



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2016 – 07:45 AM EDT

PDB ID : 5DOD
Title : Human A20 OTU domain with I325N and alkylated C103 to 2.5A resolution
Authors : Langley, D.B.; Christ, D.; Grey, S.T.
Deposited on : 2015-09-11
Resolution : 2.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

i

X-RAY DIFFRACTION

A.

Ramachandran outliers

electron density. The numeric value is given above the bar.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13160 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 Tumor necrosis factor alpha-induced protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2356	1526	404	412	14			
1	B	298	Total	C	N	O	S	0	0	0
			2297	1488	392	404	13			
1	C	304	Total	C	N	O	S	0	0	0
			2299	1484	403	400	12			
1	D	306	Total	C	N	O	S	0	0	0
			2317	1496	401	407	13			
1	E	280	Total	C	N	O	S	0	0	0
			2026	1302	351	362	11			
1	F	260	Total	C	N	O	S	0	0	0
			1841	1180	329	319	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P21580
A	-3	PRO	-	expression tag	UNP P21580
A	-2	LEU	-	expression tag	UNP P21580
A	-1	GLY	-	expression tag	UNP P21580
A	0	SER	-	expression tag	UNP P21580
A	325	ASN	ILE	engineered mutation	UNP P21580
B	-4	GLY	-	expression tag	UNP P21580
B	-3	PRO	-	expression tag	UNP P21580
B	-2	LEU	-	expression tag	UNP P21580
B	-1	GLY	-	expression tag	UNP P21580
B	0	SER	-	expression tag	UNP P21580
B	325	ASN	ILE	engineered mutation	UNP P21580
C	-4	GLY	-	expression tag	UNP P21580
C	-3	PRO	-	expression tag	UNP P21580
C	-2	LEU	-	expression tag	UNP P21580
C	-1	GLY	-	expression tag	UNP P21580
C	0	SER	-	expression tag	UNP P21580

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	325	ASN	ILE	engineered mutation	UNP P21580
D	-4	GLY	-	expression tag	UNP P21580
D	-3	PRO	-	expression tag	UNP P21580
D	-2	LEU	-	expression tag	UNP P21580
D	-1	GLY	-	expression tag	UNP P21580
D	0	SER	-	expression tag	UNP P21580
D	325	ASN	ILE	engineered mutation	UNP P21580
E	-4	GLY	-	expression tag	UNP P21580
E	-3	PRO	-	expression tag	UNP P21580
E	-2	LEU	-	expression tag	UNP P21580
E	-1	GLY	-	expression tag	UNP P21580
E	0	SER	-	expression tag	UNP P21580
E	325	ASN	ILE	engineered mutation	UNP P21580
F	-4	GLY	-	expression tag	UNP P21580
F	-3	PRO	-	expression tag	UNP P21580
F	-2	LEU	-	expression tag	UNP P21580
F	-1	GLY	-	expression tag	UNP P21580
F	0	SER	-	expression tag	UNP P21580
F	325	ASN	ILE	engineered mutation	UNP P21580

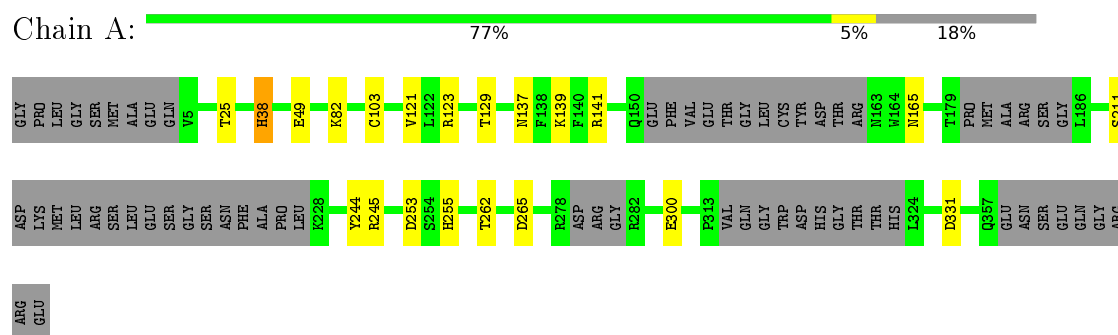
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	7	Total O 7 7	0	0
2	C	3	Total O 3 3	0	0
2	D	7	Total O 7 7	0	0
2	F	3	Total O 3 3	0	0

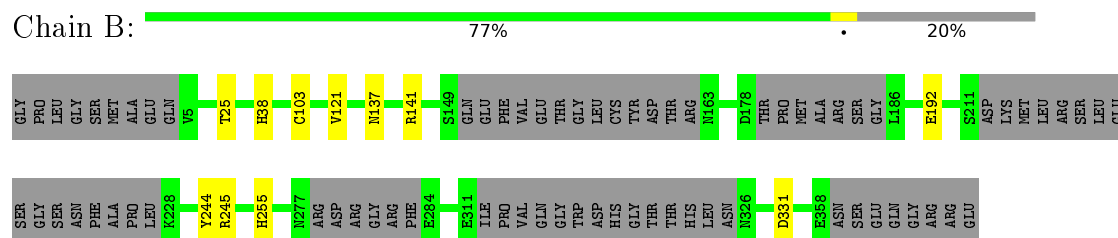
3 Residue-property plots [i](#)

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.

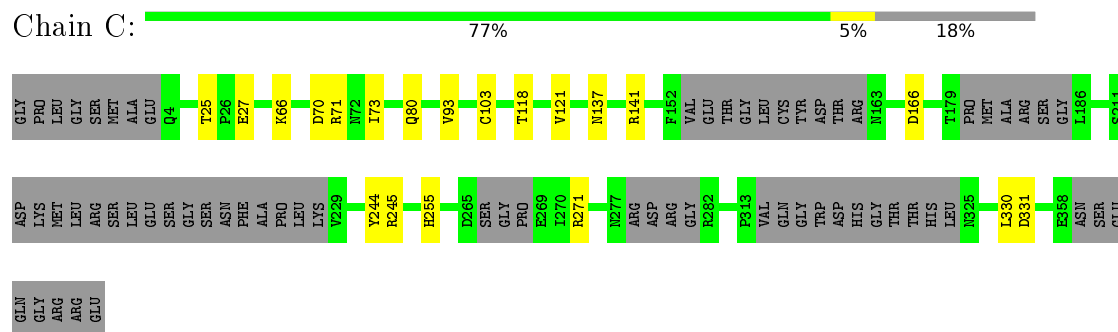
- Molecule 1: Tumor necrosis factor alpha-induced protein 3



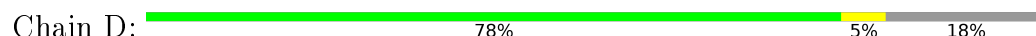
- Molecule 1: Tumor necrosis factor alpha-induced protein 3

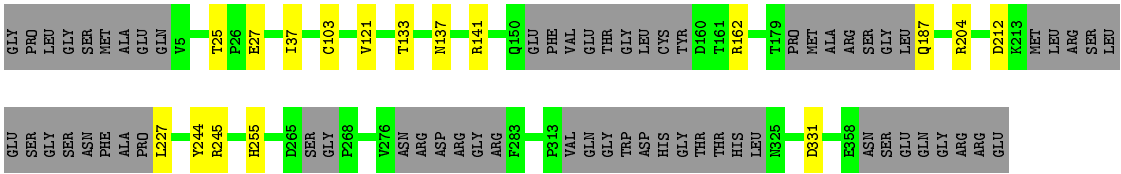


- Molecule 1: Tumor necrosis factor alpha-induced protein 3

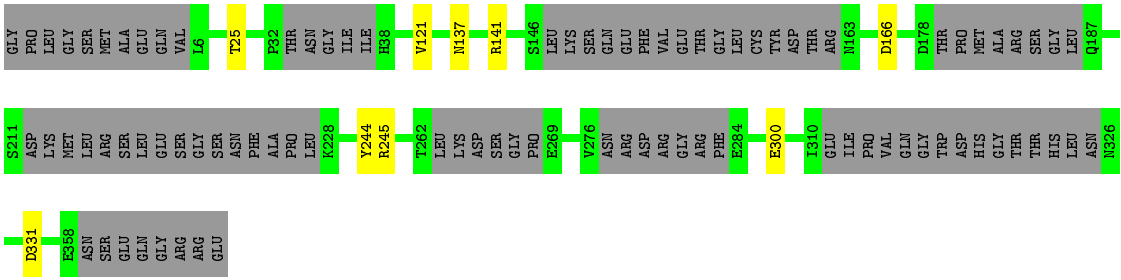


- Molecule 1: Tumor necrosis factor alpha-induced protein 3

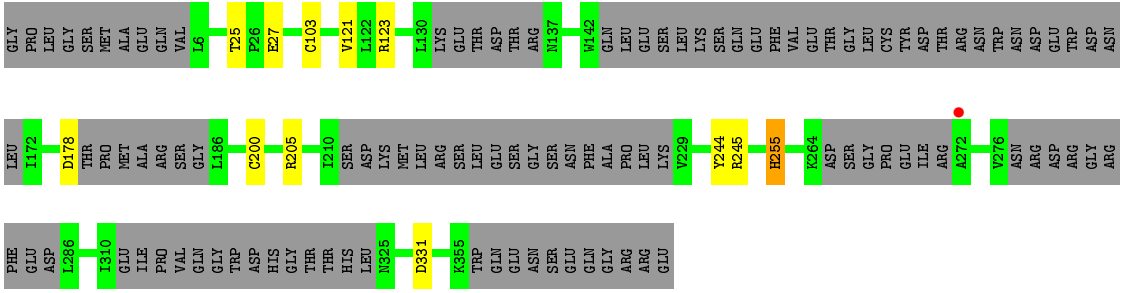




• Molecule 1: Tumor necrosis factor alpha-induced protein 3



• Molecule 1: Tumor necrosis factor alpha-induced protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	81.87Å 81.87Å 297.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.47 – 2.50 39.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.47-2.50) 99.7 (39.47-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.203 0.173 , 0.199	Depositor DCC
R_{free} test set	3843 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 16.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l 0.438 for h,-h-k,-l 0.437 for -k,-h,-l	Xtriage
Reported twinning fraction	0.261 for H, K, L 0.214 for -K, -H, -L 0.308 for -H, -K, L 0.217 for K, H, -L	Depositor
Outliers	0 of 76879 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13160	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: YCM

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	0.68	1/2401 (0.0%)	0.76	4/3272 (0.1%)
1	B	0.64	0/2340	0.77	3/3190 (0.1%)
1	C	0.61	0/2341	0.75	1/3193 (0.0%)
1	D	0.63	0/2361	0.73	1/3221 (0.0%)
1	E	0.55	0/2063	0.66	1/2820 (0.0%)
1	F	0.53	0/1870	0.70	3/2554 (0.1%)
All	All	0.61	1/13376 (0.0%)	0.73	13/18250 (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
1	A	0	1
1	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ASP	CB-CG	9.95	1.72	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	GLU	N-CA-CB	-6.58	98.76	110.60
1	A	253	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	192	GLU	CA-CB-CG	6.34	127.34	113.40
1	B	245	ARG	NE-CZ-NH1	6.05	123.33	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	245	ARG	NE-CZ-NH1	5.85	123.22	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ASP	Peptide
1	D	162	ARG	Peptide
1	D	227	LEU	Peptide

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	2356	0	2183	10	0
1	B	2297	0	2113	4	0
1	C	2299	0	2053	8	0
1	D	2317	0	2082	7	0
1	E	2026	0	1672	3	0
1	F	1841	0	1519	5	0
2	A	4	0	0	0	0
2	B	7	0	0	0	0
2	C	3	0	0	0	0
2	D	7	0	0	1	0
2	F	3	0	0	0	0
All	All	13160	0	11622	37	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 1.

The worst 5 of 37 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)
1:F:25:THR:HG22	1:F:121:VAL:HG11	1.62	0.81
1:E:25:THR:HG22	1:E:121:VAL:HG11	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:THR:HG22	1:C:121:VAL:HG11	1.64	0.78
1:D:25:THR:HG22	1:D:121:VAL:HG11	1.64	0.78
1:B:25:THR:HG22	1:B:121:VAL:HG11	1.66	0.77

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	293/371 (79%)	286 (98%)	7 (2%)	0	100	100
1	B	285/371 (77%)	278 (98%)	7 (2%)	0	100	100
1	C	289/371 (78%)	281 (97%)	8 (3%)	0	100	100
1	D	291/371 (78%)	283 (97%)	8 (3%)	0	100	100
1	E	263/371 (71%)	256 (97%)	7 (3%)	0	100	100
1	F	243/371 (66%)	237 (98%)	6 (2%)	0	100	100
All	All	1664/2226 (75%)	1621 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	228/337 (68%)	227 (100%)	1 (0%)	93	98
1	B	220/337 (65%)	219 (100%)	1 (0%)	92	98
1	C	208/337 (62%)	203 (98%)	5 (2%)	57	82
1	D	215/337 (64%)	212 (99%)	3 (1%)	74	91
1	E	164/337 (49%)	162 (99%)	2 (1%)	78	93
1	F	143/337 (42%)	141 (99%)	2 (1%)	74	91
All	All	1178/2022 (58%)	1164 (99%)	14 (1%)	78	93

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	ASP
1	D	27	GLU
1	E	300	GLU
1	C	118	THR
1	E	166	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	YCM	A	103	1	7,9,10	0.78	0	5,10,12	2.30	2 (40%)
1	YCM	B	103	1	7,9,10	1.06	0	5,10,12	2.27	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	YCM	C	103	1	7,9,10	1.24	1 (14%)	5,10,12	2.20	2 (40%)
1	YCM	D	103	1	7,9,10	1.05	1 (14%)	5,10,12	2.25	2 (40%)
1	YCM	E	103	1	7,9,10	1.44	1 (14%)	5,10,12	2.82	4 (80%)
1	YCM	F	103	1	7,9,10	1.04	0	5,10,12	2.12	2 (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
1	YCM	A	103	1	-	0/6/8/10	0/0/0/0
1	YCM	B	103	1	-	0/6/8/10	0/0/0/0
1	YCM	C	103	1	-	0/6/8/10	0/0/0/0
1	YCM	D	103	1	-	0/6/8/10	0/0/0/0
1	YCM	E	103	1	-	0/6/8/10	0/0/0/0
1	YCM	F	103	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	YCM	CB-SG	-2.46	1.76	1.81
1	D	103	YCM	CB-SG	-2.13	1.77	1.81
1	E	103	YCM	CD-CE	3.17	1.60	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	YCM	O-C-CA	-2.46	119.12	125.72
1	C	103	YCM	O-C-CA	-2.44	119.17	125.72
1	B	103	YCM	O-C-CA	-2.44	119.18	125.72
1	A	103	YCM	O-C-CA	-2.33	119.46	125.72
1	E	103	YCM	OZ1-CE-NZ2	-2.32	115.94	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	103	YCM	1	0
1	B	103	YCM	1	0
1	C	103	YCM	2	0
1	D	103	YCM	2	0
1	F	103	YCM	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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(Å²)	Q<0.9	
1	A	305/371 (82%)	-0.80	0	100	100	21, 44, 66, 80	0
1	B	297/371 (80%)	-0.77	0	100	100	22, 44, 67, 78	0
1	C	303/371 (81%)	-0.74	0	100	100	32, 50, 71, 82	0
1	D	305/371 (82%)	-0.77	0	100	100	29, 49, 73, 88	0
1	E	279/371 (75%)	-0.72	0	100	100	39, 60, 82, 95	0
1	F	259/371 (69%)	-0.69	1 (0%)	93	93	39, 60, 87, 99	0
All	All	1748/2226 (78%)	-0.75	1 (0%)	95	96	21, 51, 76, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	272	ALA	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	YCM	F	103	10/11	0.98	0.07	-	53,57,58,61	0
1	YCM	B	103	10/11	0.96	0.11	-	45,51,69,71	0
1	YCM	D	103	10/11	0.97	0.10	-	33,39,56,58	0
1	YCM	E	103	10/11	0.95	0.11	-	57,61,63,65	0
1	YCM	A	103	10/11	0.97	0.10	-	35,39,56,57	0
1	YCM	C	103	10/11	0.98	0.08	-	38,45,58,60	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.