



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:32 AM GMT

PDB ID : 2XCR
Title : THE 3.5A CRYSTAL STRUCTURE OF THE CATALYTIC CORE (B'A' REGION) OF STAPHYLOCOCCUS AUREUS DNA GYRASE COMPLEXED WITH GSK299423 AND DNA
Authors : Bax, B.D.; Chan, P.F.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.W.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.F.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on : 2010-04-25
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

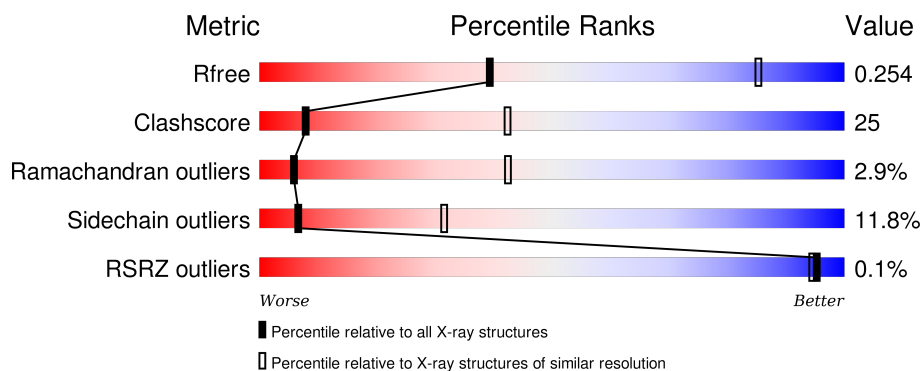
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

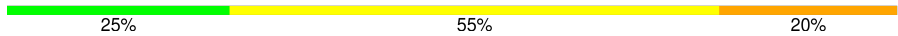
The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	726	
1	D	726	
1	S	726	
1	U	726	
2	E	20	

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Mol	Chain	Length	Quality of chain
2	F	20	
3	V	20	
3	W	20	

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
4	RXV	E	1021[A]	-	-	-	X
4	RXV	E	1021[B]	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 24495 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5689	3556	1018	1090	25			
1	D	719	Total	C	N	O	S	0	0	0
			5692	3556	1021	1090	25			
1	S	718	Total	C	N	O	S	0	0	0
			5694	3561	1022	1086	25			
1	U	717	Total	C	N	O	S	0	0	0
			5689	3558	1020	1086	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	EXPRESSION TAG	UNP Q99XG5
B	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
D	409	MET	-	EXPRESSION TAG	UNP Q99XG5
D	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
S	409	MET	-	EXPRESSION TAG	UNP Q99XG5
S	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
U	409	MET	-	EXPRESSION TAG	UNP Q99XG5
U	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5

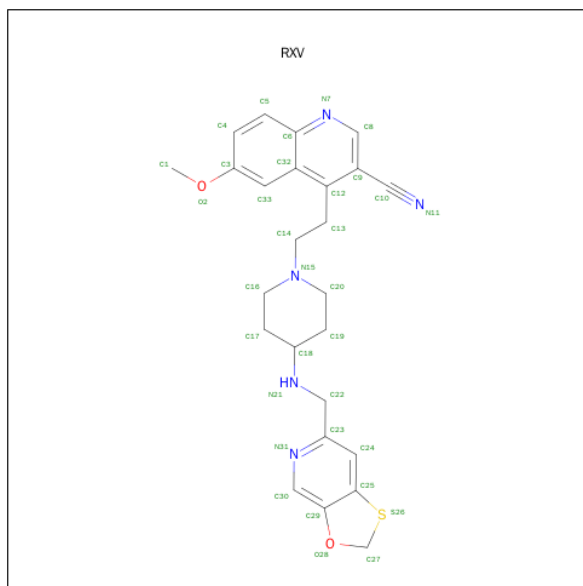
- Molecule 2 is a DNA chain called 5'-D(*5UA*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			
2	F	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			

- Molecule 3 is a DNA chain called 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*C P*CP*TP*AP*CP*GP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
3	W	18	Total	C	N	O	P	0	0	0
			369	173	70	108	18			

- Molecule 4 is 6-METHOXY-4-(2-{4-[(1,3]OXATHIOLO[5,4-C]PYRIDIN-6-YLMETHYL) AMINO]PIPERIDIN-1-YL}ETHYL)QUINOLINE-3-CARBONITRILE (three-letter code: RXV) (formula: C₂₅H₂₇N₅O₂S).

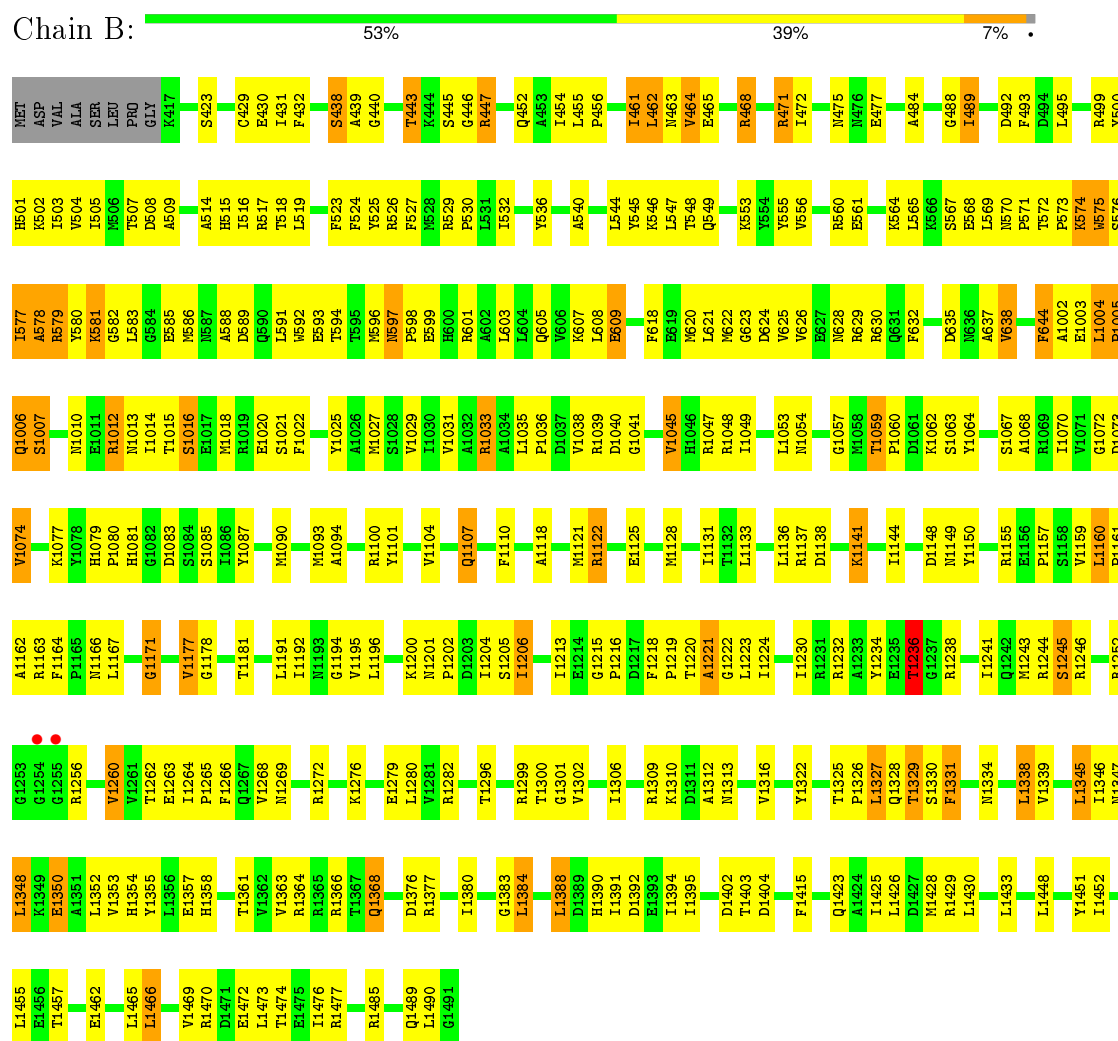


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	1
			66	50	10	4	2		
4	W	1	Total	C	N	O	S	0	1
			66	50	10	4	2		

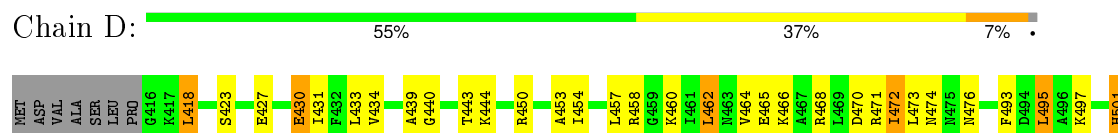
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A



L1468	D1376	L1292	I1192	V1104	E1020	S576	K502
V1469	I1380	R1293	V1195	D1105	S1021	I577	I503
R1470	I1384	R1294	V1196	D1107	F1022	A578	I504
L1473	L1385	E1295	S1197	A1119	D1024	Y580	I505
T1474	L1386	L1296	L1198	A1120	H1027	K581	K506
E1475	I1387	S1297	I1206	H1121	H1031	S582	T507
I1476	L1388	L1298	I1206	R1122	V1031	S583	D508
R1477	L1389	V1302	I1213	F1123	A1032	D590	A509
G1481	H1390	I1306	I1224	M1128	R1033	S591	V511
R1485	D1392	D1307	L1225	L1035	A1034	S592	A514
G1491	R1399	V1308	G1226	I1131	L1036	S593	S515
	L1411	R1309	K1227	T1132	P1036	T594	S516
	F1415	K1310	E1229	E1133	D1040	T595	S517
	L1416	K1311	G1230	E1134	L1042	L604	S518
	S1418	A1312	I1231	L1135	L1043	E609	F523
	E1419	H1313	R1232	L1136	P1044	E610	F524
	K1420	K1314	A1233	R1137	P1045	T617	S525
	Q1421	I1315	R1234	L1138	H1046	F618	F528
	A1422	L1316	E1235	I1139	R1047	E619	L531
	L1426	Y1322	G1239	D1144	L1048	L621	L532
	L1430	L1327	M1243	D1145	L1049	L622	P530
	R1431	Q1328	R1244	D1151	N1054	G623	L531
	L1432	T1329	R1245	D1152	Q1056	V625	
	T1434	S1330	V1248	P1157	Q1057	N628	Y536
	R1438	I1336	I1249	S1158	H1058	R629	Y537
	I1441	L1342	Q1257	V1159	T1059	F632	Y538
	E1444	R1343	R1258	L1160	P1060	I633	A540
	V1445	K1344	I1259	P1161	Y1064	F633	Q541
	N1446	L1347	I1264	A1162	N636	N636	L544
	E1447	L1348	F1266	F1164	S1067	A637	Y545
	L1448	K1349	V1268	N1165	A1068	V638	S546
	L1449	L1352	I1269	L1167	R1069	A640	L547
	N1450	V1353	K1270	L1168	V1074	N641	Q549
	Y1451	L1356	A1271	G1171	H1079	A1002	Y555
	L1455	Q1359	N1272	I1175	P1080	E1003	Y556
	E1456	K1360	I1274	I1176	H1081	L1004	Y557
	T1457	T1361	I1277	A1177	P1082	P1005	L562
	I1458	V1362	E1278	V1177	D1083	Q1006	D563
	E1459	R1364	L1280	G1178	S1084	S1007	K564
	L1464	L1365	V1281	N1179	S1085	R1008	L565
	L1465	Q1369	R1282	A1180	I1086	I1009	K566
	L1466	L1373	I1289	I1183	V1091	N1010	S567
	Q1467	T1373		P1184	R1092	E1011	E568
				E1279	M1093	R1012	L569
				L1286	M1094	P570	K570
				V1281	Q1095	I1014	P571
				R1282	Y1101	T1015	T572
					M1018	K574	P573
					R1019	K575	K574
							K575

• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain S: 51% 40% 8%

MET	I482	B560	V638	M1075	P1165	E1251	R1252
ASP	F485	L566	L642	G1076	L1168	R1256	R1257
VAL	F486	S567	D643	K1077	A1169	Q1257	Q1258
ALA	F493	E568	F644	P1080	S1173	R1261	R1262
SER	L494	L569	A1002	H1081	G1174	T1261	T1262
LEU	L495	N570	E1003	S1085	I1175	E1263	E1264
PRO	R499	P571	L1004	I1086	A1176	P1265	P1266
GLY	Y500	T572	Q1006	Y1087	M1179	K1270	K1271
ARG	K502	F573	S1007	E1088	A1180	M1273	M1274
ASN	S503	K574	R1008	I1089	T1181	I1277	I1278
ASP	Y504	S576	I1009	V1091	N1182	A1278	A1279
GLN	I505	A578	R1012	M1013	I1183	E1279	E1280
THR	M506	R579	I1014	M1093	P1184	I1274	I1275
LYS	T507	Y580	T1015	Y1099	H1186	I1277	I1278
GLN	D508	K581	R1019	R1100	L1188	I1279	I1280
ASP	V511	S582	D1024	Y1101	T1189	E1281	E1282
THR	H515	L583	Y1025	Q1107	E1190	R1283	R1284
LEU	I516	E585	M1027	F1110	L1191	G1288	G1289
GLN	T518	Q590	A1026	G1111	I1192	I1289	I1290
ASP	L519	L591	S1028	S1112	S1199		
THR	L520	M592	Y1029	D1113	I1204		
GLN	T522	T594	I1030	E1114	E1208		
GLN	F523	T595	Y1031	G1115	R1293		
GLN	F524	N596	A1032	D1116	D1294		
GLN	Y525	R597	R1033	A1120	E1295		
GLN	R526	P598	A1034	A1201	M1210		
GLN	R529	E599	L1035	F1123	I1213		
GLN	L531	R601	P1036	T1124	L1298		
GLN	I532	A602	D1040	E1125	P1219		
GLN	Y536	L603	G1041	I1131	T1220		
GLN	Y537	L604	L1042	T1132	A1221		
GLN	Y538	Q605	V1045	L1133	G1222		
GLN	A540	R606	H1046	E1134	V1304		
GLN	Q541	L608	R1047	L1135	I1224		
GLN	L544	T617	L1050	R1136	L1225		
GLN	Y545	F618	G1057	L1137	G1226		
GLN	K546		M1058	D1138	K1227		
GLN	L547		T1141	T1142	I1230		
GLN	G550		T1143	I1144	A1233		
GLN	K551		S1063	Y1150	R1238		
GLN	Q552		S1067	E1154	G1239		
GLN	K553		A1068	R1244	L1321		
GLN	Y554		R1069	S1245	Y1322		
GLN	L557		T1070	E1156	K1323		
GLN	N558		V1071	A1162	Q1324		
GLN	D559		G1072	I1163	T1325		
			D1073	A1164	P1326		
			V1074		L1327		

Chain F: 




- Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

Chain V: 



- Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

Chain W: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.26Å 165.38Å 308.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.99 – 3.50 23.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.5 (23.99-3.50) 84.6 (23.99-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.258 0.191 , 0.254	Depositor DCC
R_{free} test set	2505 reflections (4.19%)	DCC
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	1.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 52.0	EDS
Estimated twinning fraction	None for NONE	Xtriage
Reported twinning fraction	None for NONE	Depositor
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 62227 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24495	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5UA, RXV

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	B	0.40	0/5772	0.63	0/7784
1	D	0.42	0/5775	0.63	0/7792
1	S	0.43	0/5777	0.66	1/7789 (0.0%)
1	U	0.42	0/5772	0.64	0/7785
2	E	0.85	0/435	1.86	10/669 (1.5%)
2	F	0.84	0/435	1.70	9/669 (1.3%)
3	V	0.90	0/459	1.84	14/706 (2.0%)
3	W	0.94	1/413 (0.2%)	1.84	13/635 (2.0%)
All	All	0.47	1/24838 (0.0%)	0.80	47/33829 (0.1%)

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	S	0	1
1	U	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	14	DT	C1'-N1	5.28	1.56	1.49

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O4'-C1'-N9	-15.90	96.87	108.00
3	W	14	DT	O4'-C1'-N1	11.09	115.76	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	16	DC	O4'-C4'-C3'	-10.56	99.66	106.00
3	V	16	DC	O4'-C4'-C3'	-10.33	99.80	106.00
2	E	10	DG	O4'-C1'-N9	10.29	115.20	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	572	THR	Peptide
1	U	572	THR	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	B	5689	0	5712	310	0
1	D	5692	0	5704	271	0
1	S	5694	0	5731	296	0
1	U	5689	0	5721	296	0
2	E	410	0	225	24	0
2	F	410	0	225	19	0
3	V	410	0	224	26	0
3	W	369	0	201	16	0
4	E	66	0	54	9	0
4	W	66	0	54	12	0
All	All	24495	0	23851	1204	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 25.

The worst 5 of 1204 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:D:439:ALA:HB1	1:D:583:LEU:HB2	1.27	1.14
1:B:468:ARG:HG3	1:B:468:ARG:HH21	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HG2	1:B:471:ARG:HH11	0.92	1.08
1:S:1005:PRO:HA	1:S:1006:GLN:CB	1.85	1.07
1:S:1003:GLU:HA	1:S:1004:LEU:HB3	1.12	1.05

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	B	716/726 (99%)	596 (83%)	102 (14%)	18 (2%)	7	46
1	D	717/726 (99%)	599 (84%)	97 (14%)	21 (3%)	6	42
1	S	716/726 (99%)	598 (84%)	95 (13%)	23 (3%)	5	40
1	U	715/726 (98%)	607 (85%)	86 (12%)	22 (3%)	5	41
All	All	2864/2904 (99%)	2400 (84%)	380 (13%)	84 (3%)	6	42

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	ARG
1	B	644	PHE
1	B	1004	LEU
1	B	1005	PRO
1	B	1007	SER

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	B	611/624 (98%)	543 (89%)	68 (11%)	8	35
1	D	610/624 (98%)	541 (89%)	69 (11%)	7	34
1	S	611/624 (98%)	531 (87%)	80 (13%)	5	27
1	U	611/624 (98%)	539 (88%)	72 (12%)	6	31
All	All	2443/2496 (98%)	2154 (88%)	289 (12%)	6	31

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1429	ARG
1	S	600	HIS
1	U	1262	THR
1	D	1468	LEU
1	S	464	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1201	ASN
1	S	597	ASN
1	U	1313	ASN
1	D	1359	GLN
1	S	474	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	5UA	E	1	-	16,23,23	2.70	2 (12%)	17,33,33	4.76	3 (17%)
2	5UA	F	1	-	16,23,23	2.68	2 (12%)	17,33,33	4.92	4 (23%)

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	5UA	E	1	-	-	0/3/21/21	0/3/3/3
2	5UA	F	1	-	-	0/3/21/21	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	5UA	C2-N1	6.53	1.46	1.33
2	F	1	5UA	C2-N1	6.60	1.46	1.33
2	F	1	5UA	C2-N3	7.97	1.46	1.32
2	E	1	5UA	C2-N3	8.09	1.46	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	5UA	N3-C2-N1	-19.45	114.00	128.89
2	E	1	5UA	N3-C2-N1	-18.88	114.44	128.89
2	F	1	5UA	C4-C5-N7	-3.93	105.86	109.48
2	E	1	5UA	C4-C5-N7	-3.91	105.88	109.48
2	F	1	5UA	O4'-C1'-N9	2.11	111.37	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	5UA	1	0
2	F	1	5UA	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are 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	$\# Z > 2$
4	RXV	E	1021[A]	-	35,37,37	2.45	4 (11%)	40,51,51	2.52	14 (35%)
4	RXV	E	1021[B]	-	35,37,37	2.31	4 (11%)	40,51,51	1.46	10 (25%)
4	RXV	W	1020[A]	-	35,37,37	2.11	3 (8%)	40,51,51	1.46	6 (15%)
4	RXV	W	1020[B]	-	35,37,37	2.00	6 (17%)	40,51,51	1.56	8 (20%)

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	RXV	E	1021[A]	-	-	0/14/30/30	0/4/5/5
4	RXV	E	1021[B]	-	-	0/14/30/30	0/4/5/5
4	RXV	W	1020[A]	-	-	0/14/30/30	0/4/5/5
4	RXV	W	1020[B]	-	-	0/14/30/30	0/4/5/5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1021[A]	RXV	C9-C10	-11.92	1.26	1.44
4	E	1021[B]	RXV	C9-C10	-10.23	1.29	1.44
4	W	1020[B]	RXV	C9-C10	-9.80	1.29	1.44
4	W	1020[A]	RXV	C9-C10	-9.58	1.30	1.44
4	E	1021[B]	RXV	C8-C9	-7.03	1.31	1.39

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1021[A]	RXV	C9-C10-N11	-5.67	167.99	177.82
4	E	1021[A]	RXV	C4-C5-C6	-5.47	114.95	120.88
4	E	1021[A]	RXV	C9-C8-N7	-5.11	116.65	124.30
4	E	1021[A]	RXV	C32-C6-N7	-4.91	117.65	122.88
4	W	1020[B]	RXV	C9-C10-N11	-4.70	169.66	177.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1021[A]	RXV	5	0
4	E	1021[B]	RXV	4	0
4	W	1020[A]	RXV	7	0
4	W	1020[B]	RXV	5	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	B	718/726 (98%)	-0.64	2 (0%) 94 91	78, 126, 188, 218	0
1	D	719/726 (99%)	-0.65	0 100 100	63, 111, 184, 221	0
1	S	718/726 (98%)	-0.70	0 100 100	64, 116, 171, 203	0
1	U	717/726 (98%)	-0.69	1 (0%) 95 94	64, 123, 171, 222	0
2	E	19/20 (95%)	-0.46	0 100 100	103, 115, 196, 218	0
2	F	19/20 (95%)	-0.52	0 100 100	97, 112, 188, 193	0
3	V	20/20 (100%)	-0.30	0 100 100	91, 116, 209, 268	0
3	W	18/20 (90%)	-0.42	0 100 100	100, 119, 173, 202	0
All	All	2948/2984 (98%)	-0.66	3 (0%) 95 94	63, 120, 181, 268	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1254	GLY	2.6
1	B	1255	GLY	2.4
1	U	1254	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	5UA	F	1	21/21	0.89	0.42	-	220,235,239,241	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	5UA	E	1	21/21	0.89	0.30	-	193,198,206,208	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	RXV	E	1021[B]	33/33	0.88	0.29	5.32	110,128,143,146	33
4	RXV	E	1021[A]	33/33	0.88	0.29	5.18	111,129,144,148	33
4	RXV	W	1020[A]	33/33	0.94	0.20	1.63	100,108,111,111	33
4	RXV	W	1020[B]	33/33	0.94	0.20	1.50	100,108,110,110	33

6.5 Other polymers [i](#)

There are no such residues in this entry.