



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 07:25 pm BST

PDB ID : 3UA4
Title : Crystal Structure of Protein Arginine Methyltransferase PRMT5
Authors : Sun, L.; Wang, M.; Lv, Z.; Yang, N.; Liu, Y.; Bao, S.; Gong, W.; Xu, R.M.
Deposited on : 2011-10-21
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

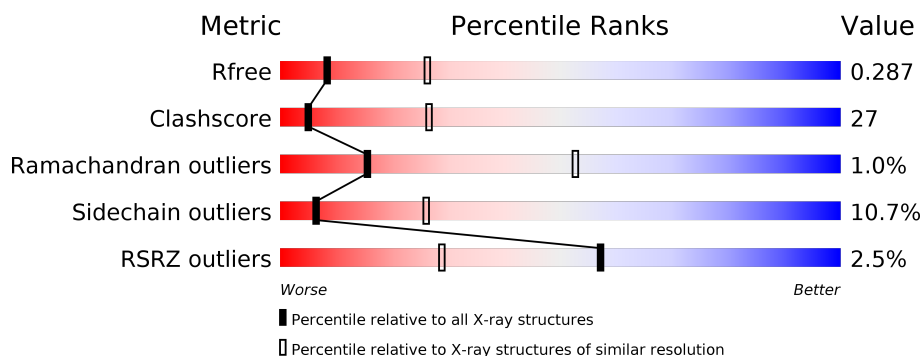
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	745	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	745	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>38%</div> <div>6%</div> <div>16%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10345 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			5143	3291	875	957	20			
1	B	628	Total	C	N	O	S	1	0	0
			5049	3238	854	937	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P46580
A	-1	ALA	-	EXPRESSION TAG	UNP P46580
A	0	SER	-	EXPRESSION TAG	UNP P46580
A	735	LEU	-	EXPRESSION TAG	UNP P46580
A	736	GLU	-	EXPRESSION TAG	UNP P46580
A	737	HIS	-	EXPRESSION TAG	UNP P46580
A	738	HIS	-	EXPRESSION TAG	UNP P46580
A	739	HIS	-	EXPRESSION TAG	UNP P46580
A	740	HIS	-	EXPRESSION TAG	UNP P46580
A	741	HIS	-	EXPRESSION TAG	UNP P46580
A	742	HIS	-	EXPRESSION TAG	UNP P46580
B	-2	MET	-	EXPRESSION TAG	UNP P46580
B	-1	ALA	-	EXPRESSION TAG	UNP P46580
B	0	SER	-	EXPRESSION TAG	UNP P46580
B	735	LEU	-	EXPRESSION TAG	UNP P46580
B	736	GLU	-	EXPRESSION TAG	UNP P46580
B	737	HIS	-	EXPRESSION TAG	UNP P46580
B	738	HIS	-	EXPRESSION TAG	UNP P46580
B	739	HIS	-	EXPRESSION TAG	UNP P46580
B	740	HIS	-	EXPRESSION TAG	UNP P46580
B	741	HIS	-	EXPRESSION TAG	UNP P46580
B	742	HIS	-	EXPRESSION TAG	UNP P46580

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	73	Total	O	0	0
			73	73		



MET	ALA	SER	MET	SER	ASN	ARG	THR	TYR	ALA	ASP	ASN	LEU	PHE	PRO	GLN	GLN	VAL	ALA	GLU	GLN	HIS	GLU	GLU	GLU	GLN	MET	SER	SER	GLY	SER	THR	PRO	LYS	SER	ASN	SER	PRO	SER	ARG	ILE	SER	SER	VAL	GLU	ALA	A44	N45	S46	R47	I50	G51	W52	N53	N54	T55	T56	L57	D58																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
V59	A60	E61	N62	L63	A68	T69	F70	R73	L74	F77	K78	Y79	N80	F81	V82	P85	I86	G87	G88	V89	R91	A92	F93	N94	T95	P96	R97	E101	N102	P105	Y106	I107	V112	Q113	L114	R115	N116	D117	E120	K126	I127	S128	D131	D134	L143	V59	A60	E61	N62	L63	A68	T69	F70	R73	L74	F77	K78	Y79	N80	F81	V82	P85	I86	G87	G88	V89	R91	A92	F93	N94	T95	P96	R97	E101	N102	P105	Y106	I107	V112	Q113	L114	R115	N116	D117	E120	K126	I127	S128	D131	D134	L143																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
E151	L152	S153	Y154	I155	C156	Y157	L158	G159	L160	M163	A164	T165	E166	S171	T172	P173	R174	I178	L179	K180	K181	W182	I183	A184	T185	R186	V187	S188	R189	W193	Q195	L196	S198	A199	I200	E201	K202	Y206	D207	A208	F209	T210	I211	E212	D215	T218	I219	W220	A221	C227	G228	N229	Y234	F235	Q236	V237	A238	L239	T240	L245	E248	N314	T250	S316	E251	L254	V255	D256	R257	W258	K259	L263	A264	T265	R266	V267	T268	E269	S270	G271	L272	F273	ILE	SER	GLY	ARG	ASN	GLY	GLY	ASP	ASN	ASP	S282	I283	P284	H287	I288	N289	L290	L291	K292	H293	L294	T297	D298																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A299	L300	R301	I302	V303	L304	R305	A306	T307	T308	D309	T310	F311	K312	Y313	N314	T315	S316	I317	K318	S319	Y321	R326	H327	A328	VAL	ARG	ASN	VAL	ASN	TYR	ARG	SER	PRO	ASP	VAL	GLY	GLY	GLY	ASN	ASP	SER	THR	HIS	TYR	LEU	ASN	VAL	ILE	GLU	TYR	LYS	ASP	VAL	GLN	L300	R301	I302	V303	L304	R305	A306	T307	T308	D309	T310	F311	K312	Y313	N314	T315	S316	I317	K318	S319	Y321	R326	H327	A328	VAL	ARG	ASN	VAL	ASN	TYR	ARG	SER	PRO	ASP	VAL	GLY	GLY	GLY	ASN	ASP	SER	THR	HIS	TYR	LEU	ASN	VAL	ILE	GLU	TYR	LYS	ASP	VAL	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
ALA	PRO	GLN	PRO	LEU	SER	GLU	ASN	LEU	ASP	SER	GLY	VAL	TYR	ASN	THR	PHE	GLU	Q381	D382	Q383	I384	D387	V388	Y389	G390	E391	A392	V393	V394	G395	K398	D399	L400	G401	A402	D403	G404	R405	K406	T407	V408	V409	I410	Y411	L412	G415	G418	P419	I420	G421	T422	K423	I424	L425	ALA	PRO	GLN	PRO	LEU	SER	GLU	ASN	LEU	ASP	SER	GLY	VAL	TYR	ASN	THR	PHE	GLU	Q381	D382	Q383	I384	D387	V388	Y389	G390	E391	A392	V393	V394	G395	K398	D399	L400	G401	A402	D403	G404	R405	K406	T407	V408	V409	I410	Y411	L412	G415	G418	P419	I420	G421	T422	K423	I424	L425																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
K426	S427	E428	R429	F430	Y431	N432	N433	F434	F435	R436	GLN	GLY	GLN	GLU	S441	L442	K443	Y444	K445	L446	Y447	L448	V449	E450	I456	V457	T458	Y461	N462	N463	R464	T466	W467	K468	R469	R470	V471	T472	L473	I474	E475	S476	D477	N478	R479	S480	L481	P482	G483	I484	A485	K486	Q492	P493	D494	K426	S427	E428	R429	F430	Y431	N432	N433	F434	F435	R436	GLN	GLY	GLN	GLU	S441	L442	K443	Y444	K445	L446	Y447	L448	V449	E450	I456	V457	T458	Y461	N462	N463	R464	T466	W467	K468	R469	R470	V471	T472	L473	I474	E475	S476	D477	N478	R479	S480	L481	P482	G483	I484	A485	K486	Q492	P493	D494																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
I495	L496	V497	L501	B506	H507	E508	L509	S510	P511	E512	C513	V517	T518	G519	F520	L521	K522	T525	I526	S527	P529	Q530	K531	Y532	W536	K537	S541	I544	L556	S557	R558	A559	F561	S562	E569	B572	D573	W576	I577	O578	K579	W585	P672	A673	I495	L496	V497	L501	B506	H507	E508	L509	S510	P511	E512	C513	V517	T518	G519	F520	L521	K522	T525	I526	S527	P529	Q530	K531	Y532	W536	K537	S541	I544	L556	S557	R558	A559	F561	S562	E569	B572	D573	W576	I577	O578	K579	W585	P672	A673																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V708	V709	V710	V711	V712	V713	V714	V715	V716	V717	V720	V721	V722	V723	V724	V727	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V150

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.56 Å 129.49 Å 149.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 3.00 30.02 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.02-3.00) 99.4 (30.02-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 3.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.232 , 0.288 0.229 , 0.287	Depositor DCC
R_{free} test set	1817 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10345	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/5272	0.47	0/7161
1	B	0.27	0/5176	0.47	0/7031
All	All	0.27	0/10448	0.47	0/14192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5143	0	5096	272	0
1	B	5049	0	5005	285	0
2	B	6	0	8	0	0
3	A	74	0	0	5	0
3	B	73	0	0	2	0
All	All	10345	0	10109	553	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 27.

The worst 5 of 553 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:724:ASN:HD21	1:B:730:TYR:HB3	1.10	1.15
1:A:533:THR:HB	1:A:612:THR:HG22	1.23	1.08
1:A:635:ARG:HH11	1:A:635:ARG:HG2	1.16	1.07
1:A:74:LEU:HB3	1:A:79:TYR:HE1	1.20	1.07
1:B:198:SER:HB2	1:B:202:LYS:HD3	1.48	0.96

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 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	636/745 (85%)	551 (87%)	77 (12%)	8 (1%)	12	45
1	B	620/745 (83%)	538 (87%)	77 (12%)	5 (1%)	19	57
All	All	1256/1490 (84%)	1089 (87%)	154 (12%)	13 (1%)	15	53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	ASN
1	A	182	TRP
1	A	284	PRO
1	B	212	GLU
1	B	509	LEU

5.3.2 Protein sidechains [i](#)

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	567/662 (86%)	511 (90%)	56 (10%)	8	30
1	B	557/662 (84%)	493 (88%)	64 (12%)	5	24
All	All	1124/1324 (85%)	1004 (89%)	120 (11%)	6	26

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	714	ASN
1	B	180	LYS
1	B	659	GLU
1	A	717	SER
1	B	95	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	195	GLN
1	B	287	HIS
1	B	649	GLN
1	A	649	GLN
1	B	563	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 ⓘ

1 ligand is modelled in this entry.

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	GOL	B	743	-	5,5,5	0.36	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	743	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	743	GOL	C1-C2-C3-O3
2	B	743	GOL	O2-C2-C3-O3
2	B	743	GOL	O1-C1-C2-C3
2	B	743	GOL	O1-C1-C2-O2

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	640/745 (85%)	-0.22	13 (2%) 65 36	14, 91, 179, 238	1 (0%)
1	B	628/745 (84%)	-0.10	19 (3%) 50 22	23, 101, 190, 251	15 (2%)
All	All	1268/1490 (85%)	-0.16	32 (2%) 57 29	14, 96, 183, 251	16 (1%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	4.6
1	A	275	SER	4.4
1	B	429	ARG	4.1
1	B	97	ASN	3.8
1	B	308	THR	3.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	743	6/6	0.91	0.45	86,91,92,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.