



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

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 (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

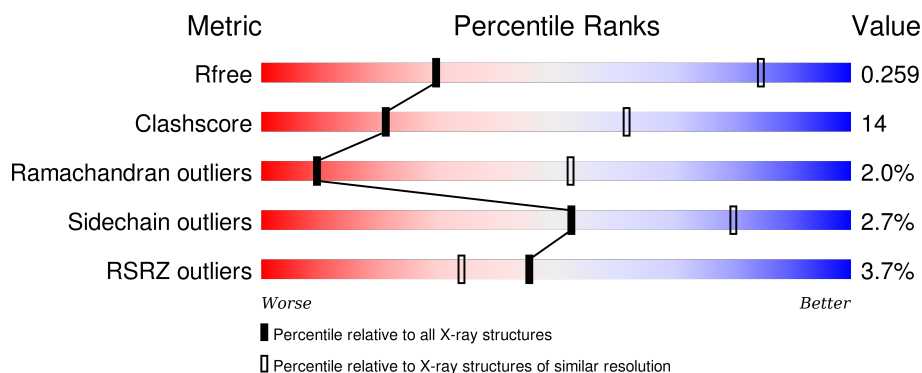
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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>3%</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
10	NDG	H	2642	X	-	-	-
10	MAN	H	2644	X	-	-	-
10	MAN	H	2645	X	-	-	-
12	NDG	I	1743	X	-	-	-
12	MAN	I	1745	X	-	-	-
12	NDG	J	1743	X	-	-	-
12	MAN	J	1745	X	-	-	-
13	NDG	I	1746	X	-	-	-
14	NDG	K	1743	X	-	-	-
14	MAN	K	1745	X	-	-	-
14	MAN	K	1746	X	-	-	-
14	MAN	K	1748	X	-	-	-
15	NDG	L	1746	X	-	-	-
16	NDG	L	1743	X	-	-	-
5	NDG	B	2642	X	-	-	-
5	NDG	D	2642	X	-	-	-
5	NDG	E	1646	X	-	-	-
7	NDG	C	1646	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NDG	G	1646	X	-	-	-

2 Entry composition

There are 17 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			

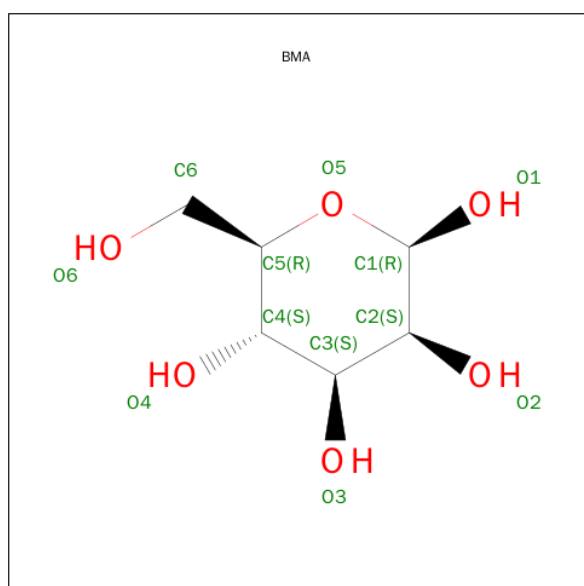
- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

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 a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		
5	D	4	Total	C	N	O	0	0
			50	28	2	20		
5	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	C	O	0	0
			11	6	5		

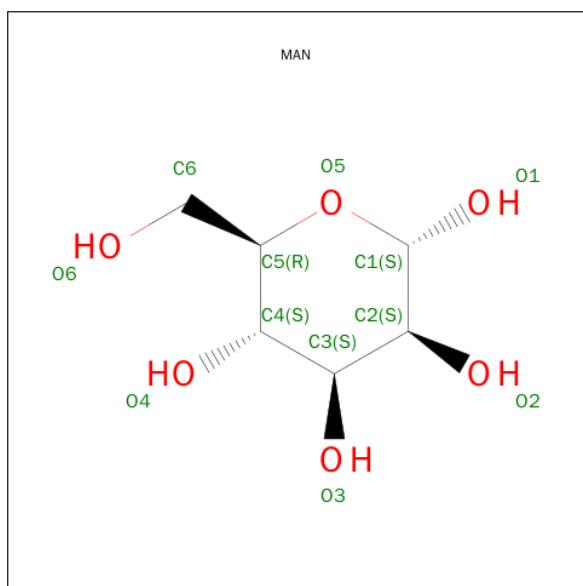
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	5	Total	C	N	O	0	0
			61	34	2	25		
7	G	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	H	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	I	3	Total	C	N	O	0	0
			39	22	2	15		
12	J	3	Total	C	N	O	0	0
			39	22	2	15		

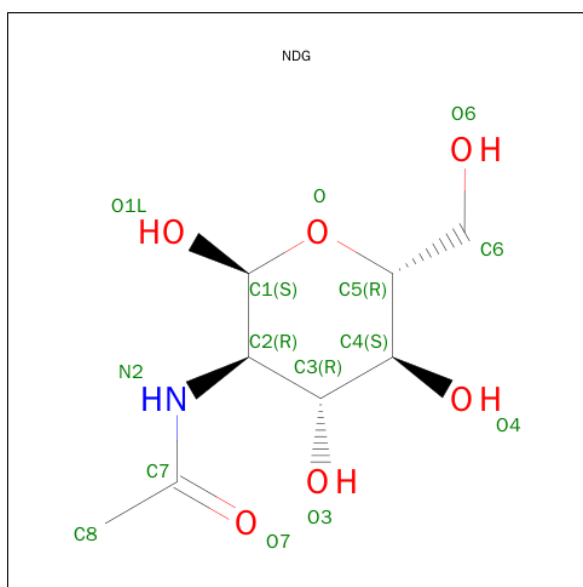
- Molecule 13 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 15 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			14	8	1	5		
15	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 16 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	L	3	Total	C	N	O	0	0
			39	22	2	15		

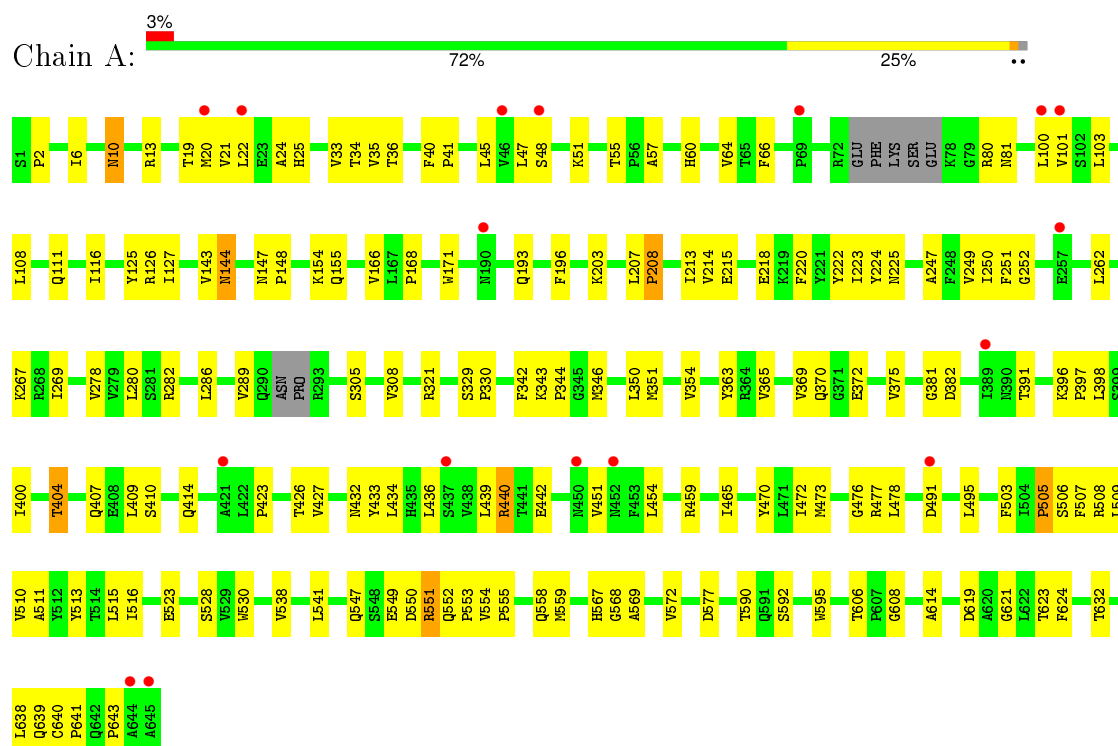
- Molecule 17 is water.

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

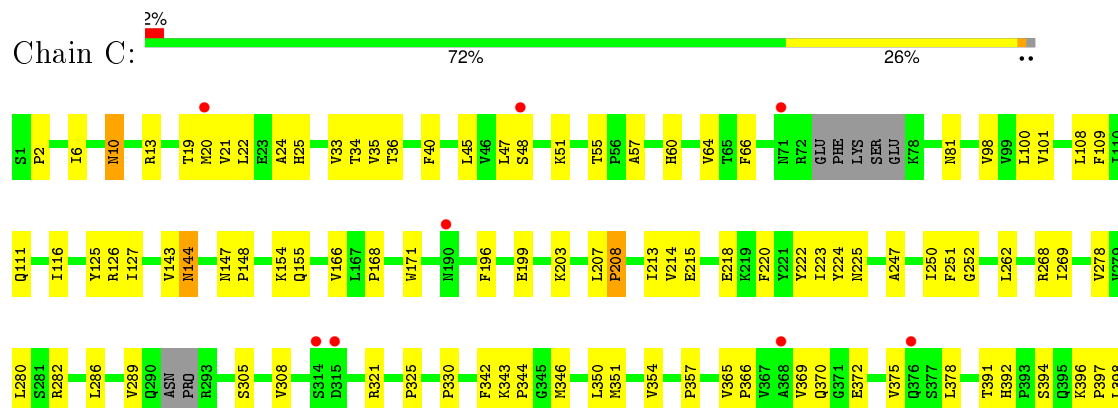
3 Residue-property plots

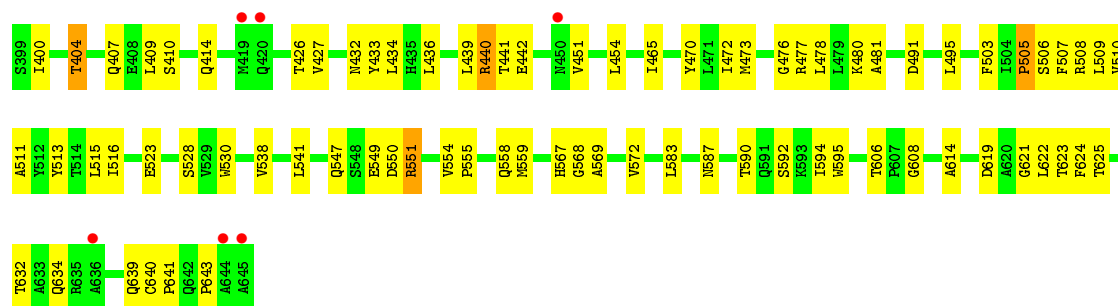
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

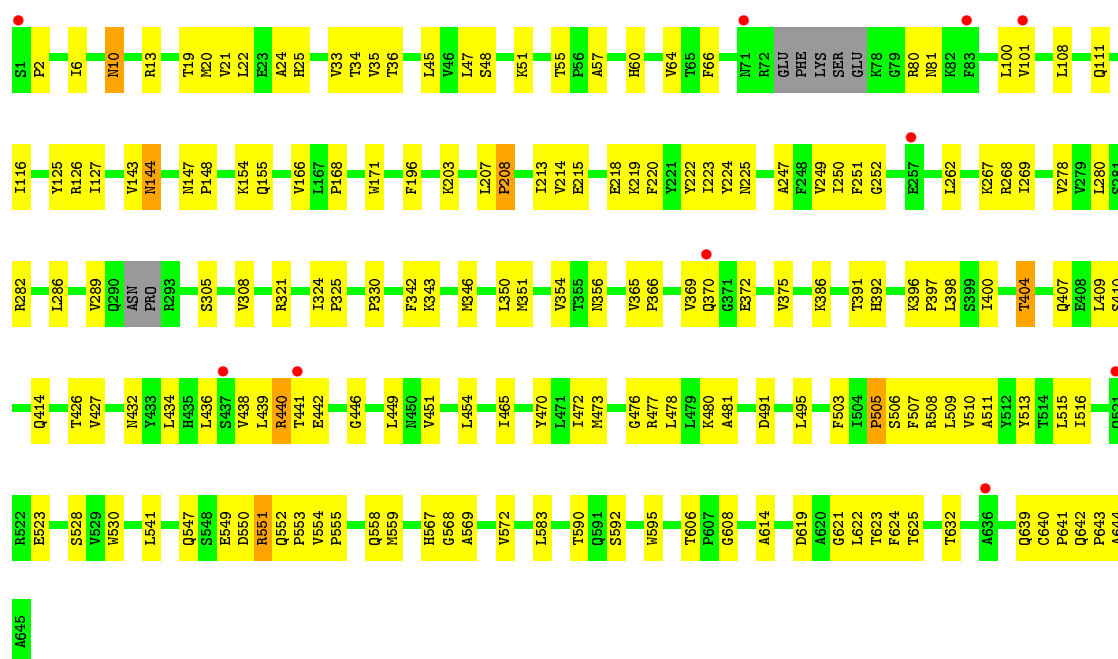


• Molecule 1: COMPLEMENT C3 BETA CHAIN

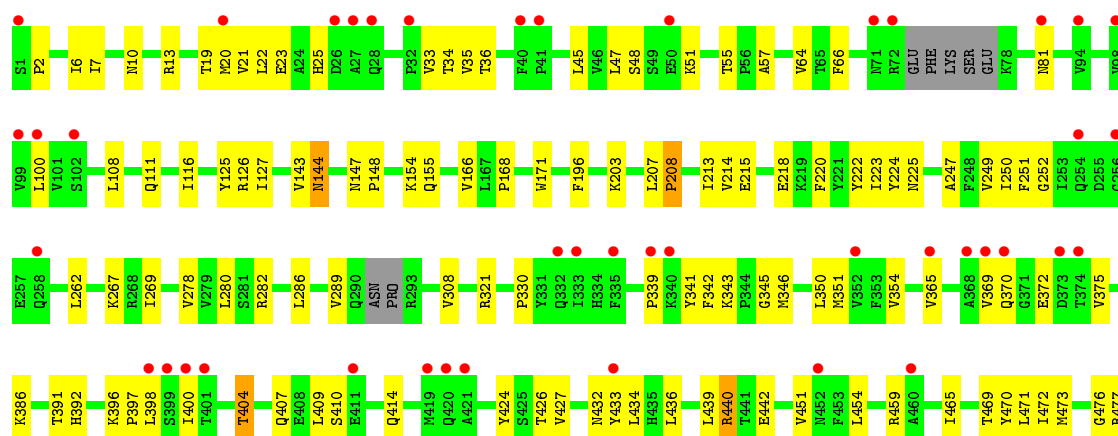


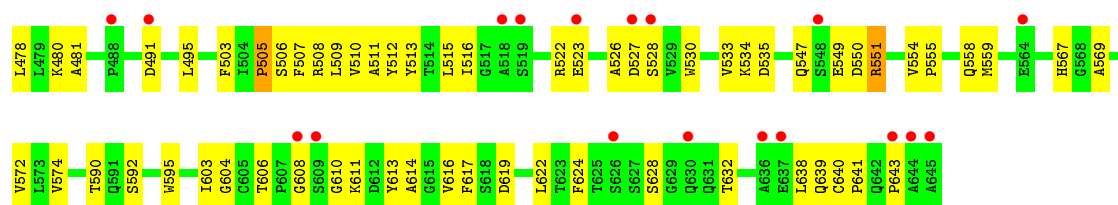


• Molecule 1: COMPLEMENT C3 BETA CHAIN

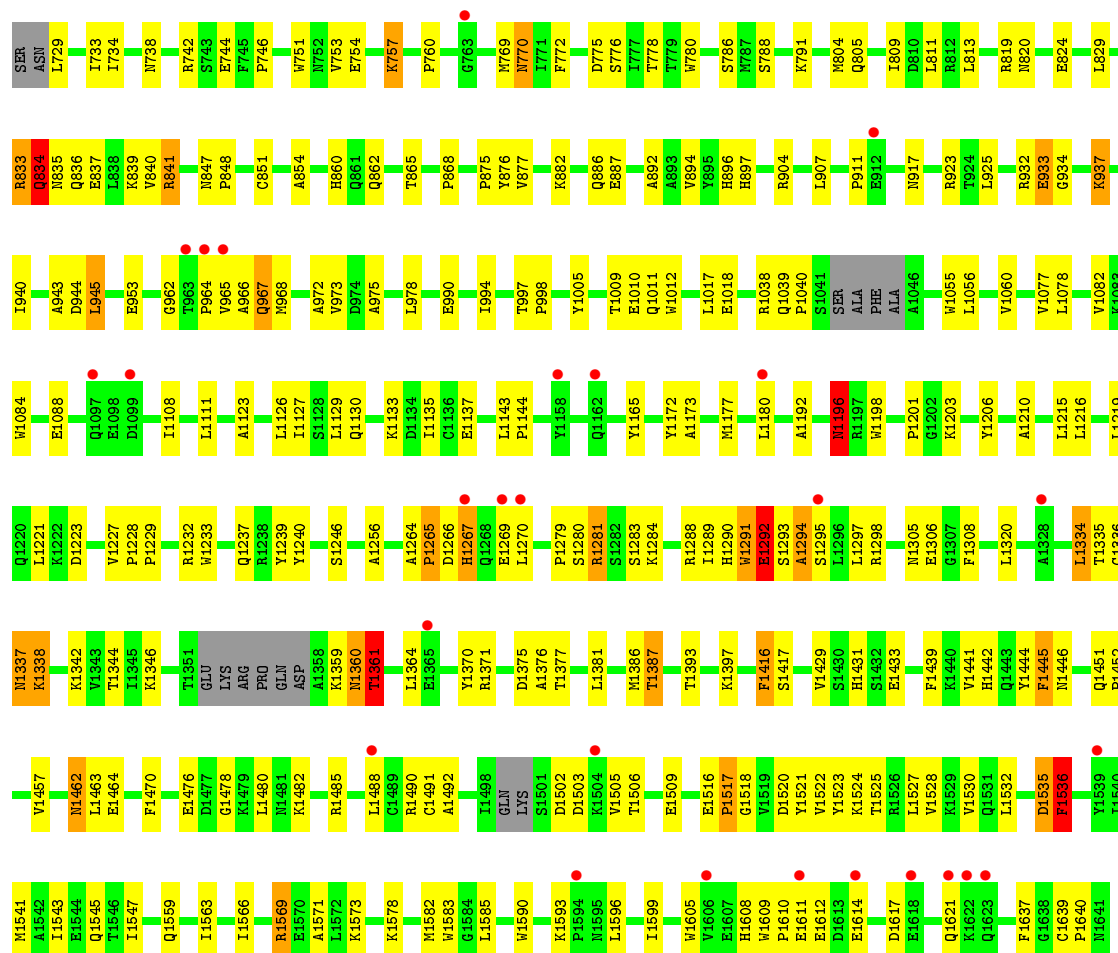


• Molecule 1: COMPLEMENT C3 BETA CHAIN

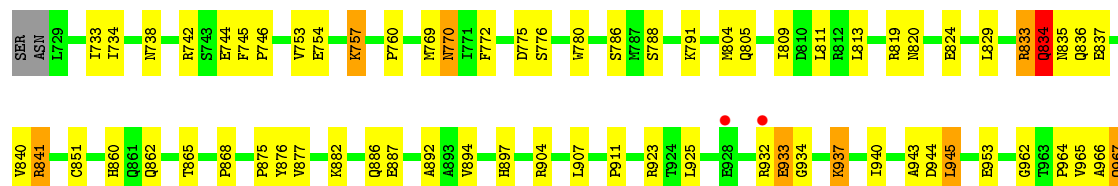


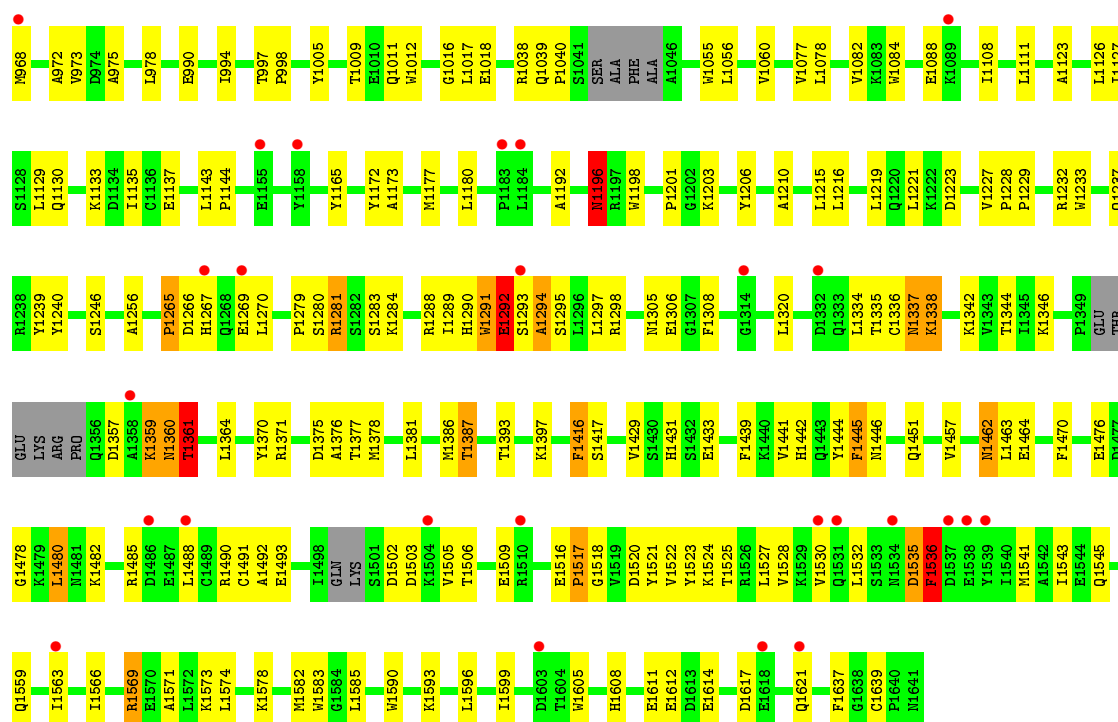


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



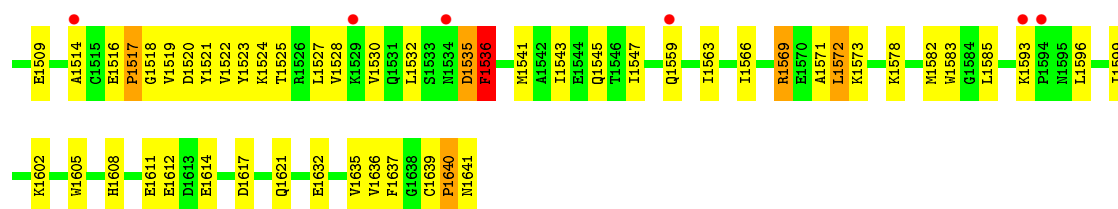
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



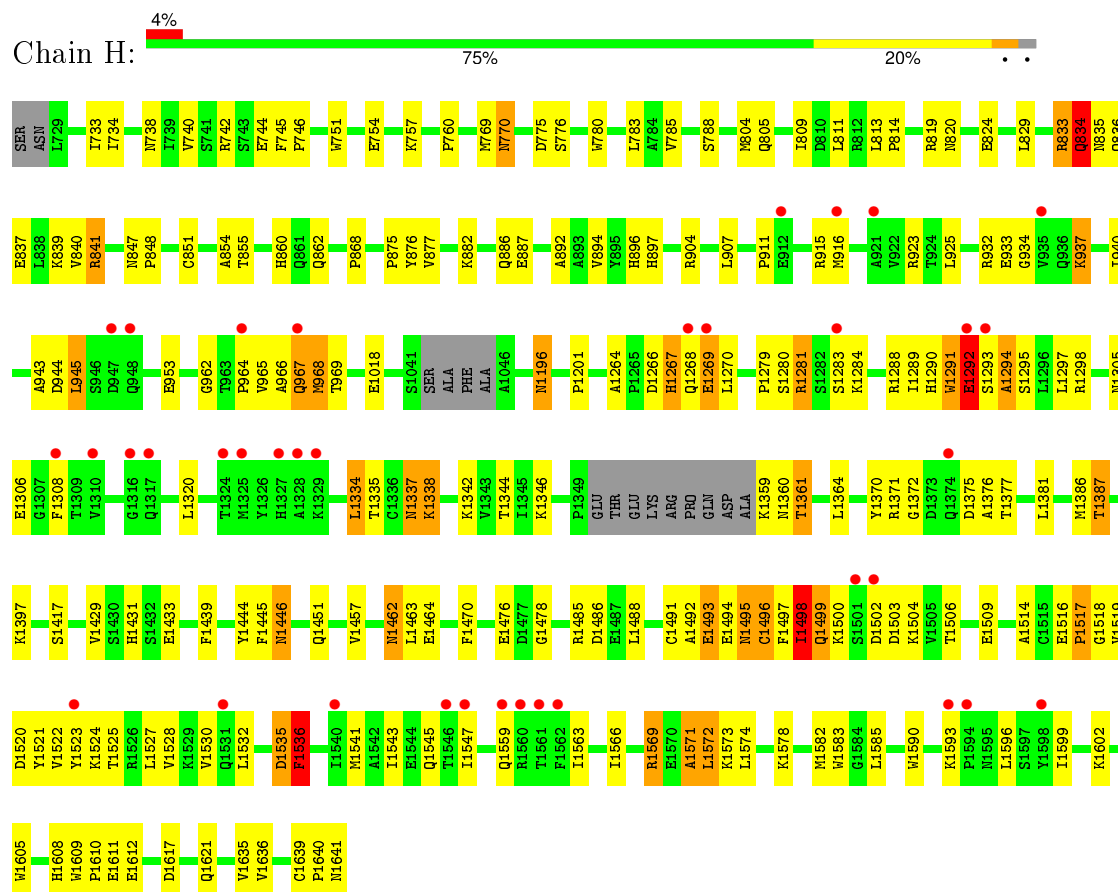


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

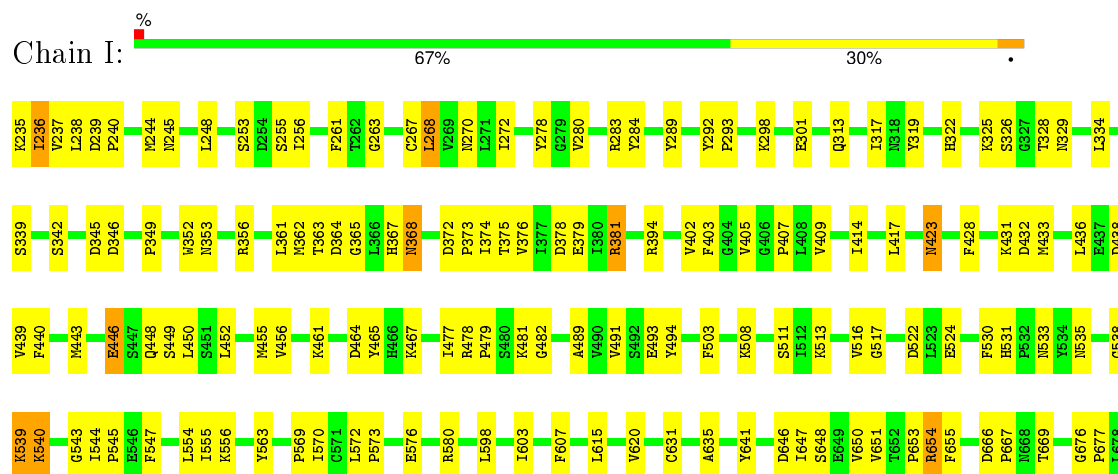




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

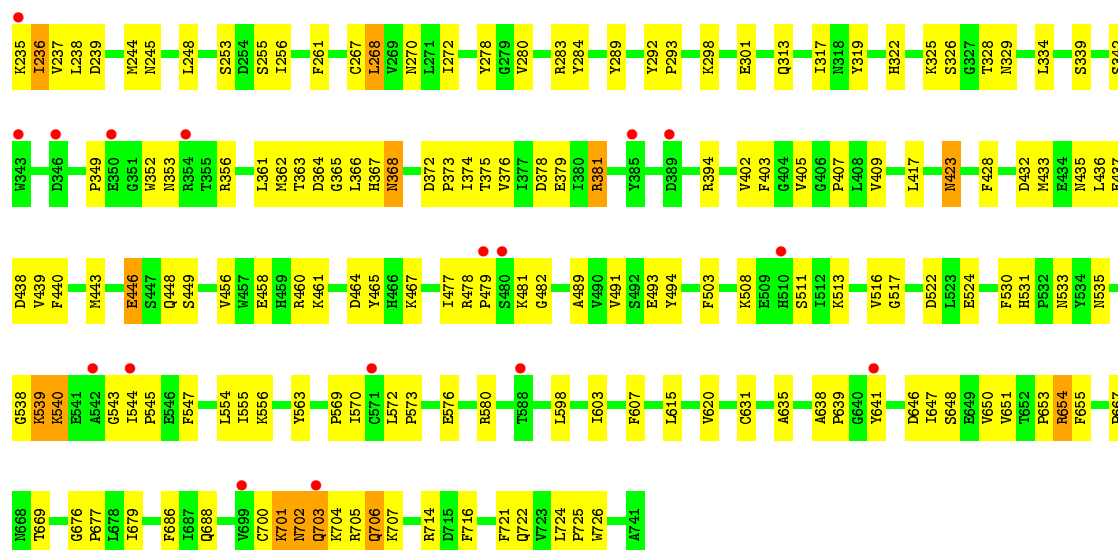


• Molecule 3: COMPLEMENT FACTOR B

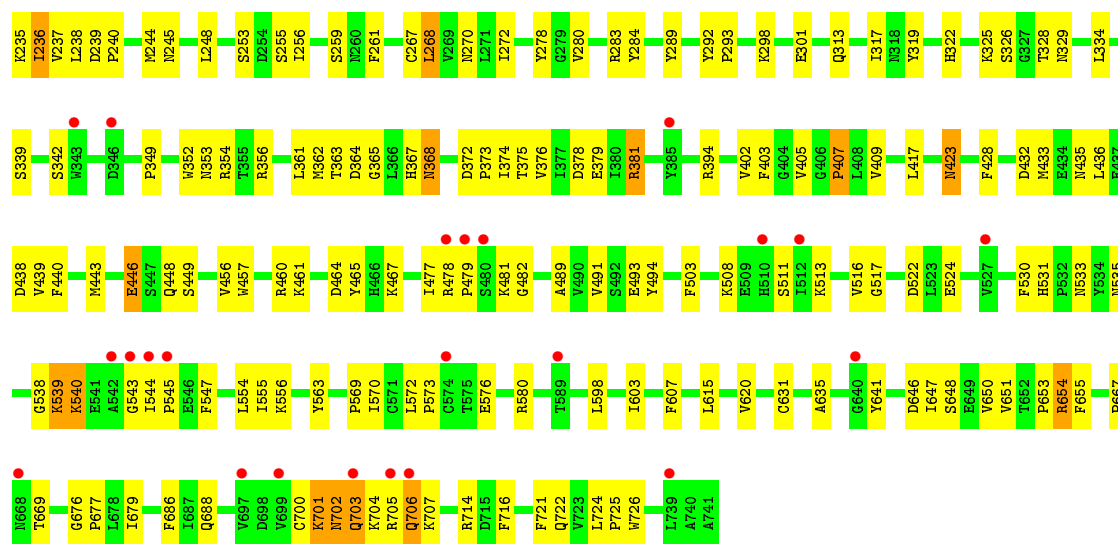




• Molecule 3: COMPLEMENT FACTOR B

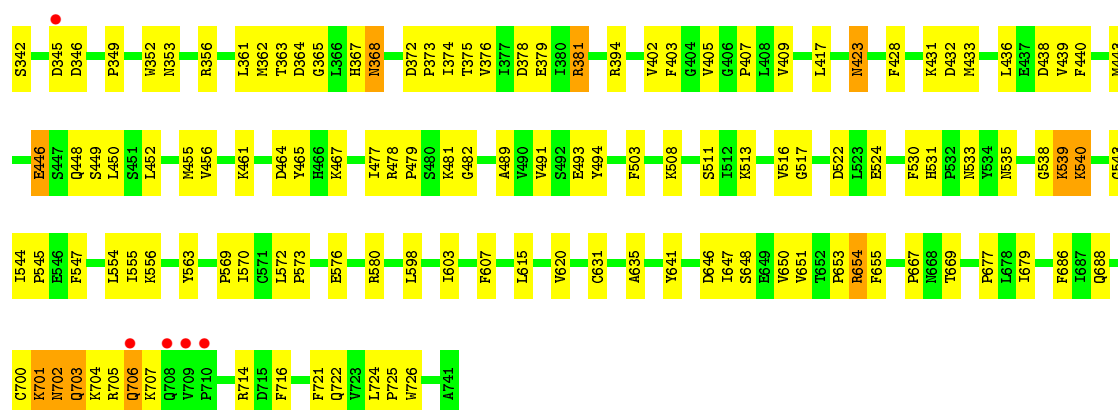


• Molecule 3: COMPLEMENT FACTOR B



• Molecule 3: COMPLEMENT FACTOR B





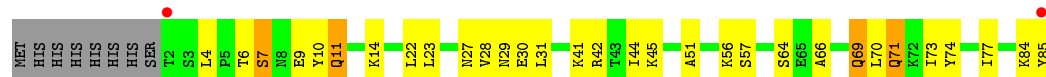
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



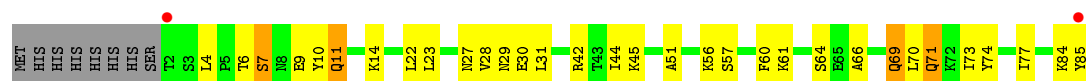
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• 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
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 137471 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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
5	B	1	0
5	D	1	0
5	E	1	0
7	C	1	0
7	G	1	0
10	H	3	0
12	I	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	2	0
13	I	1	0
14	K	4	0
16	L	1	0
All	All	18	0

There are no bond length outliers.

There are no bond angle outliers.

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	2642	NDG	C1
7	C	1646	NDG	C1
5	D	2642	NDG	C1
5	E	1646	NDG	C1
7	G	1646	NDG	C1

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	A	50	0	43	1	0
5	B	50	0	42	1	0
5	D	50	0	43	1	0
5	E	50	0	43	5	0
6	B	11	0	10	0	0
6	K	11	0	10	0	0
7	C	61	0	52	2	0
7	G	61	0	52	6	0
8	F	72	0	61	2	0
9	G	11	0	10	1	0
10	H	50	0	43	2	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
12	I	39	0	34	3	0
12	J	39	0	34	2	0
13	I	28	0	25	0	0
14	K	61	0	52	6	0
15	K	14	0	13	3	0
15	L	14	0	13	0	0
16	L	39	0	34	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	2	0	0	1	0
17	K	2	0	0	0	0
17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	30	73
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	30	73
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	30	73
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	30	73
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	5	44
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	5	44
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	5	42
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	4	39
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	12	56
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	9	52

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%)	70	88
1	C	558/567 (98%)	549 (98%)	9 (2%)	70	88
1	E	558/567 (98%)	549 (98%)	9 (2%)	70	88
1	G	558/567 (98%)	549 (98%)	9 (2%)	70	88
2	B	793/810 (98%)	769 (97%)	24 (3%)	48	78
2	D	790/810 (98%)	766 (97%)	24 (3%)	48	78
2	F	793/810 (98%)	769 (97%)	24 (3%)	48	78
2	H	793/810 (98%)	766 (97%)	27 (3%)	44	77
3	I	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	J	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	K	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	L	442/446 (99%)	429 (97%)	13 (3%)	50	79
4	M	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	N	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	P	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	Q	76/84 (90%)	73 (96%)	3 (4%)	39	74
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	52	80

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

Mol	Chain	Res	Type
2	F	1397	LYS

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Mol	Chain	Res	Type
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 ⓘ

52 carbohydrates 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	$\# Z > 2$
5	NDG	A	1646	1,5	14,14,15	0.44	0	15,19,21	0.80	1 (6%)
5	NAG	A	1647	5	14,14,15	0.61	0	15,19,21	1.85	4 (26%)
5	BMA	A	1648	5	11,11,12	0.54	0	14,15,17	1.33	2 (14%)
5	BMA	A	1649	5	11,11,12	0.64	0	14,15,17	1.39	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NDG	B	2642	2,5	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
5	NAG	B	2643	5	14,14,15	0.51	0	15,19,21	2.18	1 (6%)
5	BMA	B	2644	5	11,11,12	0.91	0	14,15,17	1.97	3 (21%)
5	BMA	B	2645	5	11,11,12	0.70	0	14,15,17	0.81	0
7	NDG	C	1646	1,7	14,14,15	0.59	0	15,19,21	1.26	2 (13%)
7	NAG	C	1647	7	14,14,15	0.64	0	15,19,21	1.04	1 (6%)
7	BMA	C	1648	7	11,11,12	0.64	0	14,15,17	1.16	1 (7%)
7	BMA	C	1649	7	11,11,12	0.73	0	14,15,17	1.63	3 (21%)
7	BMA	C	1650	7	11,11,12	0.64	0	14,15,17	1.82	4 (28%)
5	NDG	D	2642	2,5	14,14,15	0.47	0	15,19,21	0.86	0
5	NAG	D	2643	5	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
5	BMA	D	2644	5	11,11,12	0.61	0	14,15,17	1.36	2 (14%)
5	BMA	D	2645	5	11,11,12	0.64	0	14,15,17	1.31	2 (14%)
5	NDG	E	1646	1,5	14,14,15	0.53	0	15,19,21	0.85	1 (6%)
5	NAG	E	1647	5	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
5	BMA	E	1648	5	11,11,12	0.67	0	14,15,17	1.10	1 (7%)
5	BMA	E	1649	5	11,11,12	0.89	1 (9%)	14,15,17	1.81	3 (21%)
8	NDG	F	2642	8,2	14,14,15	0.37	0	15,19,21	1.10	2 (13%)
8	NAG	F	2643	8	14,14,15	0.43	0	15,19,21	1.74	3 (20%)
8	BMA	F	2644	8	11,11,12	0.57	0	14,15,17	1.58	4 (28%)
8	BMA	F	2645	8	11,11,12	0.96	1 (9%)	14,15,17	1.79	4 (28%)
8	BMA	F	2646	8	11,11,12	0.64	0	14,15,17	1.91	4 (28%)
8	BMA	F	2647	8	11,11,12	0.67	0	14,15,17	1.08	1 (7%)
7	NDG	G	1646	1,7	14,14,15	0.42	0	15,19,21	1.20	1 (6%)
7	NAG	G	1647	7	14,14,15	0.50	0	15,19,21	2.25	5 (33%)
7	BMA	G	1648	7	11,11,12	0.50	0	14,15,17	2.85	6 (42%)
7	BMA	G	1649	7	11,11,12	0.54	0	14,15,17	4.67	6 (42%)
7	BMA	G	1650	7	11,11,12	0.62	0	14,15,17	1.42	2 (14%)
10	NDG	H	2642	10,2	14,14,15	0.56	0	15,19,21	0.68	0
10	NAG	H	2643	10	14,14,15	0.46	0	15,19,21	0.78	0
10	MAN	H	2644	10	11,11,12	0.75	0	14,15,17	1.36	1 (7%)
10	MAN	H	2645	10	11,11,12	0.73	0	14,15,17	1.11	2 (14%)
12	NDG	I	1743	3,12	14,14,15	0.54	0	15,19,21	1.08	2 (13%)
12	NAG	I	1744	12	14,14,15	0.60	0	15,19,21	1.01	1 (6%)
12	MAN	I	1745	12	11,11,12	0.62	0	14,15,17	1.07	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NDG	I	1746	3,13	14,14,15	0.52	0	15,19,21	1.18	2 (13%)
13	NAG	I	1747	13	14,14,15	0.52	0	15,19,21	0.97	1 (6%)
12	NDG	J	1743	3,12	14,14,15	0.49	0	15,19,21	1.10	1 (6%)
12	NAG	J	1744	12	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
12	MAN	J	1745	12	11,11,12	0.62	0	14,15,17	1.00	1 (7%)
14	NDG	K	1743	3,14	14,14,15	0.60	0	15,19,21	1.11	1 (6%)
14	NAG	K	1744	14	14,14,15	0.67	0	15,19,21	1.41	3 (20%)
14	MAN	K	1745	14	11,11,12	0.54	0	14,15,17	1.88	5 (35%)
14	MAN	K	1746	14	11,11,12	0.72	0	14,15,17	1.66	3 (21%)
14	MAN	K	1748	14	11,11,12	0.58	0	14,15,17	1.09	2 (14%)
16	NDG	L	1743	3,16	14,14,15	0.47	0	15,19,21	0.95	0
16	NAG	L	1744	16	14,14,15	0.58	0	15,19,21	1.08	1 (6%)
16	BMA	L	1745	16	11,11,12	0.62	0	14,15,17	0.91	1 (7%)

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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1647	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1648	5	-	0/2/19/22	0/1/1/1
5	BMA	A	1649	5	-	0/2/19/22	0/1/1/1
5	NDG	B	2642	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	2643	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2644	5	-	0/2/19/22	0/1/1/1
5	BMA	B	2645	5	-	0/2/19/22	0/1/1/1
7	NDG	C	1646	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	1647	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1648	7	-	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	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	2643	5	-	0/6/23/26	0/1/1/1
5	BMA	D	2644	5	-	0/2/19/22	0/1/1/1
5	BMA	D	2645	5	-	0/2/19/22	0/1/1/1
5	NDG	E	1646	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	1647	5	-	0/6/23/26	0/1/1/1
5	BMA	E	1648	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	E	1649	5	-	0/2/19/22	0/1/1/1
8	NDG	F	2642	8,2	-	0/6/23/26	0/1/1/1
8	NAG	F	2643	8	-	0/6/23/26	0/1/1/1
8	BMA	F	2644	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2645	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2646	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2647	8	-	0/2/19/22	0/1/1/1
7	NDG	G	1646	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	G	1647	7	-	0/6/23/26	0/1/1/1
7	BMA	G	1648	7	-	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
10	NDG	H	2642	10,2	1/1/5/7	0/6/23/26	0/1/1/1
10	NAG	H	2643	10	-	0/6/23/26	0/1/1/1
10	MAN	H	2644	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	H	2645	10	1/1/4/5	0/2/19/22	0/1/1/1
12	NDG	I	1743	3,12	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	I	1744	12	-	0/6/23/26	0/1/1/1
12	MAN	I	1745	12	1/1/4/5	0/2/19/22	0/1/1/1
13	NDG	I	1746	3,13	1/1/5/7	0/6/23/26	0/1/1/1
13	NAG	I	1747	13	-	0/6/23/26	0/1/1/1
12	NDG	J	1743	3,12	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	J	1744	12	-	0/6/23/26	0/1/1/1
12	MAN	J	1745	12	1/1/4/5	0/2/19/22	0/1/1/1
14	NDG	K	1743	3,14	1/1/5/7	0/6/23/26	0/1/1/1
14	NAG	K	1744	14	-	0/6/23/26	0/1/1/1
14	MAN	K	1745	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	K	1746	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	K	1748	14	1/1/4/5	0/2/19/22	0/1/1/1
16	NDG	L	1743	3,16	1/1/5/7	0/6/23/26	0/1/1/1
16	NAG	L	1744	16	-	0/6/23/26	0/1/1/1
16	BMA	L	1745	16	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1649	BMA	O5-C1	-2.24	1.40	1.43
8	F	2645	BMA	O5-C1	-2.12	1.40	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1649	BMA	C1-C2-C3	-10.99	96.54	109.54
7	G	1649	BMA	C1-O5-C5	-7.49	102.74	112.25
7	G	1649	BMA	C3-C4-C5	-7.24	97.58	110.20
7	G	1648	BMA	C1-C2-C3	-5.62	102.89	109.54
5	E	1649	BMA	C1-O5-C5	-4.80	106.16	112.25

5 of 18 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1646	NDG	1	0
5	A	1647	NAG	1	0
5	B	2642	NDG	1	0
7	C	1646	NDG	2	0
7	C	1647	NAG	1	0
5	D	2642	NDG	1	0
5	D	2643	NAG	1	0
5	E	1646	NDG	4	0
5	E	1647	NAG	1	0
5	E	1648	BMA	1	0
5	E	1649	BMA	1	0
8	F	2644	BMA	1	0
8	F	2645	BMA	2	0
8	F	2647	BMA	1	0
7	G	1646	NDG	2	0
7	G	1647	NAG	3	0
7	G	1648	BMA	2	0
7	G	1649	BMA	2	0
10	H	2643	NAG	1	0
10	H	2644	MAN	1	0
10	H	2645	MAN	1	0
12	I	1743	NDG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	1744	NAG	2	0
12	J	1743	NDG	1	0
12	J	1744	NAG	2	0
14	K	1743	NDG	4	0
14	K	1744	NAG	1	0
14	K	1745	MAN	2	0
14	K	1746	MAN	1	0
14	K	1748	MAN	1	0

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 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	$\# Z > 2$
6	BMA	B	2646	-	11,11,12	0.70	0	14,15,17	1.46	3 (21%)
9	MAN	G	1651	-	11,11,12	0.79	0	14,15,17	1.79	4 (28%)
6	BMA	K	1747	-	11,11,12	0.77	0	14,15,17	2.04	4 (28%)
15	NDG	K	1749	3	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
15	NDG	L	1746	3	14,14,15	0.49	0	15,19,21	0.64	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
6	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
9	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
6	BMA	K	1747	-	-	0/2/19/22	0/1/1/1
15	NDG	K	1749	3	-	0/6/23/26	0/1/1/1
15	NDG	L	1746	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1747	BMA	C1-O5-C5	-5.42	105.37	112.25
9	G	1651	MAN	C1-C2-C3	-4.09	104.70	109.54
6	K	1747	BMA	C1-C2-C3	-3.83	105.01	109.54
6	B	2646	BMA	C1-C2-C3	-3.40	105.52	109.54
9	G	1651	MAN	C1-O5-C5	-3.25	108.12	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	L	1746	NDG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	1651	MAN	1	0
15	K	1749	NDG	3	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 ⓘ

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%)	0.19	17 (2%) 58 46	87, 142, 190, 237	0
1	C	638/645 (98%)	0.14	14 (2%) 65 54	80, 127, 176, 228	0
1	E	638/645 (98%)	0.13	10 (1%) 74 64	84, 142, 196, 245	0
1	G	638/645 (98%)	0.45	61 (9%) 10 7	93, 180, 241, 267	0
2	B	901/915 (98%)	0.18	27 (2%) 54 40	91, 167, 229, 260	0
2	D	901/915 (98%)	0.20	28 (3%) 52 40	81, 155, 216, 266	0
2	F	900/915 (98%)	0.39	51 (5%) 27 19	96, 179, 284, 329	0
2	H	605/915 (66%)	0.40	37 (6%) 25 16	98, 162, 231, 294	0
3	I	507/507 (100%)	0.00	4 (0%) 87 81	93, 142, 197, 240	0
3	J	507/507 (100%)	0.15	17 (3%) 49 37	127, 170, 220, 261	0
3	K	507/507 (100%)	0.23	23 (4%) 37 27	132, 183, 230, 284	0
3	L	507/507 (100%)	-0.02	5 (0%) 84 77	101, 144, 194, 239	0
4	M	84/92 (91%)	-0.05	1 (1%) 81 72	87, 110, 186, 221	0
4	N	84/92 (91%)	-0.02	2 (2%) 62 50	97, 116, 189, 227	0
4	P	84/92 (91%)	-0.00	2 (2%) 62 50	100, 124, 176, 211	0
4	Q	84/92 (91%)	-0.09	2 (2%) 62 50	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.21	301 (3%) 45 34	80, 155, 228, 329	0

The worst 5 of 301 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	5.8
1	G	399	SER	5.7
2	F	1038	ARG	5.4

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](#)

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
16	NDG	L	1743	14/15	0.87	0.36	1.80	122,147,148,148	0
14	NDG	K	1743	14/15	0.87	0.28	0.75	174,204,206,207	0
12	NDG	I	1743	14/15	0.92	0.28	0.68	122,149,151,152	0
12	NDG	J	1743	14/15	0.90	0.27	0.33	158,188,189,189	0
7	NDG	C	1646	14/15	0.82	0.28	-0.76	163,191,192,193	0
5	NDG	E	1646	14/15	0.83	0.23	-0.92	174,204,206,206	0
8	NDG	F	2642	14/15	0.86	0.22	-1.27	169,193,194,194	0
5	NDG	A	1646	14/15	0.88	0.21	-2.67	156,185,187,188	0
7	NAG	G	1647	14/15	0.83	0.25	-	213,216,216,217	0
16	NAG	L	1744	14/15	0.85	0.43	-	185,187,189,189	0
12	NAG	J	1744	14/15	0.81	0.33	-	177,179,180,180	0
8	BMA	F	2644	11/12	0.84	0.15	-	232,233,234,234	0
5	NAG	A	1647	14/15	0.82	0.23	-	199,200,201,203	0
5	NAG	D	2643	14/15	0.88	0.21	-	200,201,202,203	0
5	BMA	A	1648	11/12	0.80	0.30	-	212,214,215,216	0
14	NAG	K	1744	14/15	0.83	0.27	-	196,199,201,202	0
5	NDG	B	2642	14/15	0.91	0.23	-	163,194,194,195	0
5	NDG	D	2642	14/15	0.89	0.20	-	147,176,178,179	0
8	BMA	F	2646	11/12	0.72	0.37	-	221,222,224,224	0
16	BMA	L	1745	11/12	0.76	0.24	-	197,201,202,202	0
14	MAN	K	1746	11/12	0.87	0.52	-	229,230,232,232	0
10	NDG	H	2642	14/15	0.90	0.21	-	183,213,214,215	0
7	BMA	C	1648	11/12	0.64	0.27	-	219,220,222,223	0
12	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	BMA	D	2645	11/12	0.86	0.28	-	229,232,233,234	0
5	BMA	E	1648	11/12	0.74	0.43	-	229,230,231,232	0
8	BMA	F	2645	11/12	0.83	0.23	-	248,249,249,250	0
7	BMA	G	1650	11/12	0.55	0.68	-	229,231,232,232	0
7	BMA	C	1650	11/12	0.70	0.33	-	231,233,235,235	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	MAN	J	1745	11/12	0.61	0.36	-	206,210,211,212	0
5	NAG	E	1647	14/15	0.83	0.21	-	223,225,227,227	0
7	NAG	C	1647	14/15	0.67	0.27	-	200,202,203,203	0
13	NAG	I	1747	14/15	0.63	0.66	-	222,223,224,224	0
12	NAG	I	1744	14/15	0.94	0.36	-	178,180,181,182	0
10	NAG	H	2643	14/15	0.82	0.26	-	221,222,224,225	0
10	MAN	H	2644	11/12	0.64	0.27	-	229,230,231,232	0
8	NAG	F	2643	14/15	0.91	0.21	-	200,202,204,204	0
5	NAG	B	2643	14/15	0.91	0.28	-	193,196,196,197	0
10	MAN	H	2645	11/12	0.68	0.61	-	234,236,237,238	0
5	BMA	B	2645	11/12	0.41	0.37	-	237,239,240,241	0
5	BMA	A	1649	11/12	0.83	0.44	-	226,227,228,228	0
13	NDG	I	1746	14/15	0.79	0.65	-	198,225,227,227	0
7	BMA	G	1649	11/12	0.59	0.37	-	226,228,229,230	0
5	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
14	MAN	K	1748	11/12	0.84	0.36	-	230,232,235,235	0
8	BMA	F	2647	11/12	0.70	0.50	-	214,215,217,217	0
14	MAN	K	1745	11/12	0.73	0.34	-	249,252,253,254	0
5	BMA	B	2644	11/12	0.39	0.35	-	218,220,222,223	0
5	BMA	D	2644	11/12	0.67	0.32	-	220,221,223,223	0
7	NDG	G	1646	14/15	0.90	0.16	-	198,201,208,215	0

6.4 Ligands ⓘ

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
11	MG	L	1742	1/1	0.91	0.25	0.53	127,127,127,127	0
11	MG	I	1742	1/1	0.42	0.17	-0.61	120,120,120,120	0
11	MG	K	1742	1/1	0.84	0.11	-0.92	138,138,138,138	0
11	MG	J	1742	1/1	0.82	0.07	-2.08	148,148,148,148	0
6	BMA	B	2646	11/12	0.66	0.51	-	198,200,200,201	0
6	BMA	K	1747	11/12	0.76	0.52	-	194,195,196,196	0
15	NDG	L	1746	14/15	0.87	0.56	-	176,204,205,205	0
9	MAN	G	1651	11/12	0.45	0.54	-	222,225,227,228	0
15	NDG	K	1749	14/15	0.76	0.47	-	184,214,216,217	0

6.5 Other polymers [i](#)

There are no such residues in this entry.