	P94	G95	T96	L97	Q98	G99	Y100	D101	R102	D103	P104	R105	S106	E107	A108	M109	R110	D111	E112	D113	G114	G115	G116	G117	L118	A117	T118	G119	I120
MET	S1	A2	E3	H4	V5	L6	T7	M8	N9	N10	E11	H12	E13	V14	K15	F16	V17	D18	L19	R20	F21	T22	D23	T24	K25	G26	K27	E28	Q29	H30	V31	T32	P33	G34	A35	H36	Q37	V38	R39	A40	E41	F42	F43	E44	E45	G46	K47	M48	F49	D50	G51	S52	Y53	I54	M57	K58	G59	V60			

• Molecule 1: GLUTAMINE SYNTHETASE

Chain K: 9% 39% 31% 22%

K306	V245	V182	A121	H61	MET
A307	A246	P183	D122	E62	S1
L308	H247	P184	T123	S63	A2
N309	R248	V185	V124	D64	E3
A310	F249	D186	L125	V65	H4
L311	G250	S187	F126	V66	V5
A312	K251	A188	G127	L67	L6
N313	T252	Q189	P128	M68	T7
P314	A253	D190	E129	P69	M8
T315	T254	I191	F130	D70	L9
R316	F255	R192	E131	A71	N10
N317	H256	S193	F132	S72	E11
S318	P257	E194	F133	T73	H12
V319	K258	M195	L134	A74	E13
K320	P259	C196	F135	V75	V14
R321	M260	L197	D136	I76	K15
L322		V198	D137	D77	F16
V323	D263	M199	I138	F78	V17
P324	K264	E200	R139	F79	D18
G325	G265	Q201	F140	F80	L19
S326	S266	M202	G141	A81	L19
E327	G267	G203	A142	D82	R20
A328	K268	L204	S143	S83	F21
P329	H269	V205	I144	T84	T22
V330	C270	V206	S145	L85	D23
R331	H271	E207	G146	I86	T24
L332	N272	A208	S147	I87	K25
A333	S273	H209	H148	R88	G26
V334	L274		V149	C89	K27
S335	A275	E212		D90	E28
A336	K276	V213	D152	I91	Q29
R337	N277	A214	D153	L92	Q29
N338	G278	T215	E154	E93	H30
R339	T279	A216	E155	P94	V31
S340	N280	G217	G156	G95	I33
A341	L281	Q218	A157	T96	P34
S342	F282	N219	H158	L97	A35
R343	G283		N159	Q98	H36
L344	K284	T223	S160	G99	Q37
L345	D285	R224	F161	Y100	V38
F346	K286	F225	T162	D101	N39
V347	V287	R226	K163	R102	A40
V348	A288	T227	V164	D103	E41
A349	G289	R228	E165	P104	F42
S350	L290	T229	G166	R105	F43
P351	S291	K230	G167	S106	E44
K352	F292	R231	M168	I107	E45
A353	Q293	A232	K169	A108	G46
R354	A294	D233	G170	K109	K47
R355	L295	E234	H171	R110	M48
L356	V296	T235	A172	A111	F49
V357	Y297	Q236	P173	E112	D50
F358	I298	I237	G174	D113	G51
R359	G299	T238	V175	Y114	S52
P360	V300	K239	K176	L115	S53
P361	G301	Y240	G177	R116	I54
D362	I302	V241	F178	A117	M57
P363	K303	V242	G179	T118	K58
A364	H304	H243	V181	G119	G59
A365	L305	N244	D181	I120	V182

E386
F367
Y368
L368
K369
C370
F371
A372
A373
L374
L375
L376
A377
G378
L379
D380
G381
L382
I383
I384
L385
L386
H387
P388
G389
F390
P391
P392
D393
K394
I395
L396
L397
D398
P400
P401
E402
E403
A404
Y405
E406
L407
P408
Q409
V410
A411
G412
S413
L414
E415
E416
A417
L418
I419
A420
L421
D422
L423
D424
R425

E426
F427
L428
K429
A430
G431
G432
V433
F434
T435
D436
E437
A438
I439
D440
A441
Y442
I443
A444
L445
R446
R447
E448
E449
D450
D451
R452
V453
R454
M455
T456
P457
H458
P459
V460
E461
F462
E463
L464
Y465
Y466
S467
V468

• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 9% 39% 30% 22%

WET
S1
A2
S3
D64
H5
V66
L67
M68
P69
D70
A71
E11
S72
T73
H12
E13
V14
K15
F16
P17
D18
L19
R20
F21
S22
T23
D24
K25
G26
K27
E28
D29
I30
L31
V32
T33
G34
A35
R36
Q37
V38
R39
A40
E41
D42
F43
E44
E45
G46
K47
M48
F49
D50
G51
D52
S53
Y54
R57
K58
G59
D60

M61
E62
S63
D64
M65
V66
L67
M68
P69
D70
A71
S72
T73
H12
E13
V14
K15
F16
P17
D18
L19
R20
F21
S22
T23
D24
K25
G26
K27
E28
D29
I30
L31
V32
T33
G34
A35
R36
Q37
V38
R39
A40
E41
D42
F43
E44
E45
G46
K47
M48
F49
D50
G51
D52
S53
Y54
R57
K58
G59
D60

A121
D122
T123
V124
L125
F126
G127
P128
R129
P130
E131
F132
M133
T134
L135
F136
M137
E138
D139
F140
G141
A142
S143
I144
S145
G146
S147
H148
V149
D152
D153
E155
G156
A157
M158
I159
K163
Y164
E165
G166
G167
R168
K169
G170
H171
R172
P173
G174
V175
K176
G177
G178
Y179
F180
P181
V182
P183

P184
V185
D186
L187
A188
Q189
D190
L191
R192
E193
E194
M195
C196
L197
V198
M199
E200
Q201
N202
G203
L204
V205
G206
E207
A208
H209
E212
V213
A214
T215
A216
G217
N219
T223
R224
F225
N226
T227
R228
G229
K230
K231
A232
D233
E234
I235
Q236
I237
Y238
K239
Y240
V241
V242
H243
N244
V245
A246

H247
K248
P249
G250
K251
T252
A253
T254
F255
M256
P257
K258
P259
H260
D263
K264
G265
S266
E267
A268
H269
C270
M271
K272
S273
L274
A275
K276
N277
G278
T279
N280
A281
F282
S283
G284
D285
K286
Y287
A288
Q289
S291
E292
K293
A294
L295
Y296
Y297
L298
G299
G300
V301
I302
K303
H304
A305
K306
A307

I308
N309
A310
L311
A312
N313
P314
T315
T316
N317
S318
Y319
K320
R321
L322
V323
P324
G325
Y326
E327
A328
P329
V330
M331
L332
A333
Y334
S335
A336
R337
N338
R339
S340
A341
S342
I343
R344
I345
P346
V347
V348
A349
S350
P351
K352
A353
R354
R355
L356
E357
V358
R359
F360
P361
D362
P363
A364
A365
N366
P367

Y368
L369
C370
F371
A372
A373
L374
L375
P376
A377
G378
L379
D380
G381
L382
K383
N384
K385
L386
H387
P388
G389
E390
P391
K392
T393
N394
N395
L396
Y397
D398
L399
P400
P401
E402
E403
A404
K405
E406
P408
Q409
V410
A411
G412
S413
L414
E415
E416
A417
L418
N419
A420
L421
D422
L423
D424
R425
E426
S427

L428
K429
A430
G431
G432
V433
F434
T435
D436
E437
A438
I439
D440
A441
Y442
I443
A444
L445
R446
R447
E448
E449
D450
D451
R452
V453
R454
M455
T456
P457
H458
P459
V460
E461
F462
E463
A464
Y465
Y466
S467
V468

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.50Å 134.50Å 200.10Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.258 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	43692	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: MN

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	1.48	31/3723 (0.8%)	2.38	198/5043 (3.9%)
1	B	1.48	31/3723 (0.8%)	2.38	196/5043 (3.9%)
1	C	1.48	31/3723 (0.8%)	2.38	203/5043 (4.0%)
1	D	1.48	30/3723 (0.8%)	2.38	199/5043 (3.9%)
1	E	1.48	31/3723 (0.8%)	2.38	198/5043 (3.9%)
1	F	1.48	30/3723 (0.8%)	2.38	198/5043 (3.9%)
1	G	1.48	31/3723 (0.8%)	2.38	199/5043 (3.9%)
1	H	1.48	31/3723 (0.8%)	2.38	199/5043 (3.9%)
1	I	1.49	30/3723 (0.8%)	2.38	202/5043 (4.0%)
1	J	1.48	31/3723 (0.8%)	2.38	196/5043 (3.9%)
1	K	1.49	30/3723 (0.8%)	2.38	197/5043 (3.9%)
1	L	1.48	30/3723 (0.8%)	2.38	200/5043 (4.0%)
All	All	1.48	367/44676 (0.8%)	2.38	2385/60516 (3.9%)

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	1	3
1	B	1	3
1	C	1	3
1	D	1	3
1	E	1	3
1	F	1	3
1	G	1	3
1	H	1	3
1	I	1	3
1	J	1	3
1	K	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	1	3
All	All	12	36

The worst 5 of 367 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	156	GLY	N-CA	7.84	1.57	1.46
1	J	156	GLY	N-CA	7.79	1.57	1.46
1	I	156	GLY	N-CA	7.71	1.57	1.46
1	L	156	GLY	N-CA	7.70	1.57	1.46
1	A	156	GLY	N-CA	7.68	1.57	1.46

The worst 5 of 2385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	ARG	CD-NE-CZ	28.32	163.25	123.60
1	B	88	ARG	CD-NE-CZ	28.31	163.23	123.60
1	G	88	ARG	CD-NE-CZ	28.30	163.22	123.60
1	J	88	ARG	CD-NE-CZ	28.29	163.20	123.60
1	F	88	ARG	CD-NE-CZ	28.27	163.18	123.60

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	315	THR	CA
1	B	315	THR	CA
1	C	315	THR	CA
1	D	315	THR	CA
1	E	315	THR	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	355	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	339	ARG	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	3636	0	3538	1356	0
1	B	3636	0	3538	1357	1
1	C	3636	0	3538	1344	0
1	D	3636	0	3538	1336	0
1	E	3636	0	3538	1351	1
1	F	3636	0	3538	1353	0
1	G	3636	0	3538	1352	0
1	H	3636	0	3538	1352	0
1	I	3636	0	3538	1350	0
1	J	3636	0	3538	1337	0
1	K	3636	0	3538	1341	0
1	L	3636	0	3538	1355	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
All	All	43692	0	42456	15036	1

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 175.

The worst 5 of 15036 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:C:465:TYR:CD2	1:I:315:THR:CG2	1.94	1.50
1:E:315:THR:CG2	1:K:465:TYR:CD2	1.94	1.50
1:F:315:THR:CG2	1:L:465:TYR:CD2	1.94	1.50
1:B:465:TYR:CD2	1:H:315:THR:CG2	1.94	1.50
1:E:465:TYR:CD2	1:K:315:THR:CG2	1.94	1.49

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:OE2	1:E:1:SER:N[4_444]	1.84	0.36

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	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	B	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	C	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	D	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	E	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	F	466/469 (99%)	248 (53%)	118 (25%)	100 (22%)	0	1
1	G	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	H	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	I	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	K	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	L	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
All	All	5592/5628 (99%)	2987 (53%)	1405 (25%)	1200 (22%)	0	1

5 of 1200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	13	GLU
1	A	14	VAL
1	A	21	PHE
1	A	28	GLU

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	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	B	384/385 (100%)	227 (59%)	157 (41%)	0	1
1	C	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	D	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	E	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	F	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	G	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	H	384/385 (100%)	227 (59%)	157 (41%)	0	1
1	I	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	J	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	K	384/385 (100%)	226 (59%)	158 (41%)	0	1
1	L	384/385 (100%)	227 (59%)	157 (41%)	0	1
All	All	4608/4620 (100%)	2715 (59%)	1893 (41%)	0	1

5 of 1893 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	165	GLU
1	G	323	VAL
1	L	33	ILE
1	F	236	GLN
1	G	36	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	189	GLN
1	G	313	ASN
1	L	39	ASN
1	F	293	GLN
1	G	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 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 [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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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