



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:30 PM GMT

PDB ID : 4EZM  
Title : Crystal structure of the human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23  
Authors : Dhaliwal, B.; Yuan, D.; Sutton, B.J.  
Deposited on : 2012-05-03  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

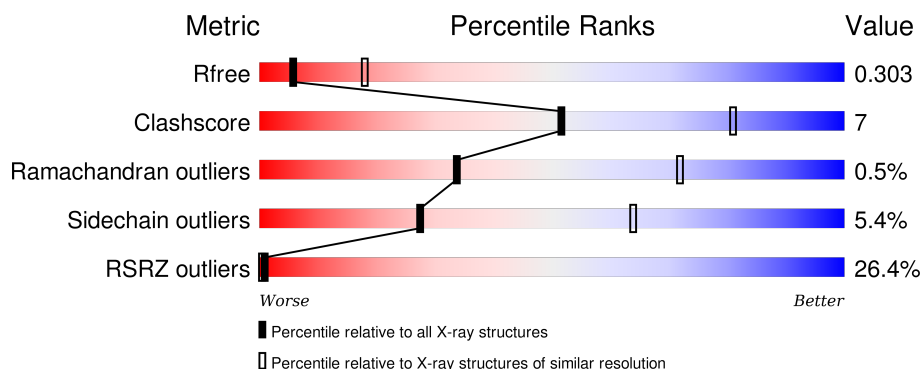
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	223	<div> <div>14%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
1	B	223	<div> <div>17%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	C	223	<div> <div>19%</div> <div>76%</div> <div>10%</div> <div>12%</div> </div>
1	D	223	<div> <div>21%</div> <div>83%</div> <div>8%</div> <div>7%</div> </div>
1	E	223	<div> <div>35%</div> <div>75%</div> <div>9%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	223	
2	G	143	
2	H	143	
2	I	143	
2	J	143	
2	K	143	
2	L	143	

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
3	NAG	A	601	-	-	-	X
3	NAG	A	602	-	-	-	X
3	NAG	C	601	-	-	-	X
3	NAG	E	601	-	-	-	X
4	MAN	C	607	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16496 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	B	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			
1	C	197	Total	C	N	O	S	0	1	0
			1565	981	284	294	6			
1	D	207	Total	C	N	O	S	0	0	0
			1639	1027	302	304	6			
1	E	191	Total	C	N	O	S	0	0	0
			1509	945	276	283	5			
1	F	208	Total	C	N	O	S	0	0	0
			1645	1030	303	306	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	EXPRESSION TAG	UNP P01854
A	326	ASP	-	EXPRESSION TAG	UNP P01854
A	327	PRO	-	EXPRESSION TAG	UNP P01854
A	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
A	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	325	ALA	-	EXPRESSION TAG	UNP P01854
B	326	ASP	-	EXPRESSION TAG	UNP P01854
B	327	PRO	-	EXPRESSION TAG	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854
C	325	ALA	-	EXPRESSION TAG	UNP P01854
C	326	ASP	-	EXPRESSION TAG	UNP P01854
C	327	PRO	-	EXPRESSION TAG	UNP P01854
C	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
C	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	325	ALA	-	EXPRESSION TAG	UNP P01854
D	326	ASP	-	EXPRESSION TAG	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	PRO	-	EXPRESSION TAG	UNP P01854
D	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854
E	325	ALA	-	EXPRESSION TAG	UNP P01854
E	326	ASP	-	EXPRESSION TAG	UNP P01854
E	327	PRO	-	EXPRESSION TAG	UNP P01854
E	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
E	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854
F	325	ALA	-	EXPRESSION TAG	UNP P01854
F	326	ASP	-	EXPRESSION TAG	UNP P01854
F	327	PRO	-	EXPRESSION TAG	UNP P01854
F	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
F	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854

- Molecule 2 is a protein called Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	H	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	I	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	J	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	K	134	Total	C	N	O	S	0	0	0
			1074	675	192	196	11			
2	L	134	Total	C	N	O	S	0	0	0
			1078	677	192	198	11			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

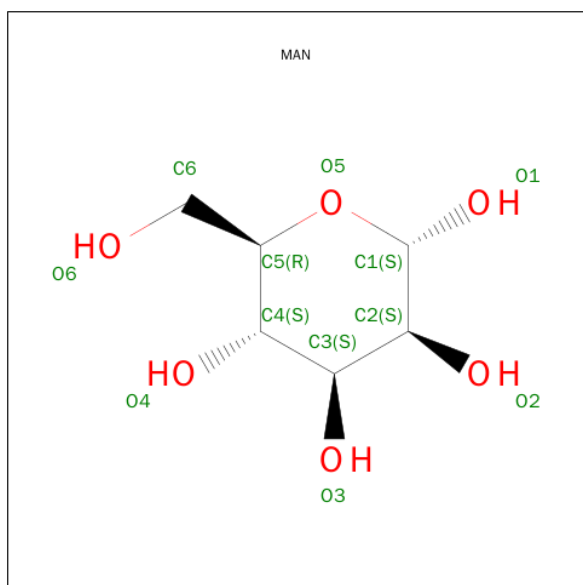
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	5	Total	C	N	O	0	0
			61	34	2	25		
3	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 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
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

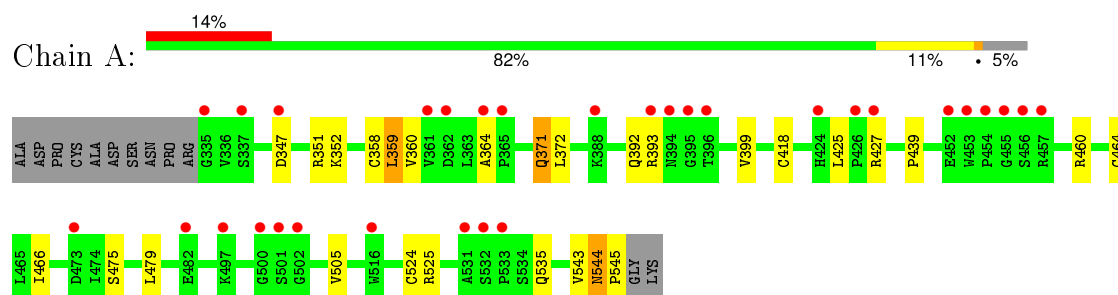
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	O	0	0
			1	1		

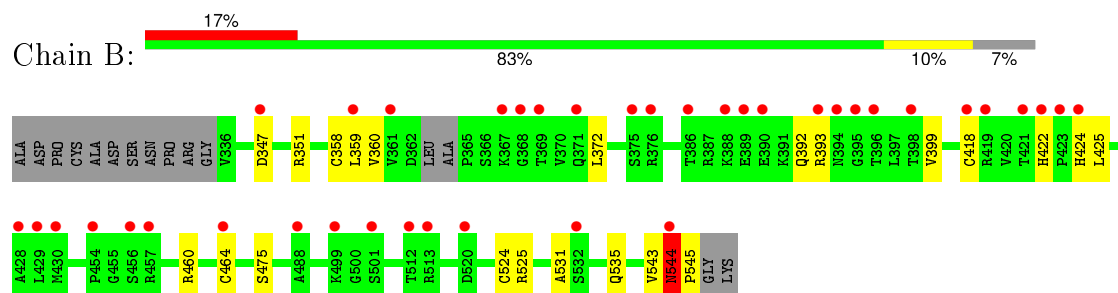
### 3 Residue-property plots

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.

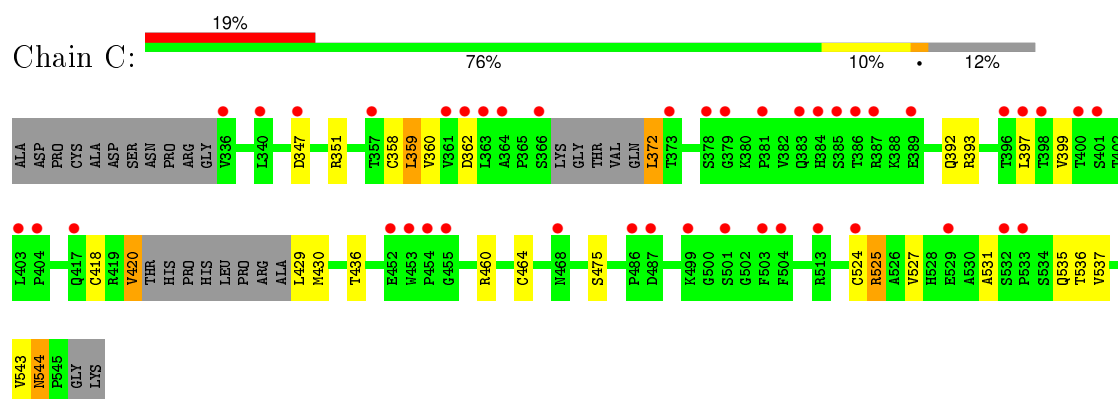
- Molecule 1: Ig epsilon chain C region



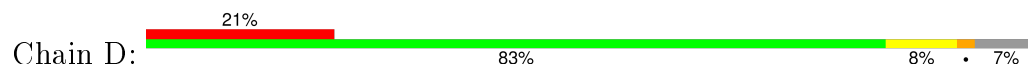
- Molecule 1: Ig epsilon chain C region

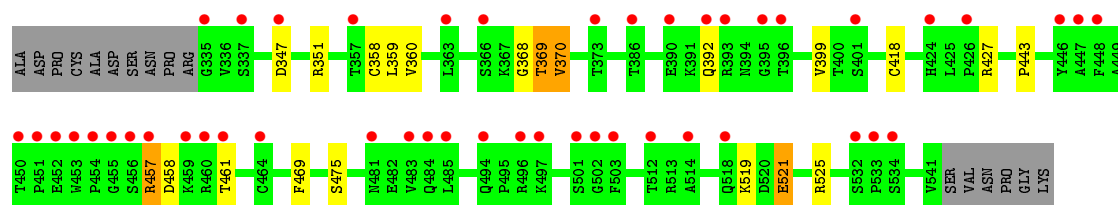


- Molecule 1: Ig epsilon chain C region

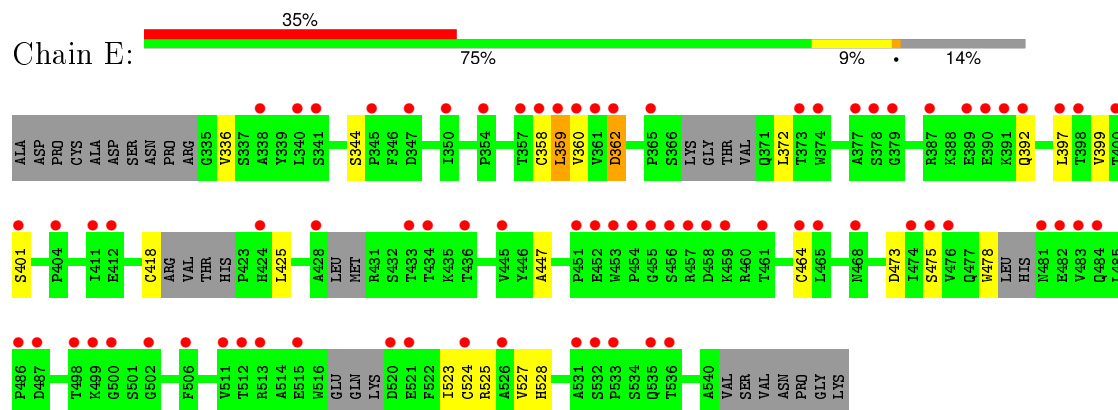


- Molecule 1: Ig epsilon chain C region

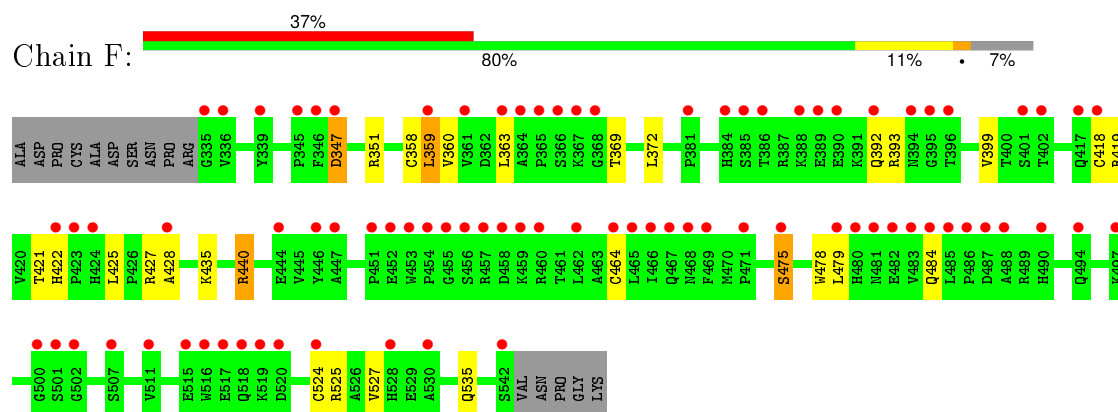




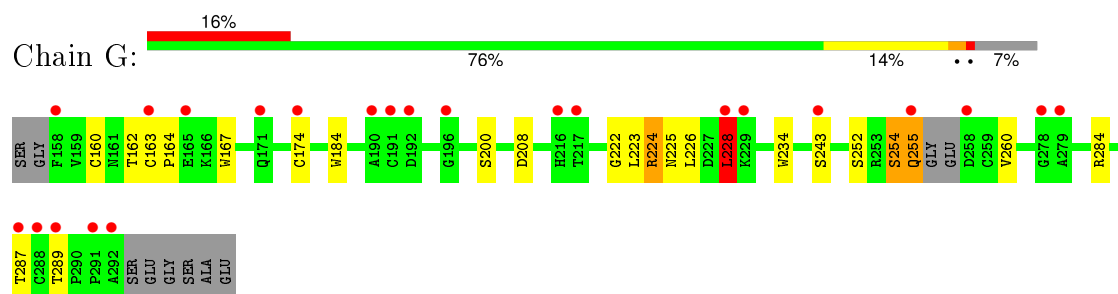
• Molecule 1: Ig epsilon chain C region



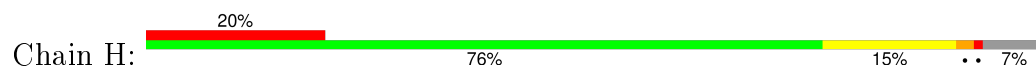
• Molecule 1: Ig epsilon chain C region



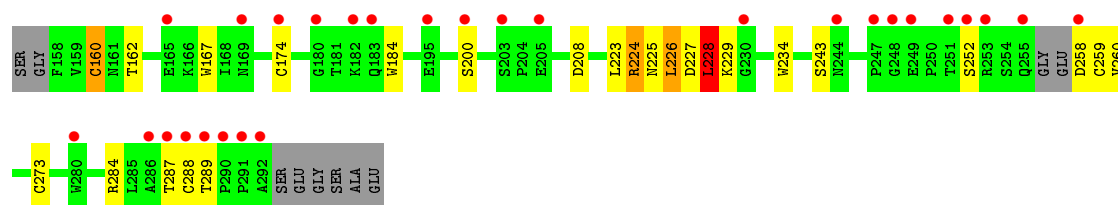
• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



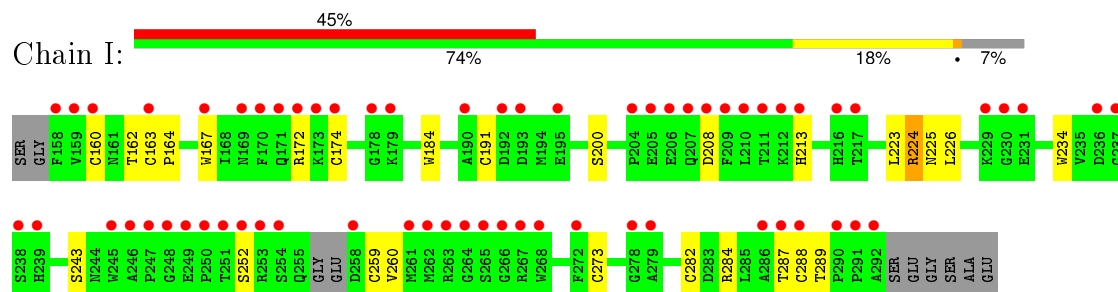
• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



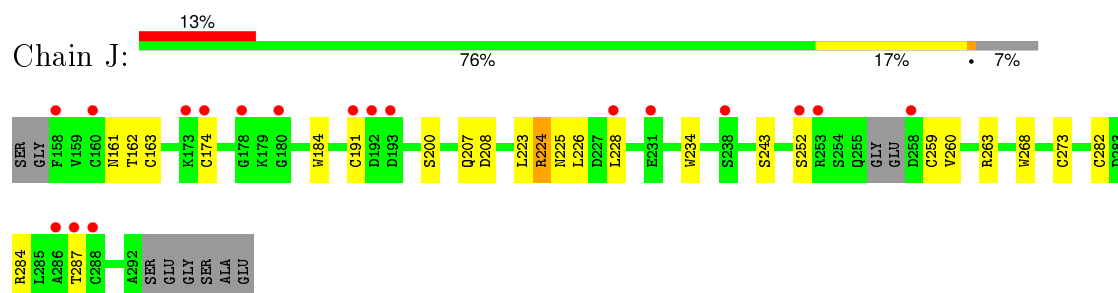




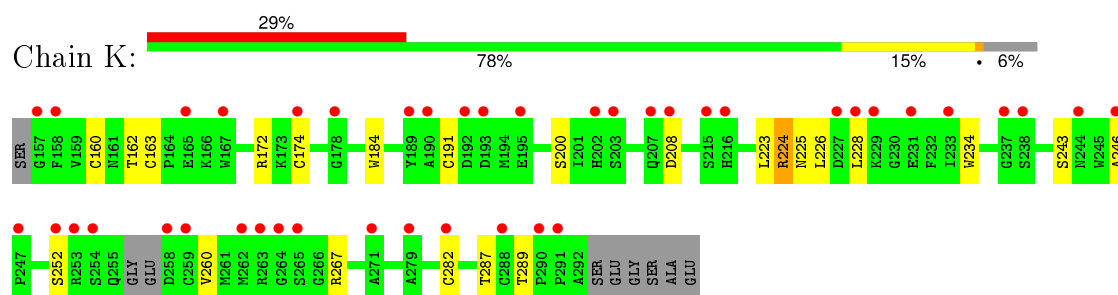
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



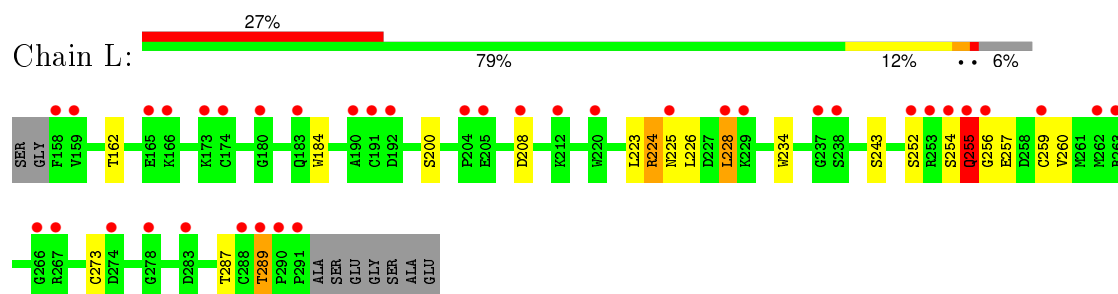
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.89Å 110.75Å 376.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.10 29.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.87-3.10) 98.7 (29.87-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 3.11Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.264 , 0.283 0.282 , 0.303	Depositor DCC
$R_{free}$ test set	2437 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 48290 reflections	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	16496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	1/1710 (0.1%)	0.72	7/2328 (0.3%)
1	B	0.39	0/1692	0.65	1/2301 (0.0%)
1	C	0.37	0/1605	0.64	0/2182
1	D	0.40	0/1681	0.76	4/2287 (0.2%)
1	E	0.37	0/1544	0.61	0/2094
1	F	0.37	0/1687	0.62	0/2295
2	G	0.42	0/1103	0.69	1/1494 (0.1%)
2	H	0.43	0/1103	0.70	0/1494
2	I	0.40	0/1103	0.68	0/1494
2	J	0.41	0/1103	0.68	0/1494
2	K	0.39	0/1107	0.68	0/1499
2	L	0.39	0/1112	0.75	3/1507 (0.2%)
All	All	0.40	1/16550 (0.0%)	0.68	16/22469 (0.1%)

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
2	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	PRO	N-CD	10.62	1.62	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	THR	CB-CA-C	13.29	147.49	111.60
2	L	256	GLY	N-CA-C	10.56	139.50	113.10
1	D	369	THR	N-CA-C	-8.64	87.67	111.00
1	A	364	ALA	N-CA-C	-6.86	92.48	111.00
1	A	371	GLN	N-CA-C	6.16	127.64	111.00
1	B	544	ASN	N-CA-C	5.97	127.12	111.00
2	G	254	SER	N-CA-C	-5.96	94.91	111.00
1	A	544	ASN	N-CA-C	5.83	126.75	111.00
1	A	545	PRO	CA-N-CD	-5.61	103.65	111.50
2	L	289	THR	N-CA-CB	5.60	120.94	110.30
1	D	369	THR	C-N-CA	5.57	135.62	121.70
1	A	544	ASN	C-N-CD	-5.56	108.36	120.60
2	L	255	GLN	CB-CA-C	-5.38	99.63	110.40
1	A	545	PRO	N-CA-C	5.25	125.75	112.10
1	A	364	ALA	CB-CA-C	5.19	117.89	110.10
1	D	368	GLY	C-N-CA	5.18	134.64	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	255	GLN	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	1667	0	1656	15	0
1	B	1650	0	1637	12	0
1	C	1565	0	1552	19	0
1	D	1639	0	1629	16	0
1	E	1509	0	1483	20	0
1	F	1645	0	1633	25	0
2	G	1070	0	994	20	0
2	H	1070	0	994	18	0
2	I	1070	0	994	17	0
2	J	1070	0	994	12	0
2	K	1074	0	996	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1078	0	999	14	0
3	A	61	0	52	5	0
3	B	61	0	52	4	0
3	C	61	0	52	9	0
3	D	61	0	52	4	0
3	E	61	0	52	6	0
3	F	61	0	52	5	0
4	C	22	0	20	3	0
5	J	1	0	0	0	0
All	All	16496	0	15893	192	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 7.

All (192) 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)
2:H:167:TRP:HB3	2:H:174:CYS:SG	1.43	1.57
1:E:478:TRP:CZ3	1:E:524:CYS:SG	2.15	1.37
2:I:163:CYS:SG	2:I:167:TRP:HB2	1.68	1.33
2:G:163:CYS:SG	2:G:167:TRP:HB2	1.72	1.27
2:H:167:TRP:CB	2:H:174:CYS:SG	2.25	1.22
1:E:478:TRP:CH2	1:E:524:CYS:SG	2.36	1.19
2:I:163:CYS:SG	2:I:167:TRP:CB	2.31	1.18
2:G:163:CYS:SG	2:G:167:TRP:CB	2.31	1.17
3:C:604:MAN:O6	4:C:607:MAN:H2	1.45	1.16
1:F:464:CYS:SG	1:F:478:TRP:CH2	2.53	1.00
2:H:259:CYS:HG	2:H:273:CYS:HG	1.07	0.97
1:E:478:TRP:CE3	1:E:524:CYS:SG	2.58	0.95
1:E:392:GLN:HG3	3:E:601:NAG:O6	1.67	0.94
1:C:392:GLN:NE2	3:C:601:NAG:O6	2.02	0.93
1:F:358:CYS:HG	1:F:418:CYS:HG	1.10	0.93
1:A:358:CYS:HG	1:A:418:CYS:HG	1.06	0.91
1:D:358:CYS:HG	1:D:418:CYS:HG	1.14	0.91
2:G:163:CYS:SG	2:G:167:TRP:HB3	2.09	0.90
2:I:191:CYS:HG	2:I:282:CYS:HG	1.21	0.89
1:D:369:THR:O	1:D:370:VAL:HG23	1.72	0.88
1:A:464:CYS:HG	1:A:524:CYS:HG	1.11	0.86
1:E:392:GLN:NE2	3:E:601:NAG:O6	2.08	0.86
1:C:392:GLN:HG3	3:C:601:NAG:O6	1.75	0.86
1:F:392:GLN:NE2	3:F:601:NAG:O6	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLN:CG	3:E:601:NAG:O6	2.25	0.84
1:F:440:ARG:NH1	2:L:255:GLN:O	2.10	0.84
2:L:254:SER:O	2:L:255:GLN:HB2	1.79	0.83
2:I:259:CYS:HG	2:I:273:CYS:HG	1.06	0.83
1:E:358:CYS:HG	1:E:418:CYS:HG	1.22	0.82
2:I:163:CYS:SG	2:I:167:TRP:HB3	2.16	0.82
1:C:544:ASN:O	1:C:544:ASN:ND2	2.13	0.82
1:D:392:GLN:NE2	3:D:601:NAG:O6	2.13	0.81
1:C:392:GLN:CG	3:C:601:NAG:O6	2.30	0.79
1:A:392:GLN:HG3	3:A:601:NAG:O6	1.81	0.79
1:B:392:GLN:NE2	3:B:601:NAG:O6	2.14	0.79
3:C:604:MAN:O6	4:C:607:MAN:C2	2.30	0.78
2:J:259:CYS:HG	2:J:273:CYS:HG	1.28	0.78
1:F:392:GLN:HG3	3:F:601:NAG:O6	1.82	0.78
2:K:191:CYS:HG	2:K:282:CYS:HG	1.28	0.78
1:C:464:CYS:HG	1:C:524:CYS:HG	1.32	0.77
1:C:544:ASN:CG	1:C:544:ASN:O	2.23	0.75
1:A:392:GLN:CG	3:A:601:NAG:O6	2.36	0.73
3:C:604:MAN:HO6	4:C:607:MAN:H2	1.52	0.73
2:H:160:CYS:HG	2:H:288:CYS:HG	1.28	0.73
1:D:521:GLU:HG3	1:F:421:THR:HG21	1.72	0.71
2:J:191:CYS:HG	2:J:282:CYS:HG	1.27	0.71
1:E:464:CYS:SG	1:E:478:TRP:CH2	2.84	0.70
1:F:392:GLN:CG	3:F:601:NAG:O6	2.38	0.70
1:B:392:GLN:HG3	3:B:601:NAG:O6	1.92	0.70
2:G:163:CYS:SG	2:G:164:PRO:HD2	2.31	0.70
1:D:392:GLN:HG3	3:D:601:NAG:O6	1.94	0.67
2:L:259:CYS:HG	2:L:273:CYS:HG	1.40	0.66
1:B:358:CYS:HG	1:B:418:CYS:HG	1.42	0.66
2:H:167:TRP:CG	2:H:174:CYS:SG	2.89	0.65
1:C:392:GLN:HE21	3:C:601:NAG:C6	2.10	0.65
1:C:543:VAL:O	1:C:544:ASN:OD1	2.16	0.64
1:B:392:GLN:CG	3:B:601:NAG:O6	2.46	0.64
1:E:478:TRP:CZ2	1:E:524:CYS:SG	2.92	0.63
2:H:167:TRP:CE3	2:H:174:CYS:SG	2.90	0.63
1:D:392:GLN:CG	3:D:601:NAG:O6	2.48	0.62
2:I:160:CYS:HG	2:I:288:CYS:HG	1.22	0.62
2:H:167:TRP:HB3	2:H:174:CYS:HG	1.55	0.62
2:L:254:SER:O	2:L:255:GLN:CB	2.48	0.62
1:D:392:GLN:HE21	3:D:601:NAG:C6	2.15	0.60
1:F:392:GLN:HE21	3:F:601:NAG:C6	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:252:SER:HB2	2:G:255:GLN:HA	1.84	0.59
1:E:392:GLN:HE21	3:E:601:NAG:C6	2.15	0.59
1:F:440:ARG:NH1	2:L:257:GLU:H	2.01	0.59
2:G:163:CYS:SG	2:G:164:PRO:CD	2.93	0.57
1:C:531:ALA:O	1:C:535:GLN:HA	2.05	0.57
1:E:475:SER:HB2	1:E:527:VAL:HB	1.86	0.56
2:J:162:THR:HB	2:J:287:THR:HG23	1.88	0.56
1:B:392:GLN:HE21	3:B:601:NAG:C6	2.16	0.56
2:K:246:ALA:HA	2:K:267:ARG:HE	1.71	0.55
1:E:359:LEU:HD11	3:E:602:NAG:O7	2.05	0.55
1:F:464:CYS:SG	1:F:478:TRP:HH2	2.18	0.55
2:I:162:THR:HB	2:I:287:THR:HG23	1.88	0.55
2:K:226:LEU:HG	2:K:226:LEU:O	2.07	0.55
1:B:464:CYS:HG	1:B:524:CYS:HG	0.59	0.55
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.89	0.55
2:H:162:THR:HB	2:H:287:THR:HG23	1.89	0.55
2:G:162:THR:HB	2:G:287:THR:HG23	1.88	0.54
2:J:174:CYS:HB2	2:J:284:ARG:HG2	1.90	0.54
1:F:464:CYS:SG	1:F:478:TRP:CZ2	2.92	0.54
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.90	0.54
2:I:163:CYS:SG	2:I:164:PRO:HD2	2.48	0.54
2:L:162:THR:HB	2:L:287:THR:HG23	1.90	0.54
1:E:336:VAL:HG12	1:E:362:ASP:HA	1.90	0.53
2:J:226:LEU:HG	2:J:226:LEU:O	2.08	0.53
2:G:184:TRP:CH2	2:G:224:ARG:HG2	2.44	0.53
2:L:226:LEU:O	2:L:226:LEU:HG	2.09	0.53
2:G:174:CYS:HB2	2:G:284:ARG:HG2	1.91	0.53
2:K:162:THR:HB	2:K:287:THR:HG23	1.89	0.53
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.91	0.52
1:D:360:VAL:HG13	1:D:399:VAL:HG13	1.91	0.52
1:F:360:VAL:HG13	1:F:399:VAL:HG13	1.91	0.52
2:J:184:TRP:CZ2	2:J:224:ARG:HG2	2.45	0.52
1:E:360:VAL:HG13	1:E:399:VAL:HG13	1.91	0.52
2:I:226:LEU:HG	2:I:226:LEU:O	2.09	0.52
1:F:347:ASP:HA	1:F:351:ARG:HB2	1.90	0.52
2:G:184:TRP:CZ2	2:G:224:ARG:HG2	2.45	0.51
1:D:443:PRO:HB3	1:D:469:PHE:HB3	1.91	0.51
2:K:184:TRP:CH2	2:K:224:ARG:HG2	2.45	0.51
1:C:359:LEU:HD11	3:C:602:NAG:O7	2.10	0.51
2:L:184:TRP:CH2	2:L:224:ARG:HG2	2.46	0.51
2:G:226:LEU:O	2:G:226:LEU:HG	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:LEU:O	2:H:226:LEU:HG	2.10	0.51
2:K:184:TRP:CZ2	2:K:224:ARG:HG2	2.46	0.51
1:C:475:SER:HB2	1:C:527:VAL:HB	1.92	0.51
1:A:535:GLN:OE1	2:G:228:LEU:HG	2.10	0.51
1:A:460:ARG:HG3	1:A:543:VAL:HG13	1.92	0.51
1:F:358:CYS:CB	1:F:418:CYS:HG	2.23	0.50
1:C:460:ARG:HG3	1:C:543:VAL:HG13	1.92	0.50
1:F:359:LEU:HD11	3:F:602:NAG:O7	2.11	0.50
2:I:184:TRP:CZ2	2:I:224:ARG:HG2	2.47	0.50
2:H:223:LEU:HB3	2:H:260:VAL:HB	1.93	0.50
1:D:358:CYS:CB	1:D:418:CYS:HG	2.25	0.50
2:G:163:CYS:HG	2:G:174:CYS:HB3	1.76	0.50
1:F:479:LEU:HG	1:F:484:GLN:HA	1.93	0.50
2:J:184:TRP:CH2	2:J:224:ARG:HG2	2.47	0.49
1:D:347:ASP:HA	1:D:351:ARG:HB2	1.94	0.49
1:B:460:ARG:HG3	1:B:543:VAL:HG13	1.94	0.49
2:L:184:TRP:CZ2	2:L:224:ARG:HG2	2.47	0.49
1:F:440:ARG:HH12	2:L:257:GLU:H	1.59	0.49
2:K:160:CYS:HB2	2:K:172:ARG:HG2	1.94	0.49
1:D:519:LYS:HD3	1:F:419:ARG:HH22	1.78	0.49
1:D:519:LYS:HA	1:F:419:ARG:HH22	1.77	0.48
2:G:252:SER:C	2:G:254:SER:H	2.17	0.48
1:C:358:CYS:CB	1:C:418:CYS:HG	2.26	0.48
1:B:347:ASP:HA	1:B:351:ARG:HB2	1.95	0.48
1:F:478:TRP:CE2	1:F:524:CYS:SG	2.99	0.48
2:K:163:CYS:CB	2:K:174:CYS:HG	2.16	0.48
1:D:369:THR:O	1:D:370:VAL:CG2	2.54	0.48
2:I:160:CYS:HB2	2:I:172:ARG:HG2	1.96	0.48
1:A:392:GLN:CD	3:A:601:NAG:HO6	2.14	0.48
2:K:163:CYS:HA	2:K:174:CYS:SG	2.54	0.48
2:I:184:TRP:CH2	2:I:224:ARG:HG2	2.48	0.48
1:C:392:GLN:CD	3:C:601:NAG:O6	2.52	0.47
2:H:167:TRP:HE3	2:H:174:CYS:SG	2.36	0.47
1:E:447:ALA:CB	1:E:464:CYS:SG	3.02	0.47
1:A:439:PRO:HA	2:G:254:SER:HA	1.96	0.47
1:D:519:LYS:HE3	1:F:428:ALA:H	1.79	0.47
1:F:535:GLN:OE1	2:L:228:LEU:HG	2.14	0.47
2:L:200:SER:HA	2:L:234:TRP:CE3	2.50	0.47
2:I:174:CYS:HB2	2:I:284:ARG:HG2	1.96	0.47
2:K:200:SER:HA	2:K:234:TRP:CE3	2.50	0.47
2:I:163:CYS:SG	2:I:174:CYS:SG	3.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:200:SER:HA	2:G:234:TRP:CE3	2.49	0.47
2:H:174:CYS:HB3	2:H:284:ARG:HG2	1.97	0.47
1:F:435:LYS:HE3	2:L:257:GLU:HG3	1.97	0.46
2:H:184:TRP:CH2	2:H:224:ARG:HG2	2.50	0.46
2:I:200:SER:HA	2:I:234:TRP:CE3	2.50	0.46
2:H:227:ASP:C	2:H:229:LYS:H	2.18	0.46
2:J:200:SER:HA	2:J:234:TRP:CE3	2.50	0.46
1:E:392:GLN:CD	3:E:601:NAG:O6	2.54	0.46
2:H:226:LEU:H	2:H:229:LYS:HG3	1.81	0.46
2:G:163:CYS:SG	2:G:174:CYS:SG	3.14	0.45
2:J:207:GLN:OE1	2:J:268:TRP:NE1	2.48	0.45
2:H:167:TRP:HB2	2:H:174:CYS:SG	2.44	0.45
1:E:447:ALA:HB2	1:E:464:CYS:SG	2.56	0.45
1:D:457:ARG:HA	1:D:457:ARG:NE	2.32	0.44
1:A:358:CYS:CB	1:A:418:CYS:HG	2.31	0.44
1:C:347:ASP:HA	1:C:351:ARG:HB2	1.99	0.44
1:B:544:ASN:HA	1:B:545:PRO:HD2	1.74	0.44
1:A:392:GLN:OE1	3:A:601:NAG:O6	2.23	0.44
1:E:362:ASP:HB3	1:E:397:LEU:O	2.18	0.44
2:K:163:CYS:CB	2:K:174:CYS:SG	3.04	0.44
2:J:163:CYS:CB	2:J:174:CYS:SG	3.06	0.44
2:I:163:CYS:SG	2:I:164:PRO:CD	3.06	0.43
1:C:525:ARG:HD2	1:C:536:THR:HG21	2.01	0.43
1:B:422:HIS:HB3	1:B:425:LEU:HB3	2.01	0.42
2:G:222:GLY:O	2:G:234:TRP:HA	2.19	0.42
1:F:422:HIS:HB3	1:F:425:LEU:HD13	2.00	0.42
2:J:163:CYS:HG	2:J:174:CYS:HG	0.42	0.42
2:L:223:LEU:HB3	2:L:260:VAL:HB	2.02	0.42
1:A:347:ASP:HA	1:A:351:ARG:HB2	2.01	0.42
1:A:460:ARG:HG3	1:A:543:VAL:CG1	2.50	0.42
1:A:359:LEU:HD11	3:A:602:NAG:O7	2.20	0.41
1:B:531:ALA:O	1:B:535:GLN:HA	2.19	0.41
2:G:254:SER:O	2:G:255:GLN:OE1	2.39	0.41
1:C:531:ALA:HB1	1:C:537:VAL:HG23	2.01	0.41
2:G:223:LEU:HB3	2:G:260:VAL:HB	2.02	0.41
1:E:478:TRP:CD2	1:E:524:CYS:SG	3.09	0.41
2:K:223:LEU:HB3	2:K:260:VAL:HB	2.03	0.41
2:I:223:LEU:HB3	2:I:260:VAL:HB	2.02	0.41
2:H:226:LEU:O	2:H:228:LEU:N	2.54	0.41
1:C:372:LEU:HA	1:C:420:VAL:HG13	2.04	0.40
1:E:473:ASP:O	1:E:528:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:223:LEU:HB3	2:J:260:VAL:HB	2.03	0.40
2:H:200:SER:HA	2:H:234:TRP:CE3	2.57	0.40
1:F:475:SER:HB2	1:F:527:VAL:HB	2.03	0.40
1:A:466:ILE:HD13	1:A:505:VAL:HG23	2.04	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	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	34	72
1	B	204/223 (92%)	190 (93%)	13 (6%)	1 (0%)	34	72
1	C	192/223 (86%)	183 (95%)	8 (4%)	1 (0%)	34	72
1	D	205/223 (92%)	193 (94%)	11 (5%)	1 (0%)	34	72
1	E	179/223 (80%)	171 (96%)	8 (4%)	0	100	100
1	F	206/223 (92%)	200 (97%)	5 (2%)	1 (0%)	34	72
2	G	129/143 (90%)	113 (88%)	15 (12%)	1 (1%)	24	63
2	H	129/143 (90%)	118 (92%)	9 (7%)	2 (2%)	12	44
2	I	129/143 (90%)	113 (88%)	16 (12%)	0	100	100
2	J	129/143 (90%)	116 (90%)	12 (9%)	1 (1%)	24	63
2	K	130/143 (91%)	118 (91%)	12 (9%)	0	100	100
2	L	132/143 (92%)	118 (89%)	14 (11%)	0	100	100
All	All	1973/2196 (90%)	1831 (93%)	133 (7%)	9 (0%)	34	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	VAL
2	H	228	LEU
1	A	393	ARG
1	B	393	ARG
1	F	393	ARG
1	C	393	ARG
2	G	228	LEU
2	H	226	LEU
2	J	161	ASN

### 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	186/195 (95%)	176 (95%)	10 (5%)	27	64
1	B	185/195 (95%)	179 (97%)	6 (3%)	46	79
1	C	176/195 (90%)	166 (94%)	10 (6%)	25	62
1	D	182/195 (93%)	174 (96%)	8 (4%)	35	71
1	E	167/195 (86%)	159 (95%)	8 (5%)	31	69
1	F	183/195 (94%)	174 (95%)	9 (5%)	31	68
2	G	114/120 (95%)	106 (93%)	8 (7%)	19	54
2	H	114/120 (95%)	105 (92%)	9 (8%)	15	49
2	I	114/120 (95%)	107 (94%)	7 (6%)	23	59
2	J	114/120 (95%)	107 (94%)	7 (6%)	23	59
2	K	114/120 (95%)	107 (94%)	7 (6%)	23	59
2	L	115/120 (96%)	108 (94%)	7 (6%)	23	59
All	All	1764/1890 (93%)	1668 (95%)	96 (5%)	27	64

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LYS
1	A	359	LEU

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Mol	Chain	Res	Type
1	A	371	GLN
1	A	372	LEU
1	A	425	LEU
1	A	427	ARG
1	A	475	SER
1	A	479	LEU
1	A	525	ARG
1	A	544	ASN
1	B	359	LEU
1	B	372	LEU
1	B	424	HIS
1	B	475	SER
1	B	525	ARG
1	B	544	ASN
1	C	359	LEU
1	C	362	ASP
1	C	372	LEU
1	C	397	LEU
1	C	420	VAL
1	C	429	LEU
1	C	430	MET
1	C	436	THR
1	C	525	ARG
1	C	544	ASN
1	D	359	LEU
1	D	427	ARG
1	D	457	ARG
1	D	458	ASP
1	D	461	THR
1	D	475	SER
1	D	521	GLU
1	D	525	ARG
1	E	344	SER
1	E	359	LEU
1	E	362	ASP
1	E	372	LEU
1	E	401	SER
1	E	425	LEU
1	E	523	ILE
1	E	525	ARG
1	F	347	ASP
1	F	359	LEU

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Mol	Chain	Res	Type
1	F	363	LEU
1	F	369	THR
1	F	372	LEU
1	F	427	ARG
1	F	440	ARG
1	F	475	SER
1	F	525	ARG
2	G	160	CYS
2	G	208	ASP
2	G	224	ARG
2	G	225	ASN
2	G	228	LEU
2	G	243	SER
2	G	255	GLN
2	G	289	THR
2	H	160	CYS
2	H	208	ASP
2	H	224	ARG
2	H	225	ASN
2	H	228	LEU
2	H	243	SER
2	H	252	SER
2	H	258	ASP
2	H	289	THR
2	I	208	ASP
2	I	213	HIS
2	I	224	ARG
2	I	225	ASN
2	I	243	SER
2	I	252	SER
2	I	289	THR
2	J	208	ASP
2	J	224	ARG
2	J	225	ASN
2	J	228	LEU
2	J	243	SER
2	J	252	SER
2	J	263	ARG
2	K	208	ASP
2	K	224	ARG
2	K	225	ASN
2	K	228	LEU

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Mol	Chain	Res	Type
2	K	243	SER
2	K	252	SER
2	K	289	THR
2	L	208	ASP
2	L	224	ARG
2	L	225	ASN
2	L	228	LEU
2	L	243	SER
2	L	252	SER
2	L	289	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	B	481	ASN
1	C	392	GLN
1	C	544	ASN
1	D	392	GLN
1	E	392	GLN
1	F	392	GLN
2	G	213	HIS
2	G	225	ASN
2	G	255	GLN
2	G	269	ASN
2	H	213	HIS
2	H	269	ASN
2	I	225	ASN
2	I	269	ASN
2	J	213	HIS
2	J	225	ASN
2	J	269	ASN
2	K	213	HIS
2	K	225	ASN
2	K	269	ASN
2	L	213	HIS
2	L	225	ASN
2	L	269	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

30 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	$\# Z  > 2$
3	NAG	A	601	3	14,14,15	0.49	0	15,19,21	1.26	1 (6%)
3	NAG	A	602	3	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
3	BMA	A	603	3	11,11,12	0.69	0	14,15,17	1.90	4 (28%)
3	MAN	A	604	3	11,11,12	0.61	0	14,15,17	1.63	3 (21%)
3	MAN	A	605	3	11,11,12	0.57	0	14,15,17	1.66	4 (28%)
3	NAG	B	601	3	14,14,15	0.49	0	15,19,21	1.25	1 (6%)
3	NAG	B	602	3	14,14,15	0.54	0	15,19,21	1.29	1 (6%)
3	BMA	B	603	3	11,11,12	0.68	0	14,15,17	1.91	4 (28%)
3	MAN	B	604	3	11,11,12	0.61	0	14,15,17	1.62	3 (21%)
3	MAN	B	605	3	11,11,12	0.58	0	14,15,17	1.65	4 (28%)
3	NAG	C	601	3	14,14,15	0.49	0	15,19,21	1.26	1 (6%)
3	NAG	C	602	3	14,14,15	0.53	0	15,19,21	1.29	2 (13%)
3	BMA	C	603	3	11,11,12	0.68	0	14,15,17	1.90	4 (28%)
3	MAN	C	604	3	11,11,12	0.61	0	14,15,17	1.62	3 (21%)
3	MAN	C	605	3	11,11,12	0.58	0	14,15,17	1.65	4 (28%)
3	NAG	D	601	3	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
3	NAG	D	602	3	14,14,15	0.54	0	15,19,21	1.29	2 (13%)
3	BMA	D	603	3	11,11,12	0.68	0	14,15,17	1.91	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	D	604	3	11,11,12	0.62	0	14,15,17	1.62	3 (21%)
3	MAN	D	605	3	11,11,12	0.58	0	14,15,17	1.65	4 (28%)
3	NAG	E	601	3	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
3	NAG	E	602	3	14,14,15	0.54	0	15,19,21	1.28	2 (13%)
3	BMA	E	603	3	11,11,12	0.68	0	14,15,17	1.91	4 (28%)
3	MAN	E	604	3	11,11,12	0.61	0	14,15,17	1.62	3 (21%)
3	MAN	E	605	3	11,11,12	0.58	0	14,15,17	1.65	4 (28%)
3	NAG	F	601	3	14,14,15	0.49	0	15,19,21	1.25	1 (6%)
3	NAG	F	602	3	14,14,15	0.54	0	15,19,21	1.28	1 (6%)
3	BMA	F	603	3	11,11,12	0.68	0	14,15,17	1.90	3 (21%)
3	MAN	F	604	3	11,11,12	0.61	0	14,15,17	1.64	3 (21%)
3	MAN	F	605	3	11,11,12	0.58	0	14,15,17	1.65	4 (28%)

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
3	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
3	BMA	A	603	3	-	0/2/19/22	0/1/1/1
3	MAN	A	604	3	-	0/2/19/22	0/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	NAG	B	601	3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	MAN	B	604	3	-	0/2/19/22	0/1/1/1
3	MAN	B	605	3	-	0/2/19/22	0/1/1/1
3	NAG	C	601	3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	3	-	0/6/23/26	0/1/1/1
3	BMA	C	603	3	-	0/2/19/22	0/1/1/1
3	MAN	C	604	3	-	0/2/19/22	0/1/1/1
3	MAN	C	605	3	-	0/2/19/22	0/1/1/1
3	NAG	D	601	3	-	0/6/23/26	0/1/1/1
3	NAG	D	602	3	-	0/6/23/26	0/1/1/1
3	BMA	D	603	3	-	0/2/19/22	0/1/1/1
3	MAN	D	604	3	-	0/2/19/22	0/1/1/1
3	MAN	D	605	3	-	0/2/19/22	0/1/1/1
3	NAG	E	601	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1
3	BMA	E	603	3	-	0/2/19/22	0/1/1/1
3	MAN	E	604	3	-	0/2/19/22	0/1/1/1
3	MAN	E	605	3	-	0/2/19/22	0/1/1/1
3	NAG	F	601	3	-	0/6/23/26	0/1/1/1
3	NAG	F	602	3	-	0/6/23/26	0/1/1/1
3	BMA	F	603	3	-	0/2/19/22	0/1/1/1
3	MAN	F	604	3	-	0/2/19/22	0/1/1/1
3	MAN	F	605	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	MAN	O5-C1-C2	-3.20	105.67	110.86
3	A	604	MAN	O5-C1-C2	-3.18	105.70	110.86
3	F	605	MAN	O5-C1-C2	-3.18	105.70	110.86
3	F	604	MAN	O5-C1-C2	-3.18	105.70	110.86
3	E	603	BMA	O3-C3-C4	-3.17	103.20	110.34
3	A	603	BMA	O3-C3-C4	-3.17	103.21	110.34
3	B	603	BMA	O3-C3-C4	-3.17	103.21	110.34
3	D	605	MAN	O5-C1-C2	-3.17	105.72	110.86
3	B	605	MAN	O5-C1-C2	-3.16	105.72	110.86
3	D	603	BMA	O3-C3-C4	-3.16	103.22	110.34
3	C	604	MAN	O5-C1-C2	-3.16	105.74	110.86
3	D	604	MAN	O5-C1-C2	-3.15	105.74	110.86
3	E	605	MAN	O5-C1-C2	-3.15	105.74	110.86
3	E	604	MAN	O5-C1-C2	-3.15	105.75	110.86
3	C	603	BMA	O3-C3-C4	-3.15	103.25	110.34
3	F	603	BMA	O3-C3-C4	-3.15	103.25	110.34
3	B	604	MAN	O5-C1-C2	-3.14	105.77	110.86
3	C	605	MAN	O5-C1-C2	-3.13	105.78	110.86
3	C	603	BMA	C6-C5-C4	-2.85	105.99	113.02
3	F	603	BMA	C6-C5-C4	-2.85	105.99	113.02
3	B	603	BMA	C6-C5-C4	-2.84	106.01	113.02
3	E	603	BMA	C6-C5-C4	-2.83	106.03	113.02
3	D	603	BMA	C6-C5-C4	-2.83	106.03	113.02
3	A	603	BMA	C6-C5-C4	-2.83	106.04	113.02
3	B	605	MAN	C3-C4-C5	-2.81	105.30	110.20
3	A	605	MAN	C3-C4-C5	-2.80	105.31	110.20
3	D	605	MAN	C3-C4-C5	-2.79	105.33	110.20
3	F	605	MAN	C3-C4-C5	-2.78	105.34	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	605	MAN	C3-C4-C5	-2.78	105.35	110.20
3	E	605	MAN	C3-C4-C5	-2.78	105.36	110.20
3	B	604	MAN	O4-C4-C3	-2.60	104.48	110.34
3	D	604	MAN	O4-C4-C3	-2.60	104.49	110.34
3	C	604	MAN	O4-C4-C3	-2.59	104.50	110.34
3	A	604	MAN	O4-C4-C3	-2.59	104.51	110.34
3	E	604	MAN	O4-C4-C3	-2.58	104.52	110.34
3	F	604	MAN	O4-C4-C3	-2.58	104.52	110.34
3	C	605	MAN	C2-C3-C4	-2.49	106.81	111.04
3	A	605	MAN	C2-C3-C4	-2.48	106.83	111.04
3	B	605	MAN	C2-C3-C4	-2.47	106.85	111.04
3	D	605	MAN	C2-C3-C4	-2.47	106.85	111.04
3	E	605	MAN	C2-C3-C4	-2.47	106.85	111.04
3	F	605	MAN	C2-C3-C4	-2.45	106.88	111.04
3	B	605	MAN	C1-C2-C3	-2.04	107.12	109.54
3	C	605	MAN	C1-C2-C3	-2.03	107.14	109.54
3	F	605	MAN	C1-C2-C3	-2.03	107.14	109.54
3	E	602	NAG	O7-C7-C8	-2.03	118.34	122.06
3	E	605	MAN	C1-C2-C3	-2.03	107.14	109.54
3	D	602	NAG	O7-C7-C8	-2.02	118.35	122.06
3	D	605	MAN	C1-C2-C3	-2.02	107.15	109.54
3	A	605	MAN	C1-C2-C3	-2.02	107.15	109.54
3	C	602	NAG	O7-C7-C8	-2.01	118.37	122.06
3	C	603	BMA	C1-O5-C5	2.01	114.81	112.25
3	A	603	BMA	C1-O5-C5	2.03	114.82	112.25
3	E	603	BMA	C1-O5-C5	2.04	114.84	112.25
3	B	603	BMA	C1-O5-C5	2.04	114.84	112.25
3	D	603	BMA	C1-O5-C5	2.06	114.86	112.25
3	B	601	NAG	O5-C5-C6	2.67	113.14	107.35
3	F	601	NAG	O5-C5-C6	2.67	113.14	107.35
3	D	601	NAG	O5-C5-C6	2.68	113.14	107.35
3	A	601	NAG	O5-C5-C6	2.69	113.16	107.35
3	C	601	NAG	O5-C5-C6	2.69	113.17	107.35
3	E	601	NAG	O5-C5-C6	2.69	113.18	107.35
3	E	602	NAG	C1-O5-C5	2.95	115.99	112.25
3	D	602	NAG	C1-O5-C5	2.95	116.00	112.25
3	C	602	NAG	C1-O5-C5	2.95	116.00	112.25
3	F	602	NAG	C1-O5-C5	2.96	116.01	112.25
3	B	602	NAG	C1-O5-C5	2.97	116.02	112.25
3	A	602	NAG	C1-O5-C5	3.01	116.07	112.25
3	D	604	MAN	C3-C4-C5	3.09	115.58	110.20
3	E	604	MAN	C3-C4-C5	3.09	115.59	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	MAN	C3-C4-C5	3.11	115.62	110.20
3	A	604	MAN	C3-C4-C5	3.12	115.64	110.20
3	B	604	MAN	C3-C4-C5	3.13	115.65	110.20
3	F	604	MAN	C3-C4-C5	3.15	115.69	110.20
3	C	603	BMA	O5-C5-C6	4.59	117.27	107.35
3	F	603	BMA	O5-C5-C6	4.59	117.29	107.35
3	A	603	BMA	O5-C5-C6	4.59	117.29	107.35
3	B	603	BMA	O5-C5-C6	4.61	117.32	107.35
3	D	603	BMA	O5-C5-C6	4.61	117.33	107.35
3	E	603	BMA	O5-C5-C6	4.62	117.35	107.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAG	4	0
3	A	602	NAG	1	0
3	B	601	NAG	4	0
3	C	601	NAG	5	0
3	C	602	NAG	1	0
3	C	604	MAN	3	0
3	D	601	NAG	4	0
3	E	601	NAG	5	0
3	E	602	NAG	1	0
3	F	601	NAG	4	0
3	F	602	NAG	1	0

## 5.6 Ligand geometry

2 ligands 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
4	MAN	C	606	-	11,11,12	1.39	2 (18%)	14,15,17	1.92	6 (42%)
4	MAN	C	607	-	11,11,12	1.56	3 (27%)	14,15,17	1.32	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	606	-	-	0/2/19/22	1/1/1/1
4	MAN	C	607	-	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	MAN	C1-C2	2.02	1.57	1.52
4	C	607	MAN	C4-C3	2.07	1.57	1.52
4	C	607	MAN	O5-C5	2.12	1.48	1.43
4	C	607	MAN	C4-C5	2.41	1.58	1.53
4	C	606	MAN	C4-C5	2.49	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	MAN	C3-C4-C5	-2.52	105.81	110.20
4	C	606	MAN	C6-C5-C4	2.08	118.15	113.02
4	C	606	MAN	C1-C2-C3	2.25	112.21	109.54
4	C	606	MAN	O3-C3-C4	2.37	115.68	110.34
4	C	606	MAN	O5-C1-C2	2.55	114.99	110.86
4	C	607	MAN	O3-C3-C4	2.77	116.57	110.34
4	C	606	MAN	C1-O5-C5	3.61	116.83	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	606	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	607	MAN	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	211/223 (94%)	1.09	31 (14%) 3 1	58, 83, 128, 143	0
1	B	208/223 (93%)	1.12	39 (18%) 2 1	55, 84, 162, 190	0
1	C	197/223 (88%)	1.29	43 (21%) 1 0	70, 100, 137, 178	0
1	D	207/223 (92%)	1.34	47 (22%) 1 0	65, 93, 144, 186	0
1	E	191/223 (85%)	2.23	77 (40%) 0 0	103, 134, 192, 213	0
1	F	208/223 (93%)	2.00	83 (39%) 0 0	97, 125, 172, 194	0
2	G	133/143 (93%)	1.09	23 (17%) 2 1	68, 91, 140, 176	0
2	H	133/143 (93%)	1.19	28 (21%) 1 0	66, 98, 129, 153	0
2	I	133/143 (93%)	2.56	64 (48%) 0 0	109, 140, 171, 197	0
2	J	133/143 (93%)	0.93	18 (13%) 4 2	62, 85, 120, 158	0
2	K	134/143 (93%)	1.72	42 (31%) 1 0	92, 122, 148, 168	0
2	L	134/143 (93%)	1.66	38 (28%) 1 0	91, 122, 155, 183	0
All	All	2022/2196 (92%)	1.51	533 (26%) 1 0	55, 109, 161, 213	0

All (533) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	292	ALA	23.4
2	I	264	GLY	13.0
1	E	456	SER	10.8
2	I	173	LYS	10.1
1	E	515	GLU	10.0
1	A	395	GLY	9.9
1	F	500	GLY	9.8
1	E	532	SER	9.7
2	I	291	PRO	9.5
1	D	454	PRO	9.4
2	H	292	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
2	I	205	GLU	8.7
1	D	452	GLU	8.4
1	E	424	HIS	8.3
1	A	501	SER	8.2
2	I	193	ASP	8.2
1	F	480	HIS	8.0
1	D	335	GLY	8.0
2	K	264	GLY	8.0
2	I	265	SER	7.9
1	C	533	PRO	7.8
2	K	259	CYS	7.8
1	D	533	PRO	7.7
1	B	369	THR	7.7
1	F	542	SER	7.7
1	E	359	LEU	7.4
1	D	459	LYS	7.4
1	F	464	CYS	7.3
1	D	483	VAL	7.3
1	F	396	THR	7.3
1	E	452	GLU	7.3
2	K	247	PRO	7.2
1	E	531	ALA	7.2
2	G	288	CYS	7.1
2	I	158	PHE	7.1
2	I	178	GLY	7.0
2	L	253	ARG	6.9
1	F	487	ASP	6.8
1	E	358	CYS	6.8
1	F	424	HIS	6.8
2	I	216	HIS	6.8
1	B	395	GLY	6.7
2	K	178	GLY	6.7
1	F	486	PRO	6.6
2	L	205	GLU	6.6
1	E	484	GLN	6.6
1	D	366	SER	6.6
2	L	252	SER	6.4
1	E	434	THR	6.3
2	I	231	GLU	6.3
1	F	481	ASN	6.2
1	E	457	ARG	6.2
1	C	373	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	454	PRO	6.1
1	F	455	GLY	6.0
2	H	252	SER	6.0
1	D	456	SER	6.0
1	F	483	VAL	5.9
1	B	424	HIS	5.8
1	C	417	GLN	5.8
1	E	390	GLU	5.8
2	J	193	ASP	5.8
2	H	289	THR	5.8
1	A	394	ASN	5.7
1	F	501	SER	5.7
1	A	393	ARG	5.7
1	C	378	SER	5.7
1	B	419	ARG	5.7
2	I	250	PRO	5.7
2	L	291	PRO	5.7
1	B	418	CYS	5.6
1	E	487	ASP	5.6
2	I	174	CYS	5.6
2	I	172	ARG	5.6
2	K	253	ARG	5.6
2	L	256	GLY	5.5
1	C	347	ASP	5.5
2	K	174	CYS	5.5
2	G	289	THR	5.5
1	E	458	ASP	5.5
1	F	335	GLY	5.5
1	E	454	PRO	5.4
1	A	533	PRO	5.4
1	A	454	PRO	5.4
2	I	279	ALA	5.4
2	L	266	GLY	5.4
1	F	368	GLY	5.4
1	F	402	THR	5.3
1	C	363	LEU	5.3
1	C	501	SER	5.3
2	K	165	GLU	5.3
2	G	228	LEU	5.3
1	C	336	VAL	5.2
1	B	454	PRO	5.2
2	K	229	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	378	SER	5.2
1	E	428	ALA	5.2
1	E	377	ALA	5.2
1	E	392	GLN	5.2
1	B	393	ARG	5.1
2	J	174	CYS	5.1
1	F	451	PRO	5.1
1	A	482	GLU	5.1
2	L	254	SER	5.1
2	L	191	CYS	5.1
1	D	393	ARG	5.0
2	K	238	SER	5.0
1	F	456	SER	5.0
2	L	190	ALA	4.9
1	C	389	GLU	4.9
2	L	255	GLN	4.9
1	F	390	GLU	4.9
1	E	499	LYS	4.9
2	I	249	GLU	4.9
1	F	347	ASP	4.8
2	G	192	ASP	4.8
2	I	272	PHE	4.8
2	G	216	HIS	4.8
2	K	216	HIS	4.8
1	F	365	PRO	4.8
2	K	193	ASP	4.7
1	B	347	ASP	4.7
2	G	278	GLY	4.7
1	E	533	PRO	4.7
1	C	379	GLY	4.7
1	D	460	ARG	4.7
1	B	394	ASN	4.6
1	E	373	THR	4.6
1	D	424	HIS	4.6
2	H	253	ARG	4.6
1	F	519	LYS	4.6
2	L	278	GLY	4.6
2	L	263	ARG	4.6
1	A	531	ALA	4.6
1	F	459	LYS	4.6
1	C	453	TRP	4.6
1	E	361	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	451	PRO	4.6
1	F	361	VAL	4.6
2	I	167	TRP	4.6
1	E	482	GLU	4.6
2	I	263	ARG	4.5
2	L	159	VAL	4.5
1	F	418	CYS	4.5
1	D	457	ARG	4.5
2	J	287	THR	4.5
1	E	512	THR	4.5
1	B	386	THR	4.4
1	E	464	CYS	4.4
2	I	229	LYS	4.4
2	K	263	ARG	4.4
2	I	248	GLY	4.4
2	L	289	THR	4.4
1	C	397	LEU	4.4
1	F	363	LEU	4.4
2	K	190	ALA	4.4
1	F	389	GLU	4.3
1	B	512	THR	4.3
1	E	340	LEU	4.3
1	C	383	GLN	4.3
1	F	516	TRP	4.3
1	F	345	PRO	4.3
1	B	501	SER	4.3
1	D	512	THR	4.3
1	E	341	SER	4.3
1	D	392	GLN	4.3
1	E	486	PRO	4.3
1	E	459	LYS	4.2
1	A	456	SER	4.2
1	F	417	GLN	4.2
1	A	532	SER	4.2
1	D	455	GLY	4.2
2	I	251	THR	4.2
1	E	468	ASN	4.2
2	I	266	GLY	4.2
1	F	524	CYS	4.2
1	F	460	ARG	4.2
2	I	207	GLN	4.1
2	L	212	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	487	ASP	4.1
2	L	288	CYS	4.1
1	A	335	GLY	4.1
1	E	453	TRP	4.1
2	I	290	PRO	4.1
2	I	236	ASP	4.1
2	H	291	PRO	4.1
1	A	453	TRP	4.1
1	C	364	ALA	4.0
1	F	485	LEU	4.0
2	K	262	MET	4.0
2	G	165	GLU	4.0
1	B	396	THR	4.0
2	K	228	LEU	4.0
2	K	192	ASP	4.0
1	D	373	THR	4.0
1	C	454	PRO	4.0
1	E	389	GLU	4.0
1	E	511	VAL	4.0
1	E	481	ASN	3.9
2	I	163	CYS	3.9
1	D	481	ASN	3.9
1	E	400	THR	3.9
2	K	271	ALA	3.9
1	E	401	SER	3.9
1	E	357	THR	3.9
1	D	401	SER	3.9
1	D	518	GLN	3.9
2	G	229	LYS	3.8
2	I	160	CYS	3.8
1	A	424	HIS	3.8
2	L	229	LYS	3.8
2	H	203	SER	3.8
2	K	258	ASP	3.7
1	C	503	PHE	3.7
1	B	457	ARG	3.7
2	G	279	ALA	3.7
2	H	174	CYS	3.7
1	A	455	GLY	3.7
2	K	157	GLY	3.7
1	F	458	ASP	3.7
1	E	338	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	J	238	SER	3.7
1	C	452	GLU	3.7
1	E	498	THR	3.7
1	F	446	TYR	3.7
1	E	520	ASP	3.7
1	E	354	PRO	3.6
1	C	532[A]	SER	3.6
2	K	246	ALA	3.6
1	F	490	HIS	3.6
1	F	511	VAL	3.6
1	E	536	THR	3.6
1	E	465	LEU	3.6
2	I	238	SER	3.6
2	L	173	LYS	3.6
2	L	225	ASN	3.6
1	F	482	GLU	3.6
2	J	288	CYS	3.6
1	E	535	GLN	3.6
2	L	165	GLU	3.5
2	L	238	SER	3.5
2	K	282	CYS	3.5
2	I	171	GLN	3.5
1	F	517	GLU	3.5
1	D	532	SER	3.5
2	I	288	CYS	3.5
2	G	191	CYS	3.5
1	F	385	SER	3.5
1	F	392	GLN	3.5
1	C	384	HIS	3.4
1	E	404	PRO	3.4
1	B	423	PRO	3.4
2	L	180	GLY	3.4
2	I	212	LYS	3.4
2	I	246	ALA	3.4
1	C	386	THR	3.4
2	H	183	GLN	3.4
2	L	237	GLY	3.4
1	A	364	ALA	3.4
1	E	391	LYS	3.4
2	G	292	ALA	3.3
2	L	158	PHE	3.3
1	A	365	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	346	PHE	3.3
1	A	452	GLU	3.3
1	F	364	ALA	3.3
2	H	169	ASN	3.3
1	F	465	LEU	3.3
1	B	371	GLN	3.3
1	C	499	LYS	3.3
1	A	361	VAL	3.3
1	E	362	ASP	3.3
1	F	452	GLU	3.3
2	L	192	ASP	3.3
1	A	388	LYS	3.3
1	E	374	TRP	3.3
2	L	204	PRO	3.3
1	B	389	GLU	3.3
1	A	347	ASP	3.3
2	G	287	THR	3.3
2	K	252	SER	3.3
2	K	189	TYR	3.2
2	K	231	GLU	3.2
1	C	385	SER	3.2
1	A	396	THR	3.2
1	B	421	THR	3.2
1	E	500	GLY	3.2
2	L	259	CYS	3.2
2	J	286	ALA	3.2
1	F	444	GLU	3.2
1	F	395	GLY	3.2
2	H	286	ALA	3.2
1	C	401	SER	3.2
1	D	503	PHE	3.2
2	K	233	ILE	3.2
1	B	428	ALA	3.2
1	F	497	LYS	3.2
1	E	506	PHE	3.2
1	D	464	CYS	3.1
2	H	205	GLU	3.1
1	A	516	TRP	3.1
1	F	367	LYS	3.1
1	F	494	GLN	3.1
2	I	210	LEU	3.1
2	H	230	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	I	258	ASP	3.1
2	K	207	GLN	3.1
1	E	513	ARG	3.1
1	A	502	GLY	3.1
1	D	497	LYS	3.1
1	F	339	TYR	3.1
2	I	159	VAL	3.1
1	B	398	THR	3.1
2	H	251	THR	3.1
2	H	288	CYS	3.1
2	L	228	LEU	3.1
1	E	455	GLY	3.1
1	D	451	PRO	3.1
1	F	471	PRO	3.1
2	H	247	PRO	3.1
2	L	267	ARG	3.0
1	E	347	ASP	3.0
2	K	208	ASP	3.0
1	D	461	THR	3.0
1	B	422	HIS	3.0
2	K	288	CYS	3.0
2	I	190	ALA	3.0
2	H	248	GLY	3.0
2	K	203	SER	3.0
1	A	337	SER	2.9
1	B	456	SER	2.9
2	J	191	CYS	2.9
1	F	359	LEU	2.9
2	H	255	GLN	2.9
2	J	180	GLY	2.9
1	C	400	THR	2.9
2	I	206	GLU	2.9
2	I	209	PHE	2.9
1	D	447	ALA	2.9
1	D	484	GLN	2.9
2	H	287	THR	2.9
2	J	253	ARG	2.9
1	C	361	VAL	2.9
2	H	165	GLU	2.9
1	F	388	LYS	2.9
1	E	461	THR	2.8
1	A	362	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	252	SER	2.8
2	J	158	PHE	2.8
1	C	387	ARG	2.8
1	C	362	ASP	2.8
1	A	457	ARG	2.8
1	F	507	SER	2.8
2	I	278	GLY	2.8
2	I	179	LYS	2.8
2	G	291	PRO	2.8
1	F	515	GLU	2.8
1	F	518	GLN	2.8
1	F	528	HIS	2.8
1	F	386	THR	2.8
2	I	230	GLY	2.8
2	I	254	SER	2.8
2	I	211	THR	2.8
2	K	215	SER	2.8
2	K	237	GLY	2.8
2	I	245	TRP	2.7
2	K	279	ALA	2.7
1	B	359	LEU	2.7
1	B	390	GLU	2.7
1	D	347	ASP	2.7
2	L	174	CYS	2.7
1	F	520	ASP	2.7
2	I	286	ALA	2.7
2	H	290	PRO	2.7
1	F	468	ASN	2.7
1	F	428	ALA	2.7
1	C	455	GLY	2.7
2	L	262	MET	2.7
1	B	361	VAL	2.7
1	D	446	TYR	2.7
1	F	394	ASN	2.7
2	H	195	GLU	2.7
1	A	473	ASP	2.7
1	E	387	ARG	2.7
1	B	488	ALA	2.7
1	B	367	LYS	2.7
2	H	180	GLY	2.7
2	I	237	GLY	2.7
1	E	436	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	534	SER	2.7
1	F	366	SER	2.7
2	I	252	SER	2.7
1	F	488	ALA	2.7
1	B	430	MET	2.7
1	E	365	PRO	2.7
1	F	381	PRO	2.6
2	J	178	GLY	2.6
1	D	395	GLY	2.6
1	D	357	THR	2.6
1	B	388	LYS	2.6
1	E	524	CYS	2.6
1	D	485	LEU	2.6
2	J	192	ASP	2.6
2	G	217	THR	2.6
2	J	173	LYS	2.6
1	E	397	LEU	2.6
1	F	467	GLN	2.6
1	F	484	GLN	2.6
2	G	243	SER	2.6
2	K	291	PRO	2.6
2	I	208	ASP	2.6
2	L	283	ASP	2.5
2	G	190	ALA	2.5
1	C	403	LEU	2.5
2	I	169	ASN	2.5
1	E	360	VAL	2.5
2	I	262	MET	2.5
2	H	249	GLU	2.5
1	E	398	THR	2.5
1	D	426	PRO	2.5
2	I	213	HIS	2.5
1	D	501	SER	2.5
1	F	475	SER	2.5
1	B	464	CYS	2.5
2	K	167	TRP	2.5
1	D	514	ALA	2.5
2	I	268	TRP	2.5
2	K	254	SER	2.5
2	K	202	HIS	2.5
1	E	445	VAL	2.5
1	F	401	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	524	CYS	2.4
2	G	258	ASP	2.4
2	J	160	CYS	2.4
2	K	265	SER	2.4
1	E	379	GLY	2.4
2	I	192	ASP	2.4
2	G	196	GLY	2.4
2	I	267	ARG	2.4
1	E	483	VAL	2.4
2	J	228	LEU	2.4
2	H	258	ASP	2.4
1	B	520	ASP	2.4
1	D	502	GLY	2.4
1	F	423	PRO	2.4
2	H	280	TRP	2.4
1	B	513	ARG	2.4
1	E	521	GLU	2.4
1	F	453	TRP	2.4
1	D	337	SER	2.3
2	L	290	PRO	2.3
2	H	244	ASN	2.3
1	F	336	VAL	2.3
2	K	227	ASP	2.3
1	C	504	PHE	2.3
1	D	448	PHE	2.3
1	C	513	ARG	2.3
1	E	475	SER	2.3
2	L	208	ASP	2.3
2	I	253	ARG	2.3
1	C	404	PRO	2.3
1	D	396	THR	2.3
2	G	171	GLN	2.3
2	K	158	PHE	2.3
2	L	166	LYS	2.3
1	B	375	SER	2.3
1	D	453	TRP	2.3
2	I	170	PHE	2.3
1	B	376	ARG	2.2
1	F	530	ALA	2.2
2	G	163	CYS	2.2
2	L	220	TRP	2.2
2	I	247	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	474	ILE	2.2
1	D	390	GLU	2.2
1	E	526	ALA	2.2
1	A	500	GLY	2.2
2	L	274	ASP	2.2
1	F	447	ALA	2.2
2	I	239	HIS	2.2
1	C	366	SER	2.2
1	C	357	THR	2.2
1	E	345	PRO	2.2
1	D	450	THR	2.2
1	D	494	GLN	2.2
2	K	244	ASN	2.2
2	L	183	GLN	2.2
1	B	368	GLY	2.2
1	F	422	HIS	2.2
2	J	258	ASP	2.2
1	C	340	LEU	2.2
1	F	457	ARG	2.2
2	I	195	GLU	2.2
2	K	195	GLU	2.2
2	G	174	CYS	2.2
1	E	412	GLU	2.1
1	B	429	LEU	2.1
2	H	200	SER	2.1
2	G	158	PHE	2.1
1	A	497	LYS	2.1
1	C	468	ASN	2.1
2	I	261	MET	2.1
1	C	529	GLU	2.1
1	C	396	THR	2.1
1	C	486	PRO	2.1
2	K	290	PRO	2.1
1	C	398	THR	2.1
1	D	363	LEU	2.1
1	F	462	LEU	2.1
2	I	204	PRO	2.1
2	I	287	THR	2.1
1	F	384	HIS	2.1
1	B	544	ASN	2.1
2	G	255	GLN	2.1
1	E	411	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	427	ARG	2.1
1	C	381	PRO	2.1
1	E	350	ILE	2.0
1	F	502	GLY	2.0
1	F	479	LEU	2.0
2	I	217	THR	2.0
1	E	476	VAL	2.0
1	D	496	ARG	2.0
2	H	182	LYS	2.0
2	J	231	GLU	2.0
1	D	386	THR	2.0
1	A	426	PRO	2.0
1	F	469	PHE	2.0
1	E	502	GLY	2.0
1	F	466	ILE	2.0
1	B	499	LYS	2.0
1	B	532	SER	2.0
1	E	433	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	NAG	E	601	14/15	0.67	0.80	1.62	158,160,162,164	0
3	NAG	A	602	14/15	0.88	0.51	0.75	146,148,151,152	0
3	NAG	C	601	14/15	0.40	0.59	0.63	148,155,161,164	0
3	NAG	A	601	14/15	0.72	0.44	-0.25	142,147,153,157	0
3	NAG	C	602	14/15	0.87	0.31	-0.80	135,137,142,143	0
3	NAG	D	601	14/15	0.79	0.31	-0.88	139,144,146,147	0
3	NAG	F	602	14/15	0.83	0.40	-0.97	147,150,151,151	0
3	NAG	B	602	14/15	0.84	0.31	-1.10	120,124,127,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	602	14/15	0.90	0.28	-1.22	103,105,106,107	0
3	NAG	E	602	14/15	0.76	0.21	-1.59	132,134,136,136	0
3	MAN	A	605	11/12	0.82	0.38	-	163,165,168,169	0
3	NAG	B	601	14/15	0.52	0.50	-	185,189,195,198	0
3	MAN	D	605	11/12	0.88	0.21	-	156,157,159,159	0
3	MAN	F	605	11/12	0.85	0.16	-	147,149,151,151	0
3	MAN	A	604	11/12	0.72	0.34	-	153,154,155,156	0
3	BMA	E	603	11/12	0.78	0.21	-	150,152,153,153	0
3	BMA	D	603	11/12	0.89	0.21	-	105,106,107,108	0
3	BMA	B	603	11/12	0.89	0.19	-	123,126,128,128	0
3	MAN	E	605	11/12	0.78	0.24	-	153,155,156,157	0
3	BMA	F	603	11/12	0.87	0.25	-	137,139,139,139	0
3	BMA	C	603	11/12	0.85	0.17	-	139,143,145,146	0
3	MAN	F	604	11/12	0.65	0.36	-	154,155,156,157	0
3	MAN	C	604	11/12	0.73	0.31	-	142,142,144,144	0
3	MAN	C	605	11/12	0.68	0.41	-	164,166,168,169	0
3	NAG	F	601	14/15	0.84	0.28	-	142,147,151,153	0
3	BMA	A	603	11/12	0.90	0.21	-	141,143,145,146	0
3	MAN	B	604	11/12	0.81	0.28	-	155,156,157,157	0
3	MAN	B	605	11/12	0.78	0.32	-	155,157,160,161	0
3	MAN	D	604	11/12	0.74	0.34	-	146,148,149,150	0
3	MAN	E	604	11/12	0.75	0.38	-	138,139,140,141	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	C	607	11/12	0.43	0.84	3.13	122,122,126,128	0
4	MAN	C	606	11/12	0.57	0.54	-	127,128,130,131	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.