



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2017 – 10:57 AM EDT

PDB ID : 5M6W  
Title : Properdin in complex with alternative pathway C3 convertase  
Authors : Pedersen, D.V.; Andersen, G.R.  
Deposited on : unknown  
Resolution : 6.00 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](mailto: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.

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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-20029824
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-20029824

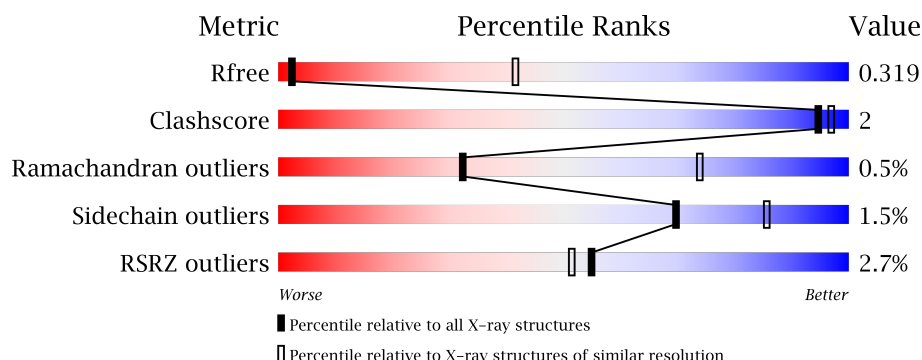
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 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.



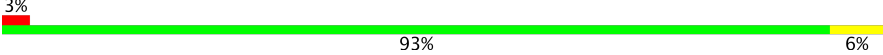
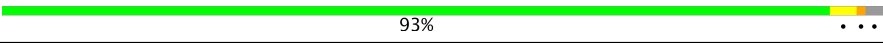

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1085 (8.30-3.70)
Clashscore	112137	1017 (8.20-3.80)
Ramachandran outliers	110173	1001 (8.20-3.72)
Sidechain outliers	110143	1085 (8.30-3.70)
RSRZ outliers	101464	1094 (8.30-3.70)

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  $\geq 3$ , 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>0.1%</div> <div>95%</div> <div>5%</div> </div>
1	G	645	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
2	B	913	<div> <div>0.1%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
2	H	913	<div> <div>5%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>
3	J	505	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	505	 3% 93% 6%
4	N	86	 93% 6% ...
4	Q	86	 91% 7% •

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	NAG	G	701	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34440 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			
1	G	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			
2	H	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			

- Molecule 3 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			
3	L	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	254	GLY	ASP	conflict	UNP P00751
J	674	ALA	SER	conflict	UNP P00751
L	254	GLY	ASP	conflict	UNP P00751
L	674	ALA	SER	conflict	UNP P00751

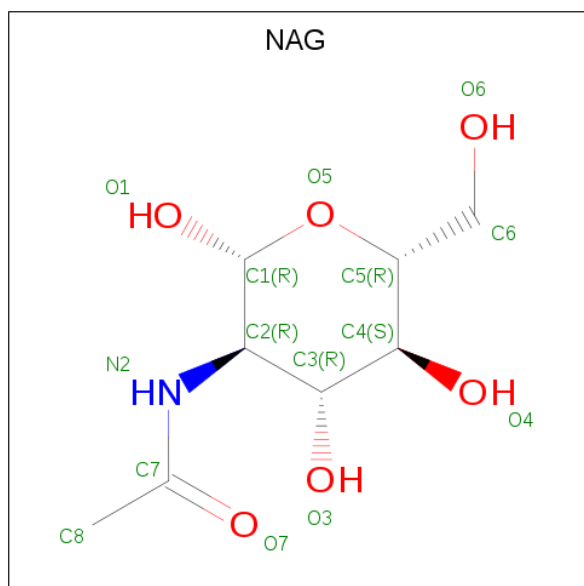
- Molecule 4 is a protein called Staphylococcal complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			
4	Q	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	0	GLY	-	expression tag	UNP Q6GFB4
Q	0	GLY	-	expression tag	UNP Q6GFB4

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



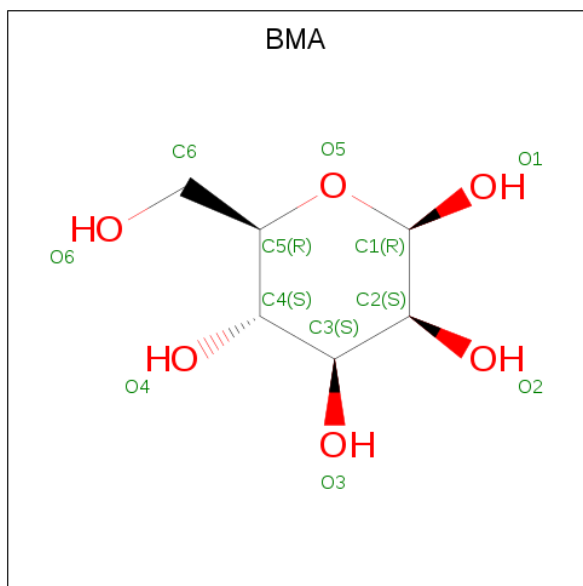
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



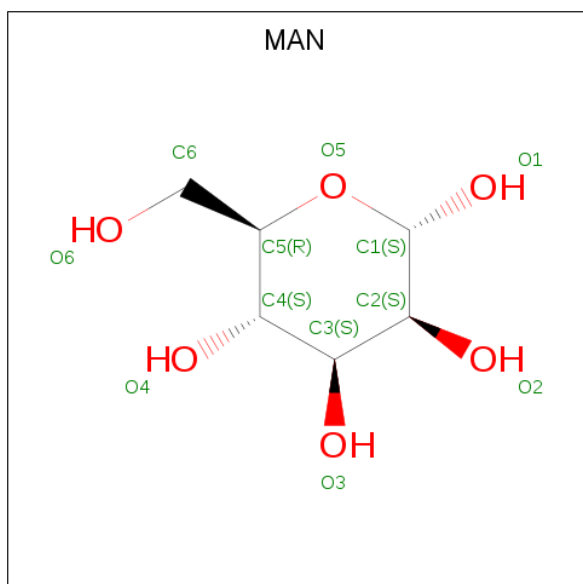
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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	G	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

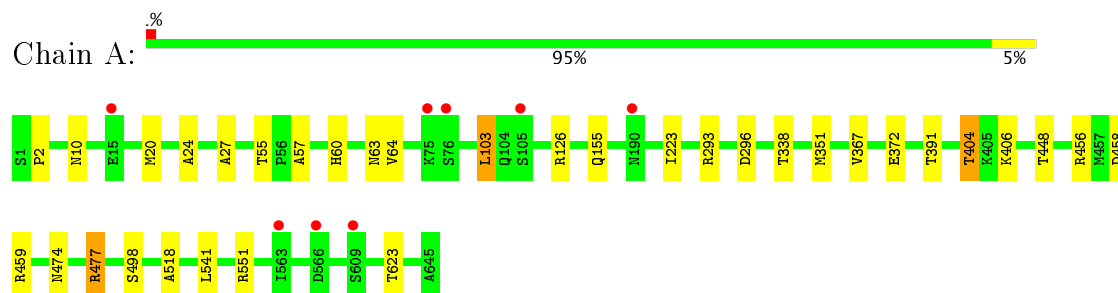
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		



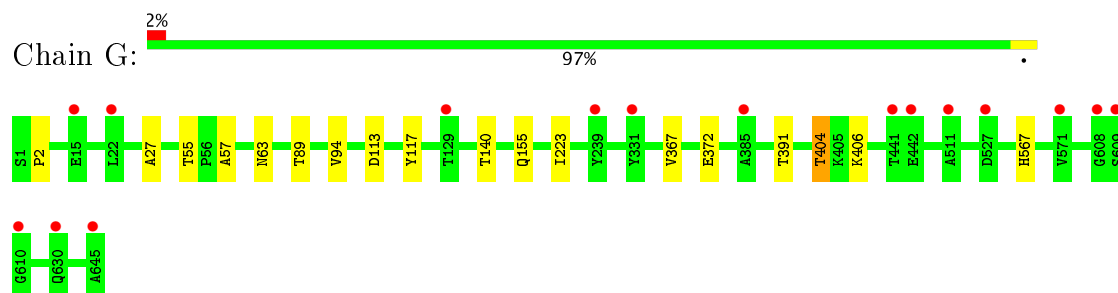
### 3 Residue-property plots [i](#)

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.

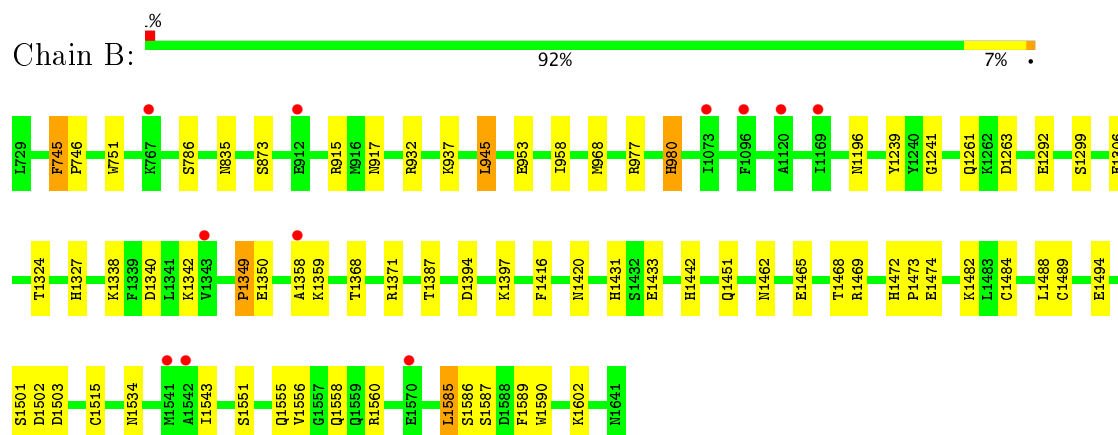
#### • Molecule 1: Complement C3



#### • Molecule 1: Complement C3

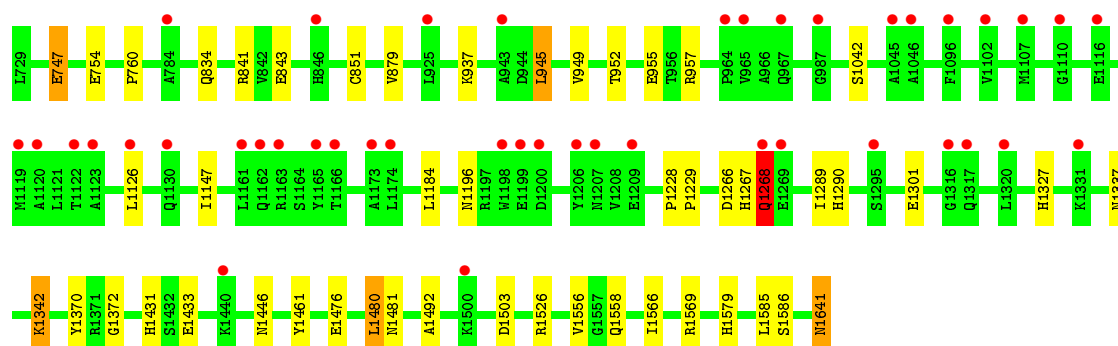


#### • Molecule 2: Complement C3

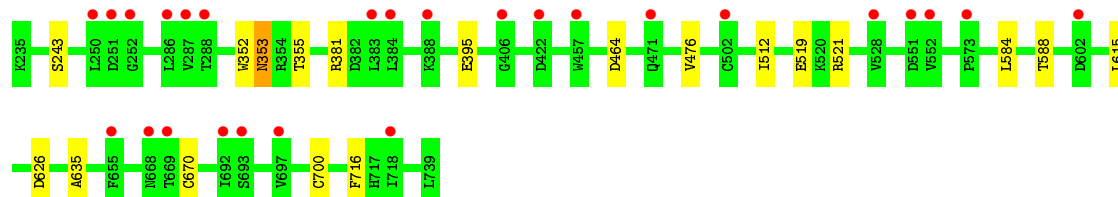


#### • Molecule 2: Complement C3

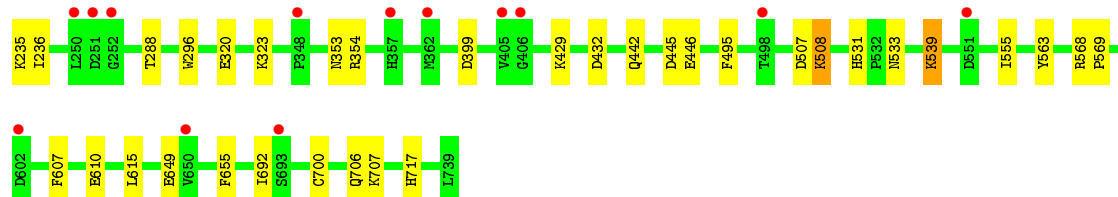




- Molecule 3: Complement factor B



- Molecule 3: Complement factor B



- Molecule 4: Staphylococcal complement inhibitor



- Molecule 4: Staphylococcal complement inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	634.87Å 121.98Å 264.42Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	48.76 – 6.00 48.76 – 5.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.76-6.00) 94.0 (48.76-5.00)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 5.10Å)	Xtriage
Refinement program	PHENIX dev_2614	Depositor
R, $R_{free}$	0.289 , 0.322 0.281 , 0.319	Depositor DCC
$R_{free}$ test set	1172 reflections (2.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	248.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 230.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.098 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	34440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	354.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [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, 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	0.28	0/5127	0.54	1/6966 (0.0%)
1	G	0.27	0/5127	0.52	0/6966
2	B	0.27	0/7439	0.53	0/10073
2	H	0.27	0/7439	0.53	0/10073
3	J	0.26	0/4095	0.50	0/5542
3	L	0.27	0/4095	0.51	1/5542 (0.0%)
4	N	0.25	0/691	0.44	0/923
4	Q	0.26	0/691	0.46	0/923
All	All	0.27	0/34704	0.52	2/47008 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	700	CYS	CA-CB-SG	5.56	124.01	114.00
1	A	518	ALA	CB-CA-C	5.12	117.78	110.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5025	0	5084	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5025	0	5084	6	0
2	B	7293	0	7217	28	0
2	H	7293	0	7216	22	0
3	J	4007	0	3996	13	0
3	L	4007	0	3996	20	0
4	N	683	0	697	2	0
4	Q	683	0	697	3	0
5	A	28	0	24	0	0
5	B	28	0	24	0	0
5	G	28	0	24	0	0
5	H	28	0	24	0	0
5	J	56	0	48	2	0
5	L	56	0	48	0	0
6	A	11	0	9	0	0
6	B	11	0	9	0	0
6	G	11	0	8	0	0
6	H	11	0	8	0	0
6	J	22	0	20	0	0
6	L	22	0	20	0	0
7	A	22	0	19	0	0
7	B	22	0	19	0	0
7	G	33	0	29	0	0
7	H	33	0	29	0	0
8	B	1	0	0	0	0
8	H	1	0	0	0	0
All	All	34440	0	34349	106	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 2.

The worst 5 of 106 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:L:508:LYS:NZ	3:L:508:LYS:HA	1.96	0.80
2:H:957:ARG:NH1	2:H:1301:GLU:OE2	2.28	0.67
2:B:1494:GLU:HB3	2:B:1602:LYS:HB3	1.78	0.66
3:L:508:LYS:HZ2	3:L:508:LYS:HA	1.64	0.63
3:L:353:ASN:OD1	3:L:354:ARG:N	2.32	0.62

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	643/645 (100%)	621 (97%)	21 (3%)	1 (0%)	51	84
1	G	643/645 (100%)	620 (96%)	22 (3%)	1 (0%)	51	84
2	B	911/913 (100%)	859 (94%)	40 (4%)	12 (1%)	14	55
2	H	911/913 (100%)	860 (94%)	45 (5%)	6 (1%)	25	68
3	J	503/505 (100%)	480 (95%)	23 (5%)	0	100	100
3	L	503/505 (100%)	480 (95%)	22 (4%)	1 (0%)	51	84
4	N	82/86 (95%)	81 (99%)	0	1 (1%)	15	57
4	Q	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
All	All	4278/4298 (100%)	4081 (95%)	175 (4%)	22 (0%)	32	74

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	968	MET
2	H	1268	GLN
4	N	7	SER
2	B	945	LEU
2	B	1349	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/567 (100%)	557 (98%)	10 (2%)	64	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	567/567 (100%)	560 (99%)	7 (1%)	75	88
2	B	808/808 (100%)	791 (98%)	17 (2%)	59	80
2	H	808/808 (100%)	791 (98%)	17 (2%)	59	80
3	J	444/444 (100%)	443 (100%)	1 (0%)	94	97
3	L	444/444 (100%)	441 (99%)	3 (1%)	87	93
4	N	76/77 (99%)	75 (99%)	1 (1%)	73	87
4	Q	76/77 (99%)	75 (99%)	1 (1%)	73	87
All	All	3790/3792 (100%)	3733 (98%)	57 (2%)	70	85

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1560	ARG
1	G	391	THR
3	L	442	GLN
2	B	1585	LEU
1	G	140	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	862	GLN
2	H	1196	ASN
3	L	459	HIS
1	G	132	HIS
3	L	466	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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	NAG	A	701	1,5	14,14,15	1.24	1 (7%)	15,19,21	2.01	2 (13%)
5	NAG	A	702	5,6	14,14,15	0.21	0	15,19,21	0.43	0
6	BMA	A	703	5,7	11,11,12	0.65	0	13,15,17	0.68	0
7	MAN	A	704	7,6	11,11,12	0.73	0	13,15,17	1.08	2 (15%)
7	MAN	A	705	7	11,11,12	0.66	0	13,15,17	1.17	2 (15%)
5	NAG	B	1702	2,5	14,14,15	1.10	1 (7%)	15,19,21	0.67	0
5	NAG	B	1703	5,6	14,14,15	0.38	0	15,19,21	0.39	0
6	BMA	B	1704	5,7	11,11,12	0.54	0	13,15,17	0.76	0
7	MAN	B	1705	7,6	11,11,12	0.82	0	13,15,17	1.03	2 (15%)
7	MAN	B	1706	7	11,11,12	0.70	0	13,15,17	1.19	2 (15%)
5	NAG	G	701	1,5	14,14,15	0.89	1 (7%)	15,19,21	2.18	2 (13%)
5	NAG	G	702	5,6	14,14,15	0.25	0	15,19,21	0.42	0
6	BMA	G	703	5,7	11,11,12	1.36	2 (18%)	13,15,17	1.59	1 (7%)
7	MAN	G	704	7,6	11,11,12	0.82	0	13,15,17	1.05	2 (15%)
7	MAN	G	705	7	11,11,12	0.71	0	13,15,17	1.20	2 (15%)
7	MAN	G	706	6	11,11,12	1.06	0	13,15,17	1.17	2 (15%)
5	NAG	H	1702	2,5	14,14,15	1.10	1 (7%)	15,19,21	1.12	2 (13%)
5	NAG	H	1703	5,6	14,14,15	0.39	0	15,19,21	0.44	0
6	BMA	H	1704	5,7	11,11,12	1.43	2 (18%)	13,15,17	1.57	2 (15%)
7	MAN	H	1705	7,6	11,11,12	0.83	0	13,15,17	1.05	2 (15%)
7	MAN	H	1706	7	11,11,12	0.70	0	13,15,17	1.19	2 (15%)
7	MAN	H	1707	6	11,11,12	0.91	0	13,15,17	1.05	1 (7%)
5	NAG	J	801	3,5	14,14,15	0.45	0	15,19,21	0.66	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	J	802	5,6	14,14,15	0.28	0	15,19,21	0.44	0
6	BMA	J	803	5	11,11,12	0.63	0	13,15,17	0.75	0
5	NAG	J	804	3,5	14,14,15	0.58	0	15,19,21	0.90	1 (6%)
5	NAG	J	805	5,6	14,14,15	0.31	0	15,19,21	0.44	0
6	BMA	J	806	5	11,11,12	0.57	0	13,15,17	0.73	0
5	NAG	L	801	3,5	14,14,15	0.39	0	15,19,21	0.70	0
5	NAG	L	802	5,6	14,14,15	0.33	0	15,19,21	0.43	0
6	BMA	L	803	5	11,11,12	0.61	0	13,15,17	0.75	0
5	NAG	L	804	3,5	14,14,15	0.30	0	15,19,21	0.64	0
5	NAG	L	805	5,6	14,14,15	0.21	0	15,19,21	0.42	0
6	BMA	L	806	5	11,11,12	0.57	0	13,15,17	0.74	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	NAG	A	701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	704	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	705	7	-	0/2/19/22	0/1/1/1
5	NAG	B	1702	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1703	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	1704	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	1705	7,6	-	0/2/19/22	0/1/1/1
7	MAN	B	1706	7	-	0/2/19/22	0/1/1/1
5	NAG	G	701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	704	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	705	7	-	0/2/19/22	0/1/1/1
7	MAN	G	706	6	-	0/2/19/22	0/1/1/1
5	NAG	H	1702	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	1703	5,6	-	0/6/23/26	0/1/1/1
6	BMA	H	1704	5,7	-	0/2/19/22	0/1/1/1
7	MAN	H	1705	7,6	-	0/2/19/22	0/1/1/1
7	MAN	H	1706	7	-	0/2/19/22	0/1/1/1
7	MAN	H	1707	6	-	0/2/19/22	0/1/1/1
5	NAG	J	801	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	802	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	J	803	5	-	0/2/19/22	0/1/1/1
5	NAG	J	804	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	805	5,6	-	0/6/23/26	0/1/1/1
6	BMA	J	806	5	-	0/2/19/22	0/1/1/1
5	NAG	L	801	3,5	-	0/6/23/26	0/1/1/1
5	NAG	L	802	5,6	-	0/6/23/26	0/1/1/1
6	BMA	L	803	5	-	0/2/19/22	0/1/1/1
5	NAG	L	804	3,5	-	0/6/23/26	0/1/1/1
5	NAG	L	805	5,6	-	0/6/23/26	0/1/1/1
6	BMA	L	806	5	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1702	NAG	O5-C1	-3.99	1.37	1.43
5	H	1702	NAG	O5-C1	-3.70	1.37	1.43
6	G	703	BMA	C2-C3	-2.33	1.49	1.52
6	H	1704	BMA	C2-C3	-2.06	1.49	1.52
6	G	703	BMA	C4-C3	2.36	1.58	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	703	BMA	O4-C4-C3	-3.84	102.01	110.36
6	H	1704	BMA	O4-C4-C3	-3.30	103.17	110.36
5	A	701	NAG	C3-C4-C5	-2.66	105.53	110.22
7	H	1707	MAN	O2-C2-C3	-2.42	105.43	110.17
7	G	705	MAN	O2-C2-C3	-2.40	105.46	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	804	NAG	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	645/645 (100%)	-0.14	8 (1%) 79 74	228, 295, 420, 581	0
1	G	645/645 (100%)	0.04	16 (2%) 58 54	260, 323, 447, 696	0
2	B	913/913 (100%)	0.06	11 (1%) 79 74	235, 333, 474, 719	0
2	H	913/913 (100%)	0.23	43 (4%) 32 33	262, 385, 578, 735	0
3	J	505/505 (100%)	0.15	26 (5%) 29 31	281, 380, 526, 634	0
3	L	505/505 (100%)	-0.02	13 (2%) 56 53	244, 316, 440, 573	0
4	N	84/86 (97%)	-0.19	0 100 100	247, 303, 418, 488	0
4	Q	84/86 (97%)	-0.22	0 100 100	261, 304, 448, 568	0
All	All	4294/4298 (99%)	0.06	117 (2%) 55 51	228, 335, 503, 735	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1199	GLU	6.2
1	G	610	GLY	6.2
1	G	609	SER	5.5
3	J	422	ASP	4.9
3	L	405	VAL	4.5

### 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 ⓘ

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	G	701	14/15	0.64	0.56	2.17	557,557,557,557	0
5	NAG	L	801	14/15	0.82	0.28	-0.42	557,557,557,557	0
5	NAG	J	801	14/15	0.88	0.19	-1.11	557,557,557,557	0
8	MG	B	1701	1/1	0.99	0.09	-1.17	328,328,328,328	0
8	MG	H	1701	1/1	0.83	0.08	-1.50	390,390,390,390	0
7	MAN	B	1705	11/12	0.77	0.51	-	557,557,557,557	0
7	MAN	H	1705	11/12	0.75	0.41	-	557,557,557,557	0
6	BMA	J	806	11/12	0.82	0.17	-	557,557,557,557	0
5	NAG	B	1703	14/15	0.79	0.50	-	557,557,557,557	0
5	NAG	B	1702	14/15	0.81	0.31	-	557,557,557,557	0
7	MAN	A	704	11/12	0.44	0.71	-	862,862,862,862	0
5	NAG	J	805	14/15	0.93	0.42	-	557,557,557,557	0
5	NAG	J	802	14/15	0.78	0.42	-	557,557,557,557	0
5	NAG	G	702	14/15	0.90	0.54	-	557,557,557,557	0
6	BMA	G	703	11/12	0.54	0.30	-	557,557,557,557	0
7	MAN	G	705	11/12	0.71	0.78	-	557,557,557,557	0
7	MAN	H	1707	11/12	0.90	0.65	-	557,557,557,557	0
7	MAN	H	1706	11/12	0.68	0.45	-	557,557,557,557	0
5	NAG	J	804	14/15	0.90	0.33	-	557,557,557,557	0
5	NAG	H	1702	14/15	0.83	0.27	-	557,557,557,557	0
7	MAN	G	704	11/12	0.59	0.44	-	557,557,557,557	0
6	BMA	H	1704	11/12	0.71	0.20	-	557,557,557,557	0
7	MAN	B	1706	11/12	0.82	0.37	-	557,557,557,557	0
5	NAG	A	701	14/15	0.63	0.62	-	862,862,862,862	0
5	NAG	L	805	14/15	0.78	0.45	-	557,557,557,557	0
7	MAN	A	705	11/12	-0.13	1.04	-	862,862,862,862	0
5	NAG	A	702	14/15	0.63	0.58	-	862,862,862,862	0
6	BMA	B	1704	11/12	0.63	0.46	-	557,557,557,557	0
5	NAG	L	804	14/15	0.89	0.35	-	557,557,557,557	0
6	BMA	L	806	11/12	0.06	0.32	-	557,557,557,557	0
6	BMA	A	703	11/12	0.50	0.50	-	862,862,862,862	0
6	BMA	L	803	11/12	0.72	0.19	-	557,557,557,557	0
6	BMA	J	803	11/12	0.48	0.39	-	557,557,557,557	0
5	NAG	L	802	14/15	0.72	0.34	-	557,557,557,557	0
5	NAG	H	1703	14/15	0.74	0.28	-	557,557,557,557	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MAN	G	706	11/12	0.43	0.69	-	557,557,557,557	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.