Full wwPDB X-ray Structure Validation Report (i)

May 31, 2016 – 04:30 PM EDT

PDB ID	:	4ZRH
Title	:	Human A20 OTU domain with I325N and alkylated C103
Authors	:	Langley, D.B.; Christ, D.; Grey, S.T.
Deposited on	:	2015-05-12
Resolution	:	2.70 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

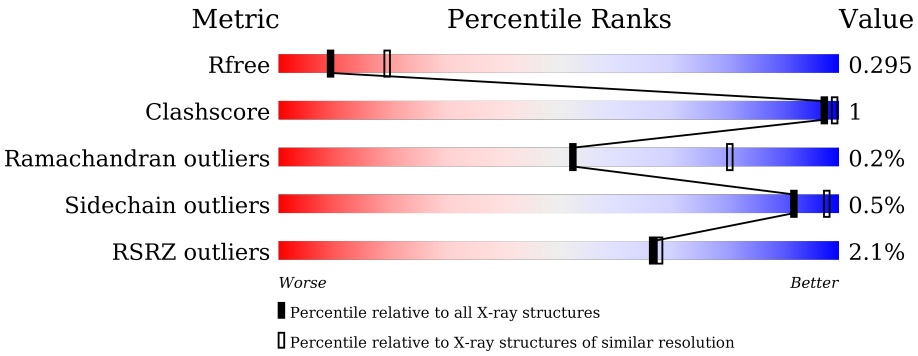
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	371	78% · · 18%
1	B	371	78% · 19%
1	C	371	2% 77% · 19%
1	D	371	% 78% · 19%
1	E	371	2% 74% · 24%
1	F	371	5% 68% · 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12938 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	303	Total	C	N	O	S	0	0	0
			2310	1496	396	404	14			
1	B	301	Total	C	N	O	S	0	0	0
			2285	1479	388	404	14			
1	C	300	Total	C	N	O	S	0	0	0
			2245	1452	382	400	11			
1	D	301	Total	C	N	O	S	0	0	0
			2251	1453	386	398	14			
1	E	282	Total	C	N	O	S	0	0	0
			2038	1311	350	363	14			
1	F	262	Total	C	N	O	S	0	0	0
			1807	1154	326	316	11			

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

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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.

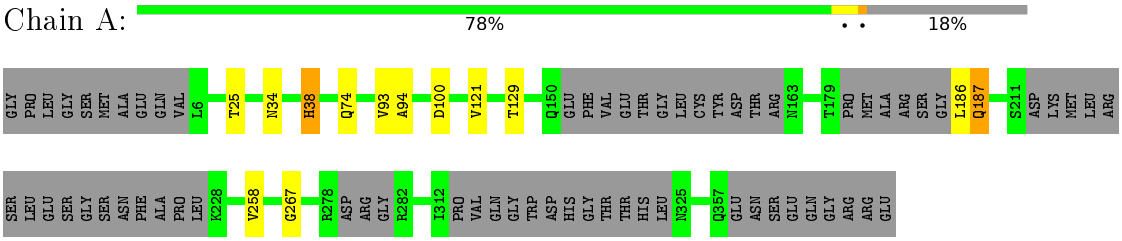
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	1	Total O 1 1	0	0

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.

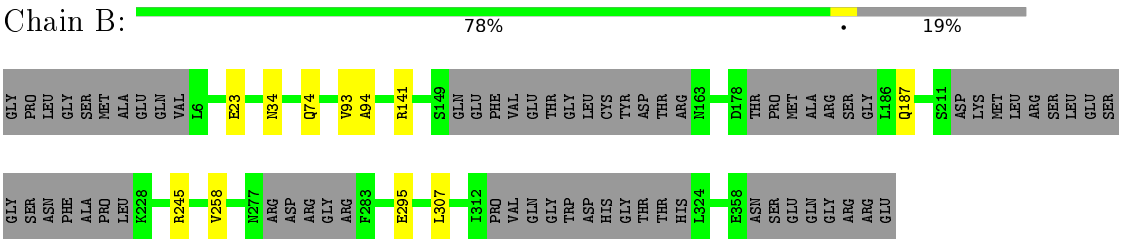
- Molecule 1: Tumor necrosis factor alpha-induced protein 3

Chain A:



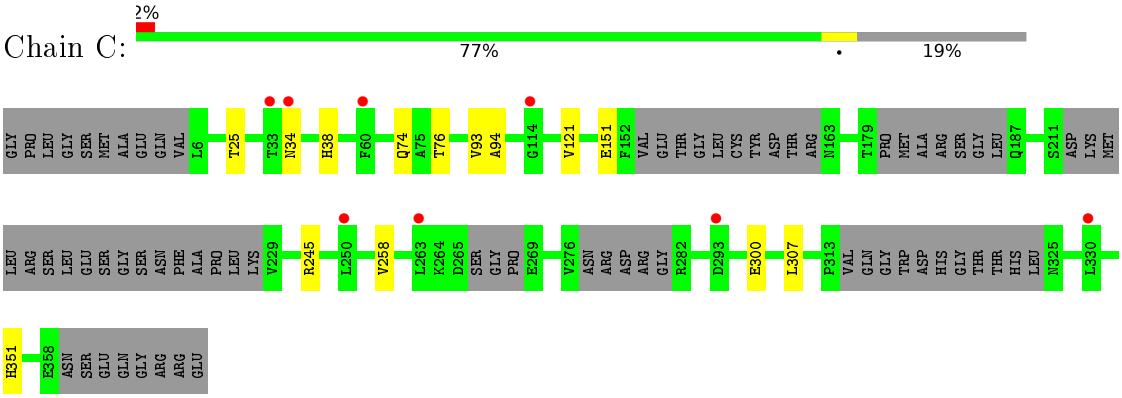
- Molecule 1: Tumor necrosis factor alpha-induced protein 3

Chain B:



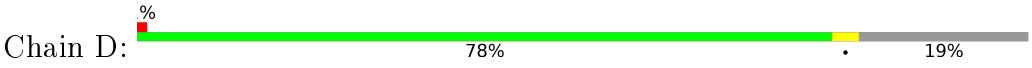
- Molecule 1: Tumor necrosis factor alpha-induced protein 3

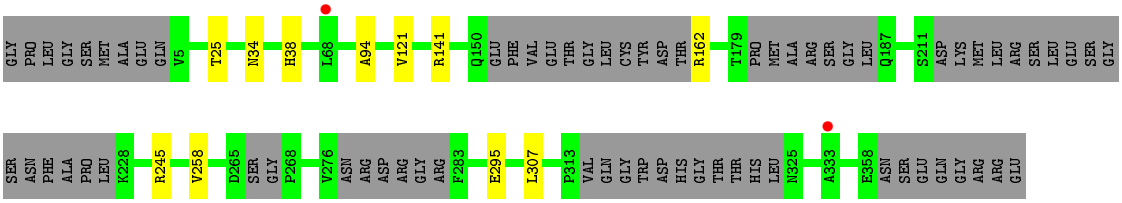
Chain C:



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

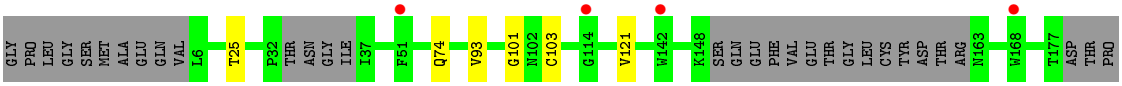
Chain D:

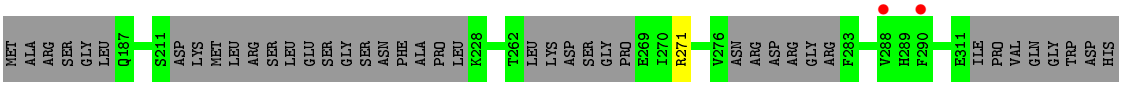


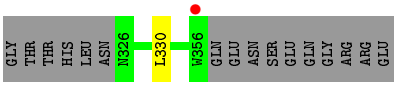


• Molecule 1: Tumor necrosis factor alpha-induced protein 3

Chain E:

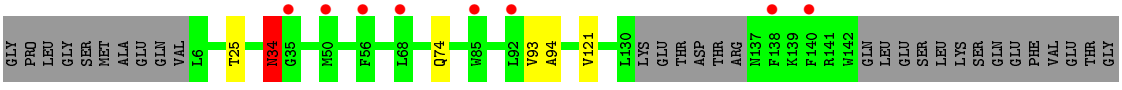


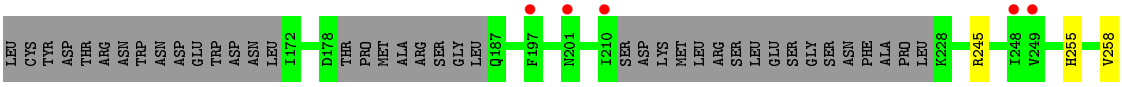


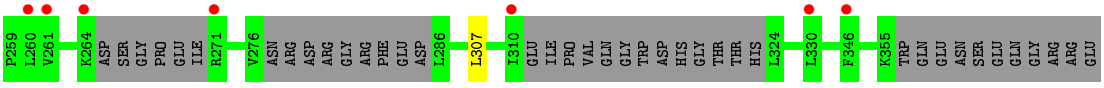


• Molecule 1: Tumor necrosis factor alpha-induced protein 3

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	80.76Å 80.76Å 297.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.33 – 2.70 45.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.33-2.70) 99.9 (45.33-2.70)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.251 , 0.300 0.251 , 0.295	Depositor DCC
R_{free} test set	2984 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.219 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12938	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.52	0/2353	0.70	1/3213 (0.0%)
1	B	0.51	0/2328	0.70	1/3180 (0.0%)
1	C	0.49	0/2287	0.66	1/3128 (0.0%)
1	D	0.49	0/2294	0.67	1/3135 (0.0%)
1	E	0.49	0/2075	0.64	0/2839
1	F	0.46	0/1838	0.65	1/2517 (0.0%)
All	All	0.50	0/13175	0.67	5/18012 (0.0%)

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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ASN	N-CA-C	5.72	126.45	111.00
1	C	34	ASN	N-CA-C	5.48	125.81	111.00
1	F	34	ASN	N-CA-C	5.39	125.56	111.00
1	B	34	ASN	N-CA-C	5.36	125.47	111.00
1	D	34	ASN	N-CA-C	5.26	125.19	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	162	ARG	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	2310	0	2113	6	0
1	B	2285	0	2067	6	0
1	C	2245	0	1969	6	1
1	D	2251	0	1988	4	0
1	E	2038	0	1684	4	0
1	F	1807	0	1401	4	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	12938	0	11222	28	1

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.

All (28) 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:D:25:THR:HG22	1:D:121:VAL:HG11	1.73	0.71
1:C:25:THR:HG22	1:C:121:VAL:HG11	1.74	0.70
1:F:25:THR:HG22	1:F:121:VAL:HG11	1.73	0.69
1:E:25:THR:HG22	1:E:121:VAL:HG11	1.73	0.68
1:A:25:THR:HG22	1:A:121:VAL:HG11	1.76	0.68
1:B:23:GLU:OE2	1:C:351:HIS:HD2	1.78	0.67
1:B:23:GLU:OE2	1:C:351:HIS:CD2	2.55	0.59
1:A:186:LEU:O	1:A:187:GLN:HB2	2.04	0.56
1:F:94:ALA:HB1	1:F:258:VAL:HG11	1.91	0.52
1:C:94:ALA:HB1	1:C:258:VAL:HG11	1.92	0.50
1:D:94:ALA:HB1	1:D:258:VAL:HG11	1.93	0.49
1:B:94:ALA:HB1	1:B:258:VAL:HG11	1.95	0.48
1:A:38:HIS:NE2	1:A:129:THR:OG1	2.47	0.47
1:A:94:ALA:HB1	1:A:258:VAL:HG11	1.95	0.47
1:E:271:ARG:NH1	1:E:330:LEU:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLN:HE21	1:C:93:VAL:HA	1.82	0.45
1:A:74:GLN:HE21	1:A:93:VAL:HA	1.82	0.44
1:B:74:GLN:HE21	1:B:93:VAL:HA	1.82	0.44
1:E:101:GLY:O	1:E:103:YCM:NZ2	2.52	0.43
1:E:74:GLN:HE21	1:E:93:VAL:HA	1.85	0.41
1:F:245:ARG:NH1	1:F:307:LEU:O	2.54	0.41
1:B:245:ARG:NH1	1:B:307:LEU:O	2.54	0.41
1:D:245:ARG:NH1	1:D:307:LEU:O	2.54	0.41
1:F:74:GLN:HE21	1:F:93:VAL:HA	1.86	0.40
1:A:100:ASP:O	1:A:187:GLN:HB3	2.21	0.40
1:B:141:ARG:NH2	1:B:295:GLU:OE2	2.54	0.40
1:C:245:ARG:NH1	1:C:307:LEU:O	2.55	0.40
1:D:141:ARG:NH2	1:D:295:GLU:OE2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:OG1	1:F:34:ASN:OD1[1_455]	1.59	0.61

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	290/371 (78%)	279 (96%)	9 (3%)	2 (1%)	26 55
1	B	288/371 (78%)	275 (96%)	12 (4%)	1 (0%)	46 75
1	C	285/371 (77%)	273 (96%)	11 (4%)	1 (0%)	39 69
1	D	286/371 (77%)	275 (96%)	11 (4%)	0	100 100
1	E	265/371 (71%)	259 (98%)	6 (2%)	0	100 100
1	F	245/371 (66%)	236 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1659/2226 (74%)	1597 (96%)	58 (4%)	4 (0%)	52 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	GLN
1	C	151	GLU
1	A	187	GLN
1	A	267	GLY

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	219/337 (65%)	218 (100%)	1 (0%)	92 98
1	B	215/337 (64%)	215 (100%)	0	100 100
1	C	202/337 (60%)	200 (99%)	2 (1%)	82 94
1	D	204/337 (60%)	203 (100%)	1 (0%)	92 98
1	E	166/337 (49%)	166 (100%)	0	100 100
1	F	128/337 (38%)	126 (98%)	2 (2%)	70 91
All	All	1134/2022 (56%)	1128 (100%)	6 (0%)	92 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	C	38	HIS
1	C	300	GLU
1	D	38	HIS
1	F	34	ASN
1	F	255	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	HIS
1	C	351	HIS
1	F	34	ASN
1	F	351	HIS

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	1.57	2 (28%)	5,10,12	6.30	3 (60%)
1	YCM	B	103	1	7,9,10	1.08	1 (14%)	5,10,12	1.53	2 (40%)
1	YCM	C	103	1	7,9,10	1.30	1 (14%)	5,10,12	1.51	2 (40%)
1	YCM	D	103	1	7,9,10	1.17	1 (14%)	5,10,12	1.42	1 (20%)
1	YCM	E	103	1	7,9,10	2.42	2 (28%)	5,10,12	3.64	4 (80%)
1	YCM	F	103	1	7,9,10	1.12	1 (14%)	5,10,12	1.43	1 (20%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	YCM	CB-SG	-3.00	1.75	1.81
1	E	103	YCM	CB-SG	-2.81	1.75	1.81
1	C	103	YCM	CB-SG	-2.51	1.76	1.81
1	A	103	YCM	CD-SG	-2.48	1.76	1.81
1	D	103	YCM	CB-SG	-2.14	1.77	1.81
1	B	103	YCM	CB-SG	-2.11	1.77	1.81
1	F	103	YCM	CB-SG	-2.05	1.77	1.81
1	E	103	YCM	CD-CE	5.09	1.65	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	YCM	OZ1-CE-CD	-4.58	110.68	120.98
1	E	103	YCM	OZ1-CE-NZ2	-4.32	110.26	122.52
1	B	103	YCM	O-C-CA	-2.46	119.13	125.72
1	E	103	YCM	O-C-CA	-2.44	119.17	125.72
1	F	103	YCM	O-C-CA	-2.36	119.39	125.72
1	C	103	YCM	O-C-CA	-2.33	119.48	125.72
1	D	103	YCM	O-C-CA	-2.29	119.59	125.72
1	A	103	YCM	O-C-CA	-2.27	119.62	125.72
1	C	103	YCM	CD-CE-NZ2	2.04	117.73	115.48
1	B	103	YCM	CD-CE-NZ2	2.05	117.74	115.48
1	E	103	YCM	OZ1-CE-CD	3.08	127.93	120.98
1	E	103	YCM	CD-CE-NZ2	5.52	121.56	115.48
1	A	103	YCM	CD-CE-NZ2	13.05	129.85	115.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	103	YCM	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	302/371 (81%)	-0.14	0 100 100	31, 51, 76, 96	0
1	B	300/371 (80%)	-0.03	0 100 100	30, 55, 79, 90	0
1	C	299/371 (80%)	0.13	8 (2%) 58 58	40, 62, 92, 114	0
1	D	300/371 (80%)	0.08	2 (0%) 89 90	38, 63, 91, 125	0
1	E	281/371 (75%)	0.18	7 (2%) 61 61	46, 71, 92, 107	0
1	F	261/371 (70%)	0.37	20 (7%) 16 14	53, 82, 108, 128	0
All	All	1743/2226 (78%)	0.09	37 (2%) 67 68	30, 64, 94, 128	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	114	GLY	5.1
1	F	50	MET	4.9
1	E	142	TRP	4.2
1	F	248	ILE	3.7
1	F	35	GLY	3.4
1	F	92	LEU	3.4
1	F	261	VAL	3.1
1	F	140	PHE	3.0
1	C	263	LEU	3.0
1	F	85	TRP	3.0
1	F	210	ILE	3.0
1	D	68	LEU	2.9
1	C	114	GLY	2.8
1	E	168	TRP	2.8
1	F	264	LYS	2.7
1	E	290	PHE	2.7
1	F	56	PHE	2.7
1	F	271	ARG	2.7
1	F	346	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	201	ASN	2.6
1	F	310	ILE	2.5
1	F	330	LEU	2.4
1	C	293	ASP	2.4
1	C	34	ASN	2.4
1	C	330	LEU	2.4
1	F	68	LEU	2.3
1	F	260	LEU	2.3
1	C	250	LEU	2.3
1	F	197	PHE	2.3
1	C	33	THR	2.2
1	E	51	PHE	2.2
1	F	138	PHE	2.2
1	E	288	VAL	2.1
1	C	60	PHE	2.1
1	D	333	ALA	2.0
1	F	249	VAL	2.0
1	E	356	TRP	2.0

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, 95^{th} 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	A	103	10/11	0.94	0.17	-	40,48,72,76	0
1	YCM	E	103	10/11	0.87	0.15	-	60,68,80,82	0
1	YCM	F	103	10/11	0.88	0.15	-	62,84,112,123	0
1	YCM	D	103	10/11	0.94	0.14	-	45,54,91,93	0
1	YCM	B	103	10/11	0.91	0.20	-	48,55,92,112	0
1	YCM	C	103	10/11	0.92	0.17	-	45,58,105,113	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.