



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 12:05 AM UTC

PDB ID : 1W63 / pdb_00001w63
Title : AP1 clathrin adaptor core
Authors : Heldwein, E.; Macia, E.; Wang, J.; Yin, H.L.; Kirchhausen, T.; Harrison, S.C.
Deposited on : 2004-08-12
Resolution : 4.00 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

<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
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

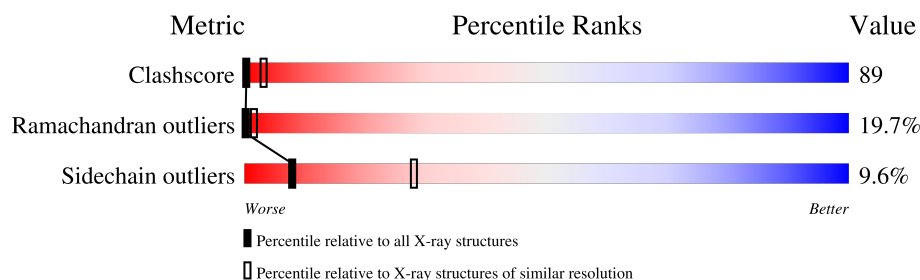
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)

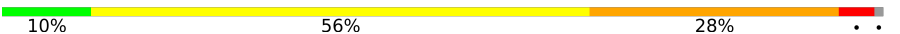
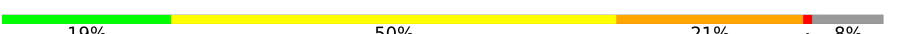
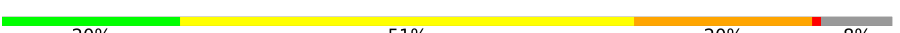
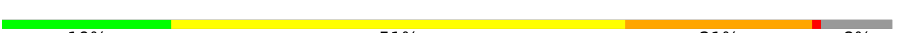
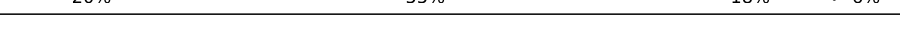
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	618	10% 59% 25% • 5%
1	C	618	10% 59% 24% • 5%
1	E	618	10% 59% 24% • 5%
1	G	618	10% 58% 25% • 5%
1	I	618	10% 58% 25% • 5%
1	K	618	9% 59% 25% • 5%
2	B	584	10% 56% 29% ••
2	D	584	11% 55% 29% ••

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Mol	Chain	Length	Quality of chain
2	F	584	 11% 55% 29% . .
2	H	584	 10% 56% 28% . .
2	J	584	 11% 56% 29% . .
2	L	584	 11% 55% 29% . .
3	M	423	 19% 50% 21% . 8%
3	N	423	 20% 51% 20% . 8%
3	O	423	 19% 51% 21% . 8%
3	P	423	 19% 51% 21% . 8%
3	R	423	 18% 52% 20% . 8%
3	V	423	 19% 51% 21% . 8%
4	Q	158	 18% 56% 18% . 6%
4	S	158	 20% 55% 18% . 6%
4	T	158	 19% 56% 18% . 6%
4	U	158	 20% 56% 18% . 6%
4	W	158	 20% 55% 18% . 6%
4	X	158	 19% 56% 18% . 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 81744 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 ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	C	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	E	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	G	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	I	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	K	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			

- Molecule 2 is a protein called ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	D	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	F	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	H	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	J	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	L	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	MET	LEU	conflict	UNP P52303
B	439	ASP	LEU	conflict	UNP P52303
B	459	SER	ILE	conflict	UNP P52303
D	155	MET	LEU	conflict	UNP P52303
D	439	ASP	LEU	conflict	UNP P52303
D	459	SER	ILE	conflict	UNP P52303
F	155	MET	LEU	conflict	UNP P52303
F	439	ASP	LEU	conflict	UNP P52303
F	459	SER	ILE	conflict	UNP P52303
H	155	MET	LEU	conflict	UNP P52303
H	439	ASP	LEU	conflict	UNP P52303
H	459	SER	ILE	conflict	UNP P52303
J	155	MET	LEU	conflict	UNP P52303
J	439	ASP	LEU	conflict	UNP P52303
J	459	SER	ILE	conflict	UNP P52303
L	155	MET	LEU	conflict	UNP P52303
L	439	ASP	LEU	conflict	UNP P52303
L	459	SER	ILE	conflict	UNP P52303

- Molecule 3 is a protein called ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	N	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	O	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	P	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	R	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	V	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	134	PHE	TYR	conflict	UNP P35585
M	406	ILE	LEU	conflict	UNP P35585
N	134	PHE	TYR	conflict	UNP P35585
N	406	ILE	LEU	conflict	UNP P35585

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Chain	Residue	Modelled	Actual	Comment	Reference
O	134	PHE	TYR	conflict	UNP P35585
O	406	ILE	LEU	conflict	UNP P35585
P	134	PHE	TYR	conflict	UNP P35585
P	406	ILE	LEU	conflict	UNP P35585
R	134	PHE	TYR	conflict	UNP P35585
R	406	ILE	LEU	conflict	UNP P35585
V	134	PHE	TYR	conflict	UNP P35585
V	406	ILE	LEU	conflict	UNP P35585

- Molecule 4 is a protein called ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT.

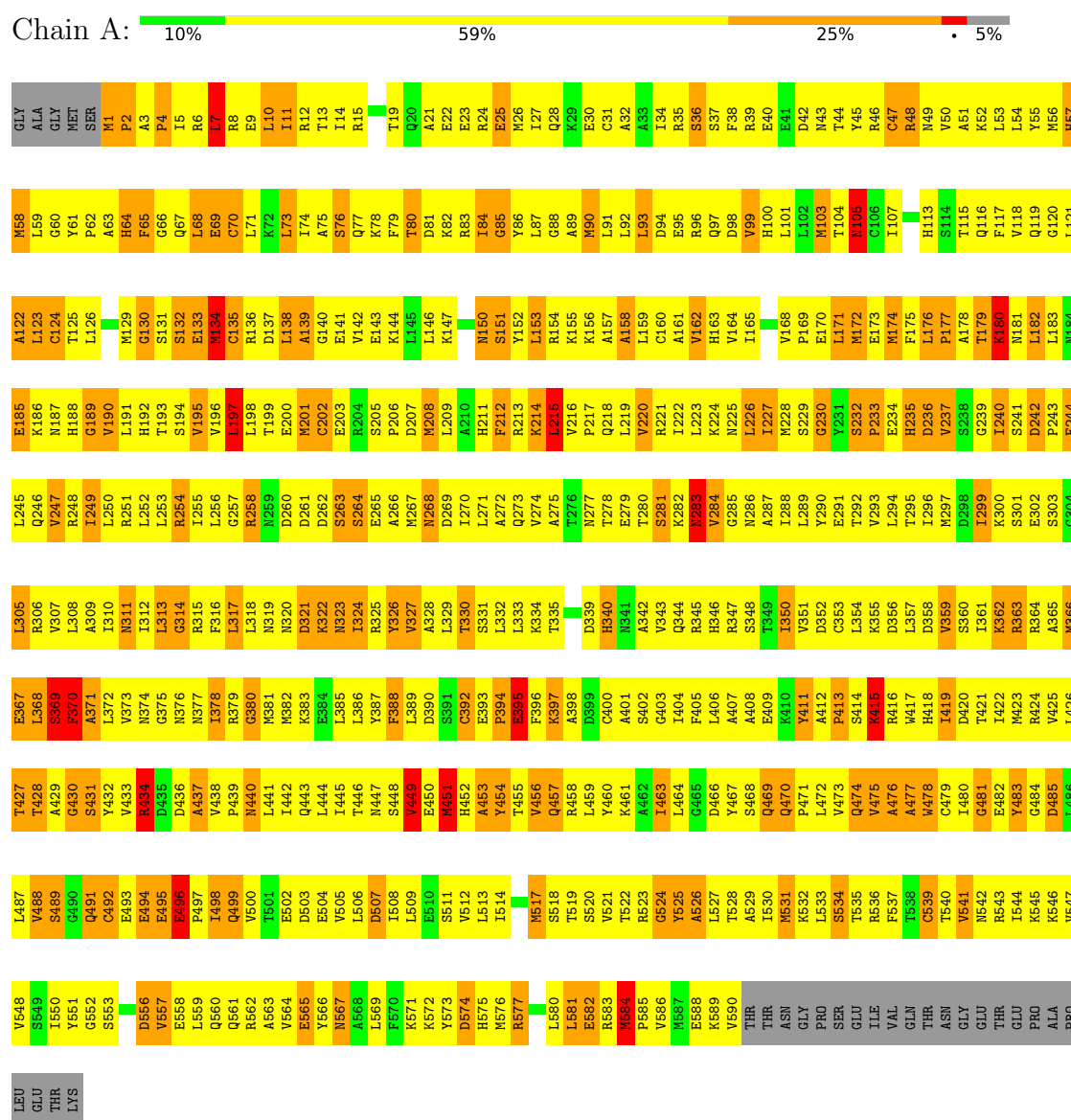
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	S	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	T	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	U	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	W	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	X	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			

3 Residue-property plots

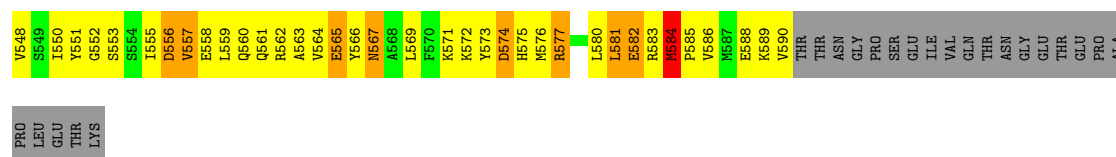
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

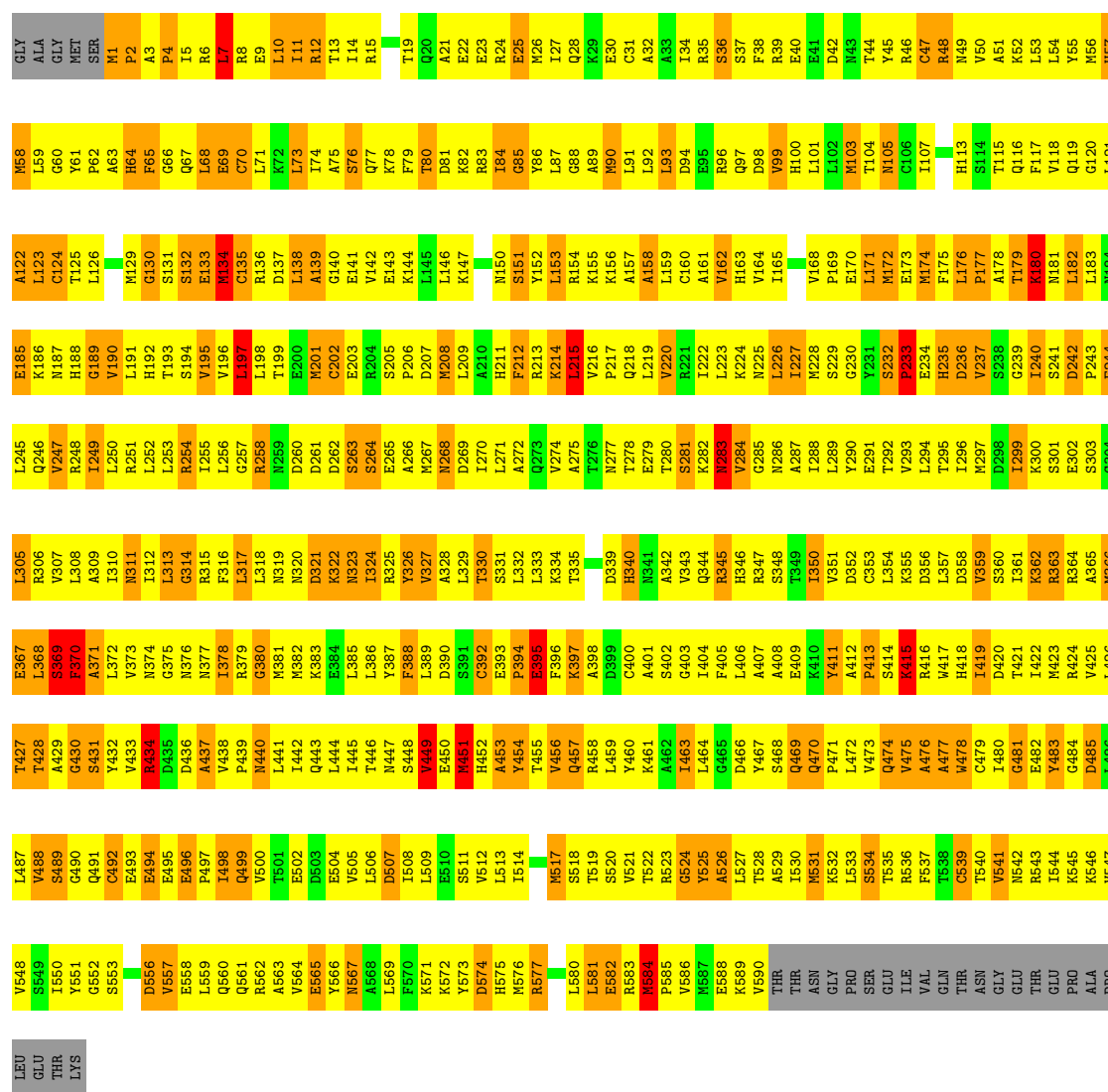


• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT



• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

Chain I: 10% 58% 25% 5%

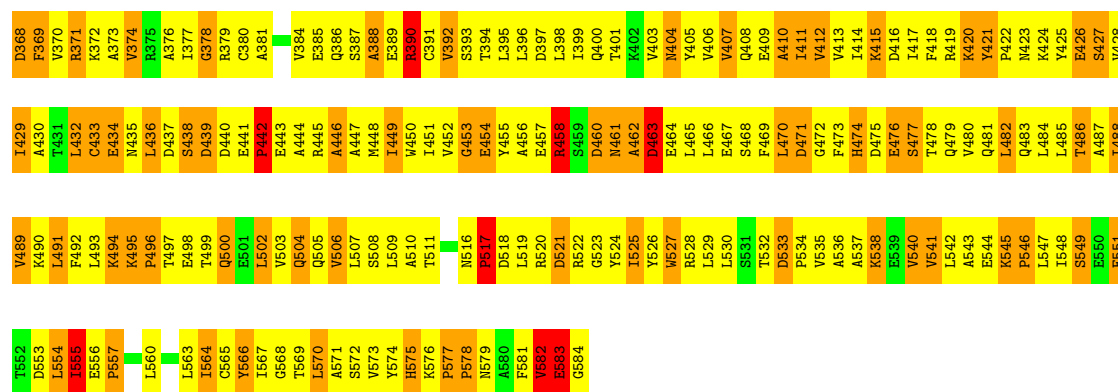


• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

Chain K: 9% 59% 25% 5%

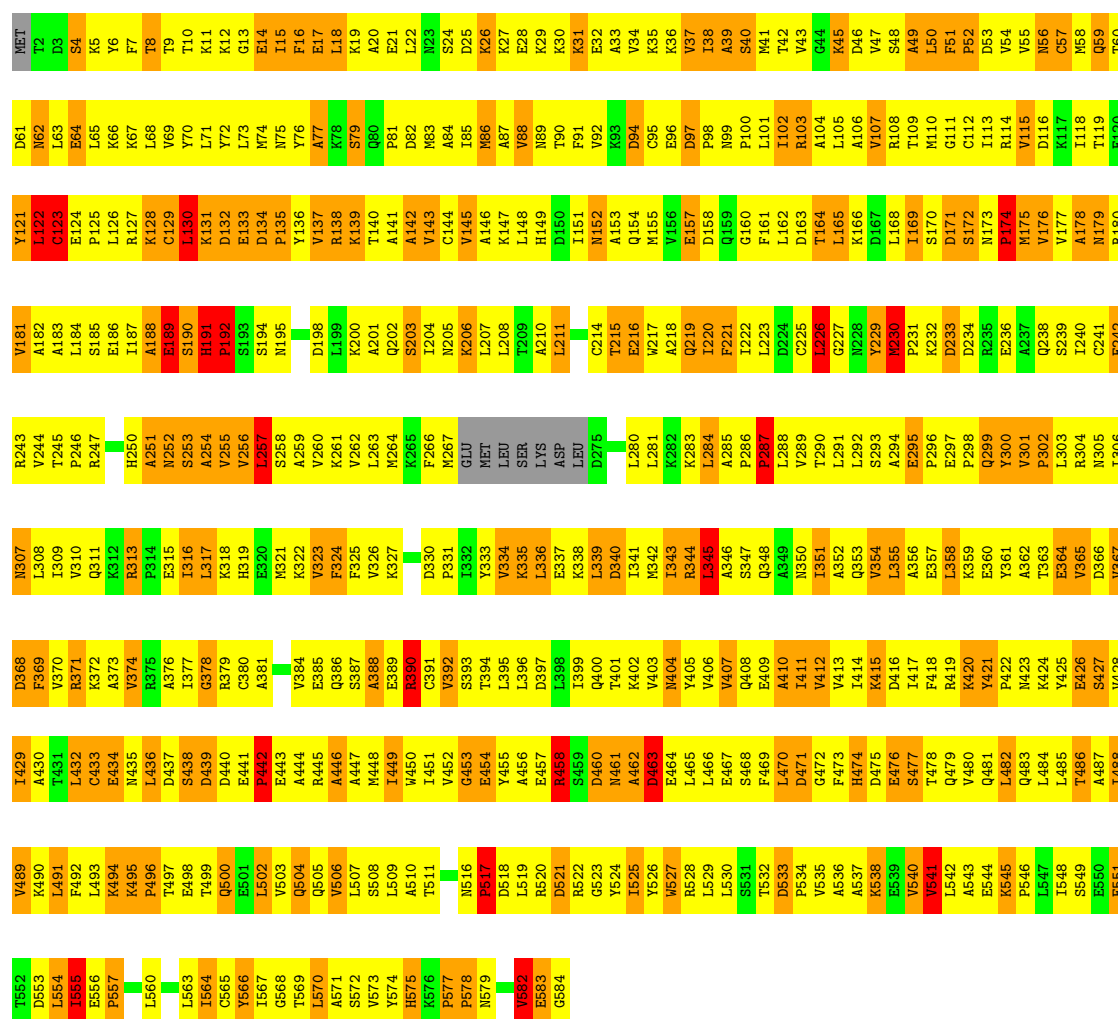


- Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT



Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

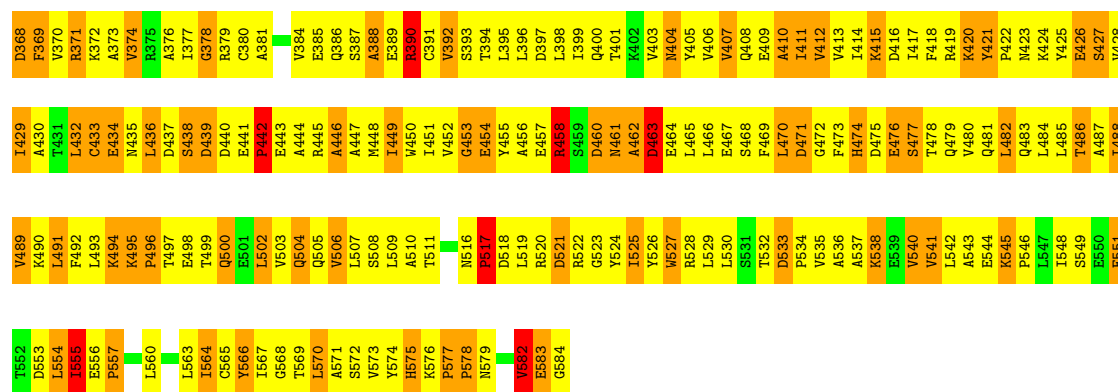
Chain D: 11% 55% 29% ..



Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

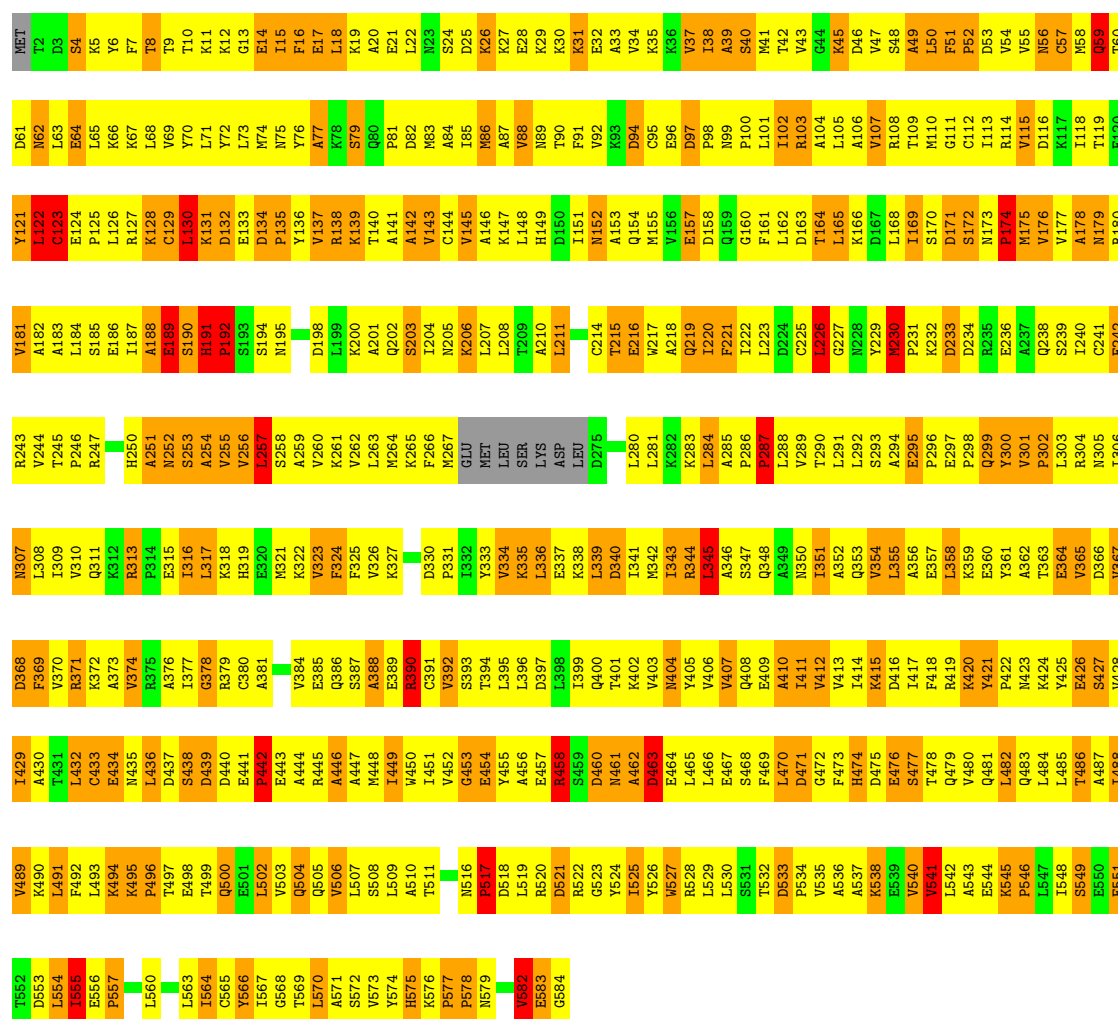
Chain F: 11% 55% 29% ..

MET	T2	D61	Y121	V181	R243	N307	D368	I429	V489	T552	D307	D308	D309	D310	D311	D312	D313	D314	D315	D316	D317	D318	D319	D320	D321	D322	D323	D324	D325	D326	D327	D328	D329	D330	D331	D332	D333	D334	D335	D336	D337	D338	D339	D340	D341	D342	D343	D344	D345	D346	D347	D348	D349	D350	D351	D352	D353	D354	D355	D356	D357	D358	D359	D360	D361	D362	D363	D364	D365	D366	D367	D368	D369	D370	D371	D372	D373	D374	D375	D376	D377	D378	D379	D380	D381	D382	D383	D384	D385	D386	D387	D388	D389	D390	D391	D392	D393	D394	D395	D396	D397	D398	D399	D400	D401	D402	D403	D404	D405	D406	D407	D408	D409	D410	D411	D412	D413	D414	D415	D416	D417	D418	D419	D420	D421	D422	D423	D424	D425	D426	D427	D428	D429	D430	D431	D432	D433	D434	D435	D436	D437	D438	D439	D440	D441	D442	D443	D444	D445	D446	D447	D448	D449	D450	D451	D452	D453	D454	D455	D456	D457	D458	D459	D460	D461	D462	D463	D464	D465	D466	D467	D468	D469	D470	D471	D472	D473	D474	D475	D476	D477	D478	D479	D480	D481	D482	D483	D484	D485	D486	D487	D488	D489	D490	D491	D492	D493	D494	D495	D496	D497	D498	D499	D500	D501	D502	D503	D504	D505	D506	D507	D508	D509	D510	D511	D512	D513	D514	D515	D516	D517	D518	D519	D520	D521	D522	D523	D524	D525	D526	D527	D528	D529	D530	D531	D532	D533	D534	D535	D536	D537	D538	D539	D540	D541	D542	D543	D544	D545	D546	D547	D548	D549	D550	D551	D552	D553	D554	D555	D556	D557	D558	D559	D560	D561	D562	D563	D564	D565	D566	D567	D568	D569	D570	D571	D572	D573	D574	D575	D576	D577	D578	D579	D580	D581	D582	D583	D584	D585	D586	D587	D588	D589	D590	D591	D592	D593	D594	D595	D596	D597	D598	D599	D600	D601	D602	D603	D604	D605	D606	D607	D608	D609	D610	D611	D612	D613	D614	D615	D616	D617	D618	D619	D620	D621	D622	D623	D624	D625	D626	D627	D628	D629	D630	D631	D632	D633	D634	D635	D636	D637	D638	D639	D640	D641	D642	D643	D644	D645	D646	D647	D648	D649	D650	D651	D652	D653	D654	D655	D656	D657	D658	D659	D660	D661	D662	D663	D664	D665	D666	D667	D668	D669	D670	D671	D672	D673	D674	D675	D676	D677	D678	D679	D680	D681	D682	D683	D684	D685	D686	D687	D688	D689	D690	D691	D692	D693	D694	D695	D696	D697	D698	D699	D700	D701	D702	D703	D704	D705	D706	D707	D708	D709	D710	D711	D712	D713	D714	D715	D716	D717	D718	D719	D720	D721	D722	D723	D724	D725	D726	D727	D728	D729	D730	D731	D732	D733	D734	D735	D736	D737	D738	D739	D740	D741	D742	D743	D744	D745	D746	D747	D748	D749	D750	D751	D752	D753	D754	D755	D756	D757	D758	D759	D760	D761	D762	D763	D764	D765	D766	D767	D768	D769	D770	D771	D772	D773	D774	D775	D776	D777	D778	D779	D780	D781	D782	D783	D784	D785	D786	D787	D788	D789	D790	D791	D792	D793	D794	D795	D796	D797	D798	D799	D800	D801	D802	D803	D804	D805	D806	D807	D808	D809	D810	D811	D812	D813	D814	D815	D816	D817	D818	D819	D820	D821	D822	D823	D824	D825	D826	D827	D828	D829	D830	D831	D832	D833	D834	D835	D836	D837	D838	D839	D840	D841	D842	D843	D844	D845	D846	D847	D848	D849	D850	D851	D852	D853	D854	D855	D856	D857	D858	D859	D860	D861	D862	D863	D864	D865	D866	D867	D868	D869	D870	D871	D872	D873	D874	D875	D876	D877	D878	D879	D880	D881	D882	D883	D884	D885	D886	D887	D888	D889	D890	D891	D892	D893	D894	D895	D896	D897	D898	D899	D900	D901	D902	D903	D904	D905	D906	D907	D908	D909	D910	D911	D912	D913	D914	D915	D916	D917	D918	D919	D920	D921	D922	D923	D924	D925	D926	D927	D928	D929	D930	D931	D932	D933	D934	D935	D936	D937	D938	D939	D940	D941	D942	D943	D944	D945	D946	D947	D948	D949	D950	D951	D952	D953	D954	D955	D956	D957	D958	D959	D960	D961	D962	D963	D964	D965	D966	D967	D968	D969	D970	D971	D972	D973	D974	D975	D976	D977	D978	D979	D980	D981	D982	D983	D984	D985	D986	D987	D988	D989	D990	D991	D992	D993	D994	D995	D996	D997	D998	D999	D1000	D1001	D1002	D1003	D1004	D1005	D1006	D1007	D1008	D1009	D1010	D1011	D1012	D1013	D1014	D1015	D1016	D1017	D1018	D1019	D1020	D1021	D1022	D1023	D1024	D1025	D1026	D1027	D1028	D1029	D1030	D1031	D1032	D1033	D1034	D1035	D1036	D1037	D1038	D1039	D1040	D1041	D1042	D1043	D1044	D1045	D1046	D1047	D1048	D1049	D1050	D1051	D1052	D1053	D1054	D1055	D1056	D1057	D1058	D1059	D1060	D1061	D1062	D1063	D1064	D1065	D1066	D1067	D1068	D1069	D1070	D1071	D1072	D1073	D1074	D1075	D1076	D1077	D1078	D1079	D1080	D1081	D1082	D1083	D1084	D1085	D1086	D1087	D1088	D1089	D1090	D1091	D1092	D1093	D1094	D1095	D1096	D1097	D1098	D1099	D1100	D1101	D1102	D1103	D1104	D1105	D1106	D1107	D1108	D1109	D1110	D1111	D1112	D1113	D1114	D1115	D1116	D1117	D1118	D1119	D1120	D1121	D1122	D1123	D1124	D1125	D1126	D1127	D1128	D1129	D1130	D1131	D1132	D1133	D1134	D1135	D1136	D1137	D1138	D1139	D1140	D1141	D1142	D1143	D1144	D1145	D1146	D1147	D1148	D1149	D1150	D1151	D1152	D1153	D1154	D1155	D1156	D1157	D1158	D1159	D1160	D1161	D1162	D1163	D1164	D1165	D1166	D1167	D1168	D1169	D1170	D1171	D1172	D1173	D1174	D1175	D1176	D1177	D1178	D1179	D1180	D1181	D1182	D1183	D1184	D1185	D1186	D1187	D1188	D1189	D1190	D1191	D1192	D1193	D1194	D1195	D1196	D1197	D1198	D1199	D1200	D1201	D1202	D1203	D1204	D1205	D1206	D1207	D1208	D1209	D1210	D1211	D1212	D1213	D1214	D1215	D1216	D1217	D1218	D1219	D1220	D1221	D1222	D1223	D1224	D1225	D1226	D1227	D1228	D1229	D1230	D1231	D1232	D1233	D1234	D1235	D1236	D1237	D1238	D1239	D1240	D1241	D1242	D1243	D1244	D1245	D1246	D1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• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

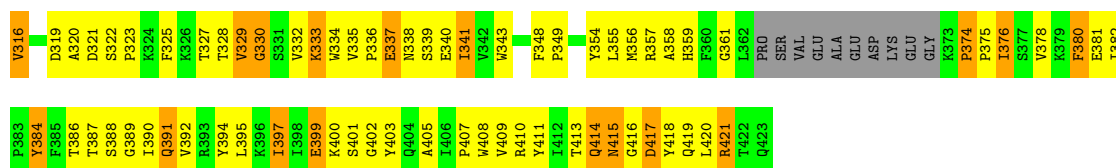
Chain J: 11% 56% 29% ..



• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

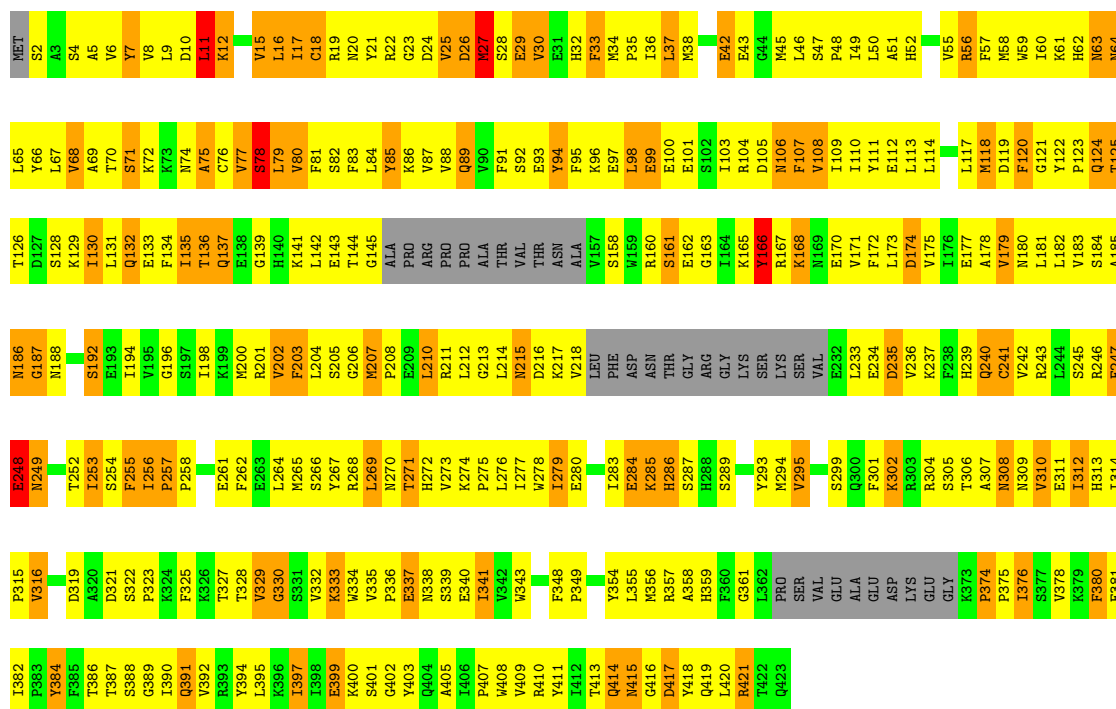
Chain L: 11% 55% 29% ..

- Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT



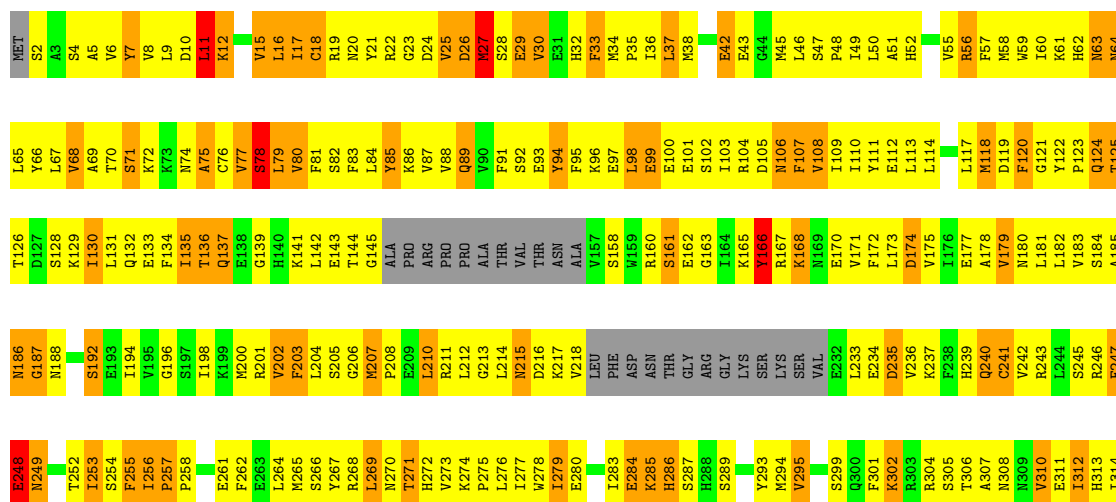
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

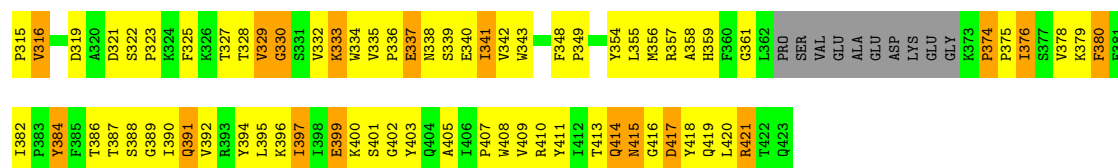
Chain P: 19% 51% 21% 8%



• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

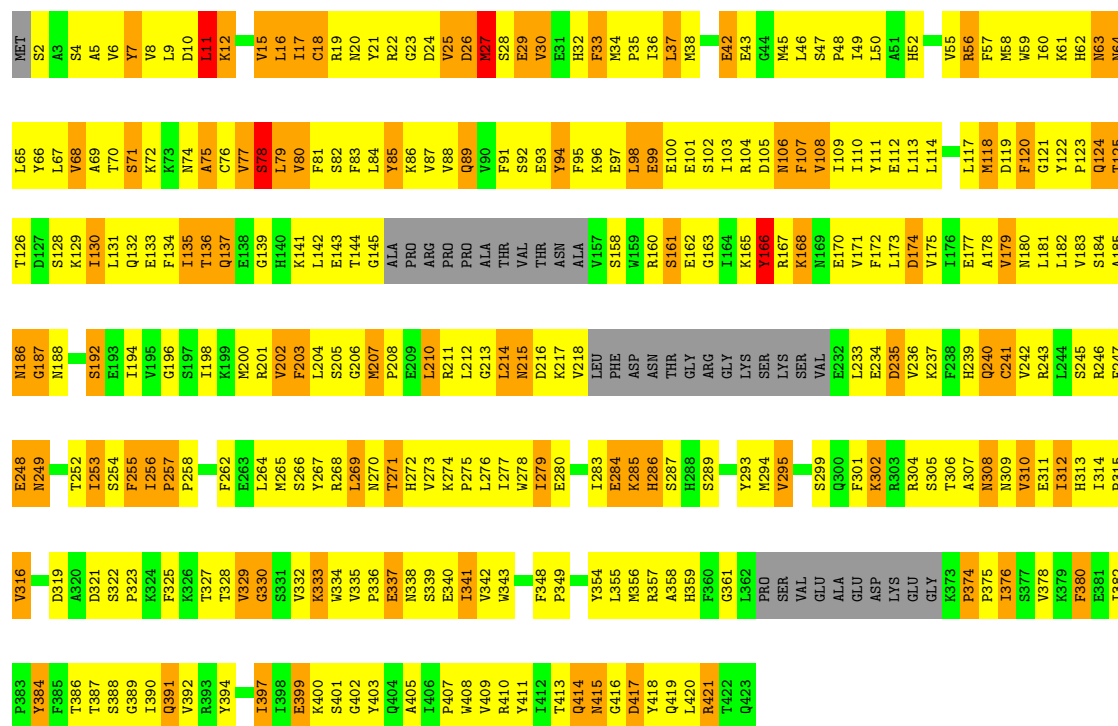
Chain R: 18% 52% 20% 8%





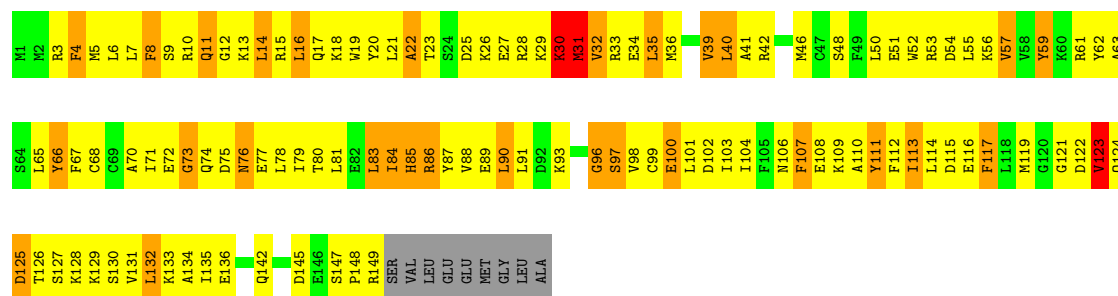
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

Chain V: 19% 51% 21% 8%



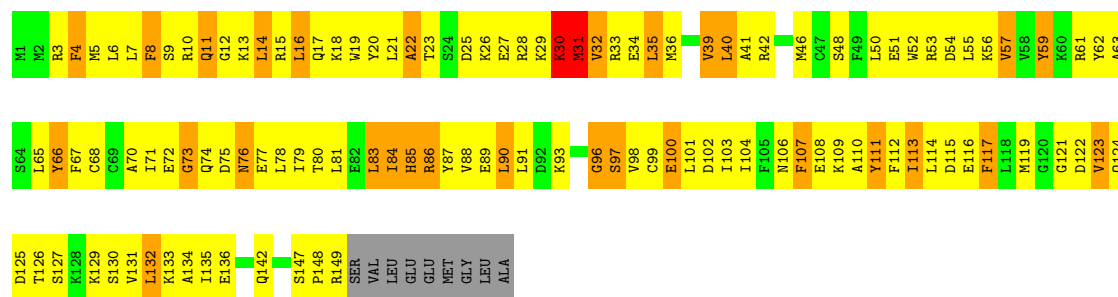
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain Q: 18% 56% 18% 6%



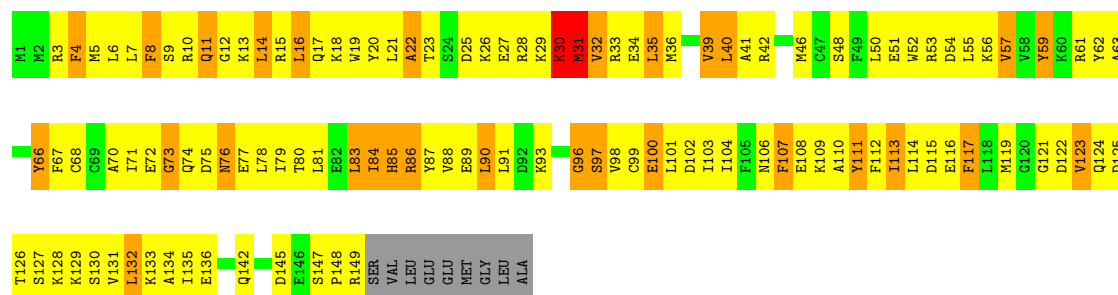
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain S: 20% 55% 18% 6%



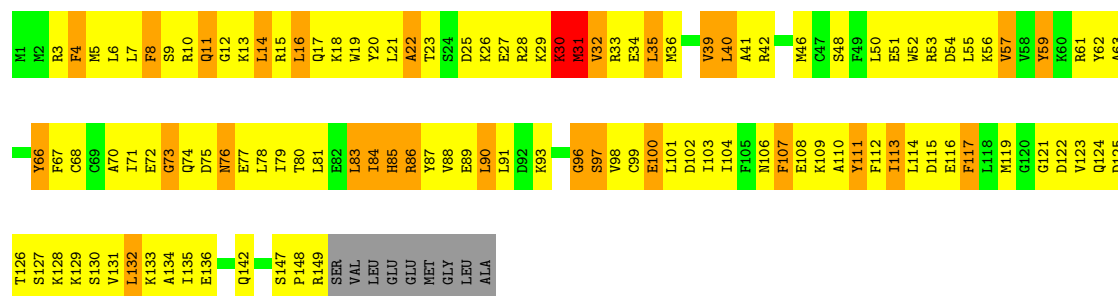
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain T: 19% 56% 18% • 6%



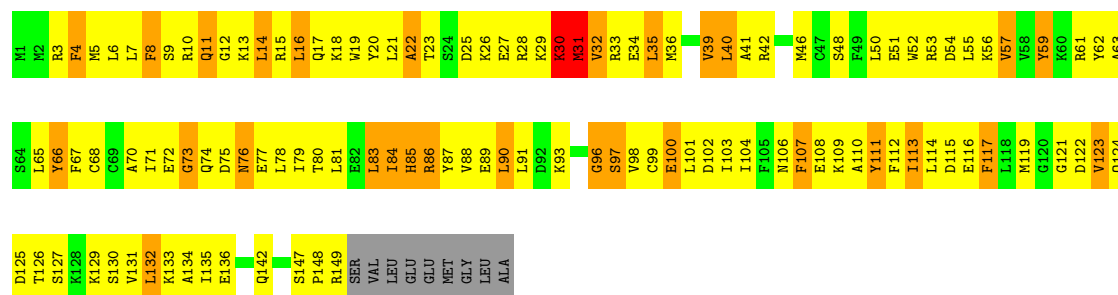
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain U: 20% 56% 18% • 6%



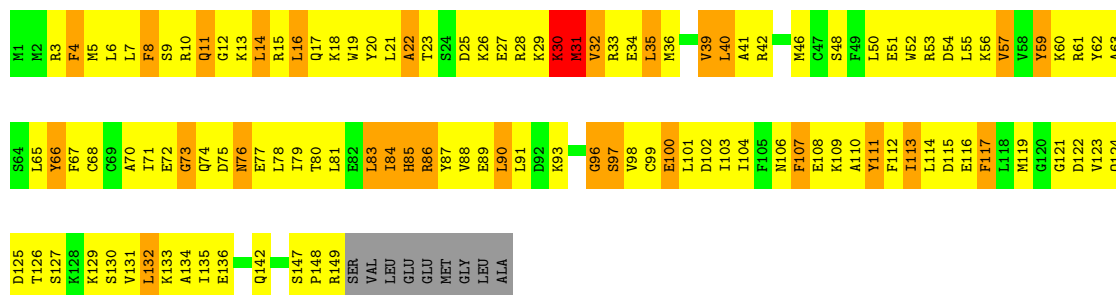
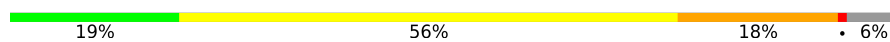
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain W: 20% 55% 18% • 6%



• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain X:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	178.14Å 178.14Å 1134.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 4.00	Depositor
% Data completeness (in resolution range)	78.8 (40.00-4.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.297 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	81744	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.77	5/4728 (0.1%)	1.13	46/6381 (0.7%)
1	C	0.77	5/4728 (0.1%)	1.13	46/6381 (0.7%)
1	E	0.77	5/4728 (0.1%)	1.13	46/6381 (0.7%)
1	G	0.77	6/4728 (0.1%)	1.13	47/6381 (0.7%)
1	I	0.77	6/4728 (0.1%)	1.13	46/6381 (0.7%)
1	K	0.77	5/4728 (0.1%)	1.13	46/6381 (0.7%)
2	B	0.80	1/4630 (0.0%)	1.28	69/6278 (1.1%)
2	D	0.80	1/4630 (0.0%)	1.28	65/6278 (1.0%)
2	F	0.80	1/4630 (0.0%)	1.28	67/6278 (1.1%)
2	H	0.80	1/4630 (0.0%)	1.28	67/6278 (1.1%)
2	J	0.80	1/4630 (0.0%)	1.28	67/6278 (1.1%)
2	L	0.80	1/4630 (0.0%)	1.28	67/6278 (1.1%)
3	M	0.89	2/3237 (0.1%)	1.36	44/4366 (1.0%)
3	N	0.89	2/3237 (0.1%)	1.36	43/4366 (1.0%)
3	O	0.89	2/3237 (0.1%)	1.36	44/4366 (1.0%)
3	P	0.90	2/3237 (0.1%)	1.36	44/4366 (1.0%)
3	R	0.89	2/3237 (0.1%)	1.36	44/4366 (1.0%)
3	V	0.90	2/3237 (0.1%)	1.36	43/4366 (1.0%)
4	Q	0.78	1/1259 (0.1%)	1.00	3/1686 (0.2%)
4	S	0.78	1/1259 (0.1%)	1.00	3/1686 (0.2%)
4	T	0.78	1/1259 (0.1%)	1.00	3/1686 (0.2%)
4	U	0.78	0/1259	0.99	3/1686 (0.2%)
4	W	0.78	1/1259 (0.1%)	1.00	3/1686 (0.2%)
4	X	0.78	0/1259	1.00	3/1686 (0.2%)
All	All	0.81	54/83124 (0.1%)	1.23	959/112266 (0.9%)

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
3	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	2
3	O	0	2
3	P	0	2
3	R	0	2
3	V	0	2
All	All	0	12

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	232	SER	C-O	-6.32	1.17	1.24
1	E	232	SER	C-O	-6.31	1.17	1.24
1	G	232	SER	C-O	-6.30	1.17	1.24
1	C	232	SER	C-O	-6.29	1.17	1.24
1	A	232	SER	C-O	-6.29	1.17	1.24

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	256	ILE	CA-C-N	16.72	131.70	119.66
3	V	256	ILE	C-N-CA	16.72	131.70	119.66
3	P	256	ILE	CA-C-N	16.71	131.69	119.66
3	P	256	ILE	C-N-CA	16.71	131.69	119.66
3	R	256	ILE	CA-C-N	16.70	131.68	119.66

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	166	TYR	Sidechain
3	M	85	TYR	Sidechain
3	N	166	TYR	Sidechain
3	N	85	TYR	Sidechain
3	O	85	TYR	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	4663	0	4792	911	0
1	C	4663	0	4792	895	6
1	E	4663	0	4792	900	12
1	G	4663	0	4792	910	0
1	I	4663	0	4792	885	7
1	K	4663	0	4792	898	12
2	B	4558	0	4674	930	0
2	D	4558	0	4674	927	0
2	F	4558	0	4674	928	3
2	H	4558	0	4674	936	0
2	J	4558	0	4674	929	0
2	L	4558	0	4674	916	4
3	M	3166	0	3178	464	0
3	N	3166	0	3178	462	0
3	O	3166	0	3178	452	0
3	P	3166	0	3178	463	0
3	R	3166	0	3178	459	0
3	V	3166	0	3178	453	0
4	Q	1237	0	1261	242	0
4	S	1237	0	1261	230	0
4	T	1237	0	1261	239	0
4	U	1237	0	1261	231	0
4	W	1237	0	1261	236	0
4	X	1237	0	1261	237	0
All	All	81744	0	83430	14652	22

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 89.

The worst 5 of 14652 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)
2:B:139:LYS:HD3	2:B:175:MET:HE2	1.21	1.19
1:E:488:VAL:HA	1:E:500:VAL:HG11	1.20	1.19
2:F:139:LYS:HD3	2:F:175:MET:HE2	1.21	1.18
1:A:482:GLU:HB3	1:A:584:MET:SD	1.83	1.18
1:E:482:GLU:HB3	1:E:584:MET:SD	1.83	1.18

The worst 5 of 22 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:E:265:GLU:OE2	1:K:221:ARG:NH1[1_545]	1.07	1.13
1:E:265:GLU:OE1	1:K:221:ARG:CZ[1_545]	1.30	0.90
1:E:265:GLU:CD	1:K:221:ARG:NH2[1_545]	1.42	0.78
1:E:265:GLU:OE1	1:K:221:ARG:NH2[1_545]	1.44	0.76
1:I:345:ARG:NE	2:L:457:GLU:OE2[5_445]	1.44	0.76

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	588/618 (95%)	254 (43%)	210 (36%)	124 (21%)	0	1
1	C	588/618 (95%)	254 (43%)	210 (36%)	124 (21%)	0	1
1	E	588/618 (95%)	253 (43%)	211 (36%)	124 (21%)	0	1
1	G	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
1	I	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
1	K	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
2	B	572/584 (98%)	239 (42%)	192 (34%)	141 (25%)	0	1
2	D	572/584 (98%)	239 (42%)	191 (33%)	142 (25%)	0	1
2	F	572/584 (98%)	240 (42%)	190 (33%)	142 (25%)	0	1
2	H	572/584 (98%)	238 (42%)	193 (34%)	141 (25%)	0	1
2	J	572/584 (98%)	239 (42%)	191 (33%)	142 (25%)	0	1
2	L	572/584 (98%)	239 (42%)	192 (34%)	141 (25%)	0	1
3	M	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4
3	N	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4
3	O	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4
3	P	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4
3	R	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4
3	V	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
4	S	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
4	T	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
4	U	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
4	W	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
4	X	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	4
All	All	10122/10698 (95%)	4988 (49%)	3145 (31%)	1989 (20%)	0	1

5 of 1989 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	58	MET
1	A	76	SER
1	A	132	SER
1	A	162	VAL

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	523/546 (96%)	478 (91%)	45 (9%)	10	33
1	C	523/546 (96%)	478 (91%)	45 (9%)	10	33
1	E	523/546 (96%)	478 (91%)	45 (9%)	10	33
1	G	523/546 (96%)	478 (91%)	45 (9%)	10	33
1	I	523/546 (96%)	478 (91%)	45 (9%)	10	33
1	K	523/546 (96%)	478 (91%)	45 (9%)	10	33
2	B	515/523 (98%)	469 (91%)	46 (9%)	9	31
2	D	515/523 (98%)	469 (91%)	46 (9%)	9	31
2	F	515/523 (98%)	469 (91%)	46 (9%)	9	31
2	H	515/523 (98%)	469 (91%)	46 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	515/523 (98%)	469 (91%)	46 (9%)	9	31
2	L	515/523 (98%)	469 (91%)	46 (9%)	9	31
3	M	355/383 (93%)	317 (89%)	38 (11%)	6	24
3	N	355/383 (93%)	317 (89%)	38 (11%)	6	24
3	O	355/383 (93%)	317 (89%)	38 (11%)	6	24
3	P	355/383 (93%)	317 (89%)	38 (11%)	6	24
3	R	355/383 (93%)	317 (89%)	38 (11%)	6	24
3	V	355/383 (93%)	317 (89%)	38 (11%)	6	24
4	Q	136/144 (94%)	118 (87%)	18 (13%)	4	18
4	S	136/144 (94%)	118 (87%)	18 (13%)	4	18
4	T	136/144 (94%)	118 (87%)	18 (13%)	4	18
4	U	136/144 (94%)	118 (87%)	18 (13%)	4	18
4	W	136/144 (94%)	118 (87%)	18 (13%)	4	18
4	X	136/144 (94%)	118 (87%)	18 (13%)	4	18
All	All	9174/9576 (96%)	8292 (90%)	882 (10%)	8	28

5 of 882 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	105	ASN
3	M	255	PHE
4	X	86	ARG
4	U	59	TYR
1	K	264	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	105	ASN
1	K	100	HIS
4	S	85	HIS
1	I	187	ASN
2	J	59	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](#)

There are no ligands in this entry.

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.