



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:29 PM UTC

PDB ID : 1YNT / pdb_00001ynt
Title : Structure of the monomeric form of T. gondii SAG1 surface antigen bound to a human Fab
Authors : Graille, M.; Stura, E.A.; Bossus, M.; Muller, B.H.; Letourneur, O.; Battail-Poirot, N.; Sibai, G.; Rolland, D.; Le Du, M.H.; Ducancel, F.
Deposited on : 2005-01-25
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

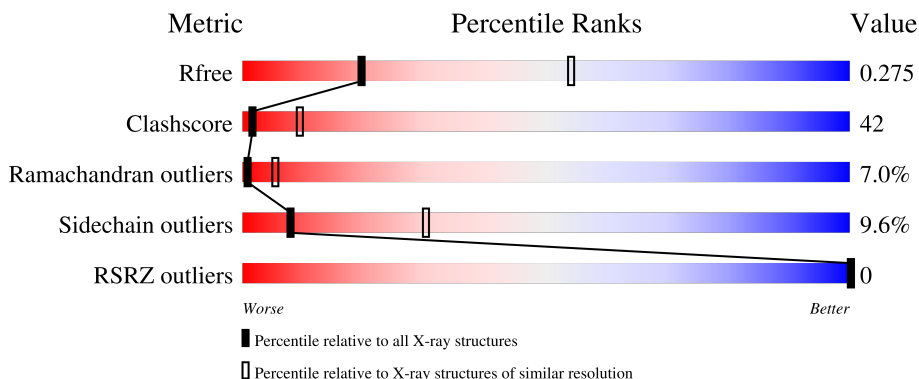
1 Overall quality at a glance

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.




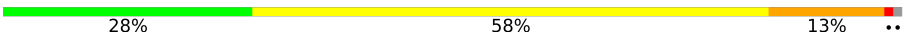
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	213	
1	C	213	
2	B	218	
2	D	218	
3	E	61	

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Mol	Chain	Length	Quality of chain	
4	F	254	 30% 56% 13% ..	
4	G	254	 28% 58% 13% ..	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10802 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 4F11E12 Fab variable light chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total	C	N	O	S	0	0	0
			1658	1027	280	346	5			
1	C	213	Total	C	N	O	S	0	0	0
			1658	1027	280	346	5			

- Molecule 2 is a protein called 4F11E12 Fab variable heavy chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	Total	C	N	O	S	0	0	0
			1657	1048	269	332	8			
2	D	218	Total	C	N	O	S	0	0	0
			1657	1048	269	332	8			

- Molecule 3 is a protein called protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	61	Total	C	N	O	S	0	0	0
			476	302	76	97	1			

- Molecule 4 is a protein called Major surface antigen p30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	252	Total	C	N	O	S	0	0	0
			1847	1151	308	374	14			
4	G	252	Total	C	N	O	S	0	0	0
			1847	1151	308	374	14			

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cd	0	0
			1	1		

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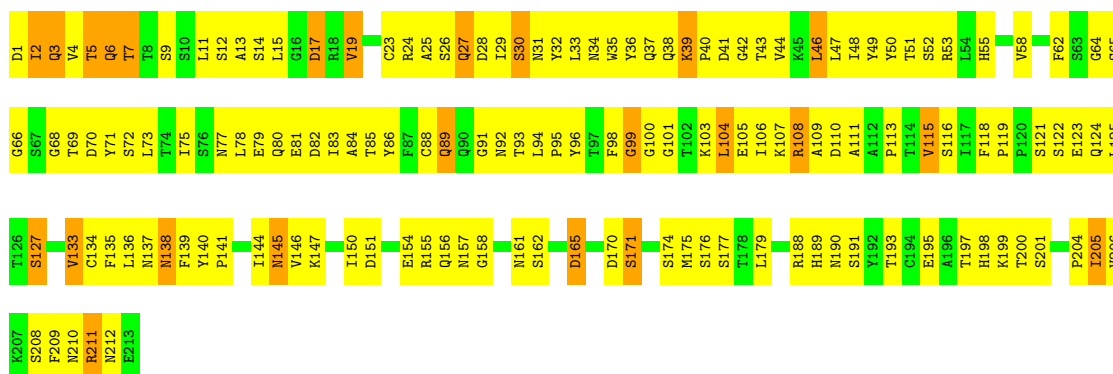
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cd	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

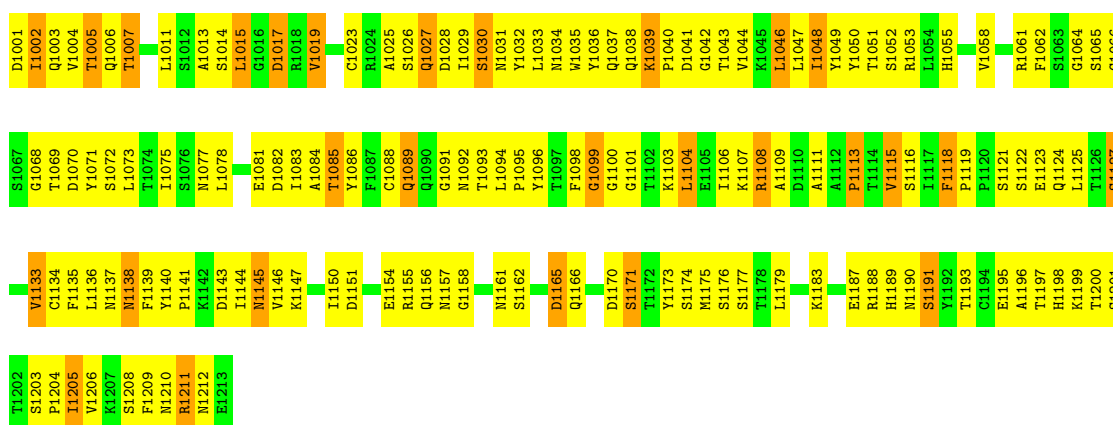
- Molecule 1: 4F11E12 Fab variable light chain region

Chain A: 



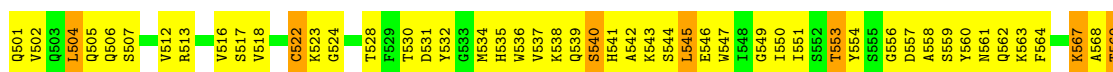
- Molecule 1: 4F11E12 Fab variable light chain region

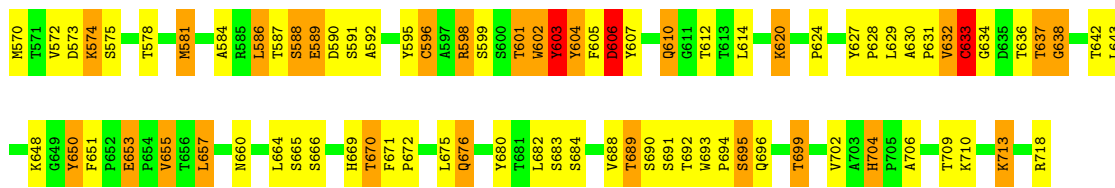
Chain C: 



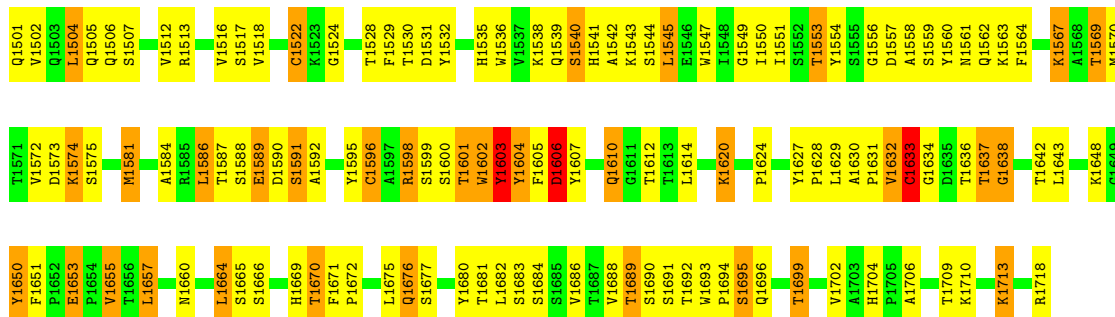
- Molecule 2: 4F11E12 Fab variable heavy chain region

Chain B: 





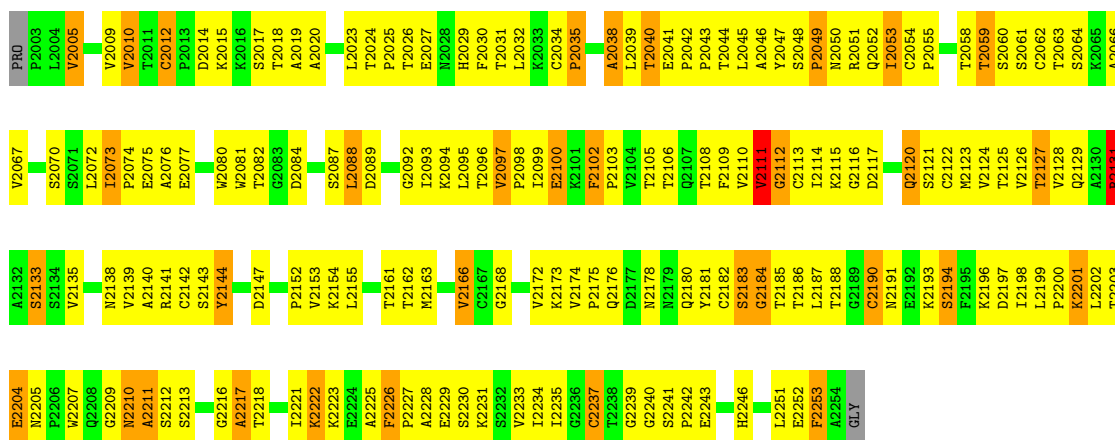
• Molecule 2: 4F11E12 Fab variable heavy chain region



• Molecule 3: protein L



• Molecule 4: Major surface antigen p30



• Molecule 4: Major surface antigen p30



L3202	S3133	S3070	PRD
T3203	S3194	S3071	P3003
E3204	V3135	L3072	L3004
N3205		I3073	V3005
W3207	N3138	P3074	V3009
Q3208	V3139	E3075	V3010
G3209	A3140	A3076	T3011
N3210	R3141	E3077	C3012
A3211	C3142	W3080	P3013
S3212	S3143	W3081	D3014
S3213	Y3144	T3082	K3015
	D3147	G3083	K3016
G3216		D3084	S3017
A3217	P3152	S3087	T3018
T3218	V3153	L3088	A3019
	K3154	D3089	
I3221	L3155		L3023
K3222	S3156	G3092	T3024
K3223	A3157	I3093	P3025
E3224	E3158	K3094	T3026
A3225		L3095	E3027
F3226	T3161	L3096	N3028
P3227	T3162	V3097	F3029
A3228	N3163	P3098	F3030
E3229	V3166	I3099	F3031
S3230	C3167	E3100	L3032
K3231	G3168	K3101	K3033
S3232		F3102	C3034
V3233	V3172	P3103	P3035
I3234	K3173	L3039	
I3235	V3174	V3104	A3038
G3236	P3175	T3105	L3040
C3237	Q3176	T3106	E3041
T3238	D3177	Q3107	P3042
G3239	N3178	T3108	P3043
G3240	N3179	F3109	T3044
S3241	Q3180	V3110	L3045
F3242	Y3181	V3111	A3046
E3243	C3182	G3112	L3047
	S3183	C3113	Y3047
L3261	G3184	I3114	S3048
E3262	T3185	K3115	P3049
F3263	T3186	G3116	N3050
A3264	L3187	D3117	R3051
GLY	T3188	Q3120	Q3052
	G3189	S3121	I3053
	C3190	C3122	C3054
	N3191	M3123	P3055
	E3192	M3124	
	K3193	V3125	T3058
	F3195	T3126	T3059
	K3196	T3127	S3060
	D3197	Q3129	S3061
	I3198	R3130	C3062
	L3199	A3131	T3063
	P3200	A3132	S3064
	K3201		K3065
			A3066
			V3067

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 198.28Å 128.37Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-3.10) 96.6 (20.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.06Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.283 0.237 , 0.275	Depositor DCC
R_{free} test set	1579 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10802	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.59	0/1692	1.07	14/2297 (0.6%)
1	C	0.59	0/1692	1.08	16/2297 (0.7%)
2	B	0.64	0/1700	1.15	23/2318 (1.0%)
2	D	0.65	0/1700	1.16	24/2318 (1.0%)
3	E	0.60	0/483	1.03	3/649 (0.5%)
4	F	0.41	0/1882	0.98	13/2568 (0.5%)
4	G	0.42	0/1882	0.98	12/2568 (0.5%)
All	All	0.56	0/11031	1.07	105/15015 (0.7%)

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	1158	GLY	N-CA-C	-9.65	101.82	115.43
1	A	158	GLY	N-CA-C	-9.54	101.97	115.43
2	D	1602	TRP	N-CA-C	8.34	120.06	110.97
2	B	602	TRP	N-CA-C	7.94	119.63	110.97
2	B	553	THR	N-CA-C	7.39	121.22	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1658	0	1583	144	0
1	C	1658	0	1580	145	0
2	B	1657	0	1607	126	0
2	D	1657	0	1607	122	0
3	E	476	0	456	43	0
4	F	1847	0	1844	175	0
4	G	1847	0	1844	183	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10802	0	10521	891	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 42.

The worst 5 of 891 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)
4:G:3133:SER:HB3	4:G:3143:SER:H	1.14	1.11
4:F:2133:SER:HB3	4:F:2143:SER:H	1.14	1.08
2:D:1624:PRO:HB3	2:D:1650:TYR:HB3	1.35	1.05
2:B:624:PRO:HB3	2:B:650:TYR:HB3	1.36	1.02
1:C:1002:ILE:HG12	1:C:1002:ILE:O	1.59	1.01

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	211/213 (99%)	165 (78%)	40 (19%)	6 (3%)	4	20
1	C	211/213 (99%)	166 (79%)	37 (18%)	8 (4%)	2	15
2	B	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1	7
3	E	59/61 (97%)	44 (75%)	9 (15%)	6 (10%)	0	3
4	F	250/254 (98%)	177 (71%)	47 (19%)	26 (10%)	0	2
4	G	250/254 (98%)	173 (69%)	50 (20%)	27 (11%)	0	2
All	All	1413/1431 (99%)	1079 (76%)	235 (17%)	99 (7%)	1	5

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	27	GLN
2	B	575	SER
2	B	633	CYS
1	C	1017	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/191 (100%)	172 (90%)	19 (10%)	7	29
1	C	191/191 (100%)	171 (90%)	20 (10%)	6	26
2	B	188/188 (100%)	163 (87%)	25 (13%)	4	17
2	D	188/188 (100%)	163 (87%)	25 (13%)	4	17
3	E	47/47 (100%)	43 (92%)	4 (8%)	10	35
4	F	214/215 (100%)	201 (94%)	13 (6%)	17	46
4	G	214/215 (100%)	202 (94%)	12 (6%)	19	49
All	All	1233/1235 (100%)	1115 (90%)	118 (10%)	8	30

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1116	SER

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Mol	Chain	Res	Type
4	G	3111	VAL
2	D	1601	THR
4	G	3053	ILE
4	F	2131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	2029	HIS
4	G	3007	ASN
4	F	2050	ASN
4	F	2178	ASN
4	G	3050	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	213/213 (100%)	-1.11	0 100 100	24, 54, 77, 89	0
1	C	213/213 (100%)	-1.12	0 100 100	23, 54, 76, 89	0
2	B	218/218 (100%)	-1.14	0 100 100	16, 50, 78, 102	0
2	D	218/218 (100%)	-1.12	0 100 100	16, 50, 78, 102	0
3	E	61/61 (100%)	-1.04	0 100 100	48, 77, 95, 103	0
4	F	252/254 (99%)	-0.65	0 100 100	67, 106, 142, 150	0
4	G	252/254 (99%)	-0.65	0 100 100	67, 106, 139, 150	0
All	All	1427/1431 (99%)	-0.95	0 100 100	16, 68, 134, 150	0

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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. 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	B-factors(\AA^2)	Q<0.9
5	CD	D	4002	1/1	0.99	0.06	115,115,115,115	0
5	CD	B	4001	1/1	1.00	0.03	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.