



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 01:07 am GMT

PDB ID : 2VZS
Title : Chitosan Product complex of Amycolatopsis orientalis exo-chitosanase CsxA
Authors : Lammerts van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B.
Deposited on : 2008-08-05
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

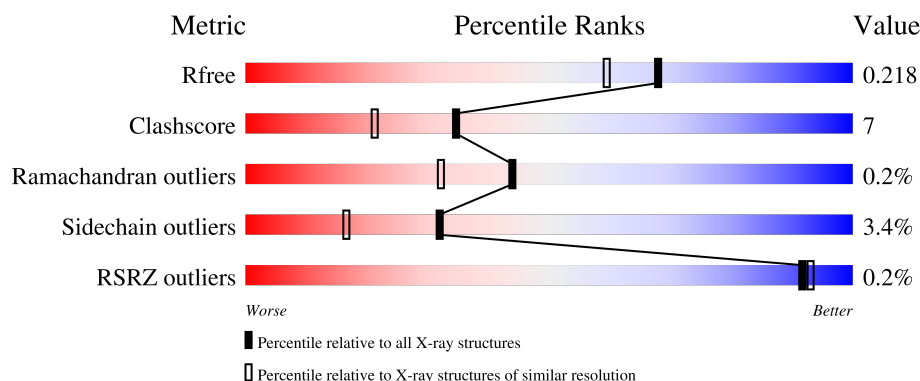
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 $\leq 5\%$. 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	1032	
1	B	1032	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CD	A	1899	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14981 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 EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	4	0	1
			6552	4115	1133	1287	17			
1	B	858	Total	C	N	O	S	0	0	1
			6552	4115	1133	1287	17			

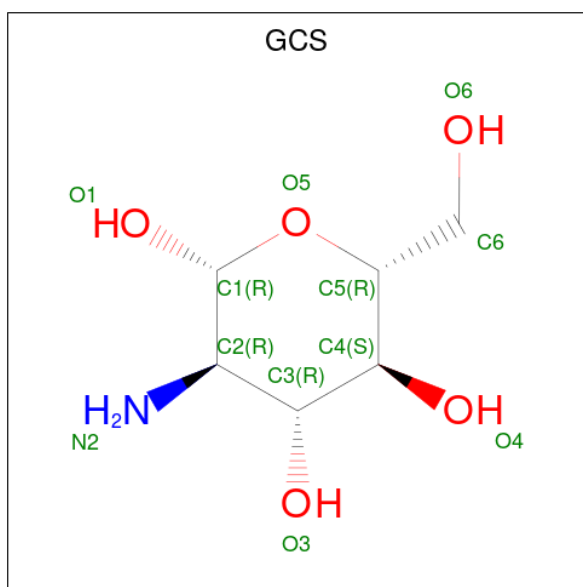
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	750	ASN	TRP	conflict	UNP Q56F26
B	750	ASN	TRP	conflict	UNP Q56F26

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cd	0	0
			3	3		
2	B	3	Total	Cd	0	0
			3	3		

- Molecule 3 is 2-amino-2-deoxy-beta-D-glucopyranose (three-letter code: GCS) (formula: C₆H₁₃NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	1	5		
3	B	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

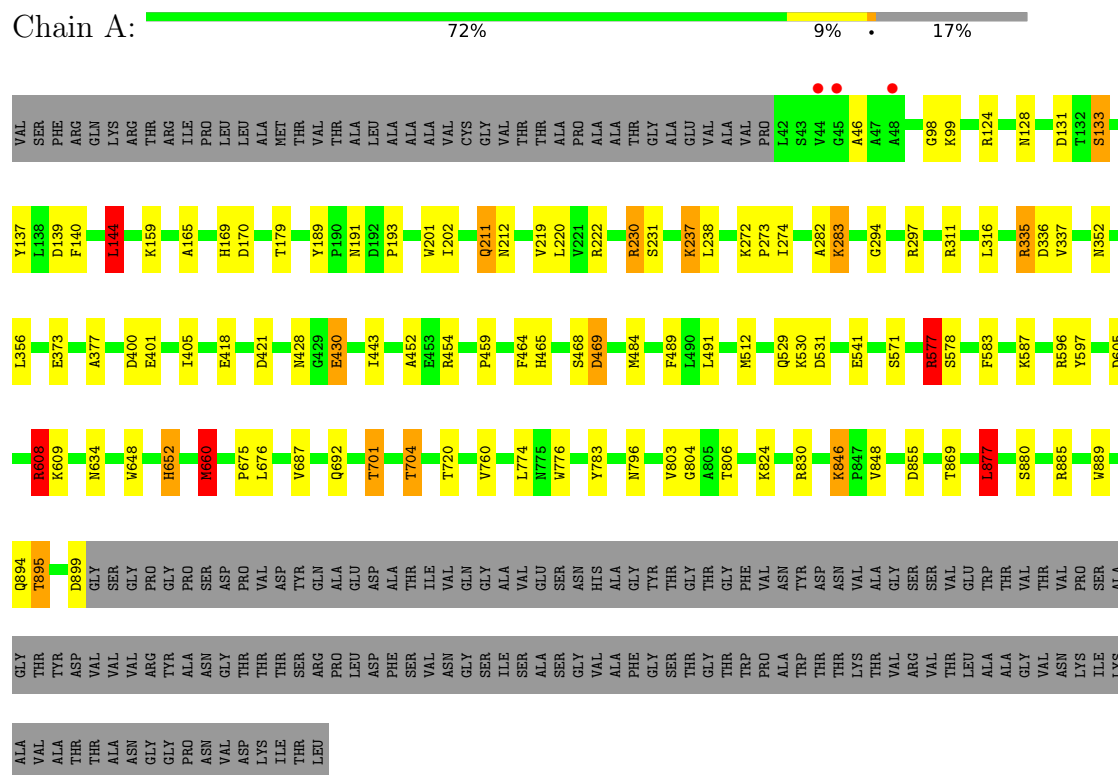
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	958	Total	O	0	0
			958	958		
5	B	871	Total	O	0	0
			871	871		

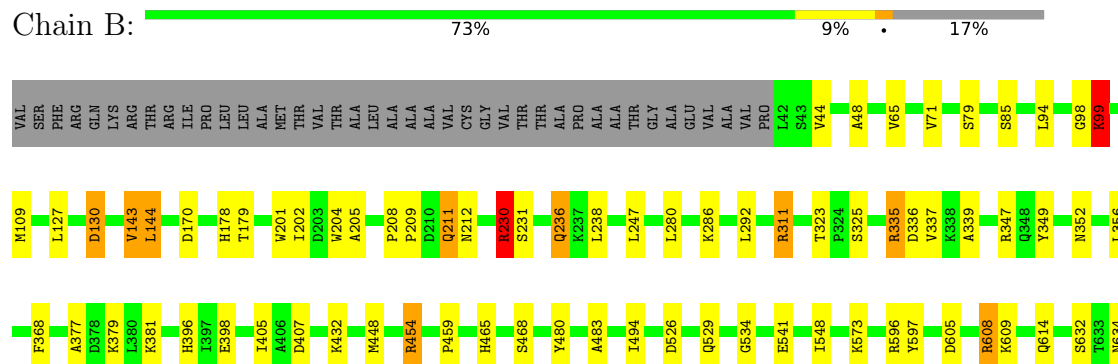
3 Residue-property plots

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 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.

• Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE



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ASN	VAL	GLY	PRO	M643	GLY	GLY	PRO	M647	GLY	GLY	PRO	M648	GLY	GLY	PRO	M652	GLY	GLY	PRO	M660	GLY	GLY	PRO	M682	GLY	GLY	PRO	M685	GLY	GLY	PRO	M686	GLY	GLY	PRO	M687	GLY	GLY	PRO	M701	GLY	GLY	PRO	M704	GLY	GLY	PRO	M736	GLY	GLY	PRO	M753	GLY	GLY	PRO	M774	GLY	GLY	PRO	M775	GLY	GLY	PRO	M776	GLY	GLY	PRO	M796	GLY	GLY	PRO	M803	GLY	GLY	PRO	M804	GLY	GLY	PRO	M808	GLY	GLY	PRO	M809	GLY	GLY	PRO	M823	GLY	GLY	PRO	M824	GLY	GLY	PRO	M827	GLY	GLY	PRO	M830	GLY	GLY	PRO	M831	GLY	GLY	PRO	M846	GLY	GLY	PRO	M847	GLY	GLY	PRO	M872	GLY	GLY	PRO	M877	GLY	GLY	PRO	M885	GLY	GLY	PRO	M889	GLY	GLY	PRO	M895	GLY	GLY	PRO	M896	GLY	GLY	PRO	M899	GLY	GLY	PRO	M904	GLY	GLY	PRO	M905	GLY	GLY	PRO	M906	GLY	GLY	PRO	M907	GLY	GLY	PRO	M908	GLY	GLY	PRO	M909	GLY	GLY	PRO	M910	GLY	GLY	PRO	M911	GLY	GLY	PRO	M912	GLY	GLY	PRO	M913	GLY	GLY	PRO	M914	GLY	GLY	PRO	M915	GLY	GLY	PRO	M916	GLY	GLY	PRO	M917	GLY	GLY	PRO	M918	GLY	GLY	PRO	M919	GLY	GLY	PRO	M920	GLY	GLY	PRO	M921	GLY	GLY	PRO	M922	GLY	GLY	PRO	M923	GLY	GLY	PRO	M924	GLY	GLY	PRO	M925	GLY	GLY	PRO	M926	GLY	GLY	PRO	M927	GLY	GLY	PRO	M928	GLY	GLY	PRO	M929	GLY	GLY	PRO	M930	GLY	GLY	PRO	M931	GLY	GLY	PRO	M932	GLY	GLY	PRO	M933	GLY	GLY	PRO	M934	GLY	GLY	PRO	M935	GLY	GLY	PRO	M936	GLY	GLY	PRO	M937	GLY	GLY	PRO	M938	GLY	GLY	PRO	M939	GLY	GLY	PRO	M940	GLY	GLY	PRO	M941	GLY	GLY	PRO	M942	GLY	GLY	PRO	M943	GLY	GLY	PRO	M944	GLY	GLY	PRO	M945	GLY	GLY	PRO	M946	GLY	GLY	PRO	M947	GLY	GLY	PRO	M948	GLY	GLY	PRO	M949	GLY	GLY	PRO	M950	GLY	GLY	PRO	M951	GLY	GLY	PRO	M952	GLY	GLY	PRO	M953	GLY	GLY	PRO	M954	GLY	GLY	PRO	M955	GLY	GLY	PRO	M956	GLY	GLY	PRO	M957	GLY	GLY	PRO	M958	GLY	GLY	PRO	M959	GLY	GLY	PRO	M960	GLY	GLY	PRO	M961	GLY	GLY	PRO	M962	GLY	GLY	PRO	M963	GLY	GLY	PRO	M964	GLY	GLY	PRO	M965	GLY	GLY	PRO	M966	GLY	GLY	PRO	M967	GLY	GLY	PRO	M968	GLY	GLY	PRO	M969	GLY	GLY	PRO	M970	GLY	GLY	PRO	M971	GLY	GLY	PRO	M972	GLY	GLY	PRO	M973	GLY	GLY	PRO	M974	GLY	GLY	PRO	M975	GLY	GLY	PRO	M976	GLY	GLY	PRO	M977	GLY	GLY	PRO	M978	GLY	GLY	PRO	M979	GLY	GLY	PRO	M980	GLY	GLY	PRO	M981	GLY	GLY	PRO	M982	GLY	GLY	PRO	M983	GLY	GLY	PRO	M984	GLY	GLY	PRO	M985	GLY	GLY	PRO	M986	GLY	GLY	PRO	M987	GLY	GLY	PRO	M988	GLY	GLY	PRO	M989	GLY	GLY	PRO	M990	GLY	GLY	PRO	M991	GLY	GLY	PRO	M992	GLY	GLY	PRO	M993	GLY	GLY	PRO	M994	GLY	GLY	PRO	M995	GLY	GLY	PRO	M996	GLY	GLY	PRO	M997	GLY	GLY	PRO	M998	GLY	GLY	PRO	M999	GLY	GLY	PRO	M1000	GLY	GLY	PRO	M1001	GLY	GLY	PRO	M1002	GLY	GLY	PRO	M1003	GLY	GLY	PRO	M1004	GLY	GLY	PRO	M1005	GLY	GLY	PRO	M1006	GLY	GLY	PRO	M1007	GLY	GLY	PRO	M1008	GLY	GLY	PRO	M1009	GLY	GLY	PRO	M1010	GLY	GLY	PRO	M1011	GLY	GLY	PRO	M1012	GLY	GLY	PRO	M1013	GLY	GLY	PRO	M1014	GLY	GLY	PRO	M1015	GLY	GLY	PRO	M1016	GLY	GLY	PRO	M1017	GLY	GLY	PRO	M1018	GLY	GLY	PRO	M1019	GLY	GLY	PRO	M1020	GLY	GLY	PRO	M1021	GLY	GLY	PRO	M1022	GLY	GLY	PRO	M1023	GLY	GLY	PRO	M1024	GLY	GLY	PRO	M1025	GLY	GLY	PRO	M1026	GLY	GLY	PRO	M1027	GLY	GLY	PRO	M1028	GLY	GLY	PRO	M1029	GLY	GLY	PRO	M1030	GLY	GLY	PRO	M1031	GLY	GLY	PRO	M1032	GLY	GLY	PRO	M1033	GLY	GLY	PRO	M1034	GLY	GLY	PRO	M1035	GLY	GLY	PRO	M1036	GLY	GLY	PRO	M1037	GLY	GLY	PRO	M1038	GLY	GLY	PRO	M1039	GLY	GLY	PRO	M1040	GLY	GLY	PRO	M1041	GLY	GLY	PRO	M1042	GLY	GLY	PRO	M1043	GLY	GLY	PRO	M1044	GLY	GLY	PRO	M1045	GLY	GLY	PRO	M1046	GLY	GLY	PRO	M1047	GLY	GLY	PRO	M1048	GLY	GLY	PRO	M1049	GLY	GLY	PRO	M1050	GLY	GLY	PRO	M1051	GLY	GLY	PRO	M1052	GLY	GLY	PRO	M1053	GLY	GLY	PRO	M1054	GLY	GLY	PRO	M1055	GLY	GLY	PRO	M1056	GLY	GLY	PRO	M1057	GLY	GLY	PRO	M1058	GLY	GLY	PRO	M1059	GLY	GLY	PRO	M1060	GLY	GLY	PRO	M1061	GLY	GLY	PRO	M1062	GLY	GLY	PRO	M1063	GLY	GLY	PRO	M1064	GLY	GLY	PRO	M1065	GLY	GLY	PRO	M1066	GLY	GLY	PRO	M1067	GLY	GLY	PRO	M1068	GLY	GLY	PRO	M1069	GLY	GLY	PRO	M1070	GLY	GLY	PRO	M1071	GLY	GLY	PRO	M1072	GLY	GLY	PRO	M1073	GLY	GLY	PRO	M1074	GLY	GLY	PRO	M1075	GLY	GLY	PRO	M1076	GLY	GLY	PRO	M1077	GLY	GLY	PRO	M1078	GLY	GLY	PRO	M1079	GLY	GLY	PRO	M1080	GLY	GLY	PRO	M1081	GLY	GLY	PRO	M1082	GLY	GLY	PRO	M1083	GLY	GLY	PRO	M1084	GLY	GLY	PRO	M1085	GLY	GLY	PRO	M1086	GLY	GLY	PRO	M1087	GLY	GLY	PRO	M1088	GLY	GLY	PRO	M1089	GLY	GLY	PRO	M1090	GLY	GLY	PRO	M1091	GLY	GLY	PRO	M1092	GLY	GLY	PRO	M1093	GLY	GLY	PRO	M1094	GLY	GLY	PRO	M1095	GLY	GLY	PRO	M1096	GLY	GLY	PRO	M1097	GLY	GLY	PRO	M1098	GLY	GLY	PRO	M1099	GLY	GLY	PRO	M1100	GLY	GLY	PRO	M1101	GLY	GLY	PRO	M1102	GLY	GLY	PRO	M1103	GLY	GLY	PRO	M1104	GLY	GLY	PRO	M1105	GLY	GLY	PRO	M1106	GLY	GLY	PRO	M1107	GLY	GLY	PRO	M1108	GLY	GLY	PRO	M1109	GLY	GLY	PRO	M1110	GLY	GLY	PRO	M1111	GLY	GLY	PRO	M1112	GLY	GLY	PRO	M1113	GLY	GLY	PRO	M1114	GLY	GLY	PRO	M1115	GLY	GLY	PRO	M1116	GLY	GLY	PRO	M1117	GLY	GLY	PRO	M1118	GLY	GLY	PRO	M1119	GLY	GLY	PRO	M1120	GLY	GLY	PRO	M1121	GLY	GLY	PRO	M1122	GLY	GLY	PRO	M1123	GLY	GLY	PRO	M1124	GLY	GLY	PRO	M1125	GLY	GLY	PRO	M1126	GLY	GLY	PRO	M1127	GLY	GLY	PRO	M1128	GLY	GLY	PRO	M1129	GLY	GLY	PRO	M1130	GLY	GLY	PRO	M1131	GLY	GLY	PRO	M1132	GLY	GLY	PRO	M1133	GLY	GLY	PRO	M1134	GLY	GLY	PRO	M1135	GLY	GLY	PRO	M1136	GLY	GLY	PRO	M1137	GLY	GLY	PRO	M1138	GLY	GLY	PRO	M1139	GLY	GLY	PRO	M1140	GLY	GLY	PRO	M1141	GLY	GLY	PRO	M1142	GLY	GLY	PRO	M1143	GLY	GLY	PRO	M1144	GLY	GLY	PRO	M1145	GLY	GLY	PRO	M1146	GLY	GLY	PRO	M1147	GLY	GLY	PRO	M1148	GLY	GLY	PRO	M1149	GLY	GLY	PRO	M1150	GLY	GLY	PRO	M1151	GLY	GLY	PRO	M1152	GLY	GLY	PRO	M1153	GLY	GLY	PRO	M1154	GLY	GLY	PRO	M1155	GLY	GLY	PRO	M1156	GLY	GLY	PRO	M1157	GLY	GLY	PRO	M1158	GLY	GLY	PRO	M1159	GLY	GLY	PRO	M1160	GLY	GLY	PRO	M1161	GLY	GLY	PRO	M1162	GLY	GLY	PRO	M1163	GLY	GLY	PRO	M1164	GLY	GLY	PRO	M1165	GLY	GLY	PRO	M1166	GLY	GLY	PRO	M1167	GLY	GLY	PRO	M1168	GLY	GLY	PRO	M1169	GLY	GLY	PRO	M1170	GLY	GLY	PRO	M1171	GLY	GLY	PRO	M1172	GLY	GLY	PRO	M1173	GLY	GLY	PRO	M1174	GLY	GLY	PRO	M1175	GLY	GLY	PRO	M1176	GLY	GLY	PRO	M1177	GLY	GLY	PRO	M1178	GLY	GLY	PRO	M1179	GLY	GLY	PRO	M1180	GLY	GLY	PRO	M1181	GLY	GLY	PRO	M1182	GLY	GLY	PRO	M1183	GLY	GLY	PRO	M1184	GLY	GLY	PRO	M1185	GLY	GLY	PRO	M1186	GLY	GLY	PRO	M1187	GLY	GLY	PRO	M1188	GLY	GLY	PRO	M1189	GLY	GLY	PRO	M1190	GLY	GLY	PRO	M1191	GLY	GLY	PRO	M1192	GLY	GLY	PRO	M1193	GLY	GLY	PRO	M1194	GLY	GLY	PRO	M1195	GLY	GLY	PRO	M1196	GLY	GLY	PRO	M1197	GLY	GLY	PRO	M1198	GLY	GLY	PRO	M1199	GLY	GLY	PRO	M1200	GLY	GLY	PRO	M1201	GLY	GLY	PRO	M1202	GLY	GLY	PRO	M1203	GLY	GLY	PRO	M1204	GLY	GLY	PRO	M1205	GLY	GLY	PRO	M1206	GLY	GLY	PRO	M1207	GLY	GLY	PRO	M1208	GLY	GLY	PRO	M1209	GLY	GLY	PRO	M1210	GLY	GLY	PRO	M1211	GLY	GLY	PRO	M1212	GLY	GLY	PRO	M1213	GLY	GLY	PRO	M1214	GLY	GLY	PRO	M1215	GLY	GLY	PRO	M1216	GLY	GLY	PRO	M1217	GLY	GLY	PRO	M1218	GLY	GLY	PRO	M1219	GLY	GLY	PRO	M1220	GLY	GLY	PRO	M1221	GLY	GLY	PRO	M1222	GLY	GLY	PRO	M1223	GLY	GLY	PRO	M1224	GLY	GLY	PRO	M1225	GLY	GLY	PRO	M1226	GLY	GLY	PRO	M1227	GLY	GLY	PRO	M1228	GLY	GLY	PRO	M1229	GLY	GLY	PRO	M1230	GLY	GLY	PRO	M1231	GLY	GLY	PRO	M1232	GLY	GLY	PRO	M1233	GLY	GLY	PRO	M1234	GLY	GLY	PRO	M1235	GLY	GLY	PRO	M1236	GLY	GLY	PRO	M1237	GLY	GLY	PRO	M1238	GLY	GLY	PRO	M1239	GLY	GLY	PRO	M1240	GLY	GLY	PRO	M1241	GLY	GLY	PRO	M1242	GLY	GLY	PRO	M1243	GLY	GLY	PRO	M1244	GLY	GLY	PRO	M1245	GLY	GLY	PRO	M1246	GLY	GLY	PRO	M1247	GLY	GLY	PRO	M1248	GLY	GLY	PRO	M1249	GLY	GLY	PRO	M1250	GLY	GLY	PRO	M1251	GLY	GLY	PRO	M1252	GLY	GLY	PRO	M1253	GLY	GLY	PRO	M1254	GLY	GLY	PRO	M1255	GLY	GLY	PRO	M1256	GLY	GLY	PRO	M1257	GLY	GLY	PRO	M1258	GLY	GLY	PRO	M1259	GLY	GLY	PRO	M1260	GLY	GLY	PRO	M1261	GLY	GLY	PRO	M1262	GLY	GLY	PRO	M1263	GLY	GLY	PRO	M1264	GLY	GLY	PRO	M1265	GLY	GLY	PRO	M1266	GLY	GLY	PRO	M1267	GLY	GLY	PRO	M1268	GLY	GLY	PRO	M1269	GLY	GLY	PRO	M1270	GLY	GLY	PRO	M1271	GLY	GLY	PRO	M1272	GLY	GLY	PRO	M1273	GLY	GLY	PRO	M1274	GLY	GLY	PRO	M1275	GLY	GLY	PRO	M1276	GLY	GLY	PRO	M1277	GLY	GLY	PRO	M1278	GLY	GLY	PRO	M1279	GLY	GLY	PRO	M1280	GLY	GLY	PRO	M1281	GLY	GLY	PRO	M1282	GLY	GLY	PRO	M1283	GLY	GLY	PRO	M1284	GLY	GLY	PRO	M1285	GLY	GLY	PRO	M1286	GLY	GLY	PRO	M1287	GLY	GLY	PRO	M1288	GLY	GLY	PRO	M1289	GLY	GLY	PRO	M1290	GLY	GLY	PRO	M1291	GLY	GLY	PRO	M1292	GLY	GLY	PRO	M1293	GLY	GLY	PRO	M1294	GLY	GLY	PRO	M1295	GLY	GLY	PRO	M1296	GLY	GLY	PRO	M1297	GLY	GLY	PRO	M1298	GLY	GLY	PRO	M1299	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.54Å 121.81Å 91.84Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.85) 99.8 (40.00-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.220 0.172 , 0.218	Depositor DCC
R_{free} test set	8098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14981	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

5.1 Standard geometry

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

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	0.90	1/6715 (0.0%)	0.97	23/9163 (0.3%)
1	B	0.90	2/6715 (0.0%)	1.04	25/9163 (0.3%)
All	All	0.90	3/13430 (0.0%)	1.00	48/18326 (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	3
1	B	0	3
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	12.05	1.75	1.52
1	B	335	ARG	CD-NE	-6.21	1.35	1.46
1	B	454	ARG	CD-NE	-5.79	1.36	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	ARG	NE-CZ-NH2	-28.58	106.01	120.30
1	B	454	ARG	NE-CZ-NH2	-27.75	106.43	120.30
1	A	335	ARG	NE-CZ-NH2	-26.63	106.99	120.30
1	A	335	ARG	NE-CZ-NH1	21.46	131.03	120.30
1	B	454	ARG	NE-CZ-NH1	21.35	130.98	120.30
1	B	335	ARG	NE-CZ-NH1	19.61	130.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	ARG	NE-CZ-NH1	17.89	129.24	120.30
1	A	230	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	A	577	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	B	311	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	A	230	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	B	230	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	B	311	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	660	MET	CG-SD-CE	-9.42	85.13	100.20
1	A	335	ARG	CD-NE-CZ	8.87	136.01	123.60
1	A	238	LEU	CA-CB-CG	8.81	135.56	115.30
1	B	454	ARG	CD-NE-CZ	8.58	135.61	123.60
1	B	335	ARG	CD-NE-CZ	8.46	135.44	123.60
1	B	597	TYR	N-CA-C	8.00	132.60	111.00
1	B	335	ARG	CG-CD-NE	-7.99	95.02	111.80
1	A	608	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	774	LEU	CA-CB-CG	-7.55	97.94	115.30
1	B	454	ARG	CG-CD-NE	-7.44	96.18	111.80
1	A	597	TYR	N-CA-C	7.40	130.99	111.00
1	A	577	ARG	CD-NE-CZ	7.25	133.75	123.60
1	B	144	LEU	CA-CB-CG	7.20	131.87	115.30
1	B	660	MET	CG-SD-CE	-7.20	88.67	100.20
1	A	774	LEU	CA-CB-CG	-7.15	98.86	115.30
1	A	335	ARG	CG-CD-NE	-7.10	96.89	111.80
1	B	230	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	144	LEU	CA-CB-CG	6.49	130.22	115.30
1	B	685	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	236	GLN	CA-CB-CG	6.40	127.48	113.40
1	A	885	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	608	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	855	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	877	LEU	CB-CG-CD1	5.62	120.56	111.00
1	B	238	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	130	ASP	CB-CA-C	-5.57	99.26	110.40
1	A	124	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	99	LYS	N-CA-C	-5.37	96.50	111.00
1	A	430	GLU	CB-CG-CD	5.30	128.51	114.20
1	B	127	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	99	LYS	N-CA-C	-5.14	97.12	111.00
1	B	143	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	A	877	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	292	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	877	LEU	CB-CG-CD1	5.01	119.51	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	SER	Peptide
1	A	596	ARG	Peptide
1	A	98	GLY	Peptide
1	B	468	SER	Peptide
1	B	596	ARG	Peptide
1	B	98	GLY	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	6552	0	6328	100	0
1	B	6552	0	6328	92	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	12	0	13	1	0
3	B	12	0	13	1	0
4	A	6	0	8	0	0
4	B	12	0	15	0	0
5	A	958	0	0	40	1
5	B	871	0	0	45	1
All	All	14981	0	12705	192	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 7.

All (192) 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:643:MET:CE	5:B:2625:HOH:O	1.81	1.26
1:B:483:ALA:HB3	5:B:2492:HOH:O	1.30	1.24
1:A:512:MET:HE1	5:A:2516:HOH:O	1.39	1.18
1:B:753:THR:HB	5:B:2719:HOH:O	1.39	1.18
1:A:846:LYS:HG2	5:A:2389:HOH:O	1.41	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:CE	1:B:209:PRO:HD3	1.78	1.12
1:B:109:MET:HE1	1:B:368:PHE:HE1	1.07	1.10
1:A:660:MET:SD	5:A:2434:HOH:O	2.07	1.10
1:B:204:TRP:HE3	5:B:2375:HOH:O	1.37	1.07
1:B:109:MET:HE2	1:B:209:PRO:CD	1.84	1.06
1:B:647:PRO:HG3	5:B:2375:HOH:O	1.55	1.05
1:B:643:MET:HE3	5:B:2625:HOH:O	1.42	1.04
1:A:401:GLU:HB3	5:A:2429:HOH:O	1.58	1.03
1:B:109:MET:CE	1:B:368:PHE:HE1	1.70	1.03
1:A:577:ARG:HD2	1:A:652:HIS:ND1	1.74	1.01
1:A:541:GLU:HG3	5:A:2596:HOH:O	1.64	0.98
1:A:660:MET:CE	5:A:2434:HOH:O	2.12	0.97
1:B:109:MET:HE1	1:B:368:PHE:CE1	1.99	0.97
1:B:109:MET:CE	1:B:368:PHE:CE1	2.48	0.96
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.07	0.96
1:A:512:MET:CE	5:A:2516:HOH:O	2.01	0.94
1:A:541:GLU:CG	5:A:2596:HOH:O	2.15	0.94
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.03	0.93
1:A:46:ALA:HB1	5:A:2094:HOH:O	1.69	0.91
1:A:846:LYS:CG	5:A:2389:HOH:O	2.09	0.89
1:B:846:LYS:HE3	5:B:2543:HOH:O	1.73	0.89
1:A:297:ARG:HG3	5:B:2018:HOH:O	1.72	0.89
1:A:634:ASN:HB3	5:A:2686:HOH:O	1.71	0.88
1:B:179:THR:CA	5:B:2183:HOH:O	2.21	0.88
1:A:297:ARG:HB2	5:A:2319:HOH:O	1.74	0.88
1:B:846:LYS:HE2	1:B:847:PRO:HD2	1.53	0.88
1:A:443:ILE:HD12	5:A:2492:HOH:O	1.73	0.87
1:A:179:THR:CA	5:A:2170:HOH:O	2.22	0.87
1:A:311:ARG:HD2	5:A:2511:HOH:O	1.74	0.87
1:B:480:TYR:HA	5:B:2492:HOH:O	1.77	0.85
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.58	0.85
1:B:109:MET:HE2	1:B:209:PRO:HD3	0.90	0.84
1:B:895:THR:HG22	5:B:2860:HOH:O	1.77	0.83
1:B:541:GLU:OE2	3:B:1903:GCS:H1	1.79	0.81
1:B:872:TYR:HB2	5:B:2814:HOH:O	1.81	0.81
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.78	0.80
1:A:846:LYS:CD	5:A:2389:HOH:O	2.30	0.79
1:A:577:ARG:HG2	1:A:583:PHE:O	1.83	0.78
1:A:128:ASN:HB2	5:A:2088:HOH:O	1.83	0.78
1:B:349:TYR:OH	1:B:494:ILE:HD11	1.84	0.77
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.20	0.77
1:B:109:MET:HE3	1:B:368:PHE:CE1	2.18	0.77
1:B:803:VAL:HB	5:B:2774:HOH:O	1.84	0.76
1:A:899:ASP:N	5:A:2954:HOH:O	2.18	0.76
1:A:220:LEU:CD1	1:A:222:ARG:HH12	1.98	0.75
1:B:311:ARG:CD	5:B:2334:HOH:O	2.34	0.75
1:B:643:MET:HE1	5:B:2625:HOH:O	1.58	0.74
1:A:846:LYS:HE2	5:A:2601:HOH:O	1.87	0.73
1:A:220:LEU:HD12	1:A:222:ARG:HH12	1.52	0.73
1:B:311:ARG:HD2	5:B:2334:HOH:O	1.88	0.71
1:A:531:ASP:HB2	5:A:2592:HOH:O	1.88	0.71
1:B:685:ARG:NH1	1:B:736:VAL:O	2.22	0.71
1:B:831:LEU:O	5:B:2798:HOH:O	2.09	0.70
1:B:109:MET:CE	1:B:208:PRO:HA	2.21	0.70
1:A:311:ARG:CD	5:A:2511:HOH:O	2.36	0.70
1:B:432:LYS:HG2	5:B:2442:HOH:O	1.92	0.70
1:A:530:LYS:HB3	5:A:2231:HOH:O	1.92	0.69
1:B:179:THR:CA	5:B:2182:HOH:O	2.40	0.68
1:A:237:LYS:HE3	1:A:237:LYS:HA	1.76	0.68
1:A:46:ALA:CB	5:A:2094:HOH:O	2.33	0.66
1:B:109:MET:HE2	1:B:208:PRO:HA	1.78	0.66
1:B:381:LYS:HD2	5:B:2400:HOH:O	1.95	0.65
1:A:541:GLU:HG2	5:A:2596:HOH:O	1.91	0.65
1:A:701:THR:HB	1:A:720:THR:HA	1.79	0.65
1:B:336:ASP:H	1:B:352:ASN:ND2	1.96	0.64
1:A:577:ARG:HD3	1:A:652:HIS:HB3	1.80	0.63
1:A:222:ARG:NE	5:A:2222:HOH:O	2.31	0.63
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.63	0.62
1:A:687:VAL:HG21	1:A:704:THR:HG21	1.80	0.62
1:A:541:GLU:OE2	3:A:1902:GCS:H1	2.01	0.60
1:A:336:ASP:H	1:A:352:ASN:ND2	1.98	0.60
1:A:634:ASN:CB	5:A:2686:HOH:O	2.37	0.59
1:B:94:LEU:O	1:B:99:LYS:HB2	2.03	0.59
1:B:335:ARG:HD3	1:B:459:PRO:O	2.03	0.59
1:A:131:ASP:OD2	1:A:133:SER:HB2	2.04	0.58
1:B:846:LYS:CE	5:B:2543:HOH:O	2.40	0.58
1:B:605:ASP:OD1	1:B:608:ARG:NH1	2.37	0.58
1:A:400:ASP:OD1	1:A:454:ARG:HD2	2.04	0.58
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.39	0.57
1:A:220:LEU:HD12	1:A:222:ARG:NH1	2.19	0.57
1:B:895:THR:HG21	5:B:2862:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.89	0.56
1:B:204:TRP:CE3	5:B:2375:HOH:O	2.25	0.56
1:A:605:ASP:HA	1:A:608:ARG:HD3	1.87	0.56
1:B:48:ALA:HB1	1:B:325:SER:O	2.06	0.56
1:A:377:ALA:HA	1:A:405:ILE:HG21	1.88	0.56
1:B:701:THR:CG2	5:B:2667:HOH:O	2.55	0.55
1:A:170:ASP:OD2	1:A:230:ARG:HD2	2.07	0.55
1:A:804:GLY:HA3	1:A:824:LYS:O	2.06	0.55
1:B:529:GLN:HG3	1:B:776:TRP:CD2	2.42	0.55
1:A:335:ARG:HD3	1:A:459:PRO:O	2.07	0.54
1:A:605:ASP:HA	1:A:608:ARG:CD	2.38	0.54
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.72	0.54
1:B:448:MET:HG2	5:B:2492:HOH:O	2.07	0.54
1:B:548:ILE:H	1:B:614:GLN:NE2	2.05	0.54
1:A:830:ARG:HD2	5:A:2750:HOH:O	2.07	0.54
1:A:577:ARG:CD	1:A:652:HIS:CG	2.91	0.53
1:B:349:TYR:OH	1:B:494:ILE:CD1	2.54	0.53
1:B:899:ASP:N	5:B:2866:HOH:O	2.41	0.53
1:A:587:LYS:HE3	5:A:2646:HOH:O	2.07	0.53
1:B:573:LYS:HG3	5:B:2579:HOH:O	2.08	0.53
1:A:220:LEU:CD1	1:A:222:ARG:NH1	2.68	0.53
1:B:548:ILE:H	1:B:614:GLN:HE22	1.56	0.53
1:A:701:THR:CG2	5:A:2740:HOH:O	2.56	0.53
1:B:211:GLN:HG3	5:B:2228:HOH:O	2.08	0.53
1:B:609:LYS:CE	1:B:796:ASN:HD21	2.21	0.53
1:B:109:MET:HE1	1:B:208:PRO:HA	1.90	0.52
1:B:130:ASP:HB2	5:B:2001:HOH:O	2.09	0.52
1:A:191:ASN:O	1:A:211:GLN:HG2	2.10	0.52
1:B:704:THR:HG23	5:B:2668:HOH:O	2.10	0.51
1:B:701:THR:HG23	5:B:2667:HOH:O	2.11	0.51
1:A:220:LEU:HD13	1:A:222:ARG:HH12	1.75	0.51
1:B:647:PRO:CG	5:B:2375:HOH:O	2.32	0.50
1:A:608:ARG:HG2	1:A:609:LYS:N	2.26	0.50
1:A:701:THR:HG22	5:A:2740:HOH:O	2.11	0.50
1:B:311:ARG:HD3	5:B:2334:HOH:O	2.03	0.49
1:B:808:ASN:HD22	1:B:809:SER:H	1.61	0.49
1:B:687:VAL:HG21	1:B:704:THR:HG21	1.93	0.49
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.95	0.48
1:A:512:MET:HG3	5:A:2596:HOH:O	2.14	0.48
1:A:282:ALA:O	1:A:283:LYS:HB2	2.14	0.48
1:B:682:HIS:HE1	5:B:2611:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:CG2	5:B:2860:HOH:O	2.46	0.48
1:A:660:MET:HE2	5:A:2434:HOH:O	1.90	0.48
1:B:804:GLY:HA3	1:B:824:LYS:O	2.13	0.48
1:B:529:GLN:HG3	1:B:776:TRP:CE3	2.49	0.47
1:A:587:LYS:NZ	5:A:2645:HOH:O	2.48	0.47
1:B:230:ARG:HG3	5:B:2245:HOH:O	2.15	0.47
1:B:65:VAL:HG11	1:B:71:VAL:CG2	2.45	0.47
1:B:753:THR:HG23	5:B:2718:HOH:O	2.14	0.47
1:A:443:ILE:CD1	5:A:2492:HOH:O	2.43	0.47
1:B:398:GLU:O	1:B:454:ARG:NH2	2.45	0.47
1:A:676:LEU:HD23	1:A:760:VAL:HG21	1.97	0.46
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.50	0.46
1:A:464:PHE:HB3	1:A:484:MET:HE1	1.97	0.46
1:A:571:SER:OG	1:A:587:LYS:HG3	2.16	0.46
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.49	0.46
1:A:159:LYS:HD3	1:A:189:TYR:CZ	2.51	0.45
1:B:377:ALA:HA	1:B:405:ILE:HG21	1.98	0.45
1:B:804:GLY:O	1:B:823:LEU:HA	2.15	0.45
1:A:144:LEU:HD22	1:A:165:ALA:CB	2.47	0.45
1:B:280:LEU:HD21	1:B:286:LYS:HB2	1.98	0.45
1:B:396:HIS:HB2	5:B:2374:HOH:O	2.15	0.45
1:B:379:LYS:HG2	1:B:660:MET:HE1	1.98	0.45
1:A:237:LYS:HE3	1:A:237:LYS:CA	2.44	0.45
1:A:609:LYS:CE	1:A:796:ASN:HD21	2.29	0.45
1:A:704:THR:HG23	5:A:2741:HOH:O	2.17	0.45
1:A:605:ASP:OD1	1:A:608:ARG:HD3	2.17	0.44
1:B:349:TYR:HH	1:B:494:ILE:HD11	1.83	0.44
1:B:336:ASP:H	1:B:352:ASN:HD22	1.63	0.44
1:A:609:LYS:NZ	1:A:796:ASN:HD21	2.16	0.43
1:A:220:LEU:HD13	1:A:222:ARG:NH1	2.33	0.43
1:A:373:GLU:HG3	5:A:2429:HOH:O	2.18	0.43
1:A:577:ARG:CD	1:A:652:HIS:HB3	2.48	0.43
1:B:846:LYS:HD2	5:B:2810:HOH:O	2.18	0.43
1:A:418:GLU:OE2	1:A:421:ASP:OD2	2.37	0.43
1:A:848:VAL:HG21	1:A:877:LEU:HD13	2.00	0.43
1:B:526:ASP:O	1:B:534:GLY:HA3	2.18	0.43
1:B:609:LYS:NZ	1:B:796:ASN:HD21	2.17	0.43
1:B:178:HIS:HD2	1:B:179:THR:O	2.01	0.43
1:B:339:ALA:HB1	1:B:347:ARG:HD2	2.01	0.43
1:A:336:ASP:H	1:A:352:ASN:HD22	1.65	0.43
1:A:803:VAL:O	1:A:894:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD11	1:A:316:LEU:HD21	2.00	0.43
1:A:577:ARG:HG3	1:A:578:SER:N	2.34	0.42
1:A:222:ARG:CZ	5:A:2222:HOH:O	2.65	0.42
1:A:895:THR:HG23	5:A:2951:HOH:O	2.19	0.42
1:B:170:ASP:OD2	1:B:230:ARG:HD3	2.20	0.42
1:A:140:PHE:HB3	1:A:219:VAL:HA	2.02	0.42
1:A:337:VAL:CG1	1:A:491:LEU:CD2	2.98	0.42
1:B:846:LYS:HE2	1:B:847:PRO:CD	2.35	0.42
1:B:465:HIS:HD2	5:B:2477:HOH:O	2.02	0.42
1:B:824:LYS:HG3	5:B:2828:HOH:O	2.19	0.42
1:A:139:ASP:HA	1:A:169:HIS:O	2.19	0.42
1:A:237:LYS:HE2	5:A:2376:HOH:O	2.20	0.42
1:A:193:PRO:O	1:A:421:ASP:HB2	2.19	0.41
1:B:704:THR:CG2	5:B:2668:HOH:O	2.66	0.41
1:B:827:SER:HB3	5:B:2798:HOH:O	2.19	0.41
1:B:885:ARG:HD3	5:B:2808:HOH:O	2.20	0.41
1:B:311:ARG:HD2	1:B:407:ASP:HB3	2.02	0.41
1:A:137:TYR:HB2	1:A:222:ARG:HB2	2.03	0.41
1:A:465:HIS:HD2	5:A:2514:HOH:O	2.04	0.40
1:A:877:LEU:HG	1:A:880:SER:O	2.21	0.40
1:A:272:LYS:HE3	1:A:294:GLY:O	2.22	0.40
1:A:273:PRO:HG3	5:B:2061:HOH:O	2.22	0.40
1:A:675:PRO:HA	1:A:692:GLN:HB2	2.03	0.40

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)
5:A:2020:HOH:O	5:B:2658:HOH:O[1_655]	2.00	0.20

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	856/1032 (83%)	838 (98%)	16 (2%)	2 (0%)	44	32
1	B	856/1032 (83%)	833 (97%)	21 (2%)	2 (0%)	44	32
All	All	1712/2064 (83%)	1671 (98%)	37 (2%)	4 (0%)	44	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	202	ILE
1	B	202	ILE
1	B	205	ALA

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	702/834 (84%)	679 (97%)	23 (3%)	33	18
1	B	702/834 (84%)	677 (96%)	25 (4%)	30	15
All	All	1404/1668 (84%)	1356 (97%)	48 (3%)	32	16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	144	LEU
1	A	211	GLN
1	A	231	SER
1	A	237	LYS
1	A	283	LYS
1	A	356	LEU
1	A	428	ASN
1	A	430	GLU
1	A	469	ASP
1	A	577	ARG
1	A	608	ARG

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Mol	Chain	Res	Type
1	A	648	TRP
1	A	652	HIS
1	A	660	MET
1	A	701	THR
1	A	704	THR
1	A	783	TYR
1	A	806	THR
1	A	846	LYS
1	A	869	THR
1	A	877	LEU
1	A	895	THR
1	B	44	VAL
1	B	79	SER
1	B	85	SER
1	B	99	LYS
1	B	143	VAL
1	B	144	LEU
1	B	211	GLN
1	B	230	ARG
1	B	231	SER
1	B	236	GLN
1	B	247	LEU
1	B	323	THR
1	B	337	VAL
1	B	356	LEU
1	B	608	ARG
1	B	632	SER
1	B	634	ASN
1	B	648	TRP
1	B	652	HIS
1	B	701	THR
1	B	704	THR
1	B	808	ASN
1	B	830	ARG
1	B	877	LEU
1	B	895	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	796	ASN
1	A	808	ASN
1	B	50	ASN
1	B	128	ASN
1	B	176	GLN
1	B	178	HIS
1	B	194	ASN
1	B	212	ASN
1	B	299	ASN
1	B	348	GLN
1	B	352	ASN
1	B	465	HIS
1	B	614	GLN
1	B	682	HIS
1	B	796	ASN
1	B	808	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1902	-	5,5,5	0.77	0	5,5,5	0.73	0
4	GOL	B	1904	-	5,5,5	0.80	0	5,5,5	1.83	2 (40%)
3	GCS	A	1902	-	12,12,12	1.05	1 (8%)	16,17,17	1.98	4 (25%)
4	GOL	A	1903	-	5,5,5	0.74	0	5,5,5	0.29	0
3	GCS	B	1903	-	12,12,12	1.31	1 (8%)	16,17,17	2.07	2 (12%)

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
4	GOL	B	1902	-	-	0/4/4/4	-
4	GOL	B	1904	-	-	3/4/4/4	-
3	GCS	A	1902	-	-	0/2/22/22	0/1/1/1
4	GOL	A	1903	-	-	0/4/4/4	-
3	GCS	B	1903	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1903	GCS	C1-C2	3.28	1.56	1.52
3	A	1902	GCS	C1-C2	2.01	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1903	GCS	O1-C1-O5	-6.01	92.33	110.38
3	B	1903	GCS	O5-C1-C2	5.10	115.47	109.51
3	A	1902	GCS	O5-C1-C2	4.23	114.44	109.51
3	A	1902	GCS	O1-C1-O5	-4.22	97.72	110.38
3	A	1902	GCS	O5-C5-C4	-3.02	104.20	109.69
4	B	1904	GOL	C3-C2-C1	2.38	120.98	111.70
3	A	1902	GCS	O1-C1-C2	-2.35	104.11	108.96
4	B	1904	GOL	O2-C2-C3	2.09	118.32	109.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1904	GOL	O1-C1-C2-C3
4	B	1904	GOL	O1-C1-C2-O2
4	B	1904	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1902	GCS	1	0
3	B	1903	GCS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	858/1032 (83%)	-0.59	3 (0%) 90 92	11, 19, 28, 42	1 (0%)
1	B	858/1032 (83%)	-0.56	0 100 100	11, 19, 29, 43	0
All	All	1716/2064 (83%)	-0.57	3 (0%) 92 93	11, 19, 28, 43	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	2.5
1	A	45	GLY	2.2
1	A	48	ALA	2.1

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 monosaccharides 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(Å ²)	Q<0.9
2	CD	A	1899	1/1	0.64	0.45	237,237,237,237	0
2	CD	A	1901	1/1	0.83	0.28	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	1903	6/6	0.93	0.07	21,22,24,25	0
4	GOL	B	1902	6/6	0.93	0.12	20,24,24,25	0
4	GOL	B	1904	6/6	0.94	0.07	20,20,23,24	0
2	CD	B	1901	1/1	0.95	0.24	76,76,76,76	0
3	GCS	B	1903	12/12	0.97	0.04	14,16,20,24	0
3	GCS	A	1902	12/12	0.97	0.04	16,18,20,25	0
2	CD	A	1900	1/1	0.99	0.15	37,37,37,37	0
2	CD	B	1899	1/1	1.00	0.01	18,18,18,18	0
2	CD	B	1900	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.