



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:51 PM 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 full wwPDB validation 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/ValidationPDFNotes.html>

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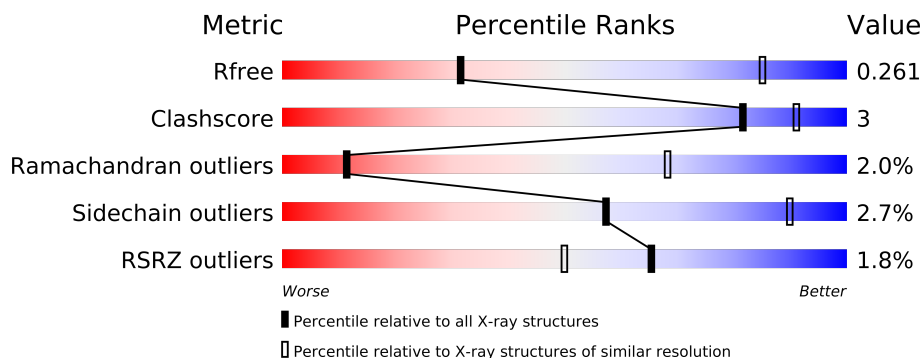
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	645	
1	C	645	
1	E	645	
1	G	645	
2	B	915	
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	

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Mol	Chain	Length	Quality of chain
4	P	92	
4	Q	92	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 67989 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

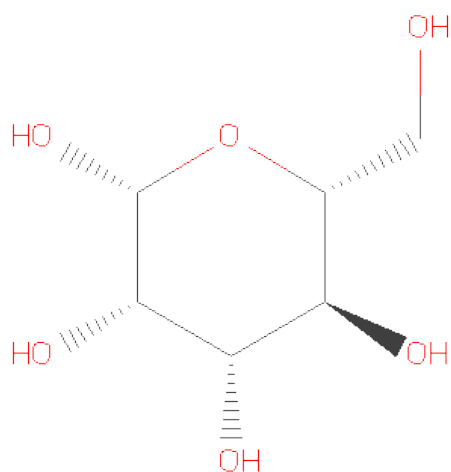
- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

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: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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		

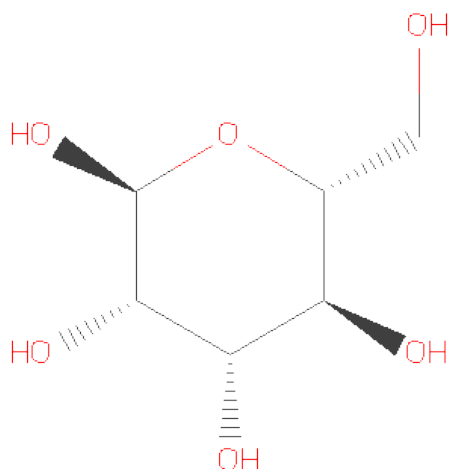
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

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: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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		

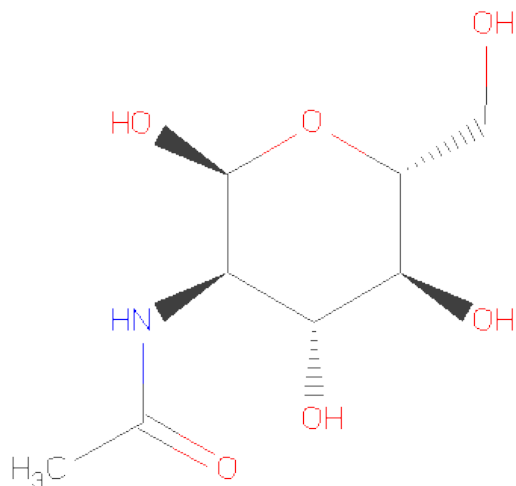
- Molecule 13 is a polymer of unknown type called SUGAR (2-MER).

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: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

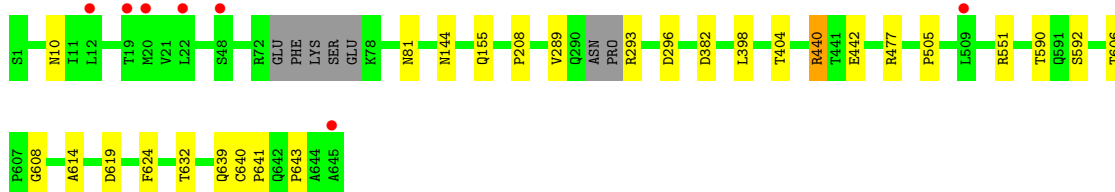


### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

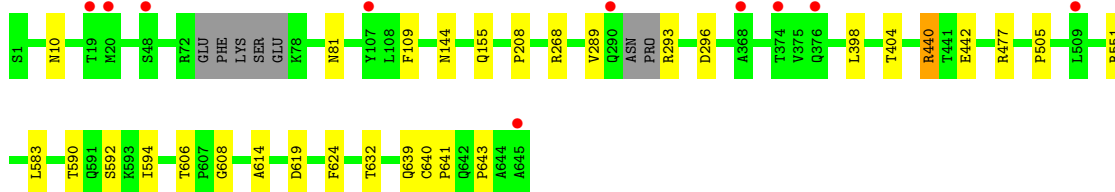
#### • Molecule 1: COMPLEMENT C3 BETA CHAIN

Chain A: 



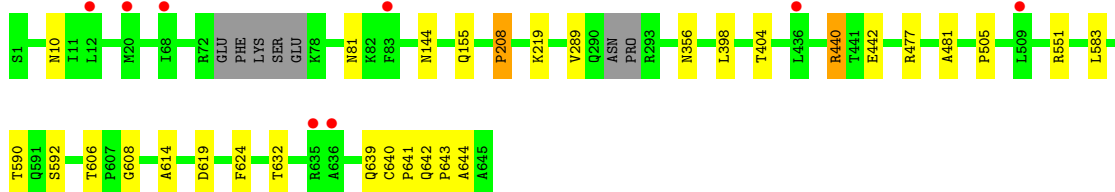
#### • Molecule 1: COMPLEMENT C3 BETA CHAIN

Chain C: 



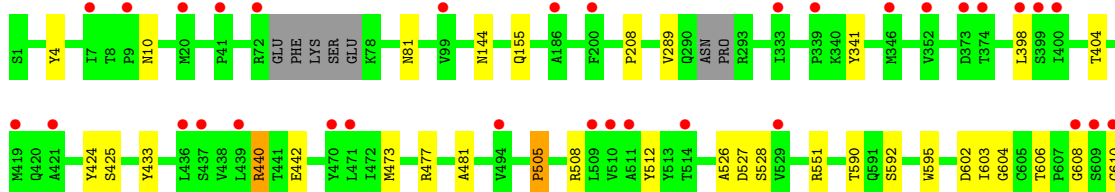
#### • Molecule 1: COMPLEMENT C3 BETA CHAIN

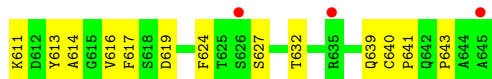
Chain E: 



#### • Molecule 1: COMPLEMENT C3 BETA CHAIN

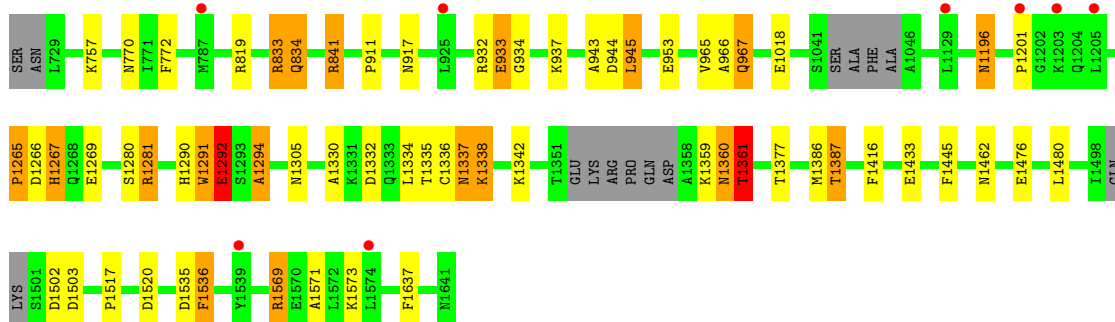
Chain G: 





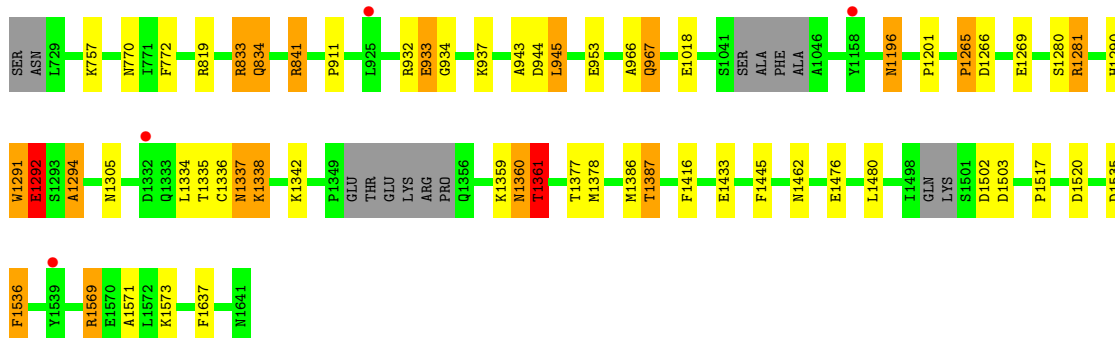
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain B:



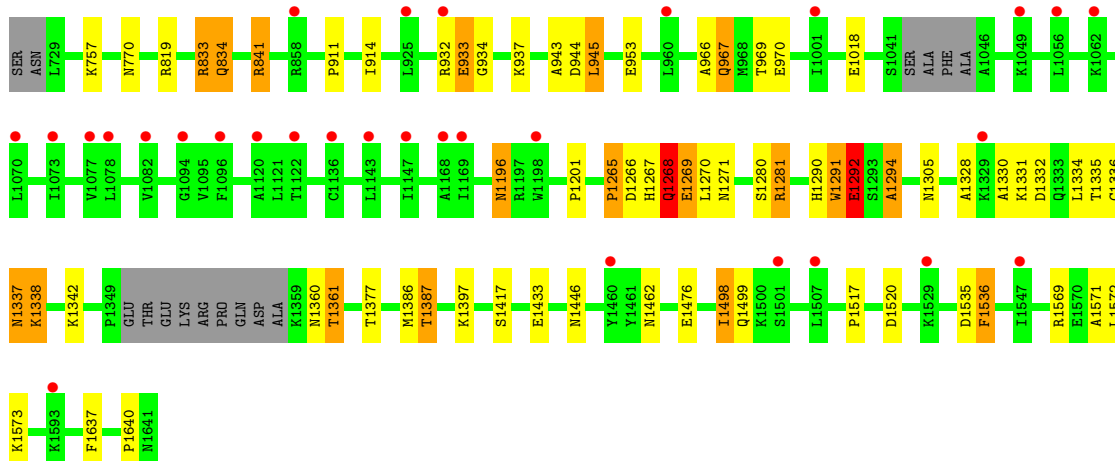
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain D:



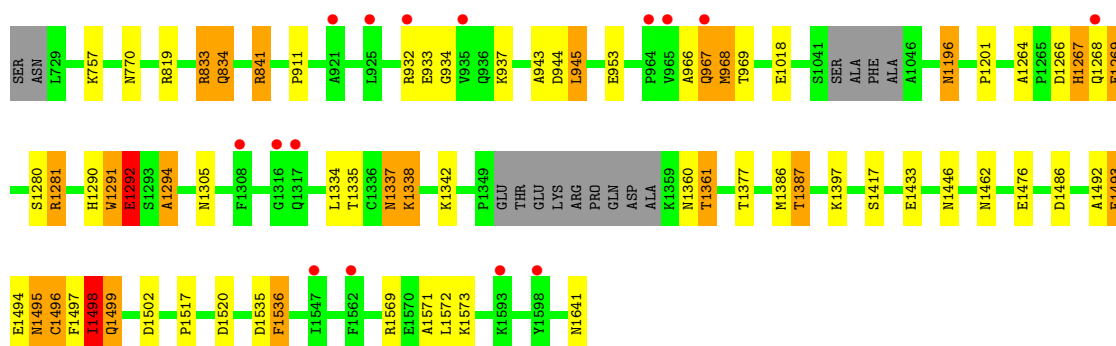
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain F:



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain H:



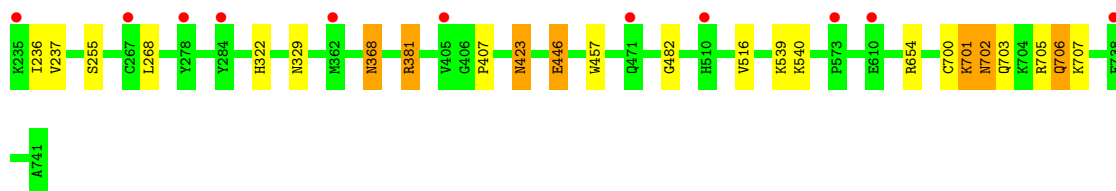
• Molecule 3: COMPLEMENT FACTOR B

Chain I:



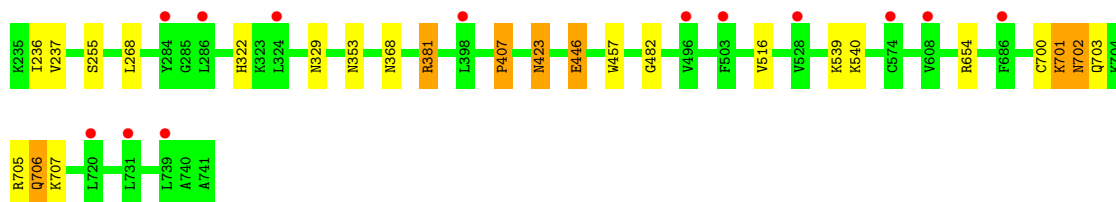
• Molecule 3: COMPLEMENT FACTOR B

Chain J:



• Molecule 3: COMPLEMENT FACTOR B

Chain K:



• Molecule 3: COMPLEMENT FACTOR B

Chain L:



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain M:



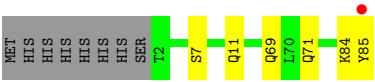
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain N: 



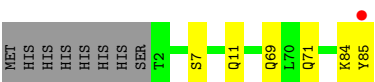
- Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain P: 



- Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain Q: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 89.7 (39.68-3.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.253 , 0.268 0.247 , 0.261	Depositor DCC
$R_{free}$ test set	2089 reflections (1.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 77.2	EDS
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 137471 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, NDG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

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.

All (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
10	H	2642	NDG	C1
10	H	2644	MAN	C1
10	H	2645	MAN	C1
12	I	1743	NDG	C1
12	I	1745	MAN	C1
13	I	1746	NDG	C1
12	J	1743	NDG	C1
12	J	1745	MAN	C1
14	K	1743	NDG	C1
14	K	1745	MAN	C1
14	K	1746	MAN	C1
14	K	1748	MAN	C1
16	L	1743	NDG	C1

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4958	0	485	11	0
1	C	4958	0	485	13	0
1	E	4958	0	485	15	0
1	G	4958	0	485	28	0
2	B	7177	0	0	24	0
2	D	7166	0	0	22	0
2	F	7172	0	0	27	0
2	H	7175	0	2299	24	0
3	I	4004	0	9	5	0
3	J	4004	0	9	8	0
3	K	4004	0	9	8	0
3	L	4004	0	9	7	0
4	M	682	0	26	3	0
4	N	682	0	26	3	0
4	P	682	0	26	2	0
4	Q	682	0	26	2	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	3	0
6	B	11	0	10	0	0
6	K	11	0	10	0	0
7	C	61	0	52	1	0
7	G	61	0	52	5	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	2	0
12	J	39	0	34	2	0
13	I	28	0	25	0	0
14	K	61	0	52	4	0
15	K	14	0	13	1	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	0	0
17	K	2	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	67989	0	4993	217	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (217) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:508:ARG:CZ	1:G:604:GLY:HA3	2.12	0.80
1:C:606:THR:HG22	1:C:608:GLY:H	1.59	0.68
1:G:606:THR:HG22	1:G:608:GLY:H	1.59	0.66
1:A:606:THR:HG22	1:A:608:GLY:H	1.59	0.66
1:E:606:THR:HG22	1:E:608:GLY:H	1.59	0.66
7:C:1646:NDG:H6C1	7:C:1647:NAG:C7	2.29	0.63
1:G:512:TYR:CZ	1:G:624:PHE:HE1	2.16	0.62
2:B:1291:TRP:CG	2:B:1292:GLU:N	2.69	0.61
2:D:1291:TRP:CG	2:D:1292:GLU:N	2.69	0.60
4:P:84:LYS:O	4:P:85:TYR:HB2	2.02	0.60
4:M:84:LYS:O	4:M:85:TYR:HB2	2.02	0.60
2:F:1291:TRP:CD1	2:F:1292:GLU:N	2.70	0.60
1:G:481:ALA:N	7:G:1646:NDG:H8C3	2.17	0.59
2:H:1291:TRP:CD1	2:H:1292:GLU:N	2.70	0.59
4:N:84:LYS:O	4:N:85:TYR:HB2	2.02	0.59
2:D:1337:ASN:O	2:D:1338:LYS:CB	2.51	0.59
4:Q:84:LYS:O	4:Q:85:TYR:HB2	2.02	0.59
2:F:1291:TRP:CG	2:F:1292:GLU:N	2.70	0.58
2:H:1268:GLN:HG3	2:H:1269:GLU:N	2.18	0.58
1:G:527:ASP:N	1:G:616:VAL:HG11	2.19	0.57
2:H:1291:TRP:CG	2:H:1292:GLU:N	2.70	0.57
1:A:614:ALA:HB1	1:A:632:THR:HA	1.86	0.57
2:B:1337:ASN:O	2:B:1338:LYS:CB	2.51	0.57
3:J:381:ARG:CG	3:J:381:ARG:NH2	2.68	0.57
1:E:614:ALA:HB1	1:E:632:THR:HA	1.86	0.57
3:I:381:ARG:CG	3:I:381:ARG:NH2	2.68	0.57
1:G:614:ALA:HB1	1:G:632:THR:HA	1.86	0.56
12:J:1743:NDG:H6C1	12:J:1744:NAG:C7	2.35	0.56
2:H:1337:ASN:O	2:H:1338:LYS:CB	2.53	0.56
1:C:614:ALA:HB1	1:C:632:THR:HA	1.86	0.56
1:G:424:TYR:O	1:G:433:TYR:CE1	2.59	0.56
3:L:381:ARG:CG	3:L:381:ARG:NH2	2.68	0.56
2:F:1337:ASN:O	2:F:1338:LYS:CB	2.53	0.56
2:D:1291:TRP:O	2:D:1292:GLU:C	2.45	0.56
3:K:381:ARG:CG	3:K:381:ARG:NH2	2.68	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:966:ALA:O	2:B:967:GLN:CB	2.54	0.55
2:D:1291:TRP:CD1	2:D:1292:GLU:N	2.75	0.55
2:B:1291:TRP:CD1	2:B:1292:GLU:N	2.75	0.55
2:D:966:ALA:O	2:D:967:GLN:CB	2.54	0.55
1:G:473:MET:CE	1:G:603:ILE:HD11	2.37	0.55
2:F:1291:TRP:O	2:F:1292:GLU:C	2.44	0.55
2:F:1268:GLN:O	2:F:1269:GLU:CG	2.55	0.55
1:G:508:ARG:NH1	1:G:604:GLY:HA3	2.22	0.54
2:H:1291:TRP:O	2:H:1292:GLU:C	2.45	0.54
2:B:1291:TRP:O	2:B:1292:GLU:C	2.45	0.54
2:H:1268:GLN:CG	2:H:1269:GLU:N	2.70	0.54
1:E:481:ALA:N	5:E:1646:NDG:H8C3	2.23	0.54
1:E:590:THR:HG22	1:E:592:SER:H	1.75	0.52
1:G:527:ASP:CA	1:G:616:VAL:HG11	2.40	0.52
2:D:1360:ASN:O	2:D:1361:THR:C	2.48	0.52
10:H:2643:NAG:O3	10:H:2643:NAG:H82	2.10	0.52
2:H:1641:ASN:O	3:J:368:ASN:ND2	2.43	0.52
2:B:1360:ASN:O	2:B:1361:THR:C	2.48	0.51
1:A:590:THR:HG22	1:A:592:SER:H	1.75	0.51
2:D:772:PHE:CD1	4:M:37:ASN:ND2	2.78	0.51
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.93	0.51
1:G:590:THR:HG22	1:G:592:SER:H	1.74	0.51
2:F:966:ALA:O	2:F:967:GLN:CB	2.57	0.51
1:G:640:CYS:HB3	1:G:641:PRO:HD2	1.93	0.51
1:C:590:THR:HG22	1:C:592:SER:H	1.75	0.51
1:C:640:CYS:HB3	1:C:641:PRO:HD2	1.93	0.51
1:E:640:CYS:HB3	1:E:641:PRO:HD2	1.93	0.50
2:F:1268:GLN:O	2:F:1269:GLU:CB	2.59	0.50
3:J:705:ARG:O	3:J:706:GLN:CB	2.60	0.49
3:L:705:ARG:O	3:L:706:GLN:CB	2.60	0.49
2:F:833:ARG:CG	2:F:833:ARG:NH1	2.75	0.49
3:I:705:ARG:O	3:I:706:GLN:CB	2.60	0.49
2:H:966:ALA:O	2:H:967:GLN:CB	2.59	0.49
2:H:1498:ILE:CG1	2:H:1499:GLN:N	2.75	0.49
3:K:705:ARG:O	3:K:706:GLN:CB	2.60	0.49
2:H:833:ARG:CG	2:H:833:ARG:NH1	2.75	0.49
2:D:833:ARG:CG	2:D:833:ARG:NH1	2.76	0.48
1:G:477:ARG:CG	1:G:477:ARG:NH1	2.76	0.48
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.76	0.48
1:C:477:ARG:CG	1:C:477:ARG:NH1	2.76	0.48
2:H:1492:ALA:O	2:H:1494:GLU:N	2.46	0.48
5:E:1646:NDG:H6C1	5:E:1647:NAG:H83	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:624:PHE:HB3	1:G:632:THR:HG23	1.96	0.48
2:D:1291:TRP:O	2:D:1294:ALA:N	2.47	0.48
1:E:477:ARG:NH1	1:E:477:ARG:CG	2.76	0.48
1:E:606:THR:HB	1:E:619:ASP:HB3	1.96	0.48
1:G:528:SER:N	1:G:616:VAL:HG13	2.29	0.48
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.96	0.48
2:H:932:ARG:O	2:H:934:GLY:N	2.47	0.48
1:A:382:ASP:OD2	1:A:440:ARG:NH2	2.47	0.47
5:A:1646:NDG:H4	5:A:1647:NAG:H2	1.61	0.47
2:B:833:ARG:NH1	2:B:833:ARG:CG	2.76	0.47
2:B:1291:TRP:O	2:B:1294:ALA:N	2.47	0.47
1:E:624:PHE:HB3	1:E:632:THR:HG23	1.96	0.47
1:C:624:PHE:HB3	1:C:632:THR:HG23	1.96	0.47
1:G:606:THR:HB	1:G:619:ASP:HB3	1.96	0.47
2:F:932:ARG:O	2:F:934:GLY:N	2.47	0.47
1:A:606:THR:HB	1:A:619:ASP:HB3	1.96	0.47
2:H:1291:TRP:O	2:H:1294:ALA:N	2.48	0.47
2:F:1265:PRO:O	2:F:1266:ASP:CB	2.64	0.46
2:F:1291:TRP:O	2:F:1294:ALA:N	2.48	0.46
3:L:700:CYS:O	3:L:701:LYS:C	2.53	0.46
14:K:1745:MAN:O3	14:K:1748:MAN:H61	2.16	0.46
3:I:700:CYS:O	3:I:701:LYS:C	2.53	0.46
3:K:700:CYS:O	3:K:701:LYS:C	2.53	0.46
3:J:700:CYS:O	3:J:701:LYS:C	2.53	0.46
1:C:639:GLN:H	1:C:639:GLN:NE2	2.14	0.46
10:H:2644:MAN:H62	10:H:2645:MAN:H2	1.43	0.46
1:C:606:THR:HB	1:C:619:ASP:HB3	1.96	0.46
3:K:407:PRO:CD	14:K:1743:NDG:H8C1	2.46	0.46
2:F:1290:HIS:O	2:F:1291:TRP:O	2.34	0.46
14:K:1743:NDG:H6C1	14:K:1744:NAG:C7	2.45	0.46
1:A:639:GLN:NE2	1:A:639:GLN:H	2.14	0.46
8:F:2645:BMA:H62	8:F:2647:BMA:H2	1.36	0.46
1:G:639:GLN:NE2	1:G:639:GLN:H	2.14	0.45
2:F:943:ALA:O	2:F:1305:ASN:ND2	2.49	0.45
2:F:1498:ILE:CG2	2:F:1499:GLN:N	2.80	0.45
5:D:2642:NDG:H6C1	5:D:2643:NAG:C7	2.46	0.45
2:D:1280:SER:O	2:D:1281:ARG:C	2.55	0.45
1:G:424:TYR:OH	1:G:613:TYR:HB3	2.16	0.45
2:H:1492:ALA:O	2:H:1493:GLU:C	2.55	0.45
2:H:1495:ASN:O	2:H:1496:CYS:C	2.54	0.45
2:B:1280:SER:O	2:B:1281:ARG:C	2.55	0.45
1:G:4:TYR:N	1:G:627:SER:HG	2.14	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:639:GLN:H	1:E:639:GLN:NE2	2.14	0.45
2:B:1330:ALA:O	2:B:1332:ASP:N	2.50	0.45
2:F:1280:SER:O	2:F:1281:ARG:C	2.55	0.45
7:G:1648:BMA:H3	9:G:1651:MAN:C1	2.46	0.45
2:D:1265:PRO:O	2:D:1266:ASP:CB	2.65	0.45
3:K:446:GLU:OE2	3:K:457:TRP:NE1	2.50	0.45
2:H:1290:HIS:O	2:H:1291:TRP:O	2.34	0.44
2:H:1497:PHE:O	2:H:1498:ILE:C	2.56	0.44
2:H:943:ALA:O	2:H:1305:ASN:ND2	2.49	0.44
2:B:1265:PRO:O	2:B:1266:ASP:CB	2.64	0.44
7:G:1647:NAG:H3	7:G:1649:BMA:O3	2.17	0.44
2:B:841:ARG:CG	2:B:841:ARG:NH1	2.81	0.44
2:D:819:ARG:NH1	2:D:819:ARG:CG	2.80	0.44
2:F:1360:ASN:O	2:F:1361:THR:O	2.36	0.44
2:H:819:ARG:CG	2:H:819:ARG:NH1	2.80	0.44
2:H:1360:ASN:O	2:H:1361:THR:O	2.36	0.44
1:G:508:ARG:NH1	1:G:602:ASP:OD2	2.51	0.44
2:H:1280:SER:O	2:H:1281:ARG:C	2.55	0.44
2:B:819:ARG:NH1	2:B:819:ARG:CG	2.80	0.44
3:L:701:LYS:O	3:L:702:ASN:ND2	2.52	0.43
12:I:1743:NDG:H6C1	12:I:1744:NAG:C7	2.48	0.43
1:G:425:SER:N	1:G:611:LYS:O	2.51	0.43
2:F:932:ARG:NH1	3:L:339:SER:CB	2.81	0.43
7:G:1647:NAG:H61	7:G:1648:BMA:H2	1.99	0.43
1:G:341:TYR:CE1	1:G:611:LYS:HB3	2.53	0.43
1:E:208:PRO:CD	1:E:583:LEU:HD11	2.48	0.43
2:B:1290:HIS:O	2:B:1291:TRP:O	2.37	0.43
2:D:1336:CYS:O	2:D:1337:ASN:O	2.36	0.43
2:B:1336:CYS:O	2:B:1337:ASN:O	2.37	0.43
3:J:701:LYS:O	3:J:702:ASN:ND2	2.52	0.43
2:B:944:ASP:O	2:B:945:LEU:C	2.57	0.43
2:D:944:ASP:O	2:D:945:LEU:C	2.57	0.43
1:G:526:ALA:O	1:G:616:VAL:HG21	2.19	0.43
2:D:841:ARG:NH1	2:D:841:ARG:CG	2.81	0.43
3:K:701:LYS:O	3:K:702:ASN:ND2	2.52	0.43
3:J:446:GLU:OE2	3:J:457:TRP:NE1	2.52	0.43
2:B:1386:MET:O	2:B:1387:THR:C	2.57	0.43
3:I:701:LYS:O	3:I:702:ASN:ND2	2.52	0.42
2:F:841:ARG:CG	2:F:841:ARG:NH1	2.81	0.42
2:B:772:PHE:CD1	4:N:37:ASN:ND2	2.87	0.42
7:G:1647:NAG:N2	7:G:1649:BMA:O3	2.52	0.42
2:B:932:ARG:O	2:B:933:GLU:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:932:ARG:O	2:D:933:GLU:C	2.57	0.42
2:F:1269:GLU:O	2:F:1271:ASN:N	2.52	0.42
12:I:1744:NAG:H2	12:I:1744:NAG:H2	1.91	0.42
2:F:969:THR:O	2:F:970:GLU:C	2.57	0.42
2:F:914:ILE:O	2:F:1328:ALA:N	2.53	0.42
2:D:1290:HIS:O	2:D:1291:TRP:O	2.37	0.42
3:K:353:ASN:OD1	15:K:1749:NDG:C7	2.67	0.42
1:G:512:TYR:CE1	1:G:624:PHE:HE1	2.37	0.42
2:H:1386:MET:O	2:H:1387:THR:C	2.58	0.42
2:F:819:ARG:CG	2:F:819:ARG:NH1	2.80	0.42
2:H:944:ASP:O	2:H:945:LEU:C	2.57	0.42
1:E:219:LYS:NZ	1:E:356:ASN:ND2	2.68	0.42
2:D:943:ALA:O	2:D:1305:ASN:ND2	2.53	0.42
2:F:944:ASP:O	2:F:945:LEU:C	2.57	0.42
4:Q:84:LYS:HG3	4:Q:84:LYS:O	2.20	0.42
2:H:841:ARG:CG	2:H:841:ARG:NH1	2.81	0.42
2:D:1386:MET:O	2:D:1387:THR:C	2.58	0.42
3:K:423:ASN:ND2	3:K:423:ASN:N	2.68	0.42
1:G:526:ALA:CB	1:G:617:PHE:CE2	3.03	0.41
2:F:1336:CYS:O	2:F:1337:ASN:C	2.59	0.41
2:B:932:ARG:O	2:B:934:GLY:N	2.53	0.41
2:D:932:ARG:O	2:D:934:GLY:N	2.53	0.41
3:I:423:ASN:ND2	3:I:423:ASN:N	2.68	0.41
2:B:943:ALA:O	2:B:1305:ASN:ND2	2.53	0.41
2:F:1330:ALA:O	2:F:1332:ASP:N	2.52	0.41
1:A:293:ARG:O	1:A:296:ASP:N	2.52	0.41
4:N:84:LYS:O	4:N:84:LYS:HG3	2.20	0.41
8:F:2644:BMA:H5	8:F:2645:BMA:H2	2.01	0.41
1:G:341:TYR:CD2	1:G:610:GLY:HA2	2.56	0.41
4:P:84:LYS:HG3	4:P:84:LYS:O	2.20	0.41
14:K:1745:MAN:H62	14:K:1746:MAN:H2	1.74	0.41
3:L:278:TYR:CE2	3:L:455:MET:SD	3.13	0.41
2:F:932:ARG:O	2:F:933:GLU:C	2.58	0.41
4:M:84:LYS:O	4:M:84:LYS:HG3	2.20	0.41
3:J:368:ASN:ND2	3:J:368:ASN:N	2.69	0.41
1:C:268:ARG:NH1	2:D:1378:MET:SD	2.94	0.41
1:G:440:ARG:O	1:G:440:ARG:CG	2.69	0.41
1:A:440:ARG:CG	1:A:440:ARG:O	2.69	0.41
1:E:440:ARG:CG	1:E:440:ARG:O	2.69	0.41
1:C:440:ARG:O	1:C:440:ARG:CG	2.69	0.41
2:F:1386:MET:O	2:F:1387:THR:C	2.58	0.41
3:L:423:ASN:N	3:L:423:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:1744:NAG:H2	12:J:1744:NAG:H82	1.91	0.41
1:E:640:CYS:HB3	1:E:641:PRO:CD	2.51	0.41
3:J:423:ASN:ND2	3:J:423:ASN:N	2.68	0.41
2:B:965:VAL:O	2:B:1267:HIS:CD2	2.74	0.41
2:B:917:ASN:OD1	5:B:2642:NDG:O	2.38	0.40
1:G:505:PRO:CG	1:G:595:TRP:CE3	3.03	0.40
1:C:109:PHE:CZ	1:C:594:ILE:HG23	2.56	0.40
5:E:1648:BMA:H62	5:E:1649:BMA:H2	1.58	0.40
1:E:583:LEU:HD12	1:E:583:LEU:N	2.36	0.40
1:C:583:LEU:HD12	1:C:583:LEU:N	2.36	0.40
1:C:293:ARG:O	1:C:296:ASP:N	2.54	0.40
2:D:1569:ARG:CB	2:D:1569:ARG:NH1	2.85	0.40
2:B:1569:ARG:NH1	2:B:1569:ARG:CG	2.84	0.40
1:E:642:GLN:O	1:E:644:ALA:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	33	86
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	33	86
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	33	86
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	33	86
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	7	58
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	7	59
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	6	56
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	5	53
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	14	72
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	14	72
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	14	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	14	72
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	19	77
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	19	77
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	19	77
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	19	77
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	11	68

All (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
2	B	1292	GLU
2	B	1294	ALA
2	B	1337	ASN
2	B	1338	LYS
2	B	1359	LYS
2	B	1377	THR
2	B	1503	ASP
2	D	933	GLU
2	D	967	GLN
2	D	1281	ARG
2	D	1291	TRP
2	D	1292	GLU
2	D	1294	ALA
2	D	1337	ASN
2	D	1338	LYS
2	D	1359	LYS
2	D	1377	THR
2	D	1503	ASP
2	F	933	GLU
2	F	967	GLN
2	F	1269	GLU
2	F	1281	ARG
2	F	1291	TRP
2	F	1292	GLU
2	F	1337	ASN

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Mol	Chain	Res	Type
2	F	1338	LYS
2	F	1361	THR
2	F	1377	THR
2	F	1417	SER
2	F	1446	ASN
2	H	933	GLU
2	H	968	MET
2	H	1281	ARG
2	H	1291	TRP
2	H	1292	GLU
2	H	1337	ASN
2	H	1338	LYS
2	H	1361	THR
2	H	1377	THR
2	H	1417	SER
2	H	1446	ASN
2	H	1493	GLU
3	I	236	ILE
3	I	407	PRO
3	I	701	LYS
3	I	706	GLN
3	J	236	ILE
3	J	407	PRO
3	J	701	LYS
3	J	706	GLN
3	K	236	ILE
3	K	407	PRO
3	K	701	LYS
3	K	706	GLN
3	L	236	ILE
3	L	407	PRO
3	L	701	LYS
3	L	706	GLN
2	B	911	PRO
2	B	1360	ASN
2	B	1361	THR
2	B	1476	GLU
2	B	1571	ALA
2	D	911	PRO
2	D	1360	ASN
2	D	1361	THR
2	D	1476	GLU

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Mol	Chain	Res	Type
2	D	1480	LEU
2	D	1571	ALA
2	F	911	PRO
2	F	1267	HIS
2	F	1294	ALA
2	F	1476	GLU
2	F	1498	ILE
2	F	1571	ALA
2	H	1266	ASP
2	H	1269	GLU
2	H	1294	ALA
2	H	1476	GLU
2	H	1496	CYS
2	H	1498	ILE
2	H	1571	ALA
1	A	442	GLU
1	A	643	PRO
2	B	1387	THR
2	B	1502	ASP
2	B	1573	LYS
1	C	442	GLU
1	C	643	PRO
2	D	1387	THR
2	D	1502	ASP
2	D	1573	LYS
1	E	442	GLU
1	E	643	PRO
2	F	1387	THR
2	F	1573	LYS
1	G	442	GLU
2	H	911	PRO
2	H	1387	THR
2	H	1573	LYS
3	I	707	LYS
3	J	516	VAL
3	J	707	LYS
3	K	516	VAL
3	K	707	LYS
3	L	707	LYS
1	A	505	PRO
2	B	1196	ASN
2	B	1265	PRO

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Mol	Chain	Res	Type
2	B	1480	LEU
1	C	505	PRO
2	D	1196	ASN
2	D	1265	PRO
2	D	1269	GLU
1	E	505	PRO
2	F	1196	ASN
2	F	1265	PRO
2	F	1268	GLN
2	F	1331	LYS
2	F	1637	PHE
1	G	505	PRO
2	H	967	GLN
2	H	1267	HIS
2	H	1486	ASP
2	H	1495	ASN
2	H	1502	ASP
3	I	516	VAL
3	L	516	VAL
4	M	7	SER
4	N	7	SER
4	P	7	SER
4	Q	7	SER
2	B	834	GLN
2	B	1201	PRO
2	B	1267	HIS
2	B	1536	PHE
2	D	834	GLN
2	D	1201	PRO
2	D	1536	PHE
2	F	834	GLN
2	F	1201	PRO
2	F	1270	LEU
2	F	1536	PHE
1	G	643	PRO
2	H	834	GLN
2	H	1196	ASN
2	H	1201	PRO
2	H	1264	ALA
2	H	1536	PHE
3	I	268	LEU
3	J	268	LEU

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Mol	Chain	Res	Type
3	K	268	LEU
3	L	268	LEU
3	I	482	GLY
3	J	482	GLY
3	K	482	GLY
3	L	482	GLY
2	B	1517	PRO
2	D	1517	PRO
2	F	1517	PRO
2	H	1517	PRO
1	A	208	PRO
1	C	208	PRO
1	E	208	PRO
1	G	208	PRO

### 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%)	75	94
1	C	558/567 (98%)	549 (98%)	9 (2%)	75	94
1	E	558/567 (98%)	549 (98%)	9 (2%)	75	94
1	G	558/567 (98%)	549 (98%)	9 (2%)	75	94
2	B	793/810 (98%)	769 (97%)	24 (3%)	53	89
2	D	790/810 (98%)	766 (97%)	24 (3%)	53	89
2	F	793/810 (98%)	769 (97%)	24 (3%)	53	89
2	H	793/810 (98%)	766 (97%)	27 (3%)	49	88
3	I	442/446 (99%)	429 (97%)	13 (3%)	55	89
3	J	442/446 (99%)	429 (97%)	13 (3%)	55	89
3	K	442/446 (99%)	429 (97%)	13 (3%)	55	89
3	L	442/446 (99%)	429 (97%)	13 (3%)	55	89
4	M	76/84 (90%)	73 (96%)	3 (4%)	43	85
4	N	76/84 (90%)	73 (96%)	3 (4%)	43	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	76/84 (90%)	73 (96%)	3 (4%)	43	85
4	Q	76/84 (90%)	73 (96%)	3 (4%)	43	85
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	57	90

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	81	ASN
1	A	144	ASN
1	A	155	GLN
1	A	289	VAL
1	A	398	LEU
1	A	404	THR
1	A	440	ARG
1	A	551	ARG
2	B	757	LYS
2	B	770	ASN
2	B	833	ARG
2	B	834	GLN
2	B	841	ARG
2	B	937	LYS
2	B	945	LEU
2	B	953	GLU
2	B	1018	GLU
2	B	1196	ASN
2	B	1292	GLU
2	B	1334	LEU
2	B	1335	THR
2	B	1342	LYS
2	B	1361	THR
2	B	1416	PHE
2	B	1433	GLU
2	B	1445	PHE
2	B	1462	ASN
2	B	1520	ASP
2	B	1535	ASP
2	B	1536	PHE
2	B	1569	ARG
2	B	1637	PHE
1	C	10	ASN

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Mol	Chain	Res	Type
1	C	81	ASN
1	C	144	ASN
1	C	155	GLN
1	C	289	VAL
1	C	398	LEU
1	C	404	THR
1	C	440	ARG
1	C	551	ARG
2	D	757	LYS
2	D	770	ASN
2	D	833	ARG
2	D	834	GLN
2	D	841	ARG
2	D	937	LYS
2	D	945	LEU
2	D	953	GLU
2	D	1018	GLU
2	D	1196	ASN
2	D	1292	GLU
2	D	1334	LEU
2	D	1335	THR
2	D	1342	LYS
2	D	1361	THR
2	D	1416	PHE
2	D	1433	GLU
2	D	1445	PHE
2	D	1462	ASN
2	D	1520	ASP
2	D	1535	ASP
2	D	1536	PHE
2	D	1569	ARG
2	D	1637	PHE
1	E	10	ASN
1	E	81	ASN
1	E	144	ASN
1	E	155	GLN
1	E	289	VAL
1	E	398	LEU
1	E	404	THR
1	E	440	ARG
1	E	551	ARG
2	F	757	LYS

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Mol	Chain	Res	Type
2	F	770	ASN
2	F	833	ARG
2	F	834	GLN
2	F	841	ARG
2	F	937	LYS
2	F	945	LEU
2	F	953	GLU
2	F	1018	GLU
2	F	1196	ASN
2	F	1268	GLN
2	F	1292	GLU
2	F	1334	LEU
2	F	1335	THR
2	F	1342	LYS
2	F	1397	LYS
2	F	1433	GLU
2	F	1462	ASN
2	F	1520	ASP
2	F	1535	ASP
2	F	1536	PHE
2	F	1569	ARG
2	F	1572	LEU
2	F	1640	PRO
1	G	10	ASN
1	G	81	ASN
1	G	144	ASN
1	G	155	GLN
1	G	289	VAL
1	G	398	LEU
1	G	404	THR
1	G	440	ARG
1	G	551	ARG
2	H	757	LYS
2	H	770	ASN
2	H	833	ARG
2	H	834	GLN
2	H	841	ARG
2	H	937	LYS
2	H	945	LEU
2	H	953	GLU
2	H	968	MET
2	H	969	THR

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Mol	Chain	Res	Type
2	H	1018	GLU
2	H	1196	ASN
2	H	1267	HIS
2	H	1292	GLU
2	H	1334	LEU
2	H	1335	THR
2	H	1342	LYS
2	H	1397	LYS
2	H	1433	GLU
2	H	1462	ASN
2	H	1498	ILE
2	H	1499	GLN
2	H	1520	ASP
2	H	1535	ASP
2	H	1536	PHE
2	H	1569	ARG
2	H	1572	LEU
3	I	237	VAL
3	I	255	SER
3	I	322	HIS
3	I	329	ASN
3	I	368	ASN
3	I	381	ARG
3	I	423	ASN
3	I	446	GLU
3	I	539	LYS
3	I	540	LYS
3	I	654	ARG
3	I	702	ASN
3	I	703	GLN
3	J	237	VAL
3	J	255	SER
3	J	322	HIS
3	J	329	ASN
3	J	368	ASN
3	J	381	ARG
3	J	423	ASN
3	J	446	GLU
3	J	539	LYS
3	J	540	LYS
3	J	654	ARG
3	J	702	ASN

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Mol	Chain	Res	Type
3	J	703	GLN
3	K	237	VAL
3	K	255	SER
3	K	322	HIS
3	K	329	ASN
3	K	368	ASN
3	K	381	ARG
3	K	423	ASN
3	K	446	GLU
3	K	539	LYS
3	K	540	LYS
3	K	654	ARG
3	K	702	ASN
3	K	703	GLN
3	L	237	VAL
3	L	255	SER
3	L	322	HIS
3	L	329	ASN
3	L	368	ASN
3	L	381	ARG
3	L	423	ASN
3	L	446	GLU
3	L	539	LYS
3	L	540	LYS
3	L	654	ARG
3	L	702	ASN
3	L	703	GLN
4	M	11	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	69	GLN
4	Q	71	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	587	ASN
1	A	634	GLN
1	A	639	GLN
1	C	587	ASN
1	C	634	GLN
1	C	639	GLN
1	E	587	ASN
1	E	639	GLN
1	G	587	ASN
1	G	634	GLN
1	G	639	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.62	0	15,19,21	0.81	1 (6%)
5	NAG	A	1647	5	12,14,15	0.77	1 (8%)	15,19,21	1.50	5 (33%)
5	BMA	A	1648	5	10,11,12	0.72	0	11,15,17	1.85	1 (9%)
5	BMA	A	1649	5	10,11,12	0.79	0	11,15,17	1.15	0
5	NDG	B	2642	2,5	12,14,15	0.73	1 (8%)	15,19,21	1.09	1 (6%)
5	NAG	B	2643	5	12,14,15	0.72	1 (8%)	15,19,21	1.18	2 (13%)
5	BMA	B	2644	5	10,11,12	1.05	1 (10%)	11,15,17	2.15	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	B	2645	5	10,11,12	0.86	1 (10%)	11,15,17	0.98	1 (9%)
7	NDG	C	1646	1,7	12,14,15	0.77	1 (8%)	15,19,21	1.16	1 (6%)
7	NAG	C	1647	7	12,14,15	0.82	1 (8%)	15,19,21	0.99	0
7	BMA	C	1648	7	10,11,12	0.81	0	11,15,17	1.23	1 (9%)
7	BMA	C	1649	7	10,11,12	0.86	1 (10%)	11,15,17	1.60	3 (27%)
7	BMA	C	1650	7	10,11,12	0.78	0	11,15,17	1.28	2 (18%)
5	NDG	D	2642	2,5	12,14,15	0.65	0	15,19,21	1.02	1 (6%)
5	NAG	D	2643	5	12,14,15	0.71	1 (8%)	15,19,21	0.83	0
5	BMA	D	2644	5	10,11,12	0.78	0	11,15,17	1.55	1 (9%)
5	BMA	D	2645	5	10,11,12	0.79	0	11,15,17	1.11	0
5	NDG	E	1646	1,5	12,14,15	0.67	1 (8%)	15,19,21	0.99	1 (6%)
5	NAG	E	1647	5	12,14,15	0.76	1 (8%)	15,19,21	0.98	0
5	BMA	E	1648	5	10,11,12	0.84	1 (10%)	11,15,17	1.08	1 (9%)
5	BMA	E	1649	5	10,11,12	0.97	1 (10%)	11,15,17	0.83	0
8	NDG	F	2642	8,2	12,14,15	0.56	0	15,19,21	1.19	2 (13%)
8	NAG	F	2643	8	12,14,15	0.52	0	15,19,21	1.58	3 (20%)
8	BMA	F	2644	8	10,11,12	0.68	0	11,15,17	1.66	4 (36%)
8	BMA	F	2645	8	10,11,12	1.05	1 (10%)	11,15,17	1.63	2 (18%)
8	BMA	F	2646	8	10,11,12	0.76	0	11,15,17	1.38	3 (27%)
8	BMA	F	2647	8	10,11,12	0.83	1 (10%)	11,15,17	0.86	0
7	NDG	G	1646	1,7	12,14,15	0.57	0	15,19,21	1.28	1 (6%)
7	NAG	G	1647	7	12,14,15	0.52	0	15,19,21	1.43	3 (20%)
7	BMA	G	1648	7	10,11,12	0.66	0	11,15,17	3.59	4 (36%)
7	BMA	G	1649	7	10,11,12	0.72	0	11,15,17	4.38	4 (36%)
7	BMA	G	1650	7	10,11,12	0.80	0	11,15,17	1.13	1 (9%)
10	NDG	H	2642	10,2	12,14,15	0.69	1 (8%)	15,19,21	0.88	1 (6%)
10	NAG	H	2643	10	12,14,15	0.61	0	15,19,21	1.05	2 (13%)
10	MAN	H	2644	10	10,11,12	0.93	1 (10%)	11,15,17	1.63	3 (27%)
10	MAN	H	2645	10	10,11,12	0.88	1 (10%)	11,15,17	0.74	0
12	NDG	I	1743	3,12	12,14,15	0.71	1 (8%)	15,19,21	1.03	1 (6%)
12	NAG	I	1744	12	12,14,15	0.76	1 (8%)	15,19,21	0.94	0
12	MAN	I	1745	12	10,11,12	0.81	0	11,15,17	1.06	1 (9%)
13	NDG	I	1746	3,13	12,14,15	0.68	1 (8%)	15,19,21	1.18	2 (13%)
13	NAG	I	1747	13	12,14,15	0.71	1 (8%)	15,19,21	0.78	0
12	NDG	J	1743	3,12	12,14,15	0.66	1 (8%)	15,19,21	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	J	1744	12	12,14,15	0.76	1 (8%)	15,19,21	0.95	0
12	MAN	J	1745	12	10,11,12	0.80	0	11,15,17	1.05	1 (9%)
14	NDG	K	1743	3,14	12,14,15	0.76	1 (8%)	15,19,21	1.19	2 (13%)
14	NAG	K	1744	14	12,14,15	0.86	1 (8%)	15,19,21	1.30	3 (20%)
14	MAN	K	1745	14	10,11,12	0.74	0	11,15,17	2.31	3 (27%)
14	MAN	K	1746	14	10,11,12	0.83	0	11,15,17	1.75	3 (27%)
14	MAN	K	1748	14	10,11,12	0.73	0	11,15,17	1.46	2 (18%)
16	NDG	L	1743	3,16	12,14,15	0.64	0	15,19,21	1.07	1 (6%)
16	NAG	L	1744	16	12,14,15	0.73	1 (8%)	15,19,21	0.97	0
16	BMA	L	1745	16	10,11,12	0.80	0	11,15,17	1.00	1 (9%)

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
5	BMA	E	1649	5	-	0/2/19/22	0/1/1/1
8	NDG	F	2642	8,2	-	0/6/23/26	1/1/1/1
8	NAG	F	2643	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	2645	BMA	O5-C5	-2.88	1.40	1.45
5	B	2644	BMA	O5-C5	-2.79	1.40	1.45
14	K	1744	NAG	O5-C5	-2.63	1.40	1.45
5	E	1649	BMA	O5-C5	-2.57	1.40	1.45
7	C	1647	NAG	O5-C5	-2.52	1.40	1.45
10	H	2644	MAN	O5-C5	-2.44	1.40	1.45
5	A	1647	NAG	O5-C5	-2.37	1.41	1.45
14	K	1743	NDG	O-C5	-2.34	1.41	1.45
12	I	1744	NAG	O5-C5	-2.33	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	1744	NAG	O5-C5	-2.33	1.41	1.45
7	C	1646	NDG	O-C5	-2.32	1.41	1.45
5	E	1647	NAG	O5-C5	-2.30	1.41	1.45
10	H	2645	MAN	O5-C5	-2.27	1.41	1.45
5	B	2643	NAG	O5-C5	-2.25	1.41	1.45
5	B	2645	BMA	O5-C5	-2.24	1.41	1.45
16	L	1744	NAG	O5-C5	-2.22	1.41	1.45
13	I	1747	NAG	O5-C5	-2.20	1.41	1.45
5	D	2643	NAG	O5-C5	-2.19	1.41	1.45
7	C	1649	BMA	O5-C5	-2.17	1.41	1.45
12	I	1743	NDG	O-C5	-2.16	1.41	1.45
10	H	2642	NDG	O-C5	-2.13	1.41	1.45
13	I	1746	NDG	O-C5	-2.12	1.41	1.45
5	B	2642	NDG	O-C5	-2.09	1.41	1.45
5	E	1648	BMA	O5-C5	-2.06	1.41	1.45
12	J	1743	NDG	O-C5	-2.05	1.41	1.45
8	F	2647	BMA	O5-C5	-2.01	1.41	1.45
5	E	1646	NDG	O-C5	-2.00	1.41	1.45

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1649	BMA	O5-C5-C6	10.46	117.96	106.98
7	G	1648	BMA	O5-C5-C6	10.09	117.57	106.98
7	G	1649	BMA	C3-C4-C5	-7.07	97.58	110.20
14	K	1745	MAN	O5-C5-C6	6.53	113.83	106.98
7	G	1649	BMA	O3-C3-C4	6.33	124.55	110.35
5	A	1648	BMA	O5-C5-C6	5.64	112.90	106.98
5	D	2644	BMA	O5-C5-C6	4.72	111.93	106.98
7	G	1648	BMA	C6-C5-C4	-4.23	102.77	113.00
5	B	2644	BMA	O5-C5-C4	-4.23	105.29	110.65
8	F	2643	NAG	O5-C5-C6	4.09	111.27	106.98
8	F	2645	BMA	C4-C3-C2	4.02	115.91	110.50
14	K	1748	MAN	O5-C5-C6	3.85	111.02	106.98
5	B	2644	BMA	O5-C5-C6	3.77	110.93	106.98
14	K	1746	MAN	C3-C4-C5	3.73	116.87	110.20
10	H	2644	MAN	O5-C5-C6	3.43	110.58	106.98
7	C	1649	BMA	O3-C3-C4	-3.38	102.78	110.35
5	B	2644	BMA	C4-C3-C2	3.33	114.97	110.50
7	G	1648	BMA	C3-C4-C5	3.16	115.85	110.20
10	H	2644	MAN	O5-C5-C4	-3.08	106.74	110.65
7	C	1649	BMA	C3-C4-C5	3.08	115.70	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	1745	MAN	O5-C5-C6	3.06	110.19	106.98
7	G	1647	NAG	O4-C4-C5	3.02	117.25	109.28
8	F	2644	BMA	O5-C5-C6	2.99	110.12	106.98
7	C	1646	NDG	C3-C4-C5	2.99	115.54	110.20
7	C	1648	BMA	O5-C5-C6	2.96	110.09	106.98
12	J	1745	MAN	O5-C5-C6	2.95	110.08	106.98
8	F	2643	NAG	O4-C4-C3	2.91	116.87	110.35
14	K	1745	MAN	O3-C3-C2	2.91	115.25	109.94
5	A	1647	NAG	C4-C3-C2	2.85	118.29	111.32
14	K	1744	NAG	C3-C4-C5	2.80	115.19	110.20
8	F	2644	BMA	C4-C3-C2	-2.75	106.81	110.50
16	L	1745	BMA	O5-C5-C6	2.73	109.85	106.98
14	K	1743	NDG	C3-C4-C5	2.72	115.05	110.20
7	G	1646	NDG	C3-C2-N2	-2.68	107.67	111.76
14	K	1746	MAN	O5-C5-C4	2.65	114.01	110.65
8	F	2644	BMA	O5-C5-C4	2.62	113.98	110.65
8	F	2646	BMA	C3-C4-C5	2.62	114.89	110.20
5	A	1647	NAG	C3-C4-C5	2.61	114.87	110.20
13	I	1746	NDG	C3-C4-C5	2.60	114.84	110.20
10	H	2642	NDG	O-C5-C6	2.57	109.68	106.98
16	L	1743	NDG	C3-C2-N2	-2.50	107.96	111.76
7	G	1648	BMA	O6-C6-C5	2.47	119.86	111.36
5	E	1648	BMA	O5-C5-C6	2.46	109.56	106.98
8	F	2642	NDG	O-C5-C6	2.43	109.53	106.98
14	K	1745	MAN	C4-C3-C2	-2.42	107.26	110.50
7	C	1650	BMA	C3-C4-C5	2.41	114.50	110.20
10	H	2643	NAG	O5-C5-C6	2.34	109.44	106.98
5	A	1647	NAG	O4-C4-C3	-2.34	105.10	110.35
5	B	2643	NAG	O5-C5-C4	2.34	113.62	110.65
7	G	1649	BMA	O3-C3-C2	2.33	114.21	109.94
14	K	1743	NDG	C3-C2-N2	-2.30	108.25	111.76
7	C	1650	BMA	O5-C5-C6	2.30	109.39	106.98
8	F	2646	BMA	O5-C5-C4	2.26	113.52	110.65
7	G	1650	BMA	O5-C5-C6	2.24	109.33	106.98
5	B	2645	BMA	O5-C5-C6	2.22	109.31	106.98
7	G	1647	NAG	C4-C3-C2	-2.20	105.92	111.32
5	A	1647	NAG	C3-C2-N2	-2.20	108.41	111.76
12	I	1743	NDG	C3-C4-C5	2.19	114.11	110.20
12	J	1743	NDG	C3-C2-N2	-2.19	108.43	111.76
8	F	2642	NDG	O4-C4-C5	2.16	114.99	109.28
10	H	2644	MAN	C4-C3-C2	2.16	113.41	110.50
14	K	1746	MAN	C6-C5-C4	-2.15	107.81	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2642	NDG	C3-C2-N2	-2.14	108.50	111.76
8	F	2645	BMA	C3-C4-C5	2.13	114.02	110.20
5	B	2642	NDG	C3-C4-C5	2.12	113.99	110.20
14	K	1744	NAG	O4-C4-C3	-2.11	105.62	110.35
5	A	1646	NDG	O-C5-C6	2.11	109.19	106.98
8	F	2643	NAG	C4-C3-C2	-2.10	106.18	111.32
8	F	2646	BMA	O5-C5-C6	2.09	109.17	106.98
14	K	1748	MAN	C3-C4-C5	2.09	113.94	110.20
13	I	1746	NDG	C3-C2-N2	-2.08	108.60	111.76
14	K	1744	NAG	C4-C3-C2	2.08	116.40	111.32
8	F	2644	BMA	C6-C5-C4	-2.06	108.03	113.00
7	G	1647	NAG	O4-C4-C3	2.04	114.92	110.35
5	E	1646	NDG	C3-C4-C5	2.02	113.81	110.20
10	H	2643	NAG	C3-C2-N2	-2.02	108.69	111.76
5	A	1647	NAG	O5-C5-C6	-2.01	104.88	106.98
5	B	2643	NAG	C6-C5-C4	-2.01	108.15	113.00
7	C	1649	BMA	O5-C5-C6	2.00	109.08	106.98

All (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
14	K	1743	NDG	C1
14	K	1746	MAN	C1
10	H	2642	NDG	C1
12	I	1745	MAN	C1
12	J	1743	NDG	C1
7	C	1646	NDG	C1
5	E	1646	NDG	C1
10	H	2644	MAN	C1
10	H	2645	MAN	C1
13	I	1746	NDG	C1
14	K	1748	MAN	C1
14	K	1745	MAN	C1
7	G	1646	NDG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:



Mol	Chain	Res	Type	Atoms
8	F	2642	NDG	C1-C2-C3-C4-C5-O

## 5.6 Ligand geometry ⓘ

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	-	10,11,12	0.83	0	11,15,17	0.94	0
9	MAN	G	1651	-	10,11,12	0.86	1 (10%)	11,15,17	1.00	1 (9%)
6	BMA	K	1747	-	10,11,12	0.83	0	11,15,17	1.11	2 (18%)
15	NDG	K	1749	3	12,14,15	0.59	0	15,19,21	1.18	1 (6%)
15	NDG	L	1746	3	12,14,15	0.66	0	15,19,21	0.84	1 (6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	1651	MAN	O5-C5	-2.05	1.41	1.45

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	1651	MAN	C3-C4-C5	2.66	114.96	110.20
15	K	1749	NDG	O-C5-C4	2.64	114.01	110.65
6	K	1747	BMA	O5-C5-C6	2.59	109.70	106.98
6	K	1747	BMA	C3-C4-C5	2.15	114.03	110.20
15	L	1746	NDG	O-C5-C6	2.13	109.22	106.98

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.

## 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	638/645 (98%)	0.41	7 (1%) 77 61	87, 142, 190, 237	0
1	C	638/645 (98%)	0.43	10 (1%) 68 53	80, 127, 176, 228	0
1	E	638/645 (98%)	0.43	8 (1%) 74 58	84, 142, 196, 245	0
1	G	638/645 (98%)	0.58	36 (5%) 24 20	93, 180, 241, 267	0
2	B	901/915 (98%)	0.35	8 (0%) 81 67	91, 167, 229, 260	0
2	D	901/915 (98%)	0.39	4 (0%) 90 81	81, 155, 216, 266	0
2	F	900/915 (98%)	0.48	30 (3%) 44 34	96, 179, 284, 329	0
2	H	605/915 (66%)	0.48	15 (2%) 54 41	98, 162, 231, 294	0
3	I	507/507 (100%)	0.34	2 (0%) 90 81	93, 142, 197, 240	0
3	J	507/507 (100%)	0.35	11 (2%) 59 44	127, 170, 220, 261	0
3	K	507/507 (100%)	0.38	13 (2%) 53 40	132, 183, 230, 284	0
3	L	507/507 (100%)	0.32	2 (0%) 90 81	101, 144, 194, 239	0
4	M	84/92 (91%)	0.47	1 (1%) 75 59	87, 110, 186, 221	0
4	N	84/92 (91%)	0.45	1 (1%) 75 59	97, 116, 189, 227	0
4	P	84/92 (91%)	0.43	1 (1%) 75 59	100, 124, 176, 211	0
4	Q	84/92 (91%)	0.38	1 (1%) 75 59	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.42	150 (1%) 65 50	80, 155, 228, 329	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	421	ALA	7.5
1	G	509	LEU	6.3
1	G	529	VAL	5.2
1	C	645	ALA	5.1
1	A	645	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	J	235	LYS	4.2
2	H	1547	ILE	4.0
2	F	1078	LEU	3.8
1	G	7	ILE	3.7
3	L	267	CYS	3.7
2	H	1593	LYS	3.7
1	G	400	ILE	3.6
1	G	470	TYR	3.6
1	G	398	LEU	3.5
2	F	1049	LYS	3.5
1	G	471	LEU	3.5
4	M	85	TYR	3.4
1	G	20	MET	3.3
1	G	373	ASP	3.3
1	G	374	THR	3.3
3	I	366	LEU	3.2
2	F	925	LEU	3.2
2	H	1317	GLN	3.1
1	G	510	VAL	3.1
2	F	1070	LEU	3.0
1	G	511	ALA	3.0
1	G	72	ARG	2.9
1	G	437	SER	2.9
1	C	376	GLN	2.9
2	B	925	LEU	2.8
2	D	925	LEU	2.8
2	H	925	LEU	2.8
3	K	324	LEU	2.8
4	P	85	TYR	2.8
4	N	85	TYR	2.8
2	H	1316	GLY	2.8
1	A	12	LEU	2.8
3	J	284	TYR	2.8
1	A	509	LEU	2.7
1	G	608	GLY	2.7
1	A	20	MET	2.7
1	C	374	THR	2.7
2	B	1574	LEU	2.7
1	G	99	VAL	2.7
2	F	1001	ILE	2.7
3	K	574	CYS	2.7
1	E	509	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	1539	TYR	2.7
3	I	267	CYS	2.7
2	H	1268	GLN	2.6
1	A	22	LEU	2.6
3	K	284	TYR	2.6
3	J	267	CYS	2.6
2	H	935	VAL	2.5
2	F	1501	SER	2.5
2	H	967	GLN	2.5
2	F	1120	ALA	2.5
3	J	738	PHE	2.5
2	F	1593	LYS	2.5
1	G	9	PRO	2.5
2	F	960	LEU	2.4
3	K	286	LEU	2.4
2	B	1205	LEU	2.4
3	L	286	LEU	2.4
2	F	1547	ILE	2.4
1	G	333	ILE	2.4
1	E	436	LEU	2.4
1	G	339	PRO	2.4
2	H	1598	TYR	2.4
4	Q	85	TYR	2.4
1	G	436	LEU	2.4
1	E	20	MET	2.4
2	H	932	ARG	2.4
2	F	1062	LYS	2.3
1	E	636	ALA	2.3
1	E	68	ILE	2.3
2	F	1147	ILE	2.3
3	K	398	LEU	2.3
3	J	573	PRO	2.3
2	F	1198	TRP	2.3
2	F	1143	LEU	2.3
2	F	1460	TYR	2.3
2	H	1308	PHE	2.3
3	K	731	LEU	2.3
1	C	20	MET	2.3
1	G	626	SER	2.3
2	H	1562	PHE	2.3
2	B	1129	LEU	2.3
1	G	645	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	J	510	HIS	2.2
1	C	19	THR	2.2
1	G	346	MET	2.2
1	G	200	PHE	2.2
3	J	610	GLU	2.2
3	K	608	VAL	2.2
1	G	635	ARG	2.2
2	B	1539	TYR	2.2
2	H	964	PRO	2.2
1	C	368	ALA	2.2
2	F	932	ARG	2.2
3	J	471	GLN	2.2
3	K	503	PHE	2.2
1	G	514	THR	2.2
2	B	787	MET	2.2
1	C	48	SER	2.2
3	K	686	PHE	2.2
1	G	352	VAL	2.2
3	K	528	VAL	2.2
1	C	509	LEU	2.2
2	H	921	ALA	2.2
1	G	494	VAL	2.2
1	G	610	GLY	2.2
2	F	1077	VAL	2.2
3	J	405	VAL	2.2
3	K	720	LEU	2.2
2	F	1136	CYS	2.2
2	F	1056	LEU	2.1
2	D	1332	ASP	2.1
1	A	19	THR	2.1
1	C	290	GLN	2.1
1	E	83	PHE	2.1
3	J	362	MET	2.1
2	F	1073	ILE	2.1
2	F	1529	LYS	2.1
2	H	965	VAL	2.1
3	K	739	LEU	2.1
1	C	107	TYR	2.1
1	A	48	SER	2.1
2	F	1169	ILE	2.1
2	F	1168	ALA	2.1
3	K	496	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	439	LEU	2.1
2	F	1096	PHE	2.1
2	F	1122	THR	2.1
3	J	278	TYR	2.1
1	G	609	SER	2.1
2	F	1094	GLY	2.1
2	F	1329	LYS	2.1
1	G	186	ALA	2.1
2	B	1201	PRO	2.1
2	B	1203	LYS	2.0
1	G	41	PRO	2.0
2	F	858	ARG	2.0
1	E	12	LEU	2.0
1	G	419	MET	2.0
2	F	1082	VAL	2.0
1	E	635	ARG	2.0
2	D	1158	TYR	2.0
2	F	1507	LEU	2.0
1	G	399	SER	2.0

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	NAG	I	1747	14/15	0.36	8.19	222,223,224,224	0
8	BMA	F	2647	11/12	0.42	2.62	214,215,217,217	0
13	NDG	I	1746	14/15	0.32	1.57	198,225,227,227	0
16	NDG	L	1743	14/15	0.25	-0.16	122,147,148,148	0
14	NDG	K	1743	14/15	0.20	-0.28	174,204,206,207	0
12	NDG	J	1743	14/15	0.23	-0.29	158,188,189,189	0
12	NDG	I	1743	14/15	0.24	-0.70	122,149,151,152	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	NDG	H	2642	14/15	0.17	-0.72	183,213,214,215	0
7	NDG	C	1646	14/15	0.27	-0.92	163,191,192,193	0
8	NDG	F	2642	14/15	0.23	-0.93	169,193,194,194	0
5	NDG	B	2642	14/15	0.22	-0.97	163,194,194,195	0
5	NDG	D	2642	14/15	0.22	-1.13	147,176,178,179	0
5	NDG	A	1646	14/15	0.22	-2.02	156,185,187,188	0
7	NDG	G	1646	14/15	0.15	-2.23	198,201,208,215	0
5	NDG	E	1646	14/15	0.17	-2.36	174,204,206,206	0
8	NAG	F	2643	14/15	0.17	-25.80	200,202,204,204	0
16	BMA	L	1745	11/12	0.22	-	197,201,202,202	0
7	BMA	G	1650	11/12	0.41	-	229,231,232,232	0
8	BMA	F	2646	11/12	0.23	-	221,222,224,224	0
12	MAN	J	1745	11/12	0.23	-	206,210,211,212	0
14	MAN	K	1746	11/12	0.22	-	229,230,232,232	0
12	NAG	I	1744	14/15	0.14	-	178,180,181,182	0
7	BMA	C	1648	11/12	0.25	-	219,220,222,223	0
12	MAN	I	1745	11/12	0.30	-	205,207,208,209	0
7	BMA	G	1648	11/12	0.34	-	247,249,250,251	0
5	BMA	D	2645	11/12	0.14	-	229,232,233,234	0
5	BMA	E	1648	11/12	0.20	-	229,230,231,232	0
8	BMA	F	2645	11/12	0.17	-	248,249,249,250	0
10	NAG	H	2643	14/15	0.16	-	221,222,224,225	0
7	BMA	C	1650	11/12	0.30	-	231,233,235,235	0
7	NAG	G	1647	14/15	0.13	-	213,216,216,217	0
5	NAG	E	1647	14/15	0.15	-	223,225,227,227	0
7	NAG	C	1647	14/15	0.24	-	200,202,203,203	0
16	NAG	L	1744	14/15	0.21	-	185,187,189,189	0
12	NAG	J	1744	14/15	0.19	-	177,179,180,180	0
8	BMA	F	2644	11/12	0.17	-	232,233,234,234	0
10	MAN	H	2644	11/12	0.18	-	229,230,231,232	0
5	NAG	A	1647	14/15	0.20	-	199,200,201,203	0
5	NAG	B	2643	14/15	0.12	-	193,196,196,197	0
10	MAN	H	2645	11/12	0.36	-	234,236,237,238	0
5	BMA	B	2645	11/12	0.28	-	237,239,240,241	0
5	BMA	A	1649	11/12	0.24	-	226,227,228,228	0
5	NAG	D	2643	14/15	0.17	-	200,201,202,203	0
7	BMA	G	1649	11/12	0.21	-	226,228,229,230	0
5	BMA	E	1649	11/12	0.20	-	209,212,214,215	0
7	BMA	C	1649	11/12	0.26	-	235,237,239,240	0
14	MAN	K	1748	11/12	0.21	-	230,232,235,235	0
5	BMA	A	1648	11/12	0.21	-	212,214,215,216	0
14	MAN	K	1745	11/12	0.18	-	249,252,253,254	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	B	2644	11/12	0.19	-	218,220,222,223	0
5	BMA	D	2644	11/12	0.18	-	220,221,223,223	0
14	NAG	K	1744	14/15	0.18	-	196,199,201,202	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	NDG	L	1746	14/15	0.28	0.27	176,204,205,205	0
11	MG	L	1742	1/1	0.22	0.14	127,127,127,127	0
15	NDG	K	1749	14/15	0.23	0.02	184,214,216,217	0
11	MG	I	1742	1/1	0.20	-0.38	120,120,120,120	0
11	MG	K	1742	1/1	0.13	-0.62	138,138,138,138	0
11	MG	J	1742	1/1	0.14	-0.77	148,148,148,148	0
6	BMA	B	2646	11/12	0.35	-	198,200,200,201	0
9	MAN	G	1651	11/12	0.26	-	222,225,227,228	0
6	BMA	K	1747	11/12	0.28	-	194,195,196,196	0

## 6.5 Other polymers

There are no such residues in this entry.