



## wwPDB EM Map/Model Validation Report

Sep 14, 2016 – 11:39 AM EDT

PDB ID : 5GKZ  
EMDB ID: : EMD-9519  
Title : Structure of RyR1 in a closed state (C3 conformer)  
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.  
Deposited on : 2016-07-07  
Resolution : 4.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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) : rb-20027939

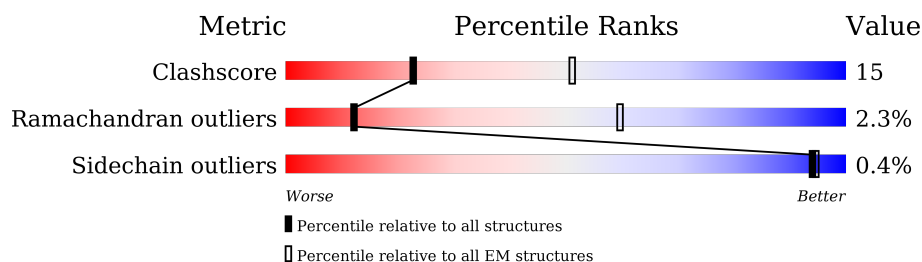
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	5037	
1	C	5037	
1	E	5037	
1	G	5037	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	C	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	E	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	G	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

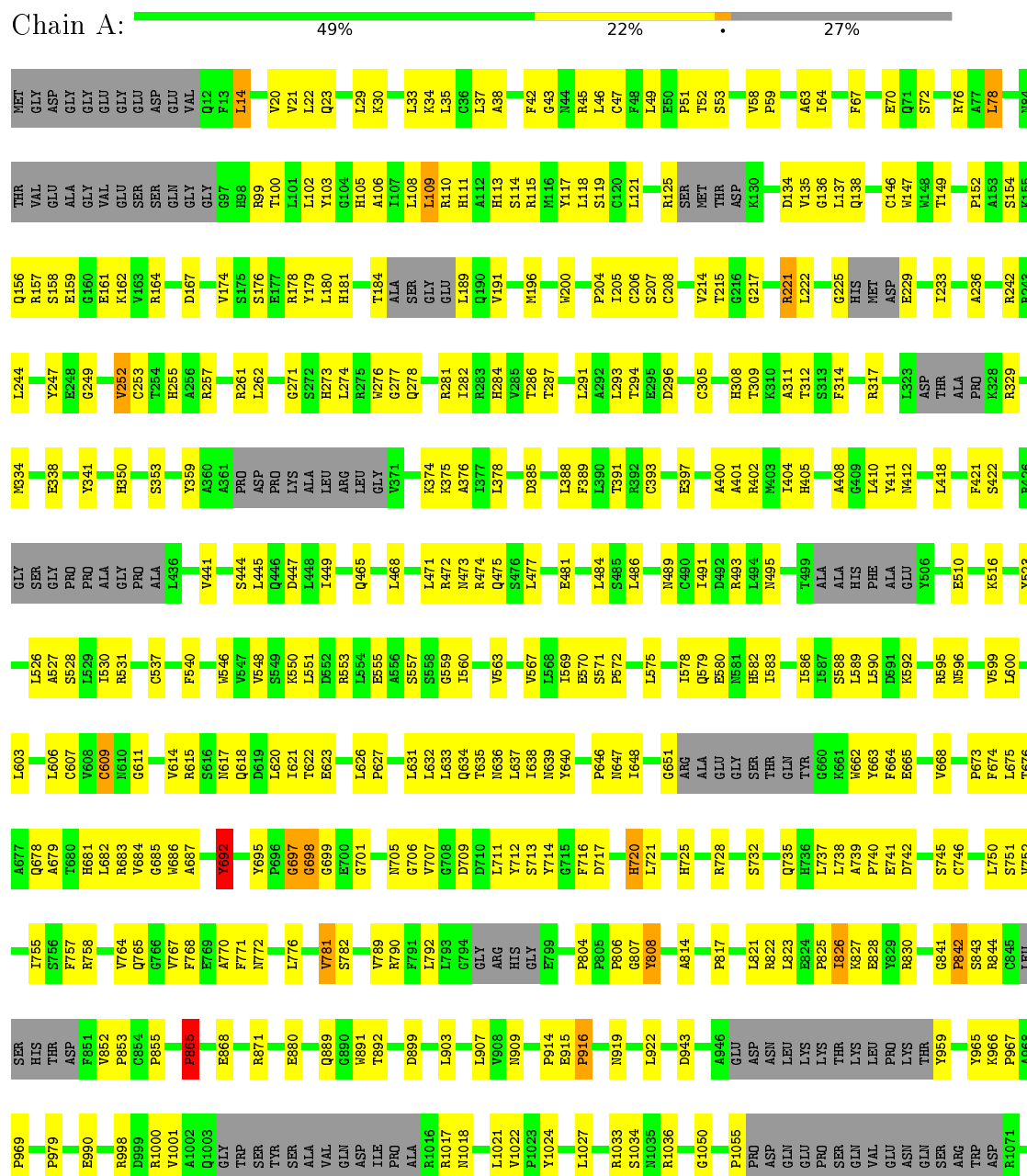
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

### 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. 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.

- Molecule 1: Ryanodine receptor 1



P2236	Y2142	GLU	F1836	G1761	V1689	F1612	A1531	V1453	LYS	ALA	P1253	F1162	R1076
K2227	T2143	LYS	V1839	L1762	D1690	L1613	M1532	T1454	ARG	GLU	H1254	E1167	A1077
T2230	I2144	GLU	P1840	P1763	G1691	Q1614	E1535	H1458	GLY	PRO	D1261	V1168	E1078
S2231	S2145	ASP	P1840	G1764	A1692	Q1693	E1535	H1459	PHE	ASP	GLY	L1169	K1079
R2234	V2149	ALA	L1844	V1765	G1693	R1623	Q1541	H1460	LEU	PRO	THR	MET	Y1081
F2239	T2152	LYS	L1848	G1766	L1695	V1626	P1544	F1464	LYS	TYR	VAL	SER	T1082
T2242	L2156	GLU	L1849	T1769	E1699	V1628	M1545	D1465	ALA	GLU	ASP	ASP	R1087
S2243	E2157	GLU	L1849	S1770	E1699	V1628	M1545	L1466	LYS	ASN	THR	SER	W1088
R2244	C2158	ALA	M1851	L1771	L1703	C1630	K1547	S1467	LEU	PRO	PRO	GLY	W1089
Q2245	L2169	ARG	G1852	R1772	P1704	Q1631	L1548	LYS	ALA	ARG	CYS	GLU	F1090
N2246	G2160	THR	L1853	P1773	L1707	D1632	F1549	VAL	MET	SER	LEU	THR	E1091
Q2247	Q2161	ARG	F1854	P1774	L1708	P1633	P1550	ARG	ALA	ALA	ARG	A1178	F1092
R2248	L2162	GLY	L1855	H1775	A1709	M1637	A1551	ALA	THR	GLY	L1272	D1186	E1093
L2263	R2163	LYS	E1857	S1778	G1710	L1638	F1552	V1472	GLN	GLY	R1275	L1189	G1098
GLY	S2164	LYS	D1858	P1779	G1710	L1638	F1553	T1475	PRO	GLY	GLY	P1190	E1099
GLY	L2165	LYS	Q1861	P1780	D1713	H1640	V1554	M1476	ALA	GLU	S1279	L1191	M1100
GLY	L2166	GLU	L1862	C1781	L1714	I1641	H1558	E1479	THR	ALA	Q1280	V1191	R1101
MET	V2168	GLU	L1865	F1782	L1715	P1642	Q1559	Q1480	PRO	GLU	M1281	C1192	V1102
GLN	GLN	GLU	M1866	V1783	I1716	E1643	M1560	LEU	LEU	GLY	F1288	S1193	G1103
GLY	ILE	GLU	I1866	ALA	S1717	C1647	I1562	V1483	PRO	LYS	GLY	P1196	W1104
GLY	ASN	GLU	E1867	LEU	H1719	M1648	Q1563	H1484	ARG	GLU	R1289	G1197	A1105
SER	ASN	GLU	F1868	PRO	H1719	D1649	F1564	S1485	LEU	GLY	L1291	Q1198	L1109
T2271	L1926	LEU	E1869	ALA	R1725	L1650	LEU	M1491	PRO	THR	S1292	H1201	P1110
P2272	L1927	VAL	VAL	ALA	S1726	L1651	LEU	CYS	ALA	ALA	L1293	L1202	R1111
L2177	G1925	GLU	PHE	GLY	R1727	E1652	LYS	Y1493	ASP	LYS	P1294	N1203	L1115
L2182	L1926	ALA	THR	VAL	R1728	E1655	GLN	GLY	VAL	VAL	V1295	L1204	L1115
G2183	L1926	GLU	GLU	ALA	S1729	R1656	LYS	G1497	PRO	THR	Q1296	G1205	L1120
N2184	L1943	LYS	GLU	GLU	H1730	R1656	ASN	GLY	ALA	PRO	HIS	Q1206	L1120
N2185	E1944	LYS	GLU	ALA	L1731	L1657	ILE	ASP	GLY	GLN	GLN	D1207	V1123
N2186	Y1945	GLU	GLU	ALA	S1732	D1658	MET	PHE	ASN	GLY	HIS	F1124	F1124
L2281	F1946	GLU	GLU	ARG	E1733	L1659	PRO	VAL	ARG	THR	PHE	N1125	N1125
D2282	C1947	GLU	GLU	L1798	Y1734	Q1660	LEU	SER	PRO	ARG	ARG	L1211	G1126
N2283	Q1952	GLU	GLU	L1802	I1735	R1661	SER	PRO	ASP	GLN	CYS	R1212	G1126
L2286	H1953	GLU	GLU	P1803	P1737	F1662	A1577	GLY	PRO	PRO	THR	F1213	Q1130
A2287	R1954	GLU	GLU	L1804	L1738	H1663	A1578	GLN	GLU	GLY	ALA	F1214	R1131
V2299	V1955	GLU	GLU	R1808	T1742	T1666	M1579	GLY	ILE	VAL	GLY	P1225	W1132
L2302	E1956	GLU	GLU	L1812	R1743	L1667	S1582	ARG	ARG	GLU	ALA	P1226	H1133
L2307	S1957	GLU	GLU	L1815	A1744	A1671	E1583	ILE	ILE	LEU	THR	F1226	L1134
GLN	L1958	GLU	GLU	L1818	T1746	V1673	R1584	GLY	ASP	GLN	PRO	A1227	G1135
SER	F1961	GLU	GLU	L1819	T1747	L1676	K1585	S1510	VAL	PRO	LEU	I1228	S1136
CYS	F1969	GLU	ASP	A1818	F1748	L1677	P1587	L1514	ARG	ALA	ALA	M1229	E1137
PRO	Q1970	GLU	GLU	V1819	P1750	N1678	P1589	I1515	ALA	PRO	PRO	Q1231	P1138
GLN	Q1973	GLU	GLU	R1820	GLY	M1679	G1517	G1517	GLY	GLY	GLY	Q1231	R1141
GLN	Q1976	GLU	GLU	D1821	ARG	R1680	L1519	L1519	ASN	ASN	GLN	V1234	R1141
GLY	R1976	LYS	LYS	D1821	LYS	V1681	V1597	G1517	GLY	GLY	GLY	T1235	V1148
GLY	TYR	GLU	GLU	R1827	GLY	A1682	Q1598	ASP	GLY	ASP	PRO	T1235	V1149
GLY	ALA	GLU	ASP	D1828	GLY	H1683	M1599	LEU	GLN	ALA	ALA	W1237	G1150
GLY	ALA	GLU	GLU	P1829	ASN	A1684	L1600	THR	THR	THR	THR	F1238	I1153
TYR	LEU	GLU	GLU	V1830	ALA	L1685	P1609	G1525	GLU	GLU	ASP	K1240	I1153
ILE	MET	GLU	GLU	S1833	ARG	C1686	M1610	THR	PRO	GLY	GLU	E1157	E1157
PHE	ARG	GLU	GLU	S1833	ARG	H1688	H1611	T1530	LYS	ALA	ALA	P1243	I1160
		ARG	GLU		HIS				LYS	ALA	ALA	H1252	I1161





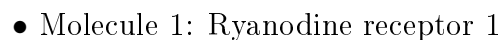

V1448	LYS	ALA	P1253	I1161	R1076	P969	SER	I755	A577	G504	A527	PRO	Y341	E248	K155	H84
V1453	ARG	GLU	H1284	F1162	A1077	P979	HIS	S756	Q678	S605	S528	ALA	H350	G249	Q156	THR
T1454	PHE	PRO	ASP	E1167	E1078	P979	THR	F757	A679	L606	L529	GLY	H350	G249	Q156	THR
H1458	PHE	ASP	THR	V1168	S1080	E930	ASP	R758	T680	C607	F757	ALA	S353	V252	S158	GLU
Q1459	LYS	TYR	GLY	L1169	Y1081	E930	ASP	V764	L681	V608	R531	ALA	S353	C253	E159	ALA
H1460	LYS	GLY	ASP	VAL	T1082	R998	ASP	Q765	L683	G509	C537	ALA	S353	T254	G160	GLY
F1464	LYS	ASN	THR	ASP	R1087	D999	ASP	Q766	V684	G511	F540	ALA	S353	H255	E161	VAL
D1465	LYS	LEU	PRO	SER	W1088	R1000	ASP	Q766	V684	V614	F540	ALA	S353	A256	K162	VAL
L1466	ALA	ARG	PRO	GLY	Y1089	A1002	ASP	F767	W686	R615	W546	ALA	S353	R257	V163	GLU
S1467	LYS	GLY	CYS	SER	F1090	G1003	ASP	F768	A687	Q618	V548	ALA	S353	R257	V163	GLU
LYS	MET	ALA	ARG	GLY	F1091	GLY	ASP	E769	V682	N617	V547	ALA	S353	R257	V163	GLU
VAL	THR	GLY	ARG	THR	F1092	TRP	ASP	A770	V682	Q618	V547	ALA	S353	R257	V163	GLU
ARG	GLN	GLY	GLY	F1179	E1093	TYR	ASP	F771	V682	L620	V547	ALA	S353	R257	V163	GLU
V1472	PRO	TRP	TRP	F1179	E1093	TYR	ASP	N772	V682	L620	V547	ALA	S353	R257	V163	GLU
T1475	PRO	GLY	GLY	D1186	G1098	SER	ASP	L776	V682	T622	V547	ALA	S353	R257	V163	GLU
M1476	THR	GLU	GLU	P1190	M1000	VAL	ASP	V781	V682	E523	V547	ALA	S353	R257	V163	GLU
E1479	LEU	GLY	GLY	V1191	R1101	GLN	ASP	S782	V682	L626	V547	ALA	S353	R257	V163	GLU
Q1480	LEU	GLY	GLY	G1192	A1103	ASP	ASP	V789	V682	P627	V547	ALA	S353	R257	V163	GLU
V1483	ARG	GLY	GLY	S1193	W1104	PRO	ASP	R790	V682	L632	V547	ALA	S353	R257	V163	GLU
S1485	PRO	GLY	GLY	G1193	A1105	ALA	ASP	R791	V682	L633	V547	ALA	S353	R257	V163	GLU
N1491	VAL	GLY	GLY	P1196	L1109	ALA	ASP	L792	V682	L633	V547	ALA	S353	R257	V163	GLU
Y1493	VAL	GLY	GLY	G1197	R1110	ALA	ASP	L793	V682	L633	V547	ALA	S353	R257	V163	GLU
G1497	ASP	GLY	GLY	Q1198	P1111	ALA	ASP	G794	V682	L633	V547	ALA	S353	R257	V163	GLU
ASP	ASN	GLY	GLY	H1201	L1115	ALA	ASP	H791	V682	L633	V547	ALA	S353	R257	V163	GLU
ARG	ARG	THR	THR	P1294	M1202	ALA	ASP	L792	V682	L633	V547	ALA	S353	R257	V163	GLU
VAL	VAL	GLY	GLY	G1295	G1116	ALA	ASP	L793	V682	L633	V547	ALA	S353	R257	V163	GLU
CYS	VAL	GLY	GLY	L1203	G1116	ALA	ASP	L793	V682	L633	V547	ALA	S353	R257	V163	GLU
PRO	PRO	THR	THR	G1296	L1120	ALA	ASP	L793	V682	L633	V547	ALA	S353	R257	V163	GLU
GLY	ASP	GLY	GLY	Q1206	V1123	ALA	ASP	P804	V682	L633	V547	ALA	S353	R257	V163	GLU
ASN	ASN	GLY	GLY	D1207	F1124	ALA	ASP	P805	V682	L633	V547	ALA	S353	R257	V163	GLU
ARG	ARG	THR	THR	P1124	M1125	ALA	ASP	G807	V682	L633	V547	ALA	S353	R257	V163	GLU
ASP	ASP	GLN	GLN	L1211	N1125	ALA	ASP	Y808	V682	L633	V547	ALA	S353	R257	V163	GLU
PRO	PRO	GLY	GLY	R1212	Q1130	ALA	ASP	A814	V682	L633	V547	ALA	S353	R257	V163	GLU
THR	THR	VAL	VAL	F1213	R1131	ALA	ASP	P817	V682	L633	V547	ALA	S353	R257	V163	GLU
ILE	ILE	GLY	GLY	F1214	W1132	ALA	ASP	A946	V682	L633	V547	ALA	S353	R257	V163	GLU
ALA	ALA	ALA	ALA	P1225	H1133	ALA	ASP	S732	V682	L633	V547	ALA	S353	R257	V163	GLU
THR	THR	ALA	ALA	F1226	L1134	ALA	ASP	Q735	V682	L633	V547	ALA	S353	R257	V163	GLU
ASN	ASN	GLN	GLN	A1227	G1135	ALA	ASP	H736	V682	L633	V547	ALA	S353	R257	V163	GLU
THR	THR	PRO	PRO	M1229	E1137	ALA	ASP	L737	V682	L633	V547	ALA	S353	R257	V163	GLU
S1436	GLY	GLY	GLY	V1234	P1138	ALA	ASP	L738	V682	L633	V547	ALA	S353	R257	V163	GLU
V1437	GLY	GLY	GLY	T1235	R1141	ALA	ASP	L739	V682	L633	V547	ALA	S353	R257	V163	GLU
V1438	GLY	GLY	GLY	T1236	V1148	ALA	ASP	E828	V682	L633	V547	ALA	S353	R257	V163	GLU
V1439	GLY	GLY	GLY	W1237	Y1149	ALA	ASP	Y829	V682	L633	V547	ALA	S353	R257	V163	GLU
F1440	GLY	GLY	GLY	F1238	G1150	ALA	ASP	R830	V682	L633	V547	ALA	S353	R257	V163	GLU
L1441	GLY	GLY	GLY	S1239	G1150	ALA	ASP	R830	V682	L633	V547	ALA	S353	R257	V163	GLU
V1450	GLY	GLY	GLY	K1240	I1153	ALA	ASP	G841	V682	L633	V547	ALA	S353	R257	V163	GLU
ASP	GLY	THR	THR	ASP	E1157	ALA	ASP	P842	V682	L633	V547	ALA	S353	R257	V163	GLU
GLY	GLY	GLY	GLY	GLY	Q1244	ALA	ASP	S843	V682	L633	V547	ALA	S353	R257	V163	GLU
LEU	GLY	GLY	GLY	LEU	Q1244	ALA	ASP	R844	V682	L633	V547	ALA	S353	R257	V163	GLU
ALA	GLY	GLY	GLY	ALA	Q1244	ALA	ASP	C845	V682	L633	V547	ALA	S353	R257	V163	GLU
THR	THR	GLY	GLY	THR	Q1244	ALA	ASP	C845	V682	L633	V547	ALA	S353	R257	V163	GLU
C1447	GLY	GLY	GLY	C1447	Q1244	ALA	ASP	C845	V682	L633	V547	ALA	S353	R257	V163	GLU
G1525	GLY	GLY	GLY	G1525	Q1244	ALA	ASP	C845	V682	L633	V547	ALA	S353	R257	V163	GLU



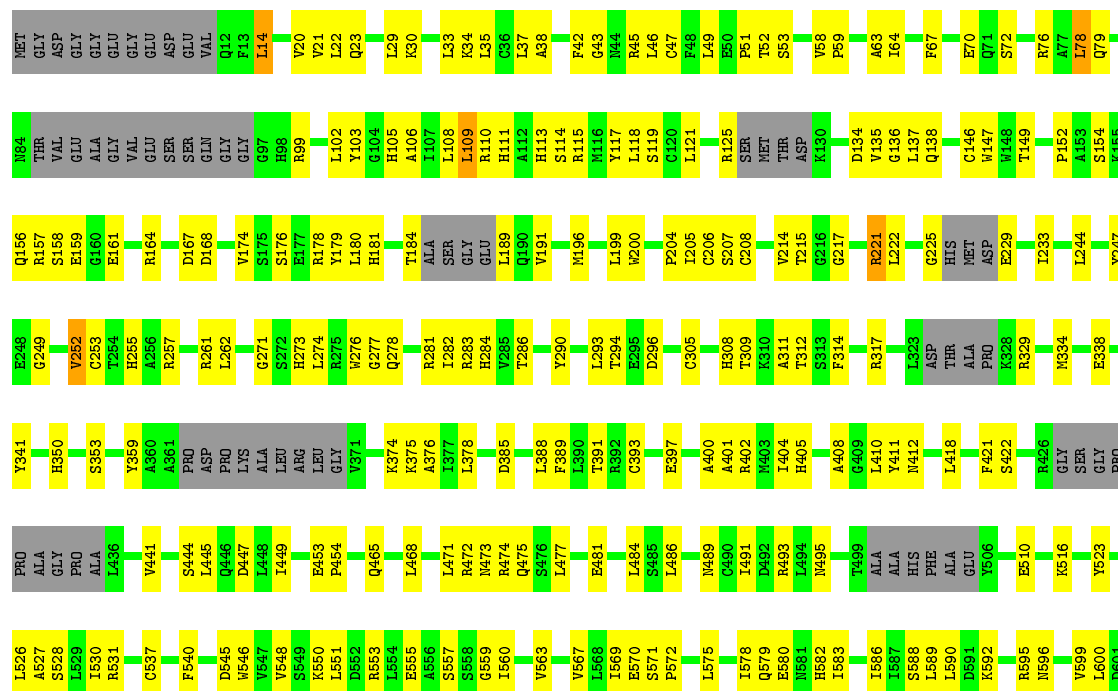








Chain E:  48% 23% . 27%

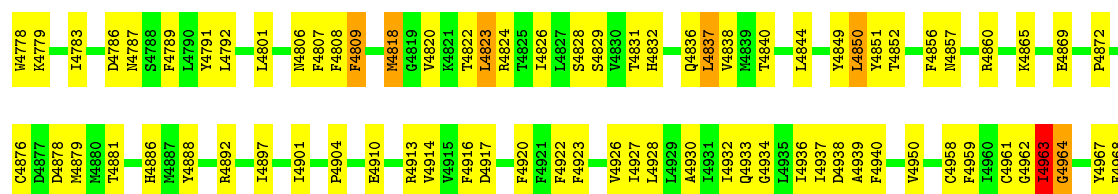






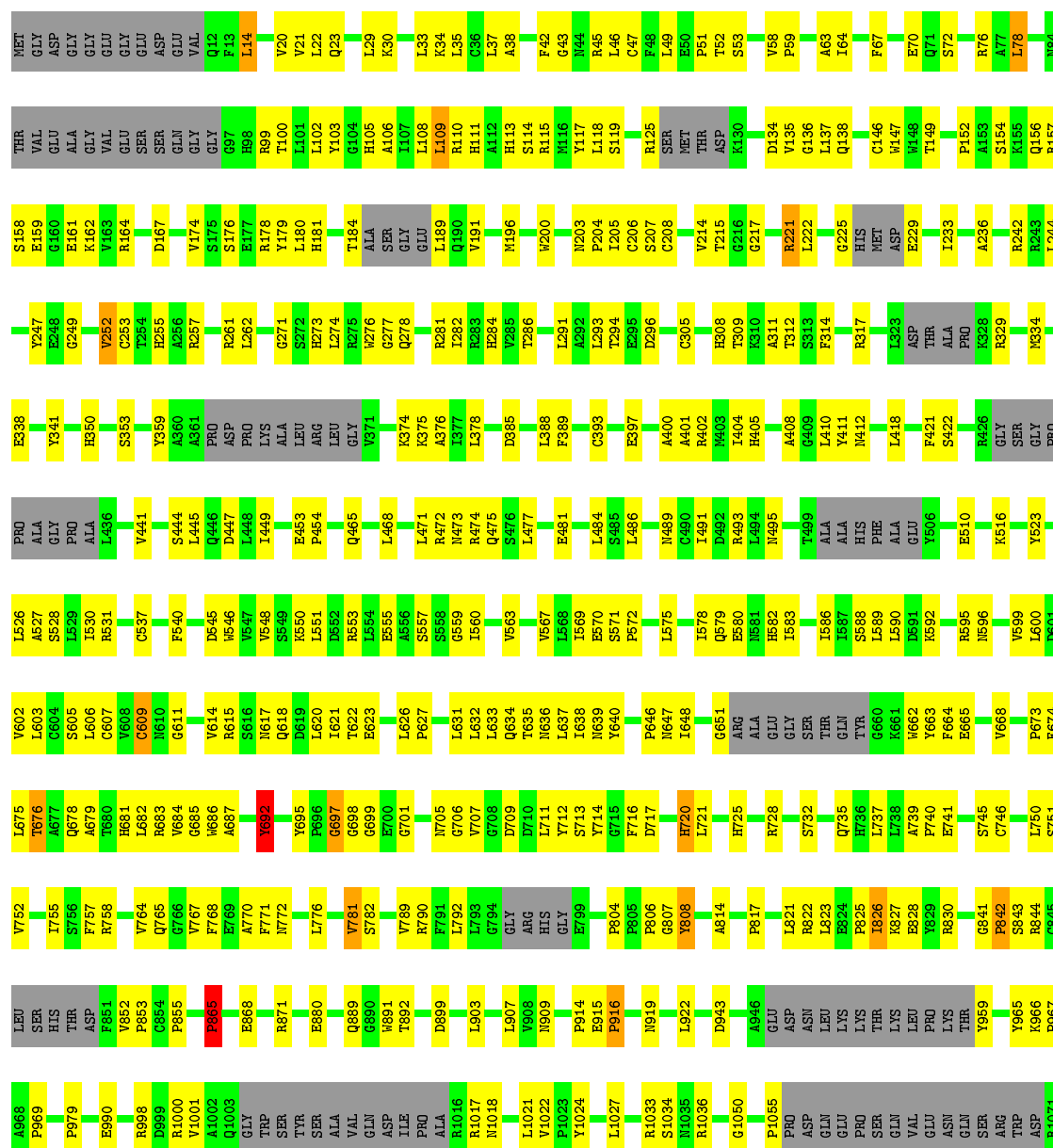




• Molecule 1: Ryanodine receptor 1

Chain G: 49% 22% 27%



M2211	R2126	GLU	V4830	LYS	H4683	M5599	LEU	PRO	LYS	ALA	Q1244	I1160	R1076
V2212	Q2127	GLU	S1833	GLY	A1684	L1600	ALA	SER	ASN	ARG	H1252	I1161	A1077
M2213	L2131	GLU	F1836	ASN	C1686	P1609	THR	V1448	LYS	ALA	H1253	F1162	E1078
L2215	G2132	GLU	F1836	ARG	S1687	H610	T1530	V1453	GLY	GLU	H1254	E1167	K1079
G2216	E2133	LYS	H688	ARG	H688	H611	A1531	T1454	PHE	ASP	D1261	L1169	S1080
GLY	L2134	THR	V1689	ARG	V1689	F1612	M1532	P1455	LEU	PRO	GLY	GLY	Y1081
GLU	L2135	ASP	D1690	HIS	D1690	R1623	E1535	H1458	PHE	ASP	THR	MET	T1082
R2136	R2136	SER	G1761	G1761	A1692	R1623	E1535	H1458	LYS	TYR	VAL	SER	R1087
A2137	A2137	ALA	L1762	L1762	G1693	W1626	E1535	Q1459	ALA	GLU	ASP	ASP	W1088
L2138	L2138	LYS	P1763	P1763	G1693	A1627	Q1541	H1460	LYS	ASN	THR	SER	R1088
P2139	P2139	THR	V1765	V1765	L1695	V1628	Q1541	H1460	LYS	LEU	PRO	SER	F1090
Y2142	Y2142	GLU	G1766	G1766	E1699	Q1629	P1544	F1464	ALA	ARG	PRO	GLU	E1091
T2143	T2143	GLU	T1768	T1768	D1700	C1630	M1545	D1465	ALA	ARG	CYS	THR	F1092
S2145	S2145	ALA	T1769	T1769	A1701	Q1631	T1546	L1466	MET	SER	LEU	THR	E1093
V2149	V2149	GLY	S1770	S1770	H1702	D1632	K1547	S1467	THR	GLY	ARG	D1186	G1098
T2152	T2152	GLY	L1771	L1771	L1703	P1633	F1549	VAL	GLN	GLY	L1272	D1186	E1099
L2156	L2156	GLY	R1772	R1772	P1704	M1637	P1550	ARG	PRO	TRP	R1275	L1189	M1100
C2158	C2158	LYS	H1775	H1775	R1707	A1638	A1551	ALA	PRO	GLY	R1275	P1190	R1101
L2159	L2159	GLY	P1781	P1781	R1707	L1639	V1552	V1472	ALA	GLU	S1279	V1191	V1102
G2160	G2160	GLU	F1782	F1782	R1708	H1640	F1553	V1472	THR	ALA	Q1280	C1192	G1103
L2161	L2161	ILE	A1784	A1784	L1714	H1641	V1554	T1475	ALA	GLY	N1281	S1193	W1104
R2162	R2162	ASN	LEU	LEU	L1715	M1648	V1554	M1476	LEU	GLY	F1288	P1196	A1105
R2163	R2163	MET	LEU	LEU	L1716	M1648	H1558	E1479	PRO	LYS	L1289	G1197	L1109
R2164	R2164	GLY	PRO	PRO	L1717	D1649	Q1563	V1483	THR	GLY	R1290	G1198	R1110
L2165	L2165	LEU	ALA	ALA	L1718	L1650	F1564	H1484	HIS	THR	L1291	H1201	V1112
L2166	L2166	LEU	ALA	ALA	H1719	L1651	E1565	S1485	ASP	LYS	L1293	L1202	L1115
L2167	L2167	HIS	GLY	GLY	R1725	E1652	LEU	M1491	VAL	GLU	V1295	L1203	G1116
V2168	V2168	VAL	VAL	VAL	R1726	E1655	LYS	Y1493	VAL	THR	Q1296	G1205	L1120
GLN	GLN	GLU	GLU	GLU	S1726	R1656	LYS	GLY	ALA	PRO	F1297	Q1206	V1123
MET	MET	GLU	GLU	GLU	R1727	R1656	GLN	GLY	ASP	GLY	HIS	D1207	F1124
GLY	GLY	GLU	GLU	GLU	R1728	L1657	LYS	G1497	ASN	GLY	HIS	S1210	N1125
PRO	PRO	GLU	GLU	GLU	S1729	D1658	ASN	GLY	ARG	THR	PHE	L1211	G1126
GLU	GLU	GLU	GLU	GLU	M1730	L1659	ILE	ASP	ASP	PRO	ARG	R1212	Q1130
C1947	C1947	ALA	ALA	ALA	L1731	Q1660	MET	PHE	ASP	GLN	CYS	F1213	W1132
Q1952	Q1952	GLY	GLY	GLY	S1732	R1661	PRO	VAL	PRO	PRO	THR	F1214	H1133
H1953	H1953	GLY	GLY	GLY	E1733	F1662	LEU	SER	GLY	GLY	ALA	P1225	W1134
R1954	R1954	GLU	GLU	GLU	Y1734	H1663	SER	PRO	ILE	VAL	GLY	F1226	L1134
V1955	V1955	GLU	GLU	GLU	L1735	T1666	A1577	GLY	ILE	GLU	ALA	A1227	G1135
E1956	E1956	GLU	GLU	GLU	V1736	L1667	A1578	GLN	ASN	ALA	THR	I1228	S1136
S1957	S1957	GLU	GLU	GLU	P1737	L1667	M1579	GLN	LEU	GLN	PRO	N1229	E1137
L1958	L1958	GLU	GLU	GLU	L1738	L1667	M1579	GLY	THR	PRO	LEU	P1138	P1138
F1961	F1961	GLY	GLY	GLY	T1742	R1671	S1582	ILE	THR	VAL	ALA	R1232	R1141
L1969	L1969	GLU	GLU	GLU	R1743	A1672	F1583	S1510	ALA	ARG	PRO	F1233	R1141
Q1970	Q1970	ASP	ASP	ASP	A1744	V1673	R1584	S1510	GLY	ALA	PRO	G1234	V1148
Q1973	Q1973	GLY	GLY	GLY	L1745	C1674	K1585	L1514	ASN	GLY	GLY	T1235	V1148
Q1976	Q1976	LYS	LYS	LYS	T1746	A1675	M1586	V1515	GLN	GLN	LEU	T1236	G1150
R1976	R1976	GLY	GLY	GLY	L1747	L1676	P1587	L1516	LYS	GLN	GLN	V1237	G1150
T1976	T1976	GLY	GLY	GLY	F1748	G1677	A1588	G1517	ASP	PRO	PRO	F1238	I1153
T1976	T1976	GLY	GLY	GLY	L1749	N1678	P1589	C1518	ALA	ALA	ALA	S1239	I1153
D1828	D1828	GLY	GLY	GLY	P1750	N1679	E1596	L1519	THR	THR	GLU	K1240	E1157
P1829	P1829	ARG	ARG	ARG	P1750	R1680	V1597	V1520	GLN	GLU	ASP	P1243	E1157



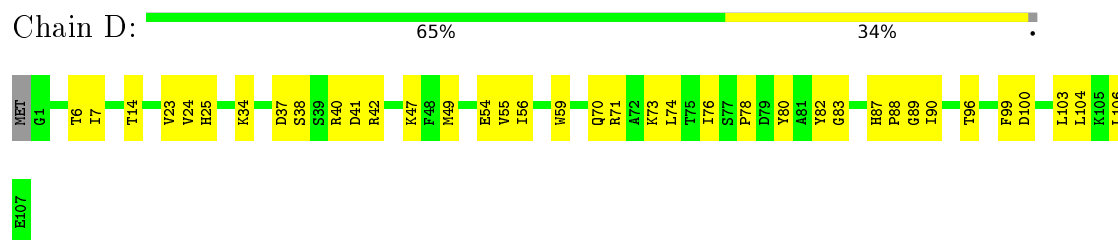



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

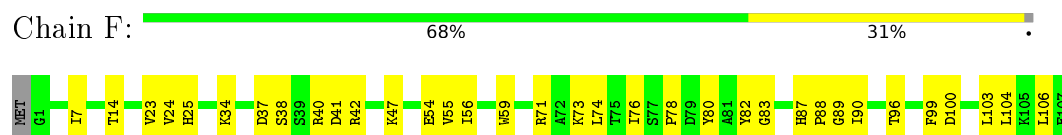
Chain B:  67% 32%



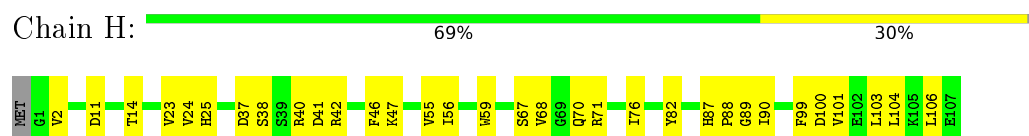
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	64000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	C	0.98	89/27385 (0.3%)	0.88	114/37104 (0.3%)
1	E	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	G	0.99	94/27385 (0.3%)	0.88	112/37104 (0.3%)
2	B	0.63	0/851	0.63	0/1146
2	D	0.63	0/851	0.63	0/1146
2	F	0.63	0/851	0.63	0/1146
2	H	0.63	0/851	0.62	0/1146
All	All	0.98	357/112944 (0.3%)	0.88	442/153000 (0.3%)

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	20
1	C	0	20
1	E	0	20
1	G	0	20
All	All	0	80

The worst 5 of 357 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-20.55	1.12	1.39
1	E	4988	TYR	CG-CD2	-19.42	1.14	1.39
1	C	4988	TYR	CG-CD2	-19.41	1.14	1.39
1	A	4988	TYR	CG-CD2	-19.37	1.14	1.39
1	G	4988	TYR	CE1-CZ	-17.94	1.15	1.38

The worst 5 of 442 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5029	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	E	5029	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	E	4988	TYR	CB-CG-CD1	10.56	127.34	121.00
1	A	4988	TYR	CB-CG-CD1	10.55	127.33	121.00
1	C	4988	TYR	CB-CG-CD1	10.53	127.32	121.00

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1464	PHE	Mainchain,Peptide
1	A	1465	ASP	Peptide
1	A	697	GLY	Mainchain,Peptide
1	A	807	GLY	Mainchain,Peptide
1	A	841	GLY	Mainchain,Peptide

## 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	26917	0	24461	801	0
1	C	26917	0	24461	789	0
1	E	26917	0	24461	787	0
1	G	26917	0	24461	770	0
2	B	832	0	831	34	0
2	D	832	0	831	35	0
2	F	832	0	831	33	0
2	H	832	0	831	28	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	3132	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 15.

The worst 5 of 3132 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:G:1782:PHE:O	2:H:82:TYR:OH	1.75	1.03
1:A:1782:PHE:O	2:B:82:TYR:OH	1.76	1.03
1:A:4888:TYR:CD1	1:G:4914:VAL:HG23	1.95	1.02
1:C:1782:PHE:O	2:D:82:TYR:OH	1.78	1.01
1:E:1782:PHE:O	2:F:82:TYR:OH	1.77	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	3496/5037 (69%)	3185 (91%)	227 (6%)	84 (2%)	7	50
1	C	3496/5037 (69%)	3185 (91%)	228 (6%)	83 (2%)	7	50
1	E	3496/5037 (69%)	3187 (91%)	226 (6%)	83 (2%)	7	50
1	G	3496/5037 (69%)	3192 (91%)	217 (6%)	87 (2%)	7	49
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	D	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	14404/20580 (70%)	13130 (91%)	937 (6%)	337 (2%)	12	51

5 of 337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	GLY
1	A	915	GLU
1	A	916	PRO

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Mol	Chain	Res	Type
1	A	969	PRO
1	A	1589	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	2503/4276 (58%)	2493 (100%)	10 (0%)	93	97
1	C	2502/4276 (58%)	2492 (100%)	10 (0%)	93	97
1	E	2500/4276 (58%)	2491 (100%)	9 (0%)	93	97
1	G	2501/4276 (58%)	2489 (100%)	12 (0%)	92	96
2	B	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	D	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	F	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10362/17464 (59%)	10318 (100%)	44 (0%)	94	97

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4850	LEU
1	E	914	PRO
1	G	4106	PRO
1	C	4972	PRO
1	E	806	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4223	ASN
1	E	596	ASN
1	G	3906	GLN

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Mol	Chain	Res	Type
1	C	4803	HIS
1	E	105	HIS

### 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 4 ligands modelled in this entry, 4 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 ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.