



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 8, 2018 – 11:38 PM EST

PDB ID : 2WIN
Title : C3 convertase (C3bBb) stabilized by SCIN
Authors : Wu, J.; Janssen, B.J.; Gros, P.
Deposited on : 2009-05-13
Resolution : 3.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

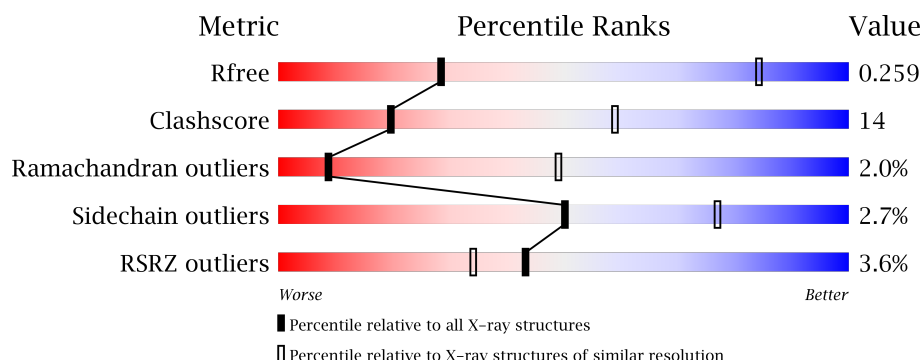
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.






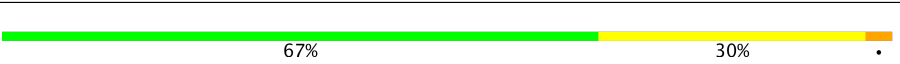
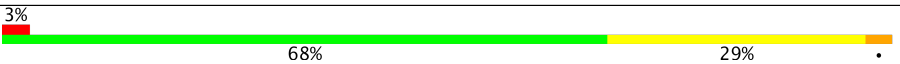

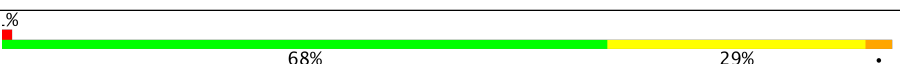
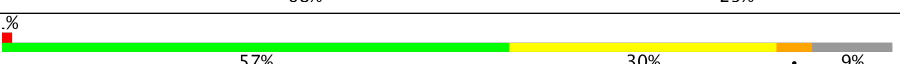
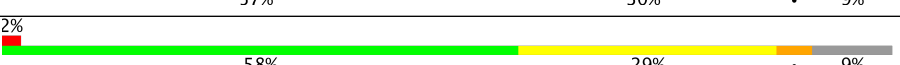
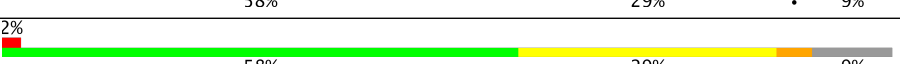
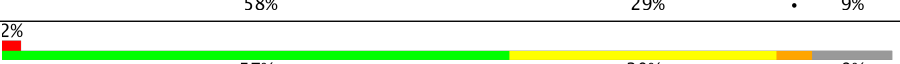
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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	A	645	<div> <div>2%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	C	645	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	E	645	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	G	645	<div> <div>9%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>
2	B	915	<div> <div>3%</div> <div>69%</div> <div>26%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	915	
2	F	915	
2	H	915	
3	I	507	
3	J	507	
3	K	507	
3	L	507	
4	M	92	
4	N	92	
4	P	92	
4	Q	92	

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
5	NDG	B	2642	X	-	-	-
5	NDG	C	1646	X	-	-	-
5	NDG	D	2642	X	-	-	-
5	NDG	E	1646	X	-	-	-
5	NDG	G	1646	X	-	-	-
5	NDG	H	2642	X	-	-	-
5	NDG	I	1743	X	-	-	-
5	NDG	I	1746	X	-	-	-
5	NDG	J	1743	X	-	-	-
5	NDG	K	1743	X	-	-	-
5	NDG	L	1743	X	-	-	-
5	NDG	L	1746	X	-	-	-
8	MAN	H	2644	X	-	-	-
8	MAN	H	2645	X	-	-	-
8	MAN	I	1745	X	-	-	-
8	MAN	J	1745	X	-	-	-
8	MAN	K	1745	X	-	-	-
8	MAN	K	1746	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MAN	K	1748	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

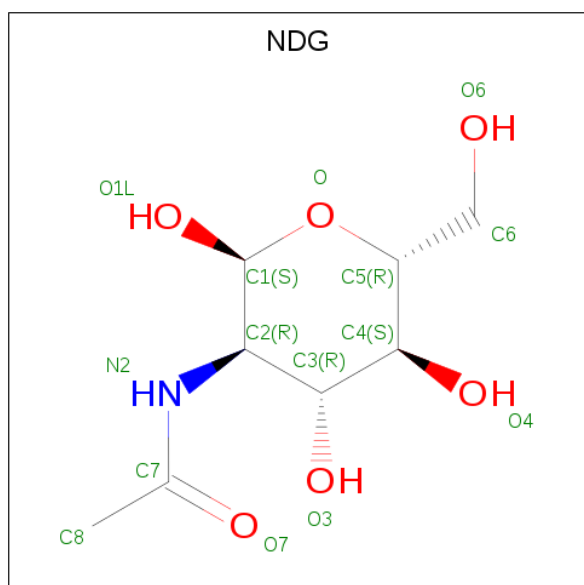
- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

- Molecule 5 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



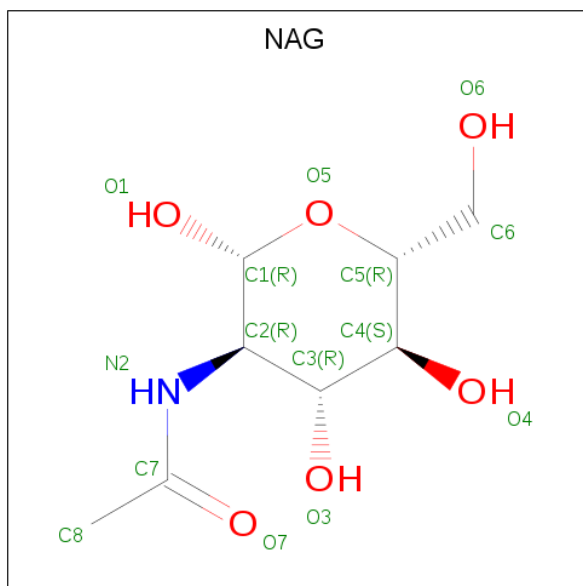
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



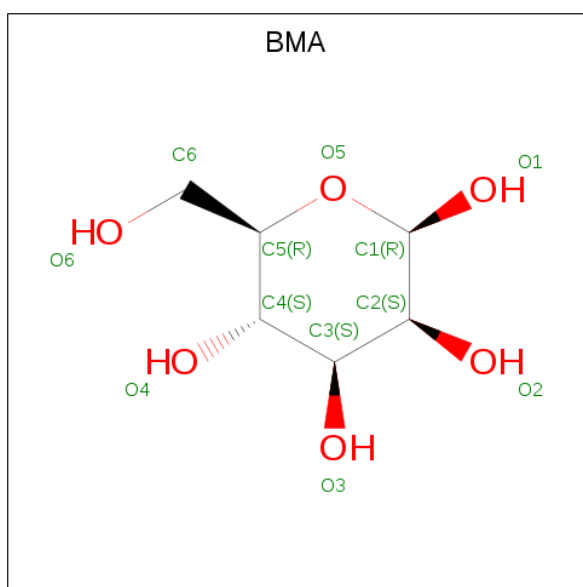
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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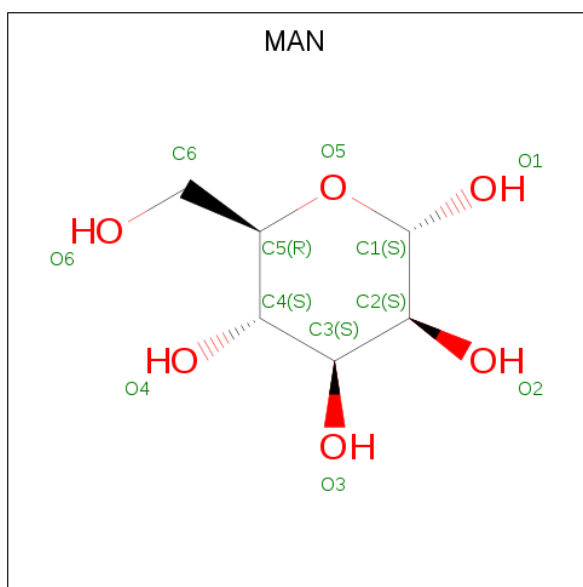
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	K	1	Total	C	O	0	0
			11	6	5		
7	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			11	6	5		
8	H	1	Total	C	O	0	0
			11	6	5		
8	H	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		
9	I	1	Total	Mg	0	0
			1	1		
9	L	1	Total	Mg	0	0
			1	1		
9	K	1	Total	Mg	0	0
			1	1		

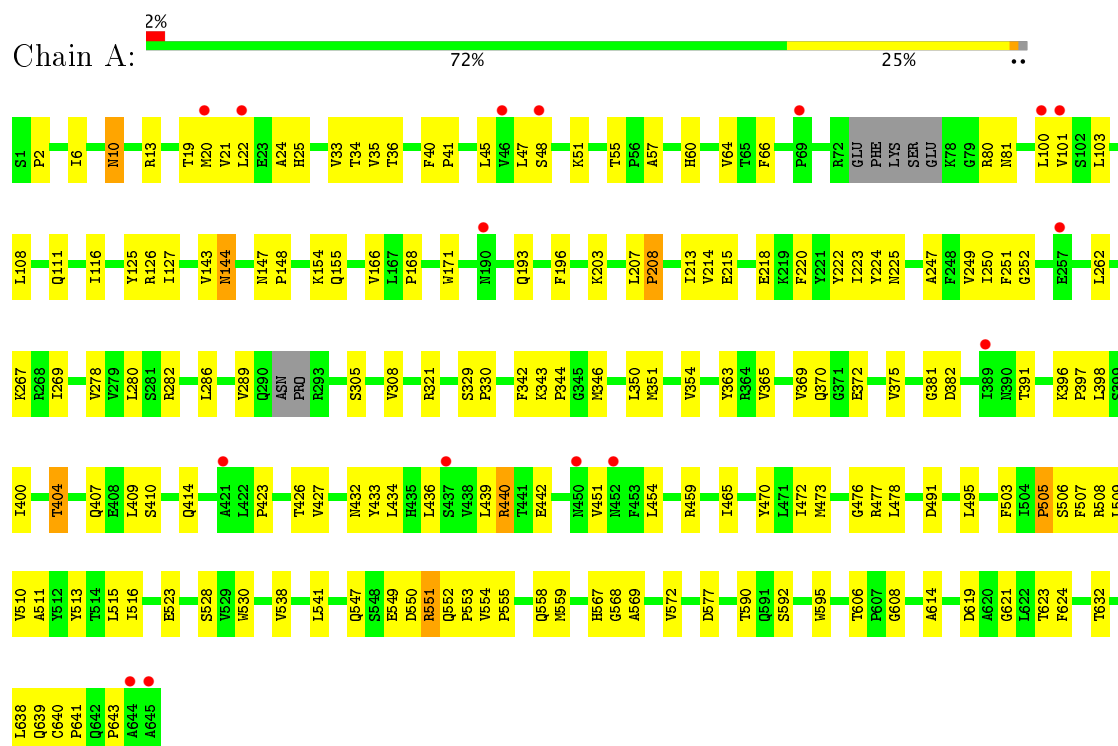
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total 1	O 1	0	0
10	I	2	Total 2	O 2	0	0
10	J	2	Total 2	O 2	0	0
10	K	2	Total 2	O 2	0	0
10	L	1	Total 1	O 1	0	0

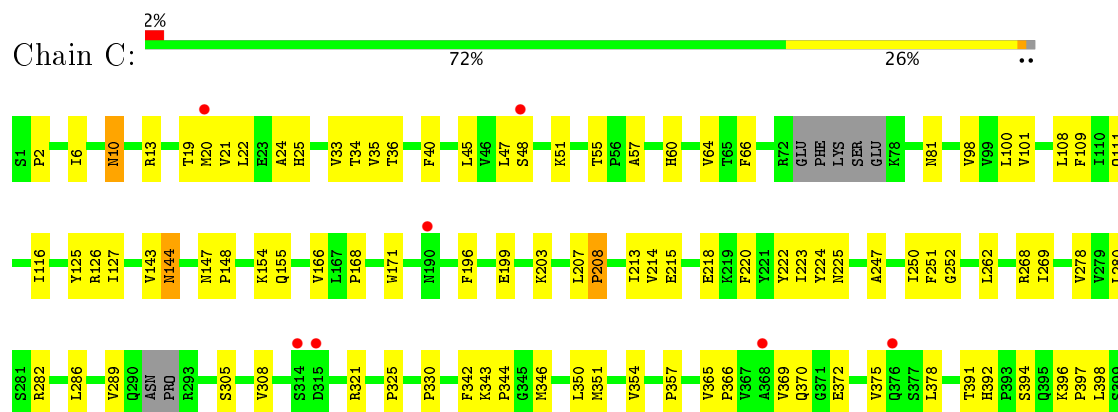
3 Residue-property plots

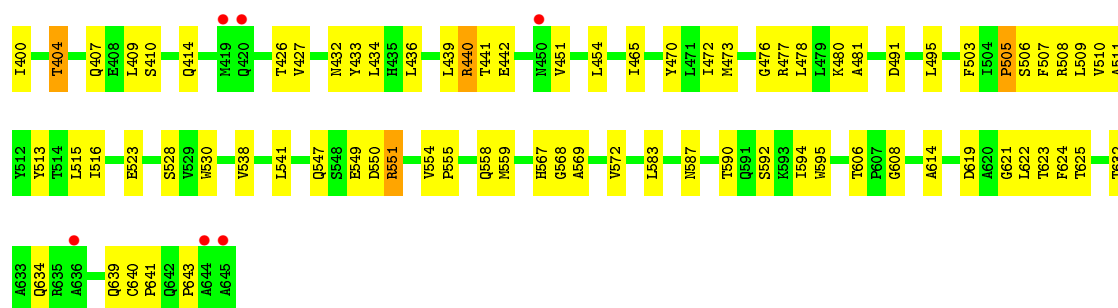
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: COMPLEMENT C3 BETA CHAIN

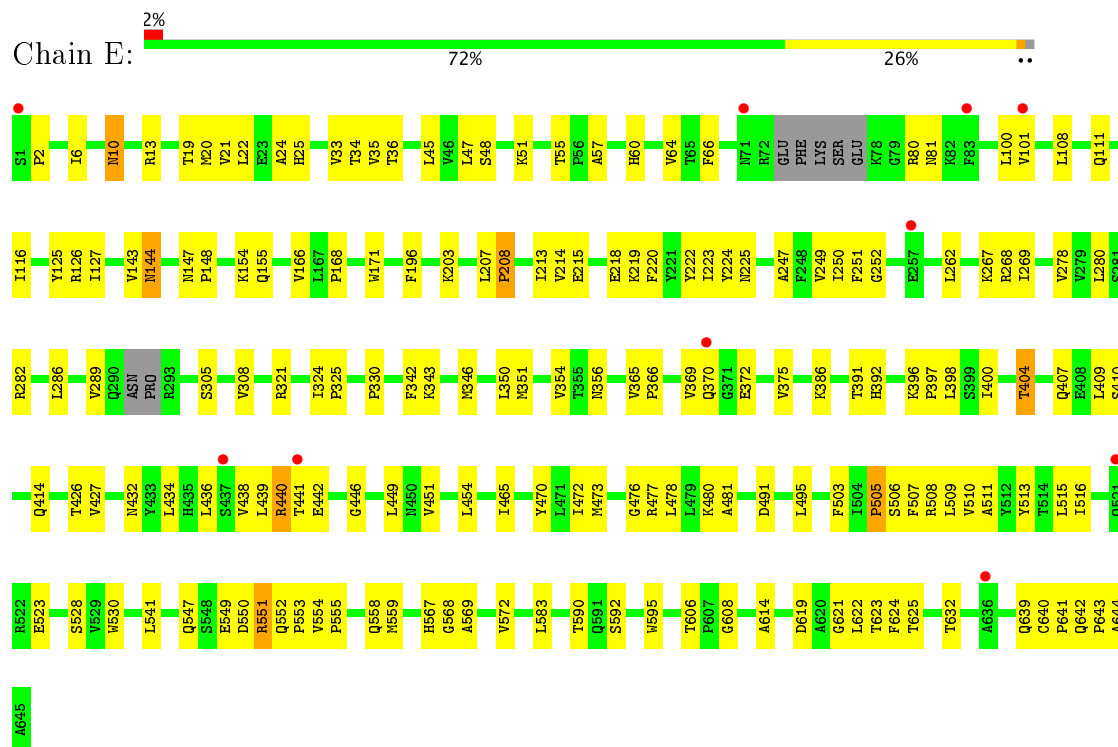


• Molecule 1: COMPLEMENT C3 BETA CHAIN

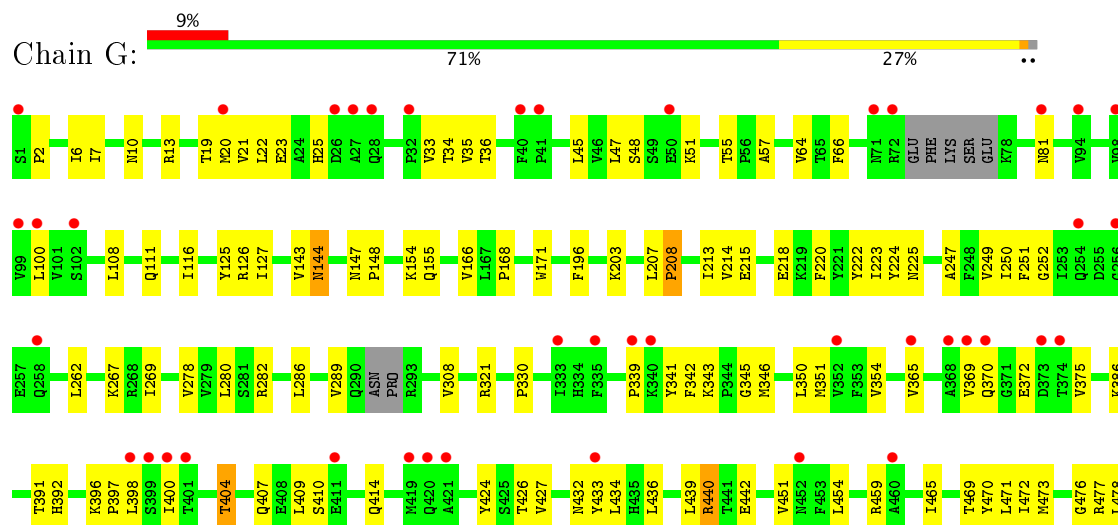


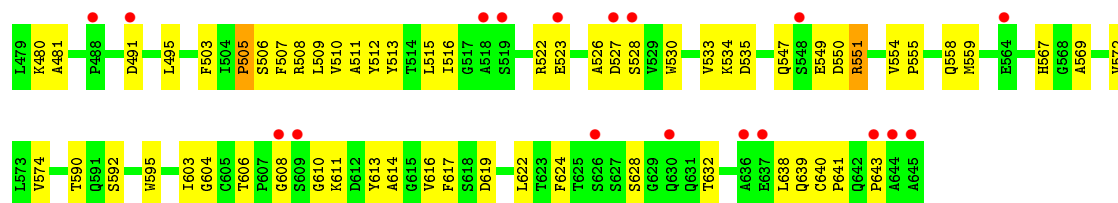


• Molecule 1: COMPLEMENT C3 BETA CHAIN

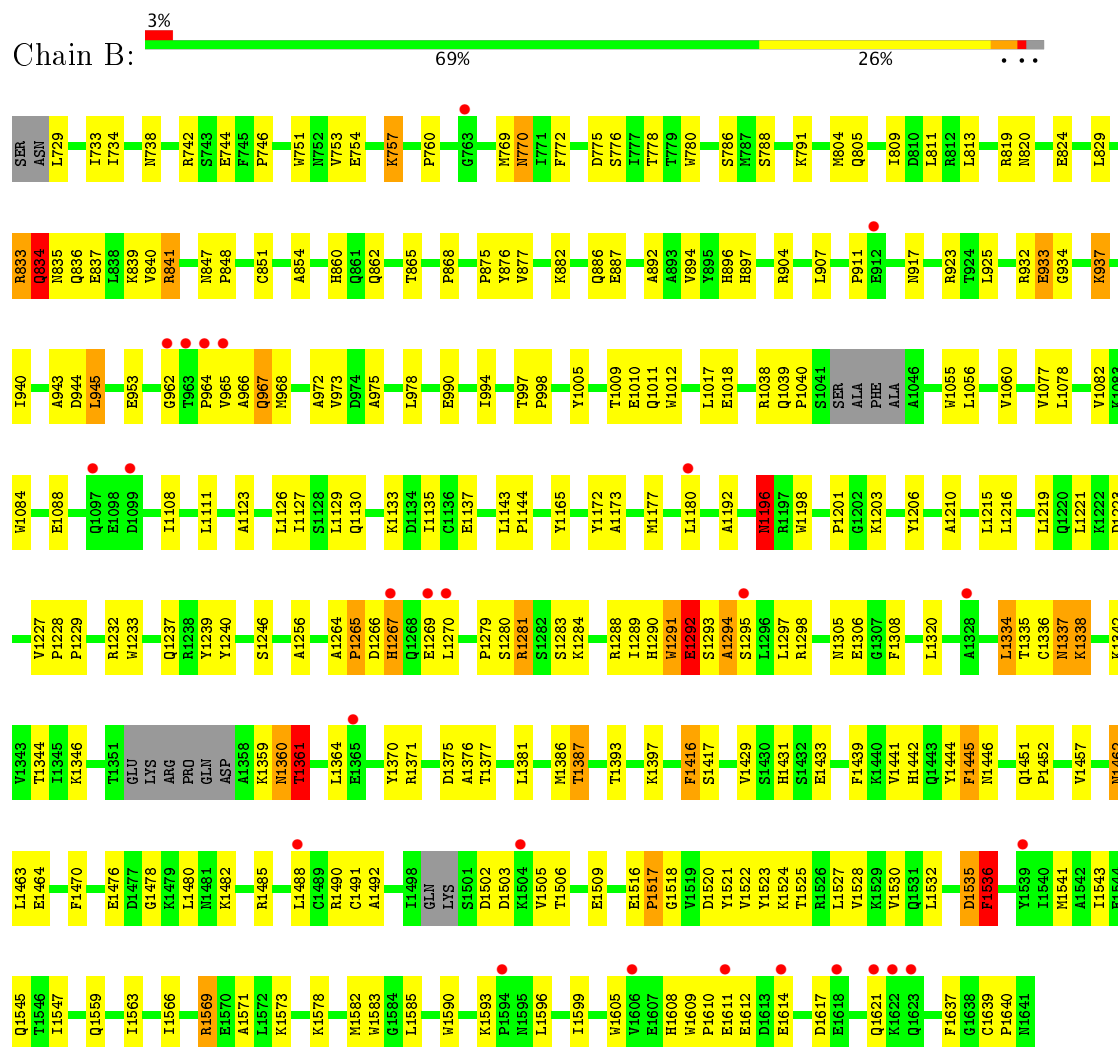


• Molecule 1: COMPLEMENT C3 BETA CHAIN

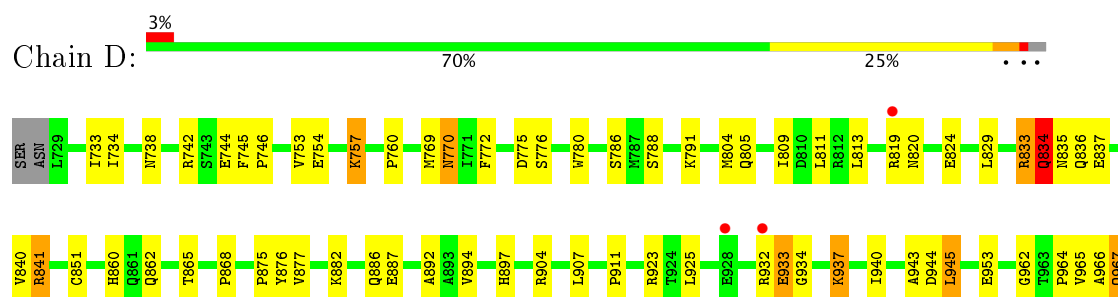




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

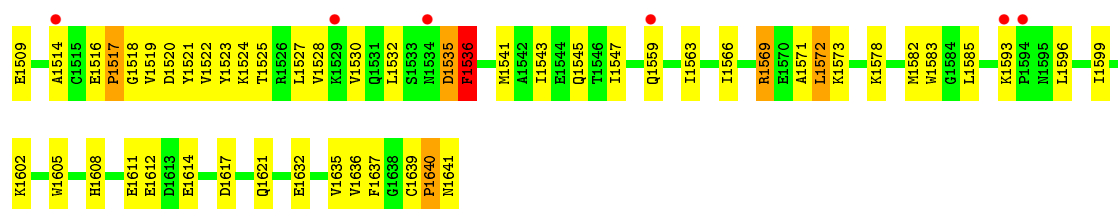


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

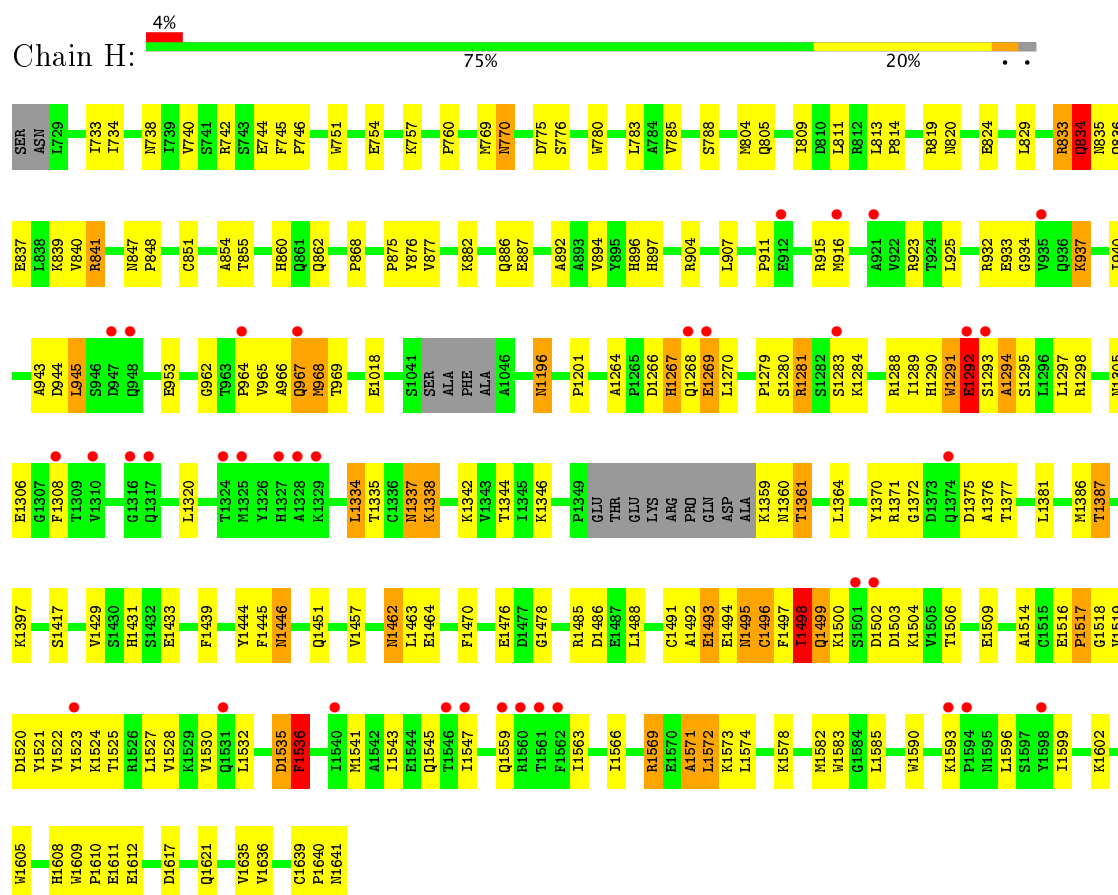




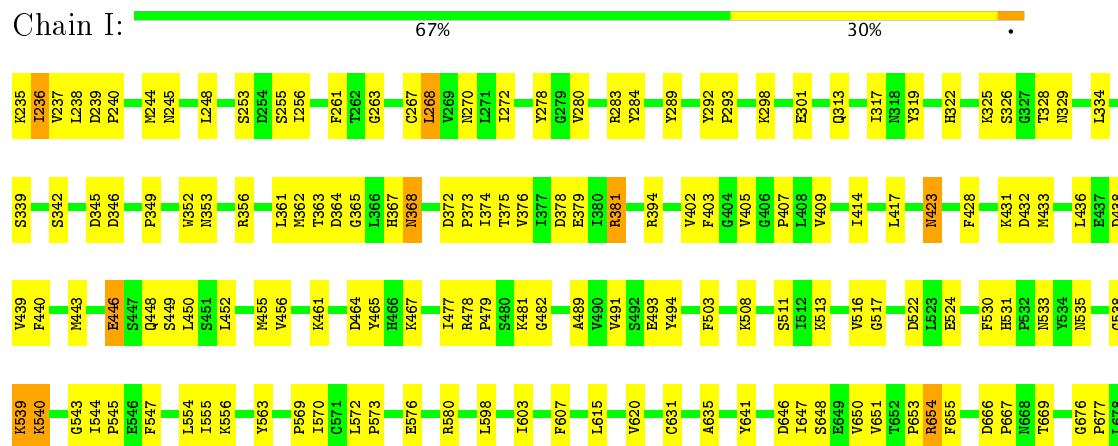
D1373	K1284	L1180	L1056	G962	V840	SER
D1375	R1288	K1181	V1060	T963	R841	ASN
A1376	I1289	P1183		P964		L729
T1377	H1290		I1073	V865	N847	I733
M1378	W1291	A1192	D1074	A868	P846	I734
	E1292	K1193	S1075	Q967		
L1381	S1293	D1194	Q1076	R968	A854	N738
	A1294	K1195	V1077	T955	T855	I739
M1386	S1295	N1196	L1078	E870	V740	V740
T1387	L1296	R1197	C1079	H860	S741	S741
	L1297	W1198		A872	Q861	R742
A1390	R1298	P1201	V1082	V973	Q862	S743
P1391	N1305	G1202	K1083	D874	E744	E744
	E1306	K1203	W1084	A975	F745	F745
K1397	G1307			P868	P746	P746
S1417	F1308	Y1206	E1088	L878	P875	V753
	K1315	A1210	D1093	G987	V876	E754
V1429	L1320	L1215	G1094	E990	K882	K757
H1430		L1216	I1108	I994	Q886	E758
H1431			L1111	T997	E987	P759
S1432	H1327	L1219	E1116	R998	A892	M769
E1433	A1328	K1329	K1117	T999	A893	N770
F1439	A1330	L1221	D1118	V1000	V894	
F1445	K1331	K1222	M1119	Y1005	H895	D775
M1446	L1334	D1223			H896	S776
	T1335	V1227	T1122		R897	
Q1451	C1336	P1228	A1123	T1009	R904	M780
V1457	N1337	P1229	L1126	Q1010	Q1011	
	K1338		S1128	W1012	L907	S786
M1462	K1342	R1232	E1128	L1017	P911	M787
L1463	V1343	W1233	L1129	E1018	E912	S788
E1464	T1344	K1237	Q1130	Q1038	R913	Q805
F1470	I1345	L1238	K1133	I1027	Y914	
Y1471	K1346	Y1239	D1134	R915	R915	L809
H1472		Y1240	I1135	Q1034	N916	D810
P1473	P1349	S1246	E1136	L1035		L811
	GLU		E1137		R923	R812
E1476	THR	A1266	L1143	Q1039	T924	L813
D1477	LVS		P1144	S1041	L925	
K1479	ARG	A1264	I1147	SER	R932	R819
	PRO	P1265	M1157	ALA	E933	N820
E1494	GLN	D1266		PHE	Q934	E821
N1495	ASP	Q1268	Y1165	ALA	R937	Q822
C1496	ALA	E1269	T1166	A1046	E924	V823
F1497	K1359	L1270	N1271	F1047		E924
L1498	N1360	L1270		V1048	Y940	L829
Q1499	T1361	M1271		A943	R833	
				D944	N835	
A1500	L1364	P1279	Y1172	K1049	L945	Q836
S1501	S1280	R1281	A1173	R1050		R837
D1502	Y1370	R1281	M1177	A1051		
	R1371	S1282		W1055		
T1506	C1372					



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

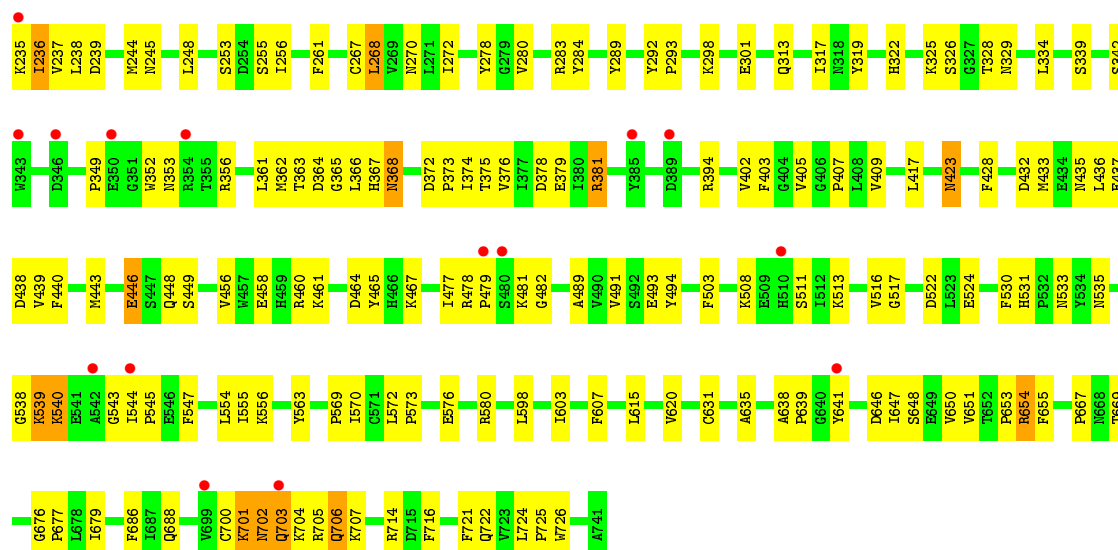


• Molecule 3: COMPLEMENT FACTOR B

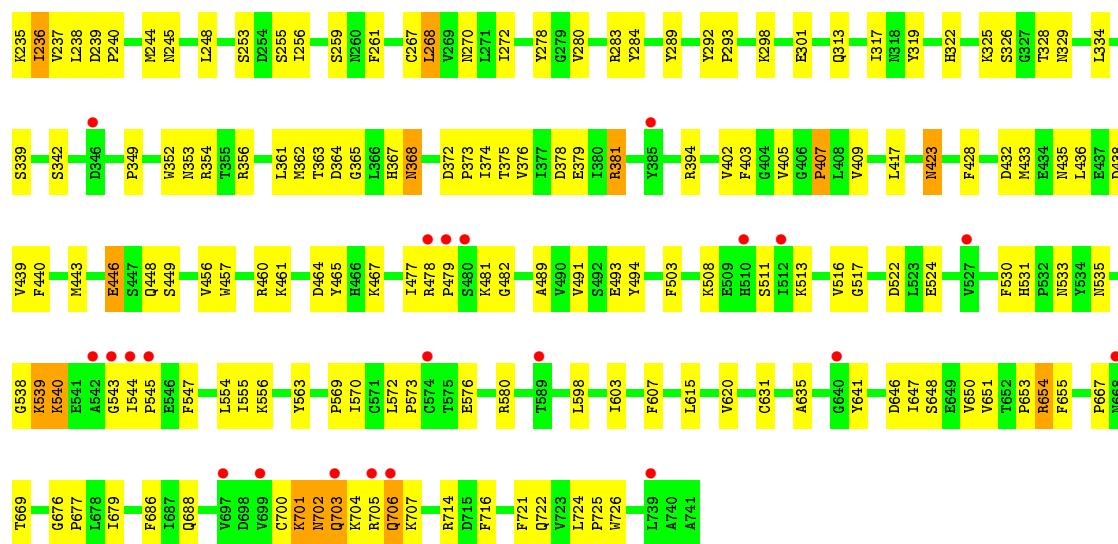




• Molecule 3: COMPLEMENT FACTOR B

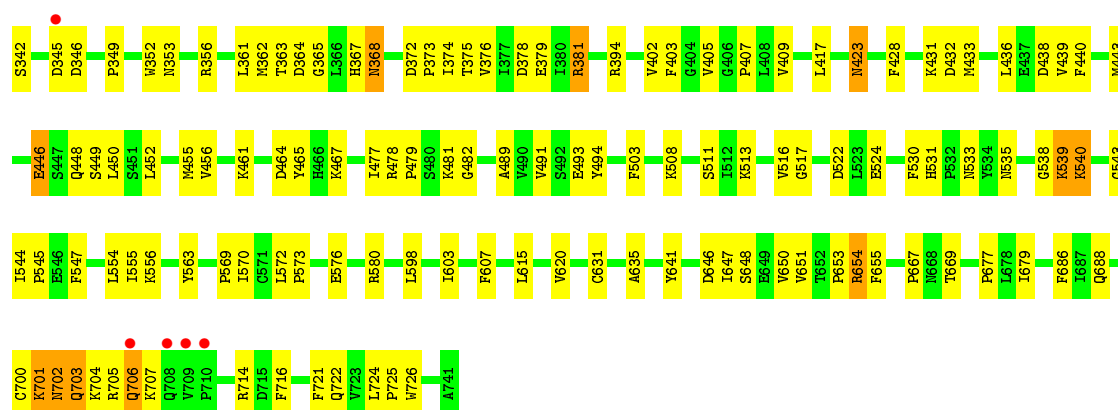


• Molecule 3: COMPLEMENT FACTOR B

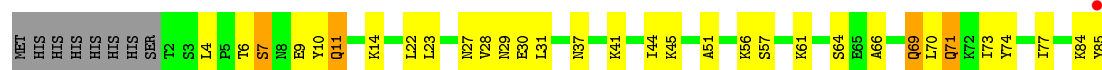


• Molecule 3: COMPLEMENT FACTOR B





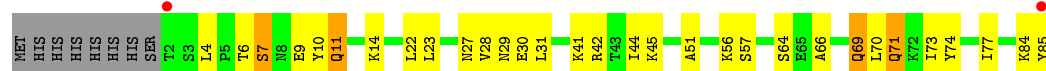
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



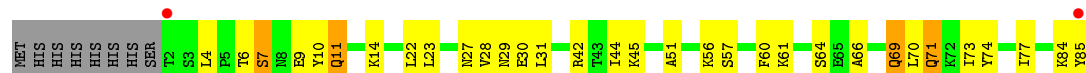
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 97.6 (39.68-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.244 , 0.259	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	DCC
Wilson B-factor (Å ²)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MG, BMA, NAG, NDG, MAN

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	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

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

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	4958	0	5017	127	0
1	C	4958	0	5017	129	0
1	E	4958	0	5017	132	0
1	G	4958	0	5016	145	0
2	B	7177	0	7085	201	0
2	D	7166	0	7062	193	0
2	F	7172	0	7080	220	0
2	H	7175	0	7087	195	0
3	I	4004	0	3966	129	0
3	J	4004	0	3967	129	0
3	K	4004	0	3965	128	0
3	L	4004	0	3966	126	0
4	M	682	0	697	35	0
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	A	14	0	12	1	0
5	B	14	0	11	1	0
5	C	14	0	12	2	0
5	D	14	0	12	1	0
5	E	14	0	12	4	0
5	F	14	0	12	0	0
5	G	14	0	12	2	0
5	H	14	0	12	0	0
5	I	28	0	24	2	0
5	J	14	0	12	1	0
5	K	28	0	25	7	0
5	L	28	0	25	0	0
6	A	14	0	12	1	0
6	B	14	0	12	0	0
6	C	14	0	12	1	0
6	D	14	0	12	1	0
6	E	14	0	12	1	0
6	F	14	0	12	0	0
6	G	14	0	12	3	0
6	H	14	0	12	1	0
6	I	28	0	25	2	0
6	J	14	0	12	2	0
6	K	14	0	12	1	0
6	L	14	0	12	0	0
7	A	22	0	19	0	0
7	B	33	0	29	0	0
7	C	33	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	22	0	19	0	0
7	E	22	0	19	1	0
7	F	44	0	37	2	0
7	G	33	0	28	4	0
7	K	11	0	10	0	0
7	L	11	0	10	0	0
8	G	11	0	10	1	0
8	H	22	0	19	1	0
8	I	11	0	10	0	0
8	J	11	0	10	0	0
8	K	33	0	28	2	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
10	B	1	0	0	0	0
10	I	2	0	0	0	0
10	J	2	0	0	1	0
10	K	2	0	0	0	0
10	L	1	0	0	0	0
All	All	67989	0	67647	1876	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 14.

The worst 5 of 1876 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:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94

There are no symmetry-related clashes.

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	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	28	70
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	28	70
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	28	70
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	28	70
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	5	40
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	5	41
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	4	39
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	4	36
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	11	53
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	9	49

5 of 170 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP

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	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	C	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	E	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	G	558/567 (98%)	549 (98%)	9 (2%)	68	86
2	B	793/810 (98%)	769 (97%)	24 (3%)	46	75
2	D	790/810 (98%)	766 (97%)	24 (3%)	46	75
2	F	793/810 (98%)	769 (97%)	24 (3%)	46	75
2	H	793/810 (98%)	766 (97%)	27 (3%)	42	73
3	I	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	J	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	K	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	L	442/446 (99%)	429 (97%)	13 (3%)	48	75
4	M	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	N	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	P	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	Q	76/84 (90%)	73 (96%)	3 (4%)	37	69
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	50	77

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	1397	LYS
2	H	834	GLN
3	L	540	LYS
2	F	1462	ASN
1	G	144	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 256 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	567	HIS
2	F	1579	HIS
4	M	11	GLN
2	F	762	ASN
2	F	1141	ASN

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 61 ligands modelled in this entry, 4 are monoatomic - leaving 57 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	$\# Z > 2$
5	NDG	A	1646	1,6	14,14,15	0.45	0	15,19,21	0.76	0
6	NAG	A	1647	5,7	14,14,15	0.63	0	15,19,21	1.89	4 (26%)
7	BMA	A	1648	7,6	11,11,12	0.56	0	13,15,17	1.10	1 (7%)
7	BMA	A	1649	7	11,11,12	0.66	0	13,15,17	1.41	2 (15%)
5	NDG	B	2642	2,6	14,14,15	0.54	0	15,19,21	1.17	2 (13%)
6	NAG	B	2643	5,7	14,14,15	0.53	0	15,19,21	2.31	3 (20%)
7	BMA	B	2644	7,6	11,11,12	0.94	0	13,15,17	1.88	4 (30%)
7	BMA	B	2645	7	11,11,12	0.71	0	13,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	B	2646	-	11,11,12	0.72	0	13,15,17	1.46	3 (23%)
5	NDG	C	1646	1,6	14,14,15	0.61	0	15,19,21	1.25	2 (13%)
6	NAG	C	1647	5,7	14,14,15	0.66	0	15,19,21	1.20	2 (13%)
7	BMA	C	1648	7,6	11,11,12	0.66	0	13,15,17	1.09	1 (7%)
7	BMA	C	1649	7	11,11,12	0.75	0	13,15,17	1.66	3 (23%)
7	BMA	C	1650	7	11,11,12	0.66	0	13,15,17	1.81	4 (30%)
5	NDG	D	2642	2,6	14,14,15	0.48	0	15,19,21	0.86	0
6	NAG	D	2643	5,7	14,14,15	0.57	0	15,19,21	1.11	2 (13%)
7	BMA	D	2644	7,6	11,11,12	0.63	0	13,15,17	1.19	1 (7%)
7	BMA	D	2645	7	11,11,12	0.66	0	13,15,17	1.33	2 (15%)
5	NDG	E	1646	1,6	14,14,15	0.55	0	15,19,21	0.95	1 (6%)
6	NAG	E	1647	5,7	14,14,15	0.59	0	15,19,21	1.22	2 (13%)
7	BMA	E	1648	7,6	11,11,12	0.69	0	13,15,17	1.06	1 (7%)
7	BMA	E	1649	7	11,11,12	0.91	1 (9%)	13,15,17	1.78	3 (23%)
5	NDG	F	2642	2,6	14,14,15	0.38	0	15,19,21	1.35	3 (20%)
6	NAG	F	2643	5,7	14,14,15	0.44	0	15,19,21	1.65	3 (20%)
7	BMA	F	2644	7,6	11,11,12	0.59	0	13,15,17	1.58	4 (30%)
7	BMA	F	2645	7	11,11,12	0.98	1 (9%)	13,15,17	1.77	4 (30%)
7	BMA	F	2646	7	11,11,12	0.66	0	13,15,17	1.91	4 (30%)
7	BMA	F	2647	7	11,11,12	0.69	0	13,15,17	1.09	1 (7%)
5	NDG	G	1646	1,6	14,14,15	0.43	0	15,19,21	1.22	1 (6%)
6	NAG	G	1647	5,7	14,14,15	0.51	0	15,19,21	2.29	5 (33%)
7	BMA	G	1648	7,6	11,11,12	0.52	0	13,15,17	2.57	5 (38%)
7	BMA	G	1649	7	11,11,12	0.56	0	13,15,17	4.47	5 (38%)
7	BMA	G	1650	7	11,11,12	0.64	0	13,15,17	1.43	2 (15%)
8	MAN	G	1651	-	11,11,12	0.82	0	13,15,17	1.79	4 (30%)
5	NDG	H	2642	2,6	14,14,15	0.57	0	15,19,21	0.78	0
6	NAG	H	2643	8,5	14,14,15	0.47	0	15,19,21	0.77	0
8	MAN	H	2644	8,6	11,11,12	0.77	0	13,15,17	1.27	1 (7%)
8	MAN	H	2645	8	11,11,12	0.75	0	13,15,17	1.08	2 (15%)
5	NDG	I	1743	3,6	14,14,15	0.55	0	15,19,21	1.06	2 (13%)
6	NAG	I	1744	8,5	14,14,15	0.61	0	15,19,21	1.08	1 (6%)
8	MAN	I	1745	6	11,11,12	0.64	0	13,15,17	0.98	1 (7%)
5	NDG	I	1746	3,6	14,14,15	0.54	0	15,19,21	1.20	2 (13%)
6	NAG	I	1747	5	14,14,15	0.54	0	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NDG	J	1743	3,6	14,14,15	0.51	0	15,19,21	1.07	1 (6%)
6	NAG	J	1744	8,5	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
8	MAN	J	1745	6	11,11,12	0.64	0	13,15,17	0.91	1 (7%)
5	NDG	K	1743	3,6	14,14,15	0.61	0	15,19,21	1.12	2 (13%)
6	NAG	K	1744	8,5	14,14,15	0.69	0	15,19,21	1.46	3 (20%)
8	MAN	K	1745	8,6	11,11,12	0.56	0	13,15,17	1.66	4 (30%)
8	MAN	K	1746	8	11,11,12	0.74	0	13,15,17	1.72	3 (23%)
7	BMA	K	1747	-	11,11,12	0.79	0	13,15,17	1.99	4 (30%)
8	MAN	K	1748	8	11,11,12	0.60	0	13,15,17	1.01	2 (15%)
5	NDG	K	1749	3	14,14,15	0.51	0	15,19,21	2.00	2 (13%)
5	NDG	L	1743	3,6	14,14,15	0.48	0	15,19,21	0.92	0
6	NAG	L	1744	5,7	14,14,15	0.60	0	15,19,21	1.10	1 (6%)
7	BMA	L	1745	6	11,11,12	0.64	0	13,15,17	0.83	1 (7%)
5	NDG	L	1746	3	14,14,15	0.51	0	15,19,21	0.66	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
5	NDG	A	1646	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	A	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	A	1649	7	-	0/2/19/22	0/1/1/1
5	NDG	B	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	B	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	B	2645	7	-	0/2/19/22	0/1/1/1
7	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
5	NDG	C	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	C	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	C	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	C	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	C	1650	7	-	0/2/19/22	0/1/1/1
5	NDG	D	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	D	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	D	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	D	2645	7	-	0/2/19/22	0/1/1/1
5	NDG	E	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	E	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	E	1649	7	-	0/2/19/22	0/1/1/1
5	NDG	F	2642	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	F	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	F	2645	7	-	0/2/19/22	0/1/1/1
7	BMA	F	2646	7	-	0/2/19/22	0/1/1/1
7	BMA	F	2647	7	-	0/2/19/22	0/1/1/1
5	NDG	G	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	G	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	G	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	G	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	G	1650	7	-	0/2/19/22	0/1/1/1
8	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
5	NDG	H	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	H	2643	8,5	-	0/6/23/26	0/1/1/1
8	MAN	H	2644	8,6	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	H	2645	8	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	I	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	I	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	I	1745	6	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	I	1746	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	I	1747	5	-	0/6/23/26	0/1/1/1
5	NDG	J	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	J	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	J	1745	6	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	K	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	K	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	K	1745	8,6	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	K	1746	8	1/1/4/5	0/2/19/22	0/1/1/1
7	BMA	K	1747	-	-	0/2/19/22	0/1/1/1
8	MAN	K	1748	8	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	K	1749	3	-	0/6/23/26	0/1/1/1
5	NDG	L	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	L	1744	5,7	-	0/6/23/26	0/1/1/1
7	BMA	L	1745	6	-	0/2/19/22	0/1/1/1
5	NDG	L	1746	3	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1649	BMA	O5-C1	-2.28	1.40	1.43
7	F	2645	BMA	O5-C1	-2.16	1.40	1.43

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1649	BMA	C1-C2-C3	-10.35	96.54	109.65
7	G	1649	BMA	C3-C4-C5	-7.17	97.58	110.22
7	G	1649	BMA	C1-O5-C5	-6.84	102.74	112.17
5	K	1749	NDG	O-C1-C2	-5.53	103.78	111.47
7	G	1648	BMA	C1-C2-C3	-5.33	102.89	109.65

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	2642	NDG	C1
8	J	1745	MAN	C1
5	L	1746	NDG	C1
5	B	2642	NDG	C1
5	I	1743	NDG	C1

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1646	NDG	1	0
6	A	1647	NAG	1	0
5	B	2642	NDG	1	0
5	C	1646	NDG	2	0
6	C	1647	NAG	1	0
5	D	2642	NDG	1	0
6	D	2643	NAG	1	0
5	E	1646	NDG	4	0
6	E	1647	NAG	1	0
7	E	1648	BMA	1	0
7	E	1649	BMA	1	0
7	F	2644	BMA	1	0
7	F	2645	BMA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	2647	BMA	1	0
5	G	1646	NDG	2	0
6	G	1647	NAG	3	0
7	G	1648	BMA	2	0
7	G	1649	BMA	2	0
8	G	1651	MAN	1	0
6	H	2643	NAG	1	0
8	H	2644	MAN	1	0
8	H	2645	MAN	1	0
5	I	1743	NDG	2	0
6	I	1744	NAG	2	0
5	J	1743	NDG	1	0
6	J	1744	NAG	2	0
5	K	1743	NDG	4	0
6	K	1744	NAG	1	0
8	K	1745	MAN	2	0
8	K	1746	MAN	1	0
8	K	1748	MAN	1	0
5	K	1749	NDG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1500:LYS	C	1501:SER	N	3.64
1	H	988:CYS	C	989:GLY	N	2.97

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	638/645 (98%)	0.17	16 (2%) 58 47	87, 142, 190, 237	0
1	C	638/645 (98%)	0.11	13 (2%) 65 56	80, 127, 176, 228	0
1	E	638/645 (98%)	0.11	10 (1%) 72 63	84, 142, 196, 245	0
1	G	638/645 (98%)	0.43	60 (9%) 9 8	93, 180, 241, 267	0
2	B	901/915 (98%)	0.16	26 (2%) 52 42	91, 167, 229, 260	0
2	D	901/915 (98%)	0.17	29 (3%) 48 38	81, 155, 216, 266	0
2	F	900/915 (98%)	0.36	50 (5%) 25 20	96, 179, 284, 329	0
2	H	605/915 (66%)	0.38	37 (6%) 22 16	98, 162, 231, 294	0
3	I	507/507 (100%)	-0.03	2 (0%) 92 88	93, 142, 197, 240	0
3	J	507/507 (100%)	0.13	15 (2%) 51 40	127, 170, 220, 261	0
3	K	507/507 (100%)	0.20	22 (4%) 36 28	132, 183, 230, 284	0
3	L	507/507 (100%)	-0.05	5 (0%) 82 74	101, 144, 194, 239	0
4	M	84/92 (91%)	-0.07	1 (1%) 79 70	87, 110, 186, 221	0
4	N	84/92 (91%)	-0.05	2 (2%) 59 49	97, 116, 189, 227	0
4	P	84/92 (91%)	-0.03	2 (2%) 59 49	100, 124, 176, 211	0
4	Q	84/92 (91%)	-0.11	2 (2%) 59 49	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.18	292 (3%) 43 34	80, 155, 228, 329	0

The worst 5 of 292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	645	ALA	9.1
1	G	421	ALA	6.8
2	F	1501	SER	5.7
2	F	1038	ARG	5.6
1	G	399	SER	5.6

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. 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
5	NDG	L	1743	14/15	0.87	0.36	1.80	122,147,148,148	0
5	NDG	K	1743	14/15	0.87	0.28	0.75	174,204,206,207	0
5	NDG	I	1743	14/15	0.92	0.28	0.68	122,149,151,152	0
9	MG	L	1742	1/1	0.91	0.25	0.53	127,127,127,127	0
5	NDG	J	1743	14/15	0.90	0.27	0.33	158,188,189,189	0
9	MG	I	1742	1/1	0.42	0.17	-0.61	120,120,120,120	0
5	NDG	C	1646	14/15	0.82	0.28	-0.76	163,191,192,193	0
9	MG	K	1742	1/1	0.84	0.11	-0.92	138,138,138,138	0
5	NDG	E	1646	14/15	0.83	0.23	-0.92	174,204,206,206	0
5	NDG	F	2642	14/15	0.86	0.22	-1.27	169,193,194,194	0
9	MG	J	1742	1/1	0.82	0.07	-2.08	148,148,148,148	0
5	NDG	A	1646	14/15	0.88	0.21	-2.67	156,185,187,188	0
7	BMA	E	1648	11/12	0.74	0.43	-	229,230,231,232	0
7	BMA	F	2644	11/12	0.84	0.15	-	232,233,234,234	0
6	NAG	A	1647	14/15	0.82	0.23	-	199,200,201,203	0
8	MAN	G	1651	11/12	0.45	0.54	-	222,225,227,228	0
6	NAG	D	2643	14/15	0.88	0.21	-	200,201,202,203	0
7	BMA	A	1648	11/12	0.80	0.30	-	212,214,215,216	0
6	NAG	K	1744	14/15	0.83	0.27	-	196,199,201,202	0
7	BMA	B	2646	11/12	0.66	0.51	-	198,200,200,201	0
5	NDG	B	2642	14/15	0.91	0.23	-	163,194,194,195	0
6	NAG	J	1744	14/15	0.81	0.33	-	177,179,180,180	0
7	BMA	F	2646	11/12	0.72	0.37	-	221,222,224,224	0
8	MAN	J	1745	11/12	0.61	0.36	-	206,210,211,212	0
7	BMA	F	2647	11/12	0.70	0.50	-	214,215,217,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BMA	L	1745	11/12	0.76	0.24	-	197,201,202,202	0
5	NDG	H	2642	14/15	0.90	0.21	-	183,213,214,215	0
8	MAN	K	1746	11/12	0.87	0.52	-	229,230,232,232	0
7	BMA	C	1648	11/12	0.64	0.27	-	219,220,222,223	0
8	MAN	I	1745	11/12	0.79	0.24	-	205,207,208,209	0
7	BMA	G	1648	11/12	0.68	0.54	-	247,249,250,251	0
5	NDG	K	1749	14/15	0.76	0.47	-	184,214,216,217	0
5	NDG	D	2642	14/15	0.89	0.20	-	147,176,178,179	0
7	BMA	F	2645	11/12	0.83	0.23	-	248,249,249,250	0
6	NAG	I	1744	14/15	0.94	0.36	-	178,180,181,182	0
7	BMA	C	1650	11/12	0.70	0.33	-	231,233,235,235	0
7	BMA	K	1747	11/12	0.76	0.52	-	194,195,196,196	0
5	NDG	L	1746	14/15	0.87	0.56	-	176,204,205,205	0
6	NAG	E	1647	14/15	0.83	0.21	-	223,225,227,227	0
6	NAG	C	1647	14/15	0.67	0.27	-	200,202,203,203	0
6	NAG	G	1647	14/15	0.83	0.25	-	213,216,216,217	0
6	NAG	I	1747	14/15	0.63	0.66	-	222,223,224,224	0
7	BMA	D	2645	11/12	0.86	0.28	-	229,232,233,234	0
7	BMA	G	1650	11/12	0.55	0.68	-	229,231,232,232	0
8	MAN	H	2644	11/12	0.64	0.27	-	229,230,231,232	0
7	BMA	B	2645	11/12	0.41	0.37	-	237,239,240,241	0
6	NAG	B	2643	14/15	0.91	0.28	-	193,196,196,197	0
6	NAG	L	1744	14/15	0.85	0.43	-	185,187,189,189	0
6	NAG	F	2643	14/15	0.91	0.21	-	200,202,204,204	0
7	BMA	A	1649	11/12	0.83	0.44	-	226,227,228,228	0
7	BMA	D	2644	11/12	0.67	0.32	-	220,221,223,223	0
7	BMA	G	1649	11/12	0.59	0.37	-	226,228,229,230	0
7	BMA	E	1649	11/12	0.81	0.27	-	209,212,214,215	0
7	BMA	C	1649	11/12	0.65	0.29	-	235,237,239,240	0
8	MAN	K	1748	11/12	0.84	0.36	-	230,232,235,235	0
6	NAG	H	2643	14/15	0.82	0.26	-	221,222,224,225	0
8	MAN	K	1745	11/12	0.73	0.34	-	249,252,253,254	0
7	BMA	B	2644	11/12	0.39	0.35	-	218,220,222,223	0
8	MAN	H	2645	11/12	0.68	0.61	-	234,236,237,238	0
5	NDG	I	1746	14/15	0.79	0.65	-	198,225,227,227	0
5	NDG	G	1646	14/15	0.90	0.16	-	198,201,208,215	0

6.5 Other polymers ⓘ

There are no such residues in this entry.