



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 12:54 PM BST

PDB ID : 2XWJ
Title : Crystal Structure of Complement C3b in Complex with Factor B
Authors : Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.
Deposited on : 2010-11-04
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

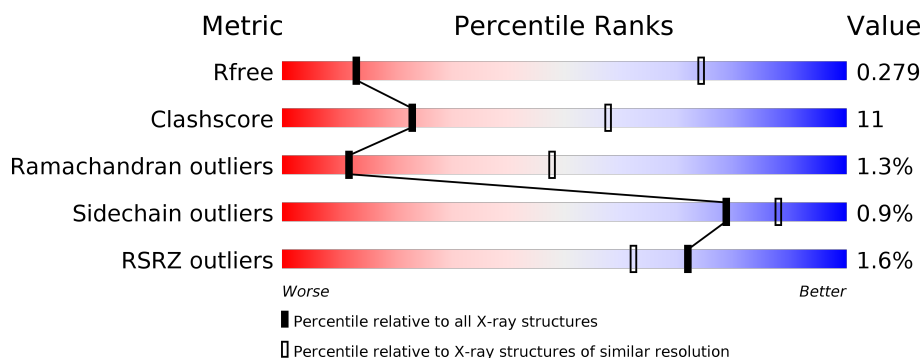
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	645	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	645	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div>.</div> </div> </div>
1	E	645	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>26%</div> <div>.</div> </div> </div>
1	G	645	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
2	B	915	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>
2	D	915	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	915	
2	H	915	
3	I	741	
3	J	741	
3	K	741	
3	L	741	

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	NAG	B	1917	-	-	-	X
4	NAG	F	1917	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 71260 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	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	C	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	E	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	G	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called COMPLEMENT C3 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	D	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	F	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	H	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	engineered mutation	UNP P01024
D	991	GLU	GLN	engineered mutation	UNP P01024
F	991	GLU	GLN	engineered mutation	UNP P01024
H	991	GLU	GLN	engineered mutation	UNP P01024

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	712	Total	C	N	O	S	0	0	0
			5593	3514	970	1076	33			
3	J	713	Total	C	N	O	S	0	0	0
			5596	3514	971	1078	33			
3	K	713	Total	C	N	O	S	0	0	0
			5603	3519	971	1080	33			
3	L	711	Total	C	N	O	S	0	0	0
			5588	3511	969	1075	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	740	ALA	-	expression tag	UNP P00751
I	741	ALA	-	expression tag	UNP P00751
I	254	GLY	ASP	engineered mutation	UNP P00751
I	260	ASP	ASN	engineered mutation	UNP P00751
J	740	ALA	-	expression tag	UNP P00751
J	741	ALA	-	expression tag	UNP P00751
J	254	GLY	ASP	engineered mutation	UNP P00751
J	260	ASP	ASN	engineered mutation	UNP P00751
K	740	ALA	-	expression tag	UNP P00751
K	741	ALA	-	expression tag	UNP P00751
K	254	GLY	ASP	engineered mutation	UNP P00751
K	260	ASP	ASN	engineered mutation	UNP P00751
L	740	ALA	-	expression tag	UNP P00751
L	741	ALA	-	expression tag	UNP P00751
L	254	GLY	ASP	engineered mutation	UNP P00751
L	260	ASP	ASN	engineered mutation	UNP P00751

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Ni	0	0
			1	1		
5	I	1	Total	Ni	0	0
			1	1		
5	L	1	Total	Ni	0	0
			1	1		
5	K	1	Total	Ni	0	0
			1	1		

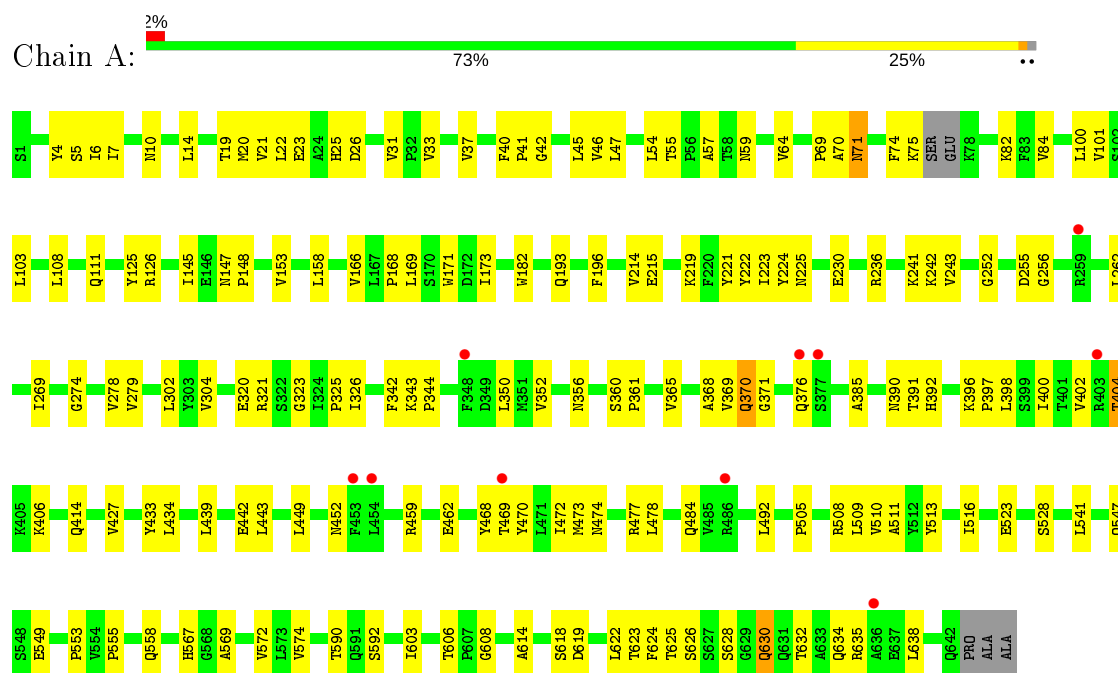
- Molecule 6 is water.

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

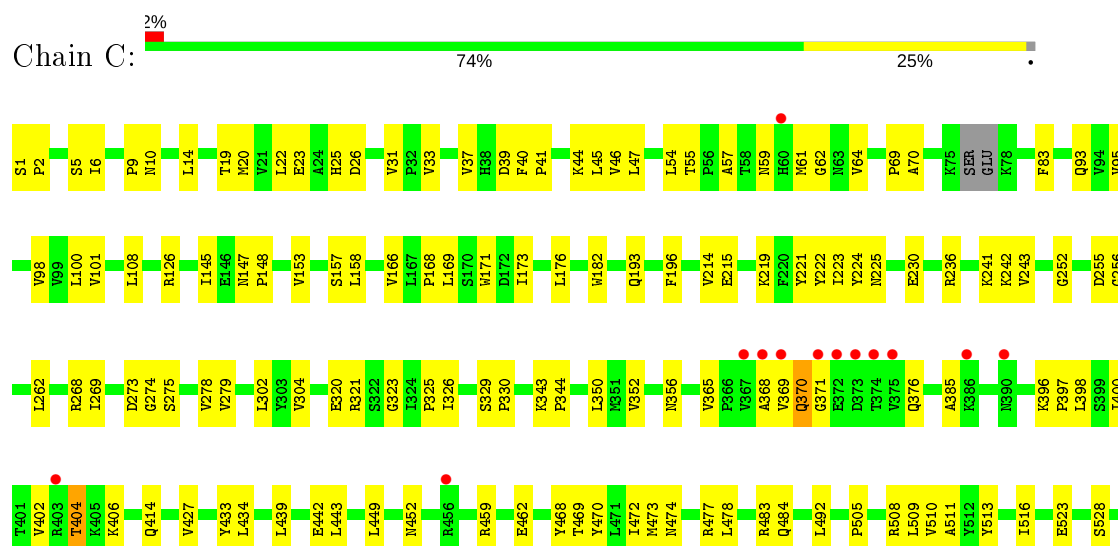
3 Residue-property plots

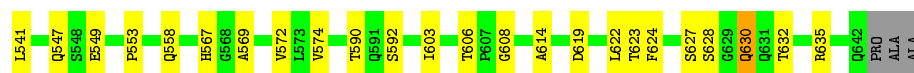
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COMPLEMENT C3 BETA CHAIN

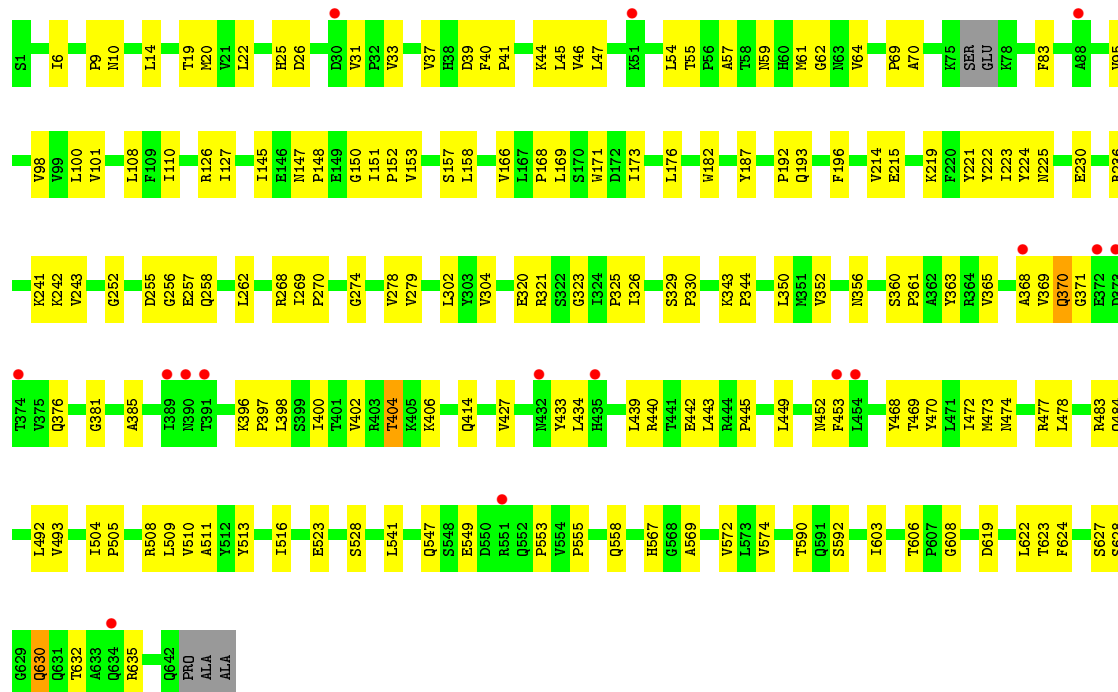
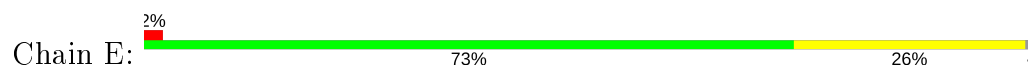


• Molecule 1: COMPLEMENT C3 BETA CHAIN

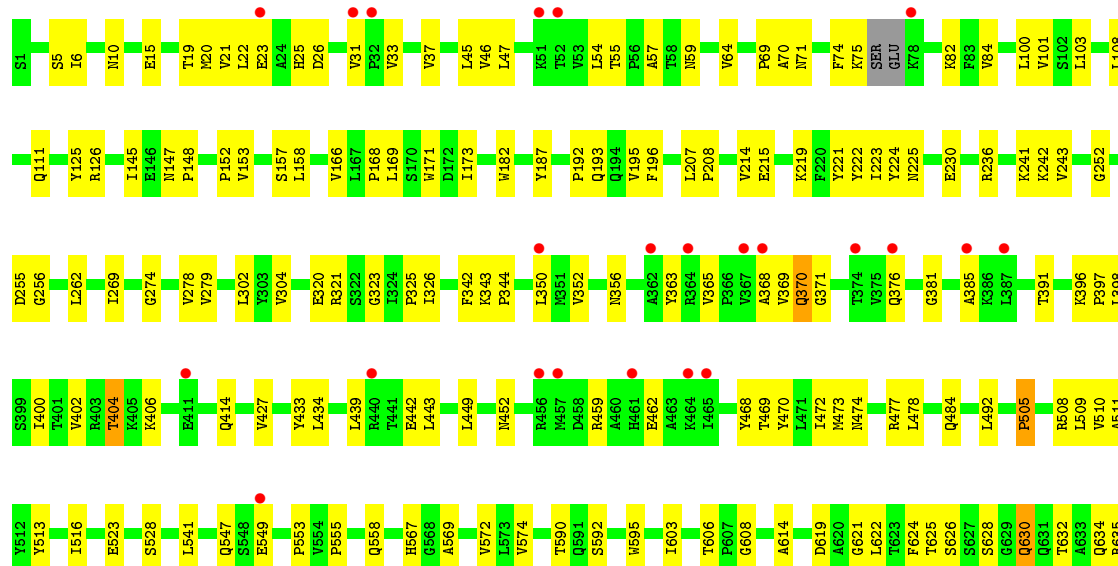
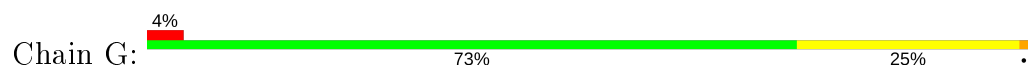


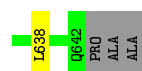


• Molecule 1: COMPLEMENT C3 BETA CHAIN

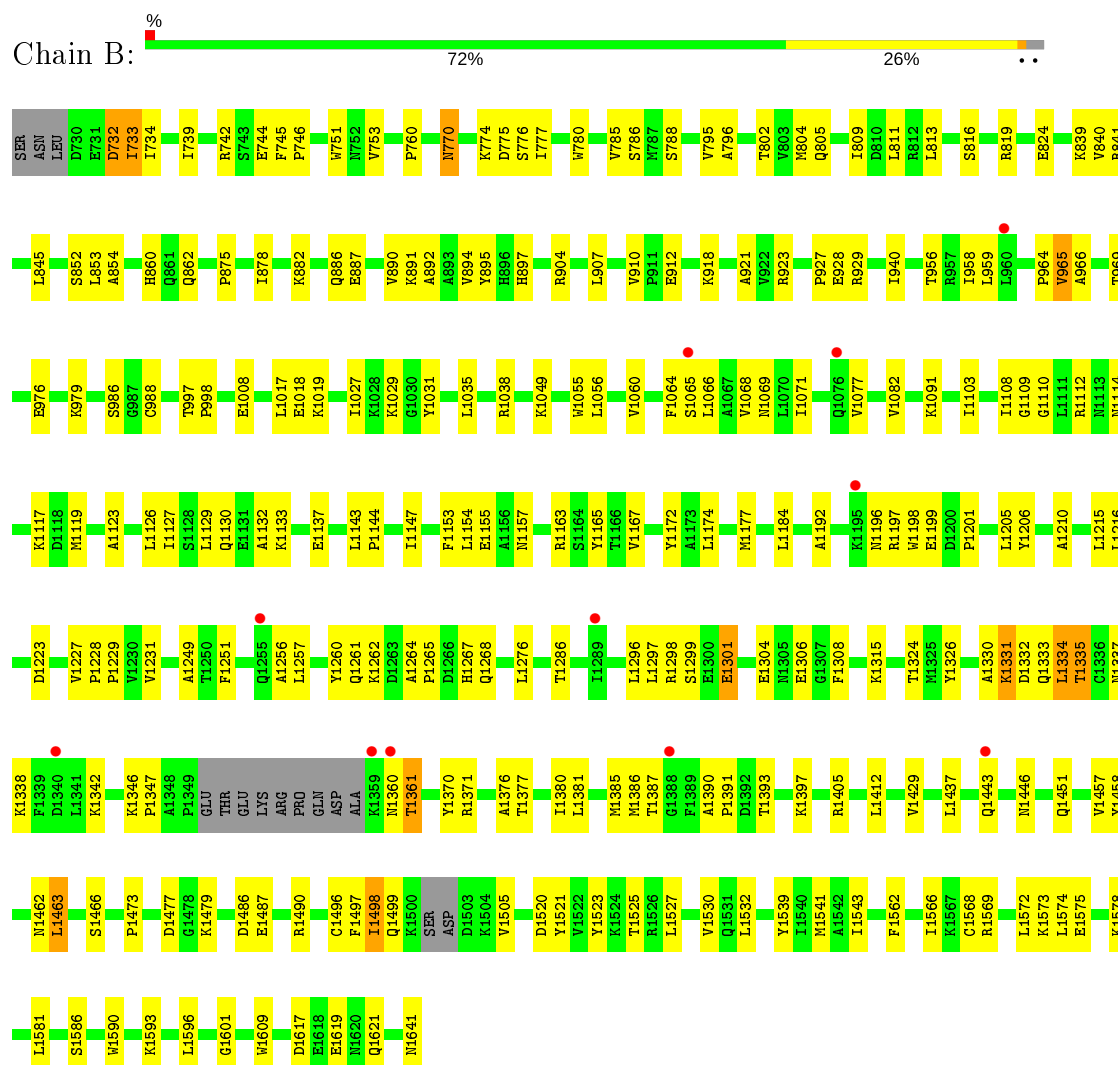


• Molecule 1: COMPLEMENT C3 BETA CHAIN

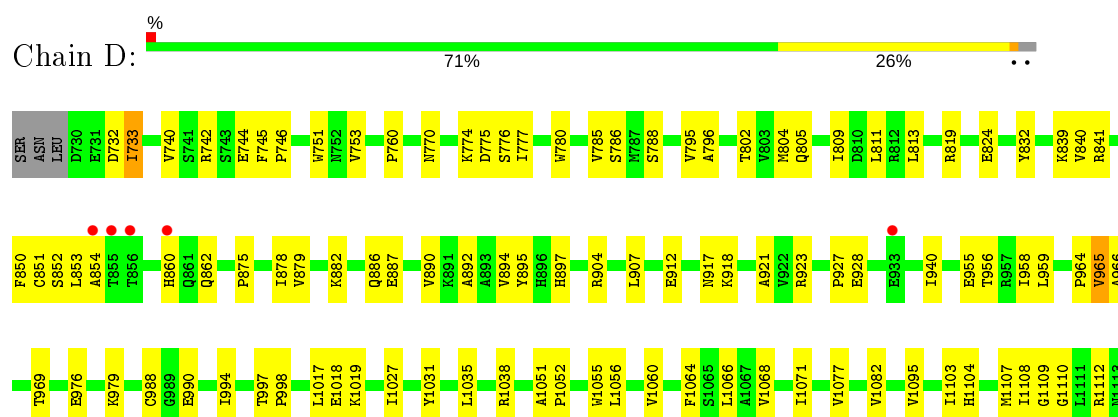


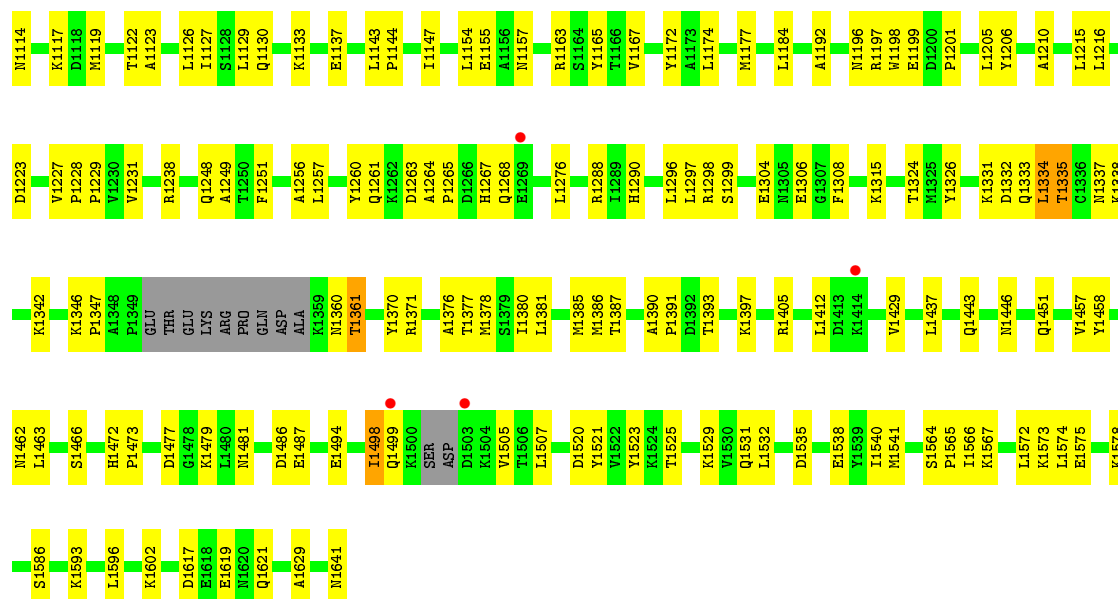


• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

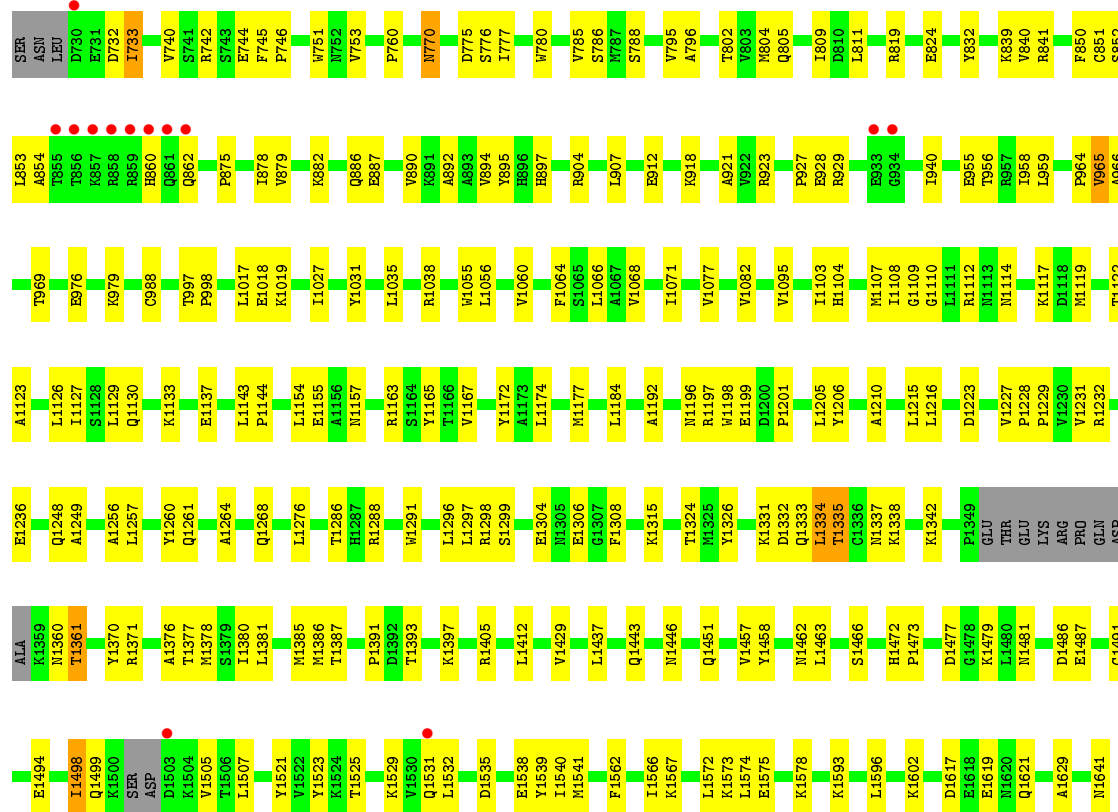


• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

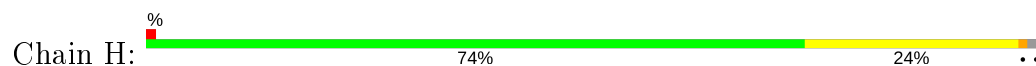


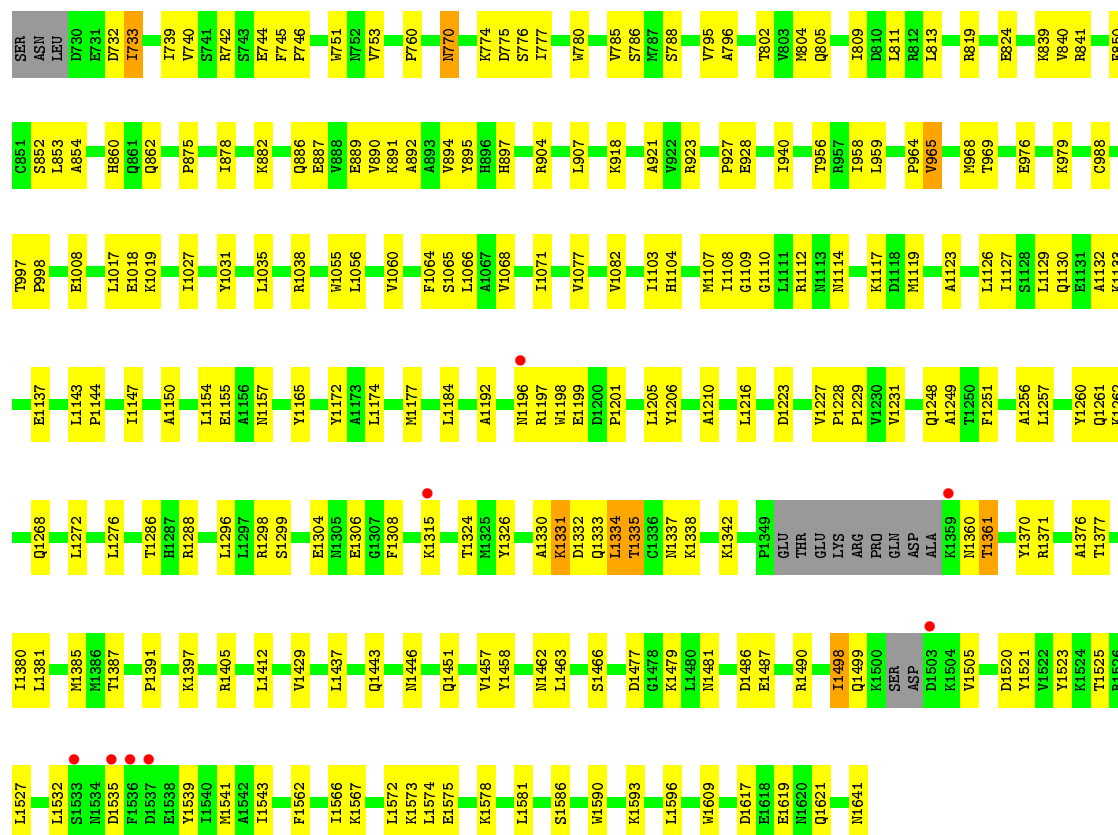


• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

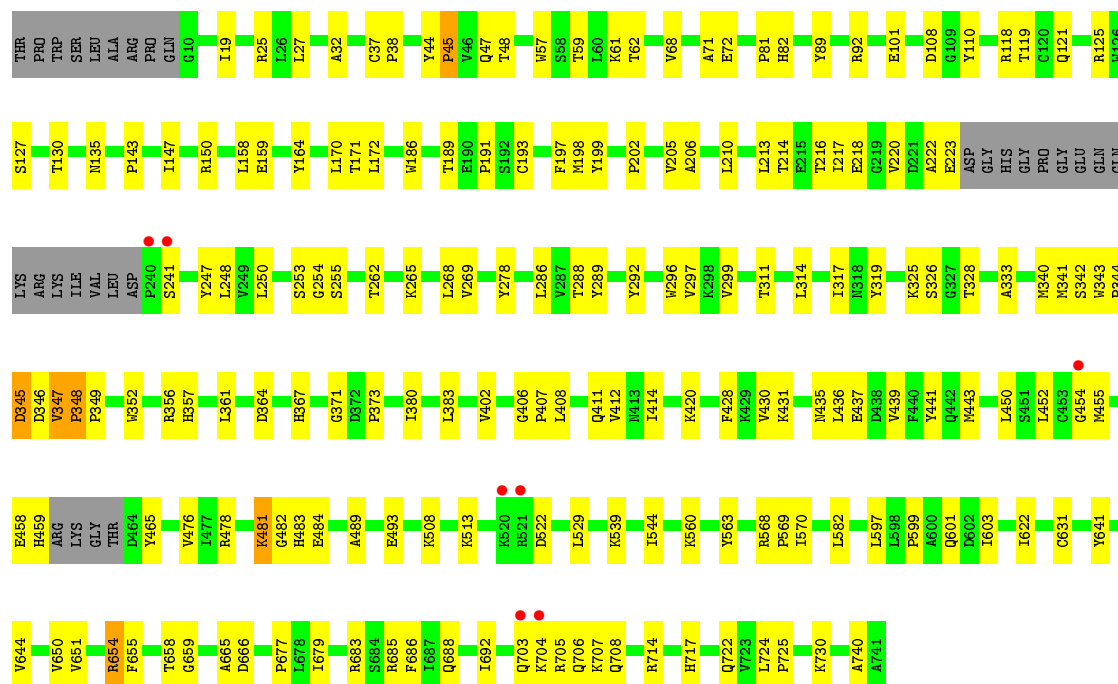


• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

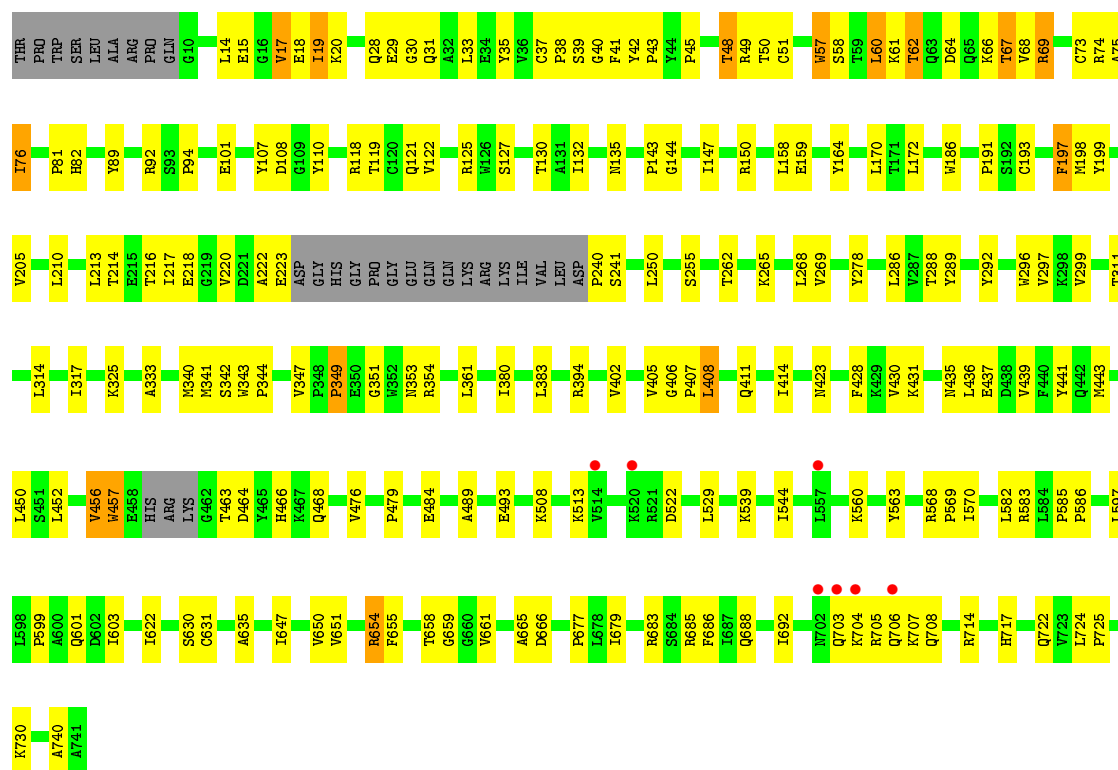




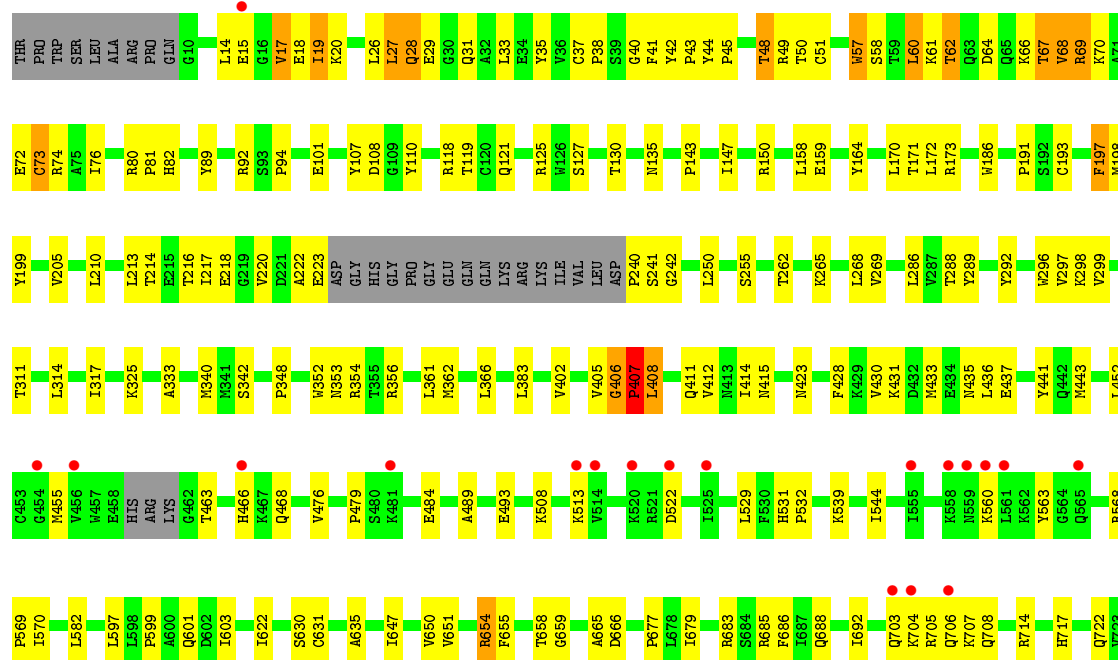
• Molecule 3: COMPLEMENT FACTOR B



• Molecule 3: COMPLEMENT FACTOR B

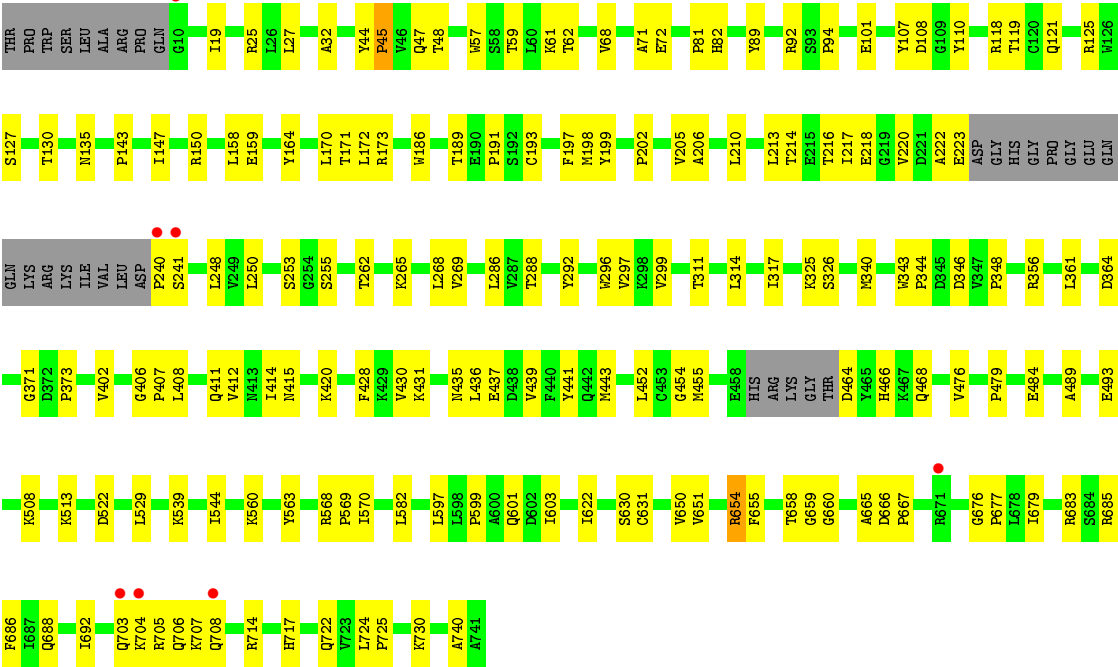


• Molecule 3: COMPLEMENT FACTOR B



L724
P725
K730
A740
A741

● Molecule 3: COMPLEMENT FACTOR B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	262.16Å 297.87Å 341.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.76 – 4.00 74.44 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (72.76-4.00) 93.2 (74.44-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 4.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.228 , 0.281 0.227 , 0.279	Depositor DCC
R_{free} test set	5250 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	71260	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4810e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NI, NAG

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	0/5092	0.37	0/6917
1	C	0.20	0/5092	0.36	0/6917
1	E	0.20	0/5092	0.36	0/6917
1	G	0.20	0/5092	0.36	0/6917
2	B	0.20	0/7340	0.35	0/9936
2	D	0.21	0/7340	0.35	0/9936
2	F	0.20	0/7340	0.35	0/9936
2	H	0.20	0/7340	0.35	0/9936
3	I	0.20	0/5717	0.36	0/7739
3	J	0.21	0/5720	0.36	0/7743
3	K	0.20	0/5727	0.36	0/7752
3	L	0.20	0/5712	0.34	0/7732
All	All	0.20	0/72604	0.35	0/98378

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
3	J	0	1
3	K	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	407	PRO	Peptide
3	K	407	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4992	0	5056	129	0
1	C	4992	0	5056	123	0
1	E	4992	0	5056	129	0
1	G	4992	0	5056	119	0
2	B	7197	0	7124	178	0
2	D	7197	0	7124	178	0
2	F	7197	0	7123	169	0
2	H	7197	0	7123	163	0
3	I	5593	0	5438	122	0
3	J	5596	0	5437	141	0
3	K	5603	0	5450	158	0
3	L	5588	0	5436	110	0
4	B	14	0	13	0	0
4	D	14	0	13	1	0
4	F	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	0	0
4	J	14	0	13	1	0
4	K	14	0	13	6	0
4	L	14	0	13	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
All	All	71260	0	70583	1615	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 11.

The worst 5 of 1615 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)
3:K:352:TRP:HZ2	4:K:1353:NAG:H82	1.05	1.19
2:F:964:PRO:HA	2:F:965:VAL:HB	1.28	1.15
2:D:964:PRO:HA	2:D:965:VAL:HB	1.27	1.13
2:H:964:PRO:HA	2:H:965:VAL:HB	1.26	1.13
1:G:69:PRO:HA	1:G:70:ALA:HB3	1.32	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/645 (99%)	574 (90%)	56 (9%)	6 (1%)	17	55
1	C	636/645 (99%)	575 (90%)	57 (9%)	4 (1%)	25	63
1	E	636/645 (99%)	573 (90%)	58 (9%)	5 (1%)	19	58
1	G	636/645 (99%)	578 (91%)	53 (8%)	5 (1%)	19	58
2	B	895/915 (98%)	785 (88%)	95 (11%)	15 (2%)	9	43
2	D	895/915 (98%)	787 (88%)	95 (11%)	13 (2%)	10	45
2	F	895/915 (98%)	785 (88%)	97 (11%)	13 (2%)	10	45
2	H	895/915 (98%)	790 (88%)	92 (10%)	13 (2%)	10	45
3	I	706/741 (95%)	636 (90%)	62 (9%)	8 (1%)	14	51
3	J	707/741 (95%)	630 (89%)	65 (9%)	12 (2%)	9	43
3	K	707/741 (95%)	627 (89%)	67 (10%)	13 (2%)	8	41
3	L	705/741 (95%)	641 (91%)	59 (8%)	5 (1%)	22	61
All	All	8949/9204 (97%)	7981 (89%)	856 (10%)	112 (1%)	12	48

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	733	ILE
2	B	965	VAL
2	B	1361	THR
2	D	733	ILE
2	D	965	VAL

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	564/567 (100%)	559 (99%)	5 (1%)	78	88
1	C	564/567 (100%)	559 (99%)	5 (1%)	78	88
1	E	564/567 (100%)	559 (99%)	5 (1%)	78	88
1	G	564/567 (100%)	559 (99%)	5 (1%)	78	88
2	B	797/810 (98%)	789 (99%)	8 (1%)	76	86
2	D	797/810 (98%)	791 (99%)	6 (1%)	81	89
2	F	797/810 (98%)	791 (99%)	6 (1%)	81	89
2	H	797/810 (98%)	791 (99%)	6 (1%)	81	89
3	I	616/643 (96%)	613 (100%)	3 (0%)	88	93
3	J	616/643 (96%)	605 (98%)	11 (2%)	59	77
3	K	618/643 (96%)	606 (98%)	12 (2%)	57	75
3	L	616/643 (96%)	614 (100%)	2 (0%)	92	95
All	All	7910/8080 (98%)	7836 (99%)	74 (1%)	78	88

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	1462	ASN
2	H	959	LEU
3	K	69	ARG
2	F	1573	LYS
1	G	404	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	770	ASN
1	G	87	GLN
3	K	591	GLN
2	F	835	ASN
2	F	1237	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1917	2	14,14,15	0.51	0	17,19,21	0.86	0
4	NAG	J	1353	3	14,14,15	0.53	0	17,19,21	0.66	0
4	NAG	B	1917	2	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
4	NAG	I	1353	3	14,14,15	0.42	0	17,19,21	1.30	1 (5%)
4	NAG	K	1353	3	14,14,15	0.57	0	17,19,21	1.98	3 (17%)
4	NAG	D	1917	2	14,14,15	0.50	0	17,19,21	1.18	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1917	2	14,14,15	0.48	0	17,19,21	1.17	2 (11%)
4	NAG	L	1353	3	14,14,15	0.54	0	17,19,21	0.63	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
4	NAG	F	1917	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1353	3	-	0/6/23/26	0/1/1/1
4	NAG	B	1917	2	-	3/6/23/26	0/1/1/1
4	NAG	I	1353	3	-	3/6/23/26	0/1/1/1
4	NAG	K	1353	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1917	2	-	2/6/23/26	0/1/1/1
4	NAG	H	1917	2	-	1/6/23/26	0/1/1/1
4	NAG	L	1353	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1353	NAG	C2-N2-C7	-6.11	114.20	122.90
4	I	1353	NAG	C1-O5-C5	4.34	118.08	112.19
4	D	1917	NAG	C2-N2-C7	-3.62	117.75	122.90
4	K	1353	NAG	O5-C1-C2	-3.56	105.67	111.29
4	K	1353	NAG	C1-C2-N2	3.37	116.25	110.49

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1353	NAG	C8-C7-N2-C2
4	K	1353	NAG	O7-C7-N2-C2
4	D	1917	NAG	C8-C7-N2-C2
4	D	1917	NAG	O7-C7-N2-C2
4	I	1353	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1353	NAG	1	0
4	K	1353	NAG	6	0
4	D	1917	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	640/645 (99%)	0.23	10 (1%) 72 62	68, 145, 225, 312	0
1	C	640/645 (99%)	0.13	13 (2%) 65 56	64, 139, 220, 312	0
1	E	640/645 (99%)	0.10	16 (2%) 57 47	69, 140, 221, 313	0
1	G	640/645 (99%)	0.23	23 (3%) 42 34	69, 146, 224, 313	0
2	B	901/915 (98%)	-0.01	11 (1%) 79 70	48, 112, 181, 342	0
2	D	901/915 (98%)	-0.09	9 (0%) 82 74	44, 110, 191, 351	0
2	F	901/915 (98%)	-0.11	13 (1%) 75 65	52, 112, 189, 337	0
2	H	901/915 (98%)	-0.03	8 (0%) 84 77	47, 112, 183, 341	0
3	I	712/741 (96%)	-0.15	7 (0%) 82 74	46, 113, 180, 276	0
3	J	713/741 (96%)	-0.09	7 (0%) 82 74	42, 110, 197, 343	0
3	K	713/741 (96%)	-0.01	19 (2%) 54 44	43, 112, 201, 357	0
3	L	711/741 (95%)	-0.13	7 (0%) 82 74	45, 112, 181, 276	0
All	All	9013/9204 (97%)	-0.01	143 (1%) 72 62	42, 119, 202, 357	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1065	SER	5.9
1	C	372	GLU	5.7
2	H	1536	PHE	5.0
2	F	860	HIS	5.0
1	C	368	ALA	4.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	K	1353	14/15	0.67	0.33	124,166,186,214	0
4	NAG	F	1917	14/15	0.71	0.45	155,176,239,261	0
4	NAG	H	1917	14/15	0.72	0.34	95,176,221,230	0
4	NAG	D	1917	14/15	0.73	0.37	103,150,180,210	0
4	NAG	B	1917	14/15	0.73	0.43	142,178,199,206	0
4	NAG	L	1353	14/15	0.77	0.34	105,162,190,209	0
4	NAG	J	1353	14/15	0.84	0.27	107,156,170,179	0
4	NAG	I	1353	14/15	0.85	0.23	111,169,185,187	0
5	NI	I	1742	1/1	0.95	0.24	209,209,209,209	0
5	NI	L	1742	1/1	0.99	0.11	85,85,85,85	0
5	NI	K	1742	1/1	1.00	0.17	102,102,102,102	0
5	NI	J	1742	1/1	1.00	0.12	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.