



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

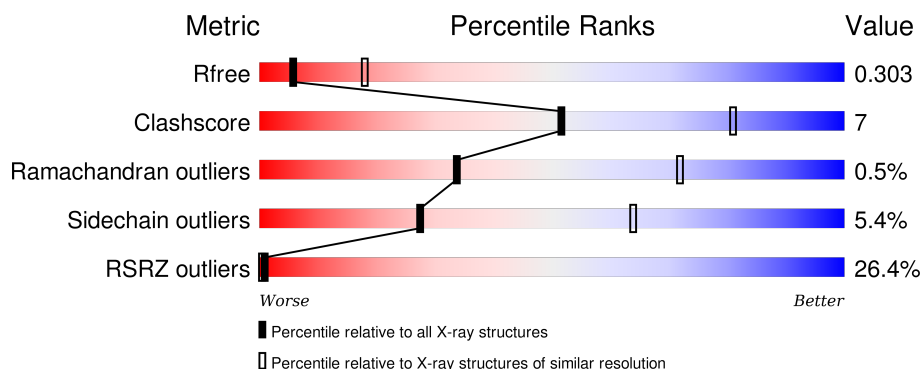
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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 ≥ 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

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).

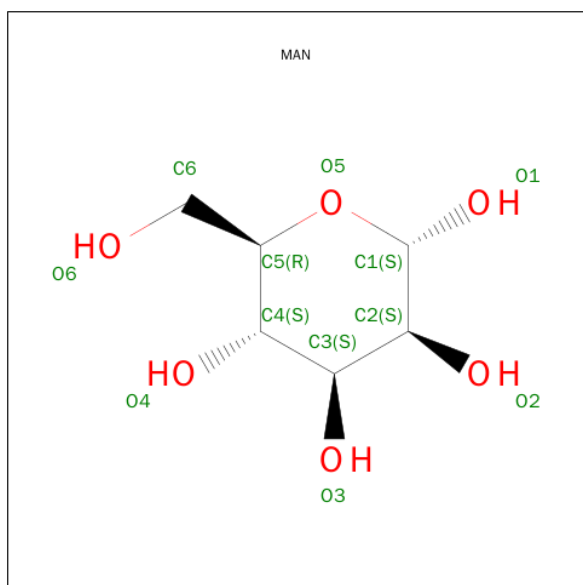
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

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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: C₆H₁₂O₆).



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		

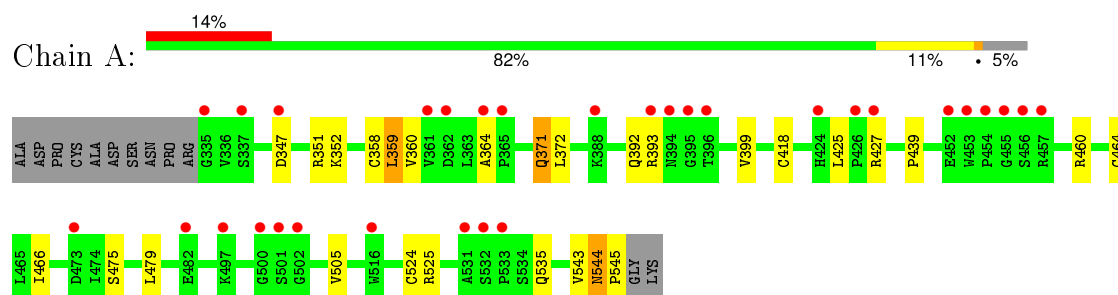
- Molecule 5 is water.

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

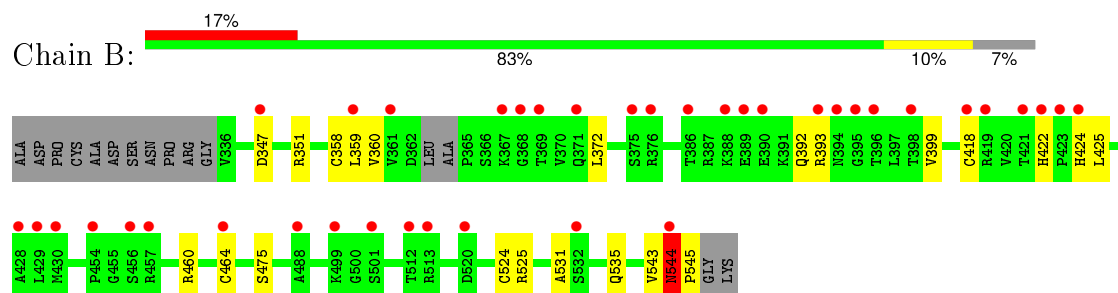
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

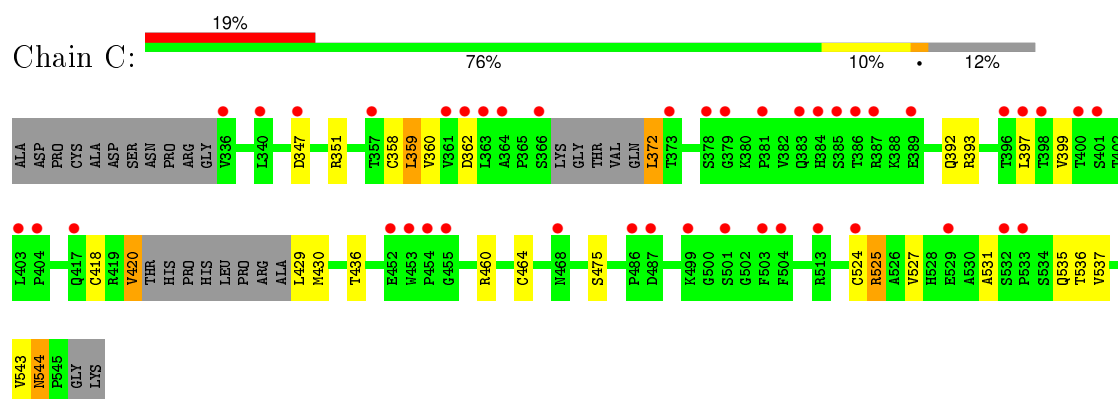
- Molecule 1: Ig epsilon chain C region



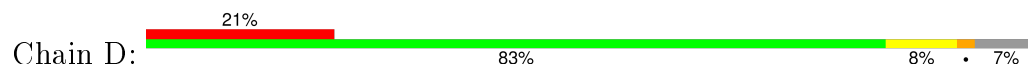
- Molecule 1: Ig epsilon chain C region

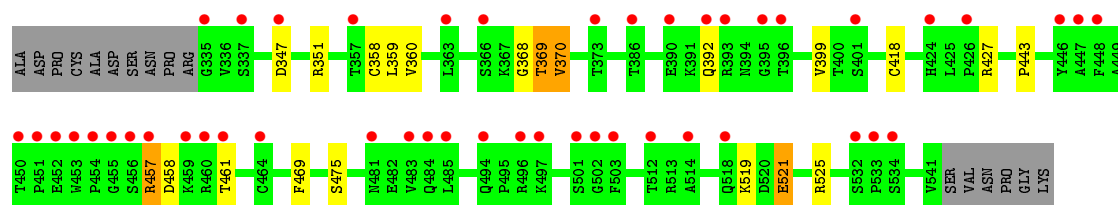


- Molecule 1: Ig epsilon chain C region

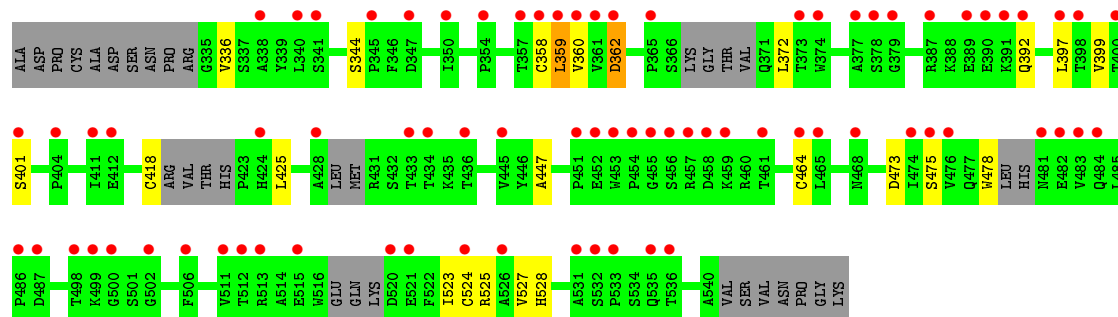
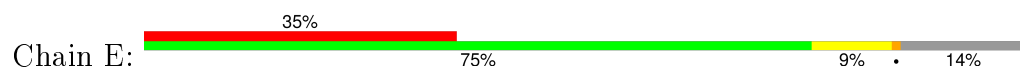


- Molecule 1: Ig epsilon chain C region

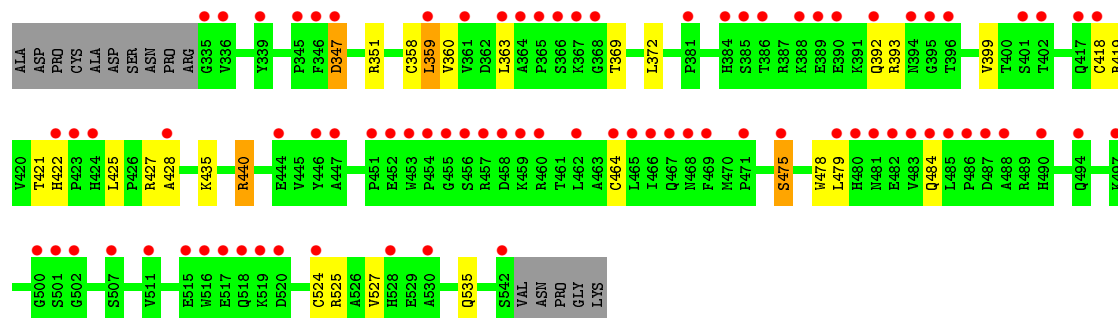
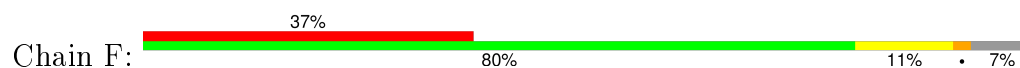




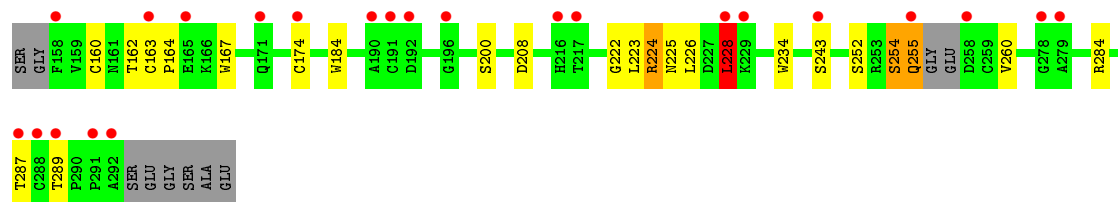
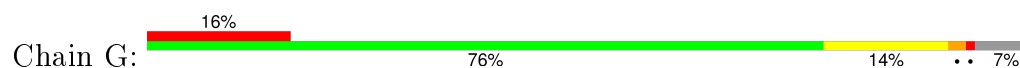
• Molecule 1: Ig epsilon chain C region



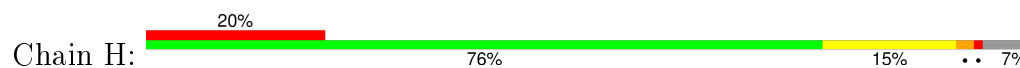
• Molecule 1: Ig epsilon chain C region

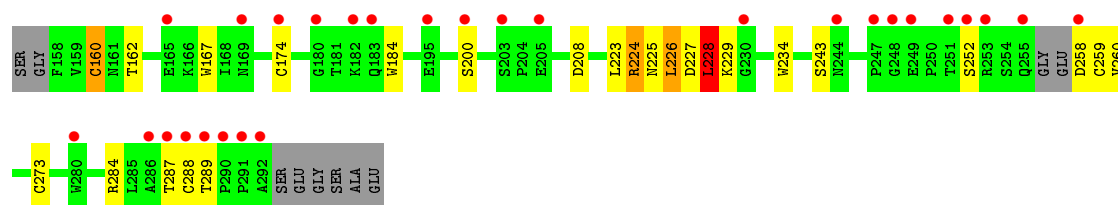


• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

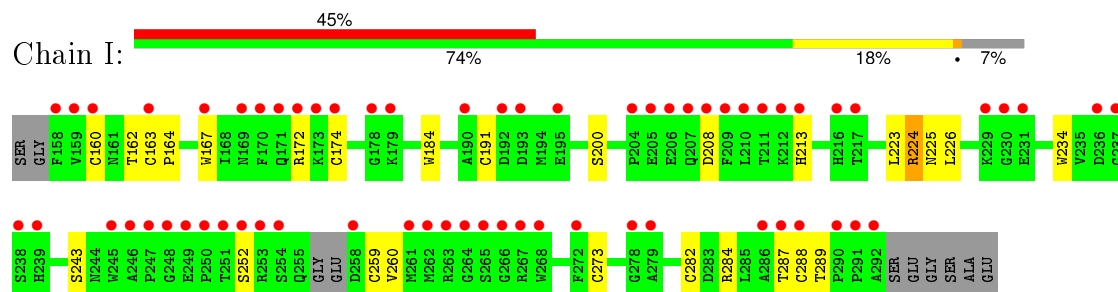


• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

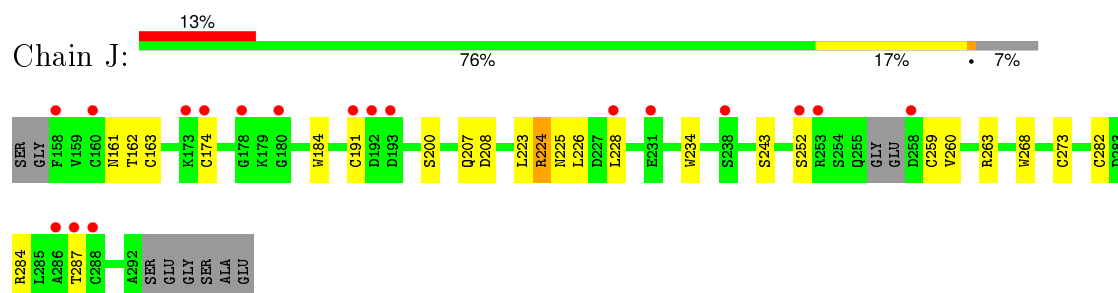




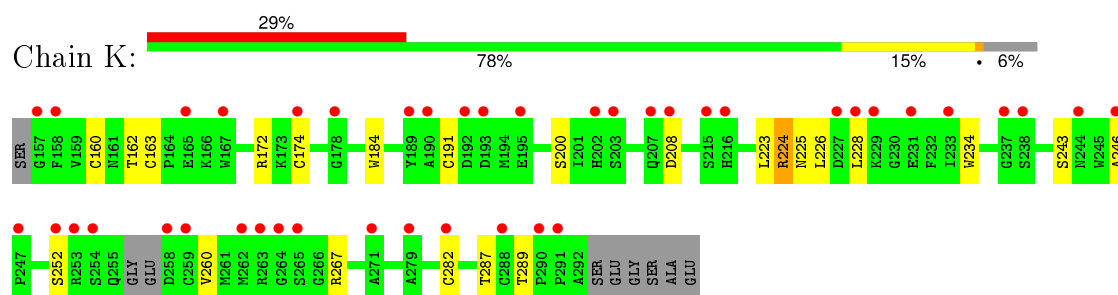
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



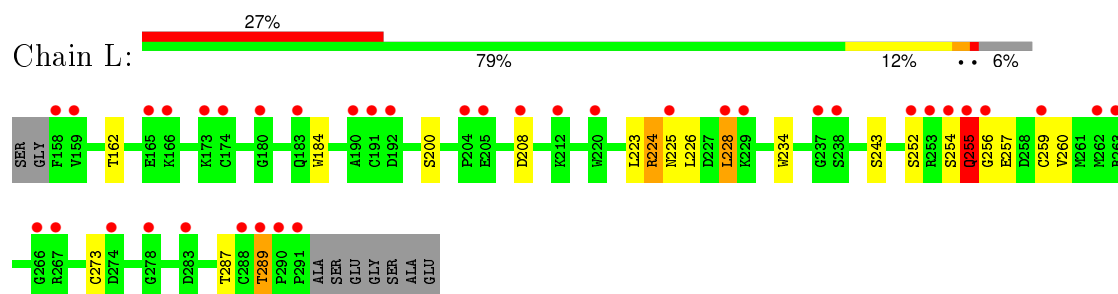
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	98.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The worst 5 of 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

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
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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

5 of 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

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

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	359	LEU
2	G	224	ARG
2	K	289	THR
1	F	363	LEU

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Mol	Chain	Res	Type
1	F	440	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	269	ASN
2	I	225	ASN
2	L	225	ASN
2	H	213	HIS
2	H	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

The worst 5 of 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

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 [i](#)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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

The worst 5 of 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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

The worst 5 of 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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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
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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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 [i](#)

There are no such residues in this entry.