



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:36 PM GMT

PDB ID : 5ANM  
Title : Crystal structure of IgE Fc in complex with a neutralizing antibody  
Authors : Cohen, E.S.; Dobson, C.L.; Kack, H.; Wang, B.; Sims, D.A.; Lloyd, C.O.; England, E.; Rees, D.G.; Guo, H.; Karagiannis, S.N.; O'Brien, S.; Persdotter, S.; Ekdahl, H.; Butler, R.; Keyes, F.; Oakley, S.; Carlsson, M.; Briend, E.; Wilkinson, T.; Anderson, I.K.; Monk, P.D.; vonWachenfeldt, K.; Eriksson, P.O.; Gould, H.J.; Vaughan, T.J.; May, R.D.  
Deposited on : 2015-09-07  
Resolution : 2.85 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

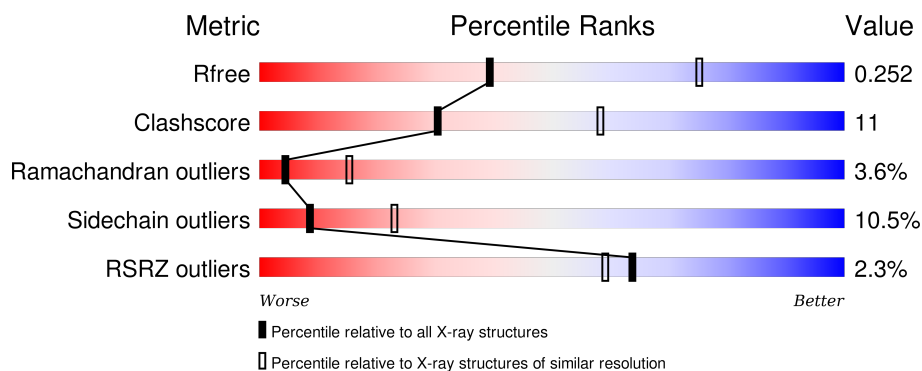
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	217	 75% 18% . . .
1	C	217	 75% 21% . . .
1	L	217	 4% 58% 24% 5% 13%
2	B	229	 1% 76% 15% . . .
2	D	229	 77% 15% . . .

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Mol	Chain	Length	Quality of chain
2	H	229	<div><div></div><div>4%</div><div>54%</div><div>29%</div><div>7%</div><div>9%</div></div>
3	E	242	<div><div></div><div>4%</div><div>47%</div><div>31%</div><div>7%</div><div>15%</div></div>
3	F	242	<div><div></div><div>2%</div><div>62%</div><div>20%</div><div></div><div>14%</div></div>
3	G	242	<div><div></div><div>2%</div><div>63%</div><div>18%</div><div>6%</div><div>13%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14788 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 IMMUNOGLOBULIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1582	991	262	325	4			
1	C	213	Total	C	N	O	S	0	0	0
			1582	991	262	325	4			
1	L	189	Total	C	N	O	S	0	0	0
			1383	865	228	286	4			

- Molecule 2 is a protein called IMMUNOGLOBULIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1673	1068	272	325	8			
2	D	219	Total	C	N	O	S	0	0	0
			1664	1062	270	324	8			
2	H	208	Total	C	N	O	S	0	0	0
			1580	1008	255	309	8			

- Molecule 3 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	206	Total	C	N	O	S	0	0	0
			1636	1026	301	303	6			
3	F	208	Total	C	N	O	S	0	0	0
			1628	1016	301	305	6			
3	G	211	Total	C	N	O	S	0	0	0
			1665	1042	307	310	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	326	ALA	-	EXPRESSION TAG	UNP P01854
E	327	ASP	-	EXPRESSION TAG	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
E	328	PRO	-	EXPRESSION TAG	UNP P01854
E	329	CYS	-	EXPRESSION TAG	UNP P01854
E	548	ASP	-	EXPRESSION TAG	UNP P01854
E	549	TYR	-	EXPRESSION TAG	UNP P01854
E	550	LYS	-	EXPRESSION TAG	UNP P01854
E	551	ASP	-	EXPRESSION TAG	UNP P01854
E	552	ASP	-	EXPRESSION TAG	UNP P01854
E	553	ASP	-	EXPRESSION TAG	UNP P01854
E	554	ASP	-	EXPRESSION TAG	UNP P01854
E	555	LYS	-	EXPRESSION TAG	UNP P01854
E	556	ALA	-	EXPRESSION TAG	UNP P01854
E	557	ALA	-	EXPRESSION TAG	UNP P01854
E	558	HIS	-	EXPRESSION TAG	UNP P01854
E	559	HIS	-	EXPRESSION TAG	UNP P01854
E	560	HIS	-	EXPRESSION TAG	UNP P01854
E	561	HIS	-	EXPRESSION TAG	UNP P01854
E	562	HIS	-	EXPRESSION TAG	UNP P01854
E	563	HIS	-	EXPRESSION TAG	UNP P01854
E	564	HIS	-	EXPRESSION TAG	UNP P01854
E	565	HIS	-	EXPRESSION TAG	UNP P01854
E	566	HIS	-	EXPRESSION TAG	UNP P01854
E	567	HIS	-	EXPRESSION TAG	UNP P01854
F	326	ALA	-	EXPRESSION TAG	UNP P01854
F	327	ASP	-	EXPRESSION TAG	UNP P01854
F	328	PRO	-	EXPRESSION TAG	UNP P01854
F	329	CYS	-	EXPRESSION TAG	UNP P01854
F	548	ASP	-	EXPRESSION TAG	UNP P01854
F	549	TYR	-	EXPRESSION TAG	UNP P01854
F	550	LYS	-	EXPRESSION TAG	UNP P01854
F	551	ASP	-	EXPRESSION TAG	UNP P01854
F	552	ASP	-	EXPRESSION TAG	UNP P01854
F	553	ASP	-	EXPRESSION TAG	UNP P01854
F	554	ASP	-	EXPRESSION TAG	UNP P01854
F	555	LYS	-	EXPRESSION TAG	UNP P01854
F	556	ALA	-	EXPRESSION TAG	UNP P01854
F	557	ALA	-	EXPRESSION TAG	UNP P01854
F	558	HIS	-	EXPRESSION TAG	UNP P01854
F	559	HIS	-	EXPRESSION TAG	UNP P01854
F	560	HIS	-	EXPRESSION TAG	UNP P01854
F	561	HIS	-	EXPRESSION TAG	UNP P01854
F	562	HIS	-	EXPRESSION TAG	UNP P01854
F	563	HIS	-	EXPRESSION TAG	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
F	564	HIS	-	EXPRESSION TAG	UNP P01854
F	565	HIS	-	EXPRESSION TAG	UNP P01854
F	566	HIS	-	EXPRESSION TAG	UNP P01854
F	567	HIS	-	EXPRESSION TAG	UNP P01854
G	326	ALA	-	EXPRESSION TAG	UNP P01854
G	327	ASP	-	EXPRESSION TAG	UNP P01854
G	328	PRO	-	EXPRESSION TAG	UNP P01854
G	329	CYS	-	EXPRESSION TAG	UNP P01854
G	548	ASP	-	EXPRESSION TAG	UNP P01854
G	549	TYR	-	EXPRESSION TAG	UNP P01854
G	550	LYS	-	EXPRESSION TAG	UNP P01854
G	551	ASP	-	EXPRESSION TAG	UNP P01854
G	552	ASP	-	EXPRESSION TAG	UNP P01854
G	553	ASP	-	EXPRESSION TAG	UNP P01854
G	554	ASP	-	EXPRESSION TAG	UNP P01854
G	555	LYS	-	EXPRESSION TAG	UNP P01854
G	556	ALA	-	EXPRESSION TAG	UNP P01854
G	557	ALA	-	EXPRESSION TAG	UNP P01854
G	558	HIS	-	EXPRESSION TAG	UNP P01854
G	559	HIS	-	EXPRESSION TAG	UNP P01854
G	560	HIS	-	EXPRESSION TAG	UNP P01854
G	561	HIS	-	EXPRESSION TAG	UNP P01854
G	562	HIS	-	EXPRESSION TAG	UNP P01854
G	563	HIS	-	EXPRESSION TAG	UNP P01854
G	564	HIS	-	EXPRESSION TAG	UNP P01854
G	565	HIS	-	EXPRESSION TAG	UNP P01854
G	566	HIS	-	EXPRESSION TAG	UNP P01854
G	567	HIS	-	EXPRESSION TAG	UNP P01854

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	6	Total	C	N	O	0	0
			72	40	2	30		

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	6	Total	C	N	O	0	0
			72	40	2	30		

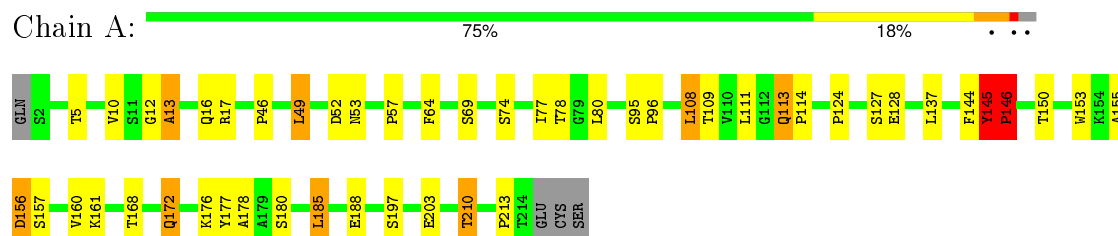
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	60	Total	O	0	0
			60	60		
7	C	16	Total	O	0	0
			16	16		
7	D	60	Total	O	0	0
			60	60		
7	E	6	Total	O	0	0
			6	6		
7	F	10	Total	O	0	0
			10	10		
7	G	22	Total	O	0	0
			22	22		
7	H	2	Total	O	0	0
			2	2		

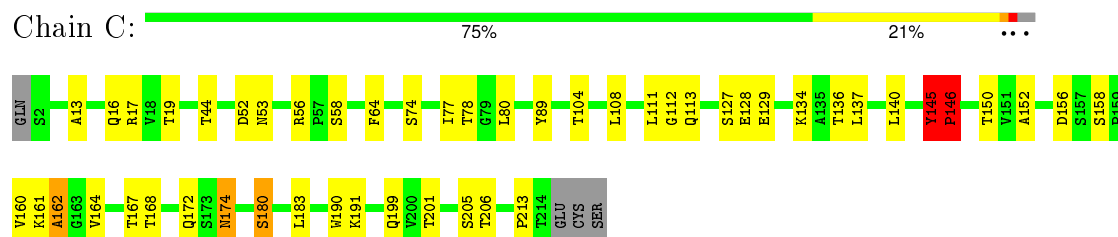
### 3 Residue-property plots

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.

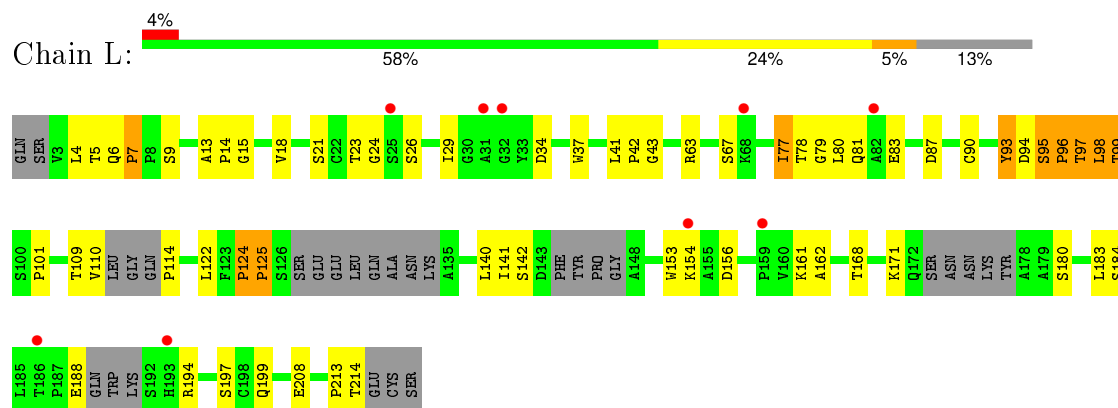
- Molecule 1: IMMUNOGLOBULIN G



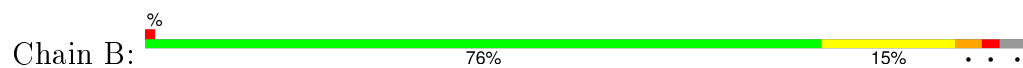
- Molecule 1: IMMUNOGLOBULIN G



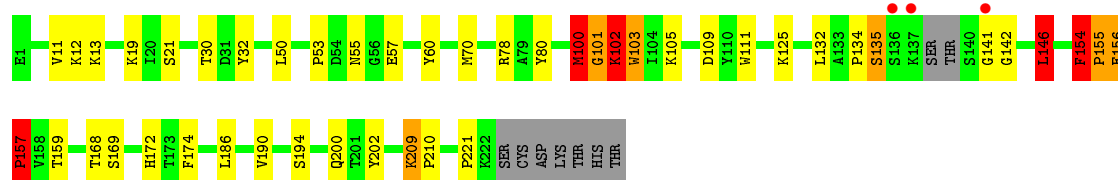
- Molecule 1: IMMUNOGLOBULIN G



- Molecule 2: IMMUNOGLOBULIN G

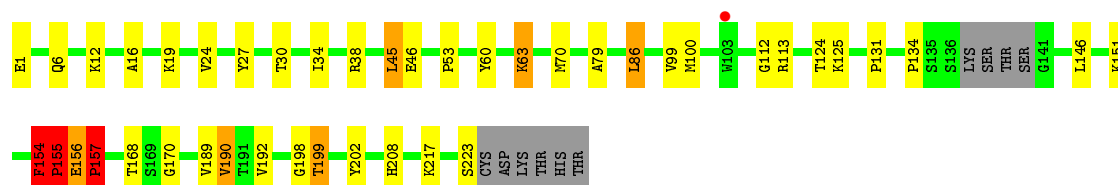






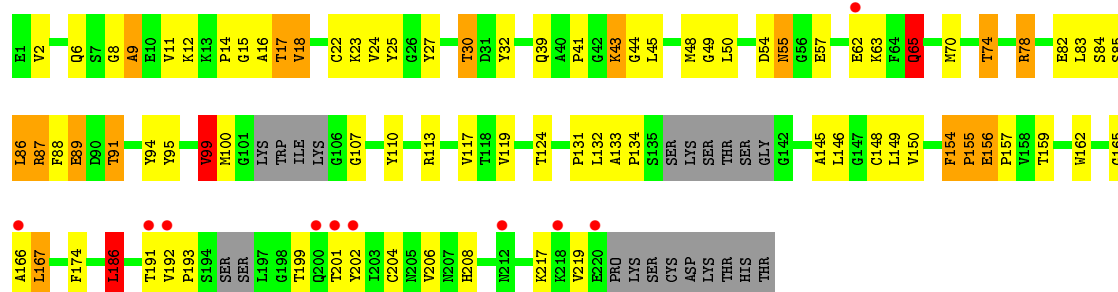
• Molecule 2: IMMUNOGLOBULIN G

Chain D: 77% 15% . . .



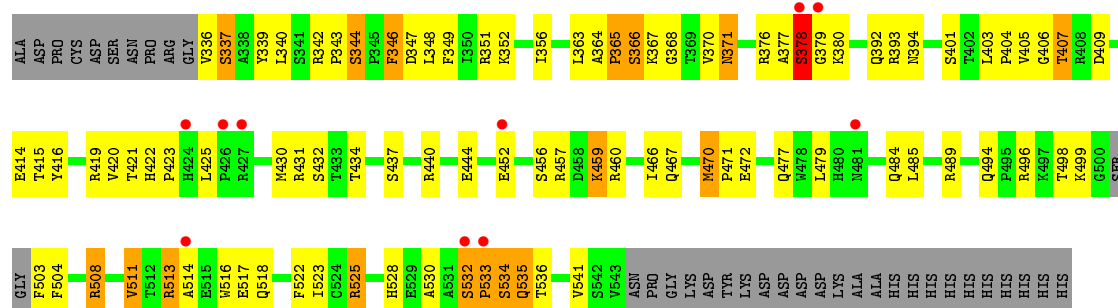
• Molecule 2: IMMUNOGLOBULIN G

Chain H: 4% 54% 29% 7% 9%



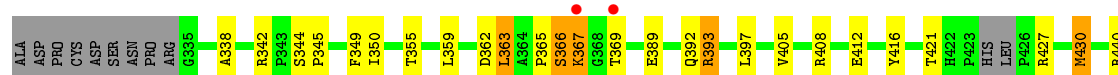
• Molecule 3: IG EPSILON CHAIN C REGION

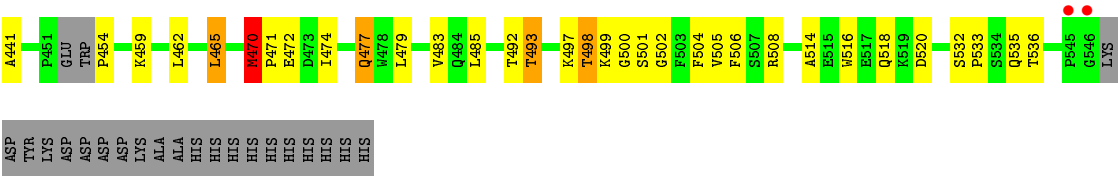
Chain E: 4% 47% 31% 7% 15%



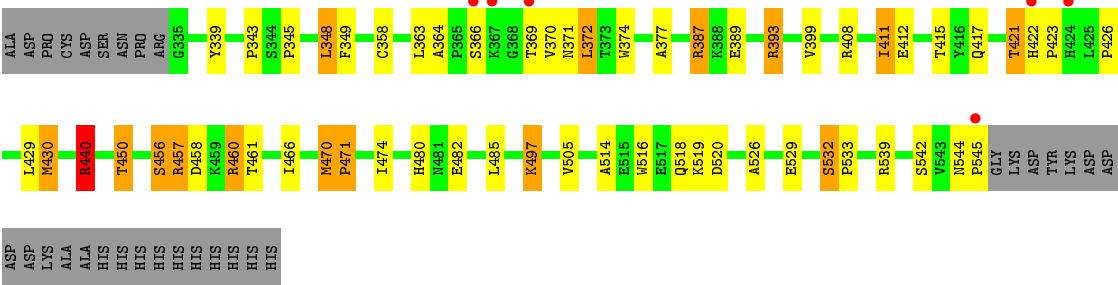
• Molecule 3: IG EPSILON CHAIN C REGION

Chain F: 2% 62% 20% 14%





● Molecule 3: IG EPSILON CHAIN C REGION



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.96Å 140.96Å 244.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.29 – 2.85 31.28 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.29-2.85) 100.0 (31.28-2.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.196 , 0.260 0.192 , 0.252	Depositor DCC
$R_{free}$ test set	3355 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.8	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66217 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 ⓘ

### 5.1 Standard geometry ⓘ

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	0.64	0/1623	0.81	2/2222 (0.1%)
1	C	0.63	0/1623	0.82	2/2222 (0.1%)
1	L	0.61	3/1413 (0.2%)	0.74	1/1930 (0.1%)
2	B	0.79	0/1715	1.02	8/2332 (0.3%)
2	D	0.78	0/1706	1.11	6/2321 (0.3%)
2	H	0.54	0/1617	0.87	3/2199 (0.1%)
3	E	0.54	0/1677	0.79	2/2282 (0.1%)
3	F	0.62	0/1666	0.93	6/2262 (0.3%)
3	G	0.70	0/1708	0.90	3/2326 (0.1%)
All	All	0.66	3/14748 (0.0%)	0.90	33/20096 (0.2%)

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
1	A	0	1
1	C	0	2
1	L	0	1
2	B	0	4
2	D	0	1
2	H	0	2
3	E	0	3
3	F	0	1
3	G	0	2
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14	PRO	C-O	7.56	1.38	1.23
1	L	14	PRO	C-N	6.41	1.44	1.33
1	L	13	ALA	C-N	-5.40	1.24	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	GLU	C-N-CD	-21.33	73.67	120.60
3	F	470	MET	C-N-CD	-16.27	84.80	120.60
2	H	156	GLU	C-N-CD	-13.12	91.74	120.60
2	D	156	GLU	C-N-CA	12.97	176.46	122.00
2	D	154	PHE	C-N-CD	-12.80	92.45	120.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Peptide
2	B	154	PHE	Mainchain,Peptide
2	B	156	GLU	Mainchain,Peptide
1	C	145	TYR	Peptide
1	C	160	VAL	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	1582	0	1528	32	0
1	C	1582	0	1528	23	0
1	L	1383	0	1339	34	0
2	B	1673	0	1642	26	0
2	D	1664	0	1629	26	0
2	H	1580	0	1537	64	0
3	E	1636	0	1622	62	0
3	F	1628	0	1616	33	0
3	G	1665	0	1647	38	0
4	E	72	0	61	0	0
5	F	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	72	0	61	1	0
7	A	14	0	0	0	0
7	B	60	0	0	2	0
7	C	16	0	0	0	0
7	D	60	0	0	2	0
7	E	6	0	0	1	0
7	F	10	0	0	0	0
7	G	22	0	0	0	0
7	H	2	0	0	0	0
All	All	14788	0	14262	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:371:ASN:HB2	3:G:421:THR:HG22	1.33	1.06
3:F:514:ALA:HB2	2:H:165:GLY:HA3	1.41	1.01
3:G:371:ASN:HB2	3:G:421:THR:CG2	1.96	0.96
3:E:508:ARG:HG3	3:E:508:ARG:HH11	1.30	0.95
2:H:30:THR:HG22	2:H:54:ASP:HA	1.48	0.92

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	211/217 (97%)	189 (90%)	16 (8%)	6 (3%)	6	21
1	C	211/217 (97%)	189 (90%)	15 (7%)	7 (3%)	5	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	177/217 (82%)	146 (82%)	21 (12%)	10 (6%)	2	6
2	B	216/229 (94%)	204 (94%)	7 (3%)	5 (2%)	8	26
2	D	215/229 (94%)	200 (93%)	12 (6%)	3 (1%)	14	40
2	H	200/229 (87%)	174 (87%)	16 (8%)	10 (5%)	3	8
3	E	202/242 (84%)	175 (87%)	14 (7%)	13 (6%)	2	4
3	F	202/242 (84%)	181 (90%)	16 (8%)	5 (2%)	7	24
3	G	209/242 (86%)	191 (91%)	10 (5%)	8 (4%)	4	14
All	All	1843/2064 (89%)	1649 (90%)	127 (7%)	67 (4%)	4	15

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	146	PRO
1	A	213	PRO
2	B	155	PRO
2	B	157	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	179/183 (98%)	165 (92%)	14 (8%)	16	39
1	C	179/183 (98%)	166 (93%)	13 (7%)	17	42
1	L	158/183 (86%)	135 (85%)	23 (15%)	4	10
2	B	184/193 (95%)	170 (92%)	14 (8%)	16	40
2	D	183/193 (95%)	172 (94%)	11 (6%)	24	53
2	H	173/193 (90%)	148 (86%)	25 (14%)	4	10
3	E	183/213 (86%)	155 (85%)	28 (15%)	3	9
3	F	182/213 (85%)	161 (88%)	21 (12%)	7	19
3	G	186/213 (87%)	166 (89%)	20 (11%)	8	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1607/1767 (91%)	1438 (90%)	169 (10%)	8 23

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	525	ARG
3	F	485	LEU
1	L	109	THR
3	E	535	GLN
3	F	421	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	392	GLN
1	L	6	GLN
3	G	480	HIS
3	E	535	GLN
3	G	535	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

17 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
4	NAG	E	1544	3,4	14,14,15	0.84	1 (7%)	15,19,21	1.02	0
4	NAG	E	1545	4	14,14,15	0.68	0	15,19,21	1.51	3 (20%)
4	BMA	E	1546	4	11,11,12	0.74	0	15,15,17	1.70	6 (40%)
4	MAN	E	1547	4	11,11,12	0.71	0	15,15,17	1.63	3 (20%)
4	MAN	E	1548	4	11,11,12	0.90	1 (9%)	15,15,17	1.77	4 (26%)
4	MAN	E	1549	4	11,11,12	0.59	0	15,15,17	0.91	0
5	NAG	F	1547	3,5	14,14,15	0.97	0	15,19,21	1.15	1 (6%)
5	NAG	F	1548	5	14,14,15	0.80	1 (7%)	15,19,21	2.47	8 (53%)
5	BMA	F	1549	5	11,11,12	0.82	0	15,15,17	1.62	2 (13%)
5	MAN	F	1550	5	11,11,12	1.01	1 (9%)	15,15,17	1.72	3 (20%)
5	BMA	F	1551	5	11,11,12	1.05	1 (9%)	15,15,17	1.88	4 (26%)
6	NAG	G	1546	3,6	14,14,15	1.34	2 (14%)	15,19,21	1.80	2 (13%)
6	NAG	G	1547	6	14,14,15	0.87	1 (7%)	15,19,21	1.26	3 (20%)
6	BMA	G	1548	6	11,11,12	1.12	0	15,15,17	2.55	5 (33%)
6	MAN	G	1549	6	11,11,12	0.71	0	15,15,17	2.94	4 (26%)
6	BMA	G	1550	6	11,11,12	0.60	0	15,15,17	1.65	2 (13%)
6	MAN	G	1551	6	11,11,12	0.78	0	15,15,17	3.18	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1544	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1545	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1546	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1547	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1548	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1549	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1547	3,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1548	5	-	0/6/23/26	0/1/1/1
5	BMA	F	1549	5	-	0/2/19/22	0/1/1/1
5	MAN	F	1550	5	-	0/2/19/22	0/1/1/1
5	BMA	F	1551	5	-	0/2/19/22	0/1/1/1
6	NAG	G	1546	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	1547	6	-	0/6/23/26	0/1/1/1
6	BMA	G	1548	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1549	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	G	1550	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1551	6	-	0/2/19/22	1/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1546	NAG	O5-C1	-3.72	1.37	1.43
6	G	1547	NAG	O5-C1	-2.49	1.39	1.43
5	F	1548	NAG	C2-N2	-2.08	1.42	1.46
6	G	1546	NAG	O5-C5	-2.04	1.39	1.43
4	E	1544	NAG	O5-C1	-2.01	1.40	1.43

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1551	MAN	C1-C2-C3	-10.58	96.73	109.55
6	G	1549	MAN	C1-C2-C3	-6.21	102.03	109.55
6	G	1548	BMA	C3-C4-C5	-4.37	102.44	110.23
6	G	1546	NAG	C3-C4-C5	-4.28	102.60	110.23
6	G	1551	MAN	C1-O5-C5	-2.88	107.91	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1551	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1547	NAG	1	0
6	G	1548	BMA	1	0

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	213/217 (98%)	-0.43	0 100 100	30, 56, 83, 105	0
1	C	213/217 (98%)	-0.43	0 100 100	31, 56, 90, 108	0
1	L	189/217 (87%)	0.21	9 (4%) 34 28	79, 118, 147, 159	0
2	B	220/229 (96%)	-0.50	3 (1%) 78 75	25, 35, 92, 148	0
2	D	219/229 (95%)	-0.51	1 (0%) 91 90	25, 37, 69, 110	0
2	H	208/229 (90%)	0.11	10 (4%) 34 28	60, 89, 127, 157	0
3	E	206/242 (85%)	0.12	10 (4%) 33 27	54, 92, 137, 165	0
3	F	208/242 (85%)	-0.20	4 (1%) 70 66	31, 67, 126, 153	0
3	G	211/242 (87%)	-0.34	6 (2%) 56 51	28, 47, 98, 161	0
All	All	1887/2064 (91%)	-0.23	43 (2%) 64 59	25, 62, 131, 165	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	546	GLY	7.4
3	E	426	PRO	5.2
1	L	159	PRO	4.6
3	G	424	HIS	4.4
3	E	532	SER	4.3

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	G	1546	14/15	0.98	0.14	-0.19	34,37,38,39	0
5	NAG	F	1547	14/15	0.96	0.17	-0.31	60,62,68,76	0
6	NAG	G	1547	14/15	0.98	0.14	-0.92	37,41,44,46	0
5	NAG	F	1548	14/15	0.97	0.13	-1.01	56,63,68,70	0
4	NAG	E	1544	14/15	0.98	0.11	-1.90	47,50,54,55	0
4	NAG	E	1545	14/15	0.96	0.11	-2.04	59,62,69,71	0
6	BMA	G	1548	11/12	0.96	0.12	-	51,57,70,76	0
6	MAN	G	1551	11/12	0.83	0.25	-	83,100,111,119	0
4	MAN	E	1548	11/12	0.87	0.17	-	89,103,107,109	0
4	MAN	E	1549	11/12	0.72	0.37	-	141,147,150,151	0
6	MAN	G	1549	11/12	0.93	0.15	-	81,83,94,97	0
5	BMA	F	1551	11/12	0.73	0.25	-	85,103,107,114	0
5	MAN	F	1550	11/12	0.83	0.18	-	91,95,102,106	0
4	MAN	E	1547	11/12	0.86	0.17	-	101,117,126,143	0
5	BMA	F	1549	11/12	0.95	0.10	-	64,72,81,87	0
6	BMA	G	1550	11/12	0.80	0.18	-	99,111,121,134	0
4	BMA	E	1546	11/12	0.95	0.09	-	74,85,96,107	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.