



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 05:50 PM BST

PDB ID : 2Y8R
Title : Crystal structure of apo AMA1 mutant (Tyr230Ala) from *Toxoplasma gondii*
Authors : Tonkin, M.L.; Roques, M.; Lamarque, M.H.; Pugniere, M.; Douguet, D.; Crawford, J.; Lebrun, M.; Boulanger, M.J.
Deposited on : 2011-02-10
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

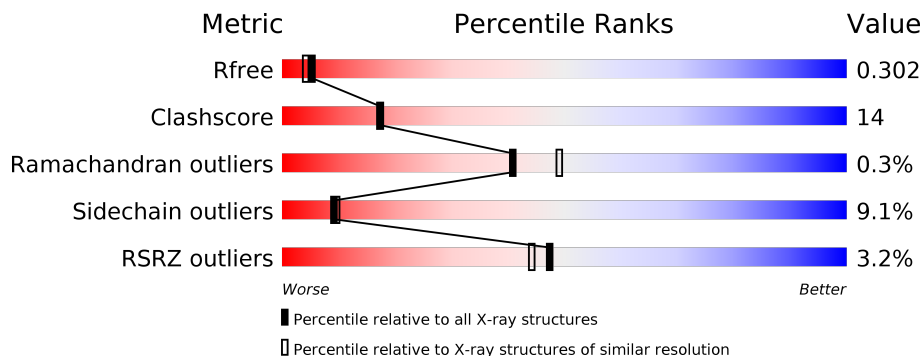
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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	432	 60% 29% 8%
1	B	432	 65% 23% 8%
1	D	432	 69% 19% 5% 6%
1	E	432	 63% 25% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13168 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 APICAL MEMBRANE ANTIGEN, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3144	1975	538	610	21	0	1	0
1	B	397	3134	1971	538	603	22	0	1	0
1	D	406	3197	2009	546	620	22	0	0	0
1	E	394	3108	1955	530	602	21	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	expression tag	UNP B9QC59
A	60	SER	-	expression tag	UNP B9QC59
A	61	ALA	-	expression tag	UNP B9QC59
A	62	MET	-	expression tag	UNP B9QC59
A	63	GLY	-	expression tag	UNP B9QC59
A	485	ALA	-	expression tag	UNP B9QC59
A	486	ALA	-	expression tag	UNP B9QC59
A	487	LEU	-	expression tag	UNP B9QC59
A	488	VAL	-	expression tag	UNP B9QC59
A	489	PRO	-	expression tag	UNP B9QC59
A	490	ARG	-	expression tag	UNP B9QC59
A	230	ALA	TYR	engineered mutation	UNP B9QC59
B	59	GLY	-	expression tag	UNP B9QC59
B	60	SER	-	expression tag	UNP B9QC59
B	61	ALA	-	expression tag	UNP B9QC59
B	62	MET	-	expression tag	UNP B9QC59
B	63	GLY	-	expression tag	UNP B9QC59
B	485	ALA	-	expression tag	UNP B9QC59
B	486	ALA	-	expression tag	UNP B9QC59
B	487	LEU	-	expression tag	UNP B9QC59
B	488	VAL	-	expression tag	UNP B9QC59

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Chain	Residue	Modelled	Actual	Comment	Reference
B	489	PRO	-	expression tag	UNP B9QC59
B	490	ARG	-	expression tag	UNP B9QC59
B	230	ALA	TYR	engineered mutation	UNP B9QC59
D	59	GLY	-	expression tag	UNP B9QC59
D	60	SER	-	expression tag	UNP B9QC59
D	61	ALA	-	expression tag	UNP B9QC59
D	62	MET	-	expression tag	UNP B9QC59
D	63	GLY	-	expression tag	UNP B9QC59
D	485	ALA	-	expression tag	UNP B9QC59
D	486	ALA	-	expression tag	UNP B9QC59
D	487	LEU	-	expression tag	UNP B9QC59
D	488	VAL	-	expression tag	UNP B9QC59
D	489	PRO	-	expression tag	UNP B9QC59
D	490	ARG	-	expression tag	UNP B9QC59
D	230	ALA	TYR	engineered mutation	UNP B9QC59
E	59	GLY	-	expression tag	UNP B9QC59
E	60	SER	-	expression tag	UNP B9QC59
E	61	ALA	-	expression tag	UNP B9QC59
E	62	MET	-	expression tag	UNP B9QC59
E	63	GLY	-	expression tag	UNP B9QC59
E	485	ALA	-	expression tag	UNP B9QC59
E	486	ALA	-	expression tag	UNP B9QC59
E	487	LEU	-	expression tag	UNP B9QC59
E	488	VAL	-	expression tag	UNP B9QC59
E	489	PRO	-	expression tag	UNP B9QC59
E	490	ARG	-	expression tag	UNP B9QC59
E	230	ALA	TYR	engineered mutation	UNP B9QC59

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	E	1	14	8	1	5	0	0

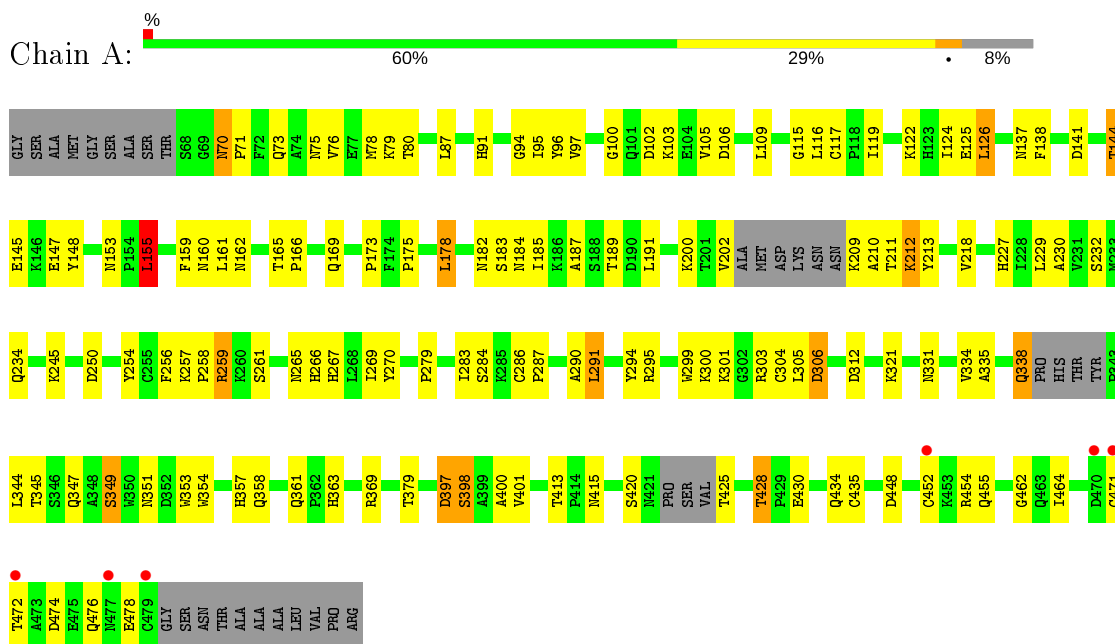
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	154	154	154	0	0
3	B	134	134	134	0	0
3	D	107	107	107	0	0
3	E	134	134	134	0	0

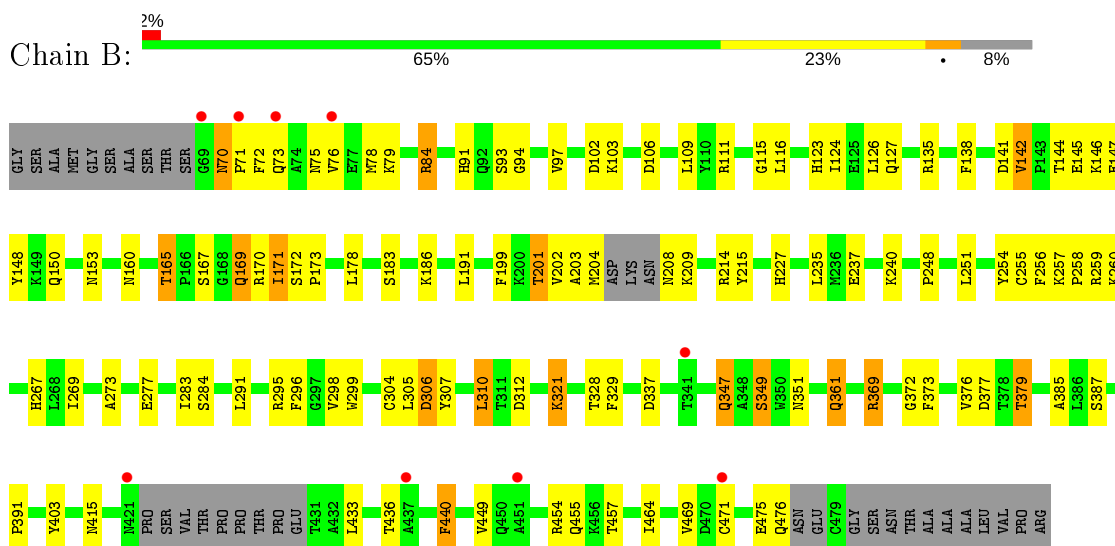
3 Residue-property plots [i](#)

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.

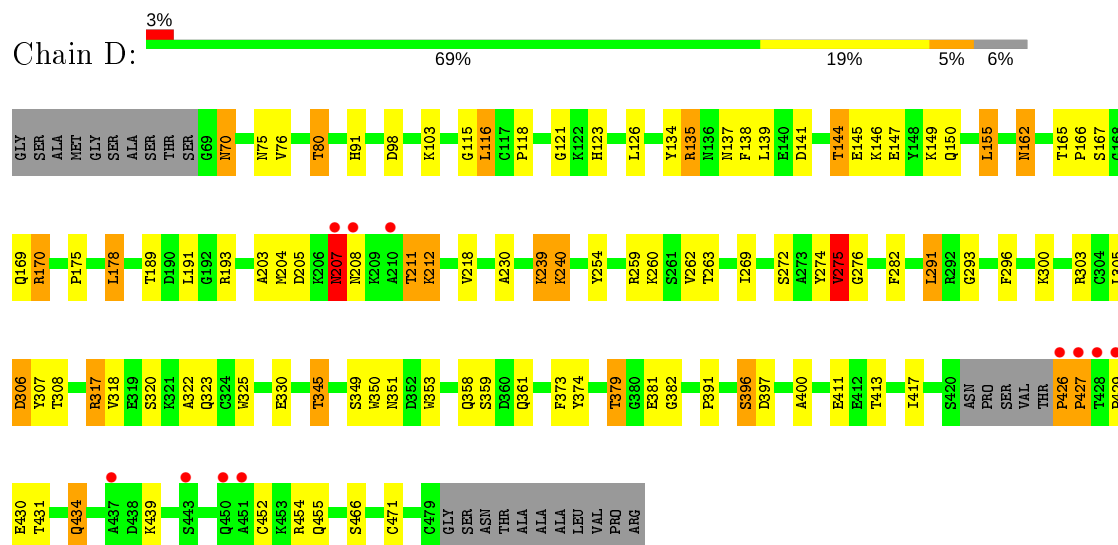
- Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



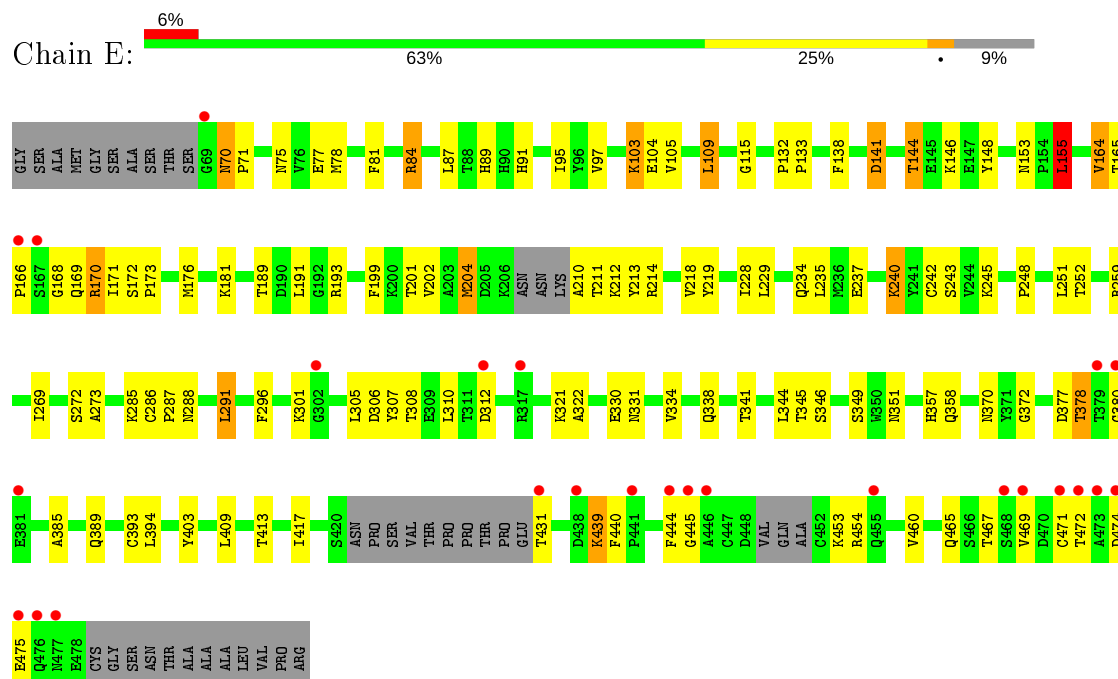
- Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



- Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



- Molecule 1: APICAL MEMBRANE ANTIGEN, PUTATIVE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.52Å 76.09Å 88.78Å 71.89° 73.37° 73.50°	Depositor
Resolution (Å)	38.59 – 2.45 38.59 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.59-2.45) 97.0 (38.59-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.305 0.212 , 0.302	Depositor DCC
R_{free} test set	2834 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13168	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.87% 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:
NAG

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	0.71	0/3229	0.80	2/4379 (0.0%)
1	B	0.68	0/3219	0.76	0/4364
1	D	0.71	1/3284 (0.0%)	0.80	8/4458 (0.2%)
1	E	0.66	0/3190	0.79	5/4325 (0.1%)
All	All	0.69	1/12922 (0.0%)	0.79	15/17526 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	426	PRO	C-N	-6.20	1.22	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	427	PRO	N-CA-CB	-7.53	94.27	103.30
1	A	305	LEU	CA-CB-CG	7.15	131.74	115.30
1	E	170	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	D	170	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	E	141	ASP	CB-CG-OD1	6.47	124.12	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	207	ASN	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	3144	0	2980	95	0
1	B	3134	0	2971	79	0
1	D	3197	0	3024	83	0
1	E	3108	0	2937	89	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	D	14	0	13	1	0
2	E	14	0	13	0	0
3	A	154	0	0	12	0
3	B	134	0	0	9	0
3	D	107	0	0	5	0
3	E	134	0	0	6	0
All	All	13168	0	11964	339	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 14.

The worst 5 of 339 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:203:ALA:O	1:D:211:THR:HG22	1.53	1.08
1:D:76:VAL:O	1:D:80:THR:HG22	1.54	1.06
1:A:105:VAL:HG13	1:A:211:THR:HG21	1.38	1.02
1:A:144:THR:HG22	1:A:147:GLU:H	1.27	1.00
1:D:203:ALA:O	1:D:211:THR:CG2	2.15	0.94

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	392/432 (91%)	370 (94%)	21 (5%)	1 (0%)	41	49
1	B	391/432 (90%)	371 (95%)	18 (5%)	2 (0%)	29	34
1	D	402/432 (93%)	376 (94%)	25 (6%)	1 (0%)	47	57
1	E	386/432 (89%)	358 (93%)	27 (7%)	1 (0%)	41	49
All	All	1571/1728 (91%)	1475 (94%)	91 (6%)	5 (0%)	41	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	369[A]	ARG
1	B	369[B]	ARG
1	E	307	TYR
1	A	397	ASP
1	D	275	VAL

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	348/371 (94%)	314 (90%)	34 (10%)	8	8
1	B	345/371 (93%)	315 (91%)	30 (9%)	10	11
1	D	353/371 (95%)	321 (91%)	32 (9%)	9	10
1	E	342/371 (92%)	312 (91%)	30 (9%)	10	11
All	All	1388/1484 (94%)	1262 (91%)	126 (9%)	9	10

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	GLN
1	D	144	THR
1	E	312	ASP
1	B	379	THR
1	B	476	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	ASN
1	B	455	GLN
1	E	358	GLN
1	B	338	GLN
1	D	70	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	NAG	A	1480	1	14,14,15	0.64	0	17,19,21	1.83	4 (23%)
2	NAG	D	1480	1	14,14,15	0.56	0	17,19,21	1.76	3 (17%)
2	NAG	B	1480	1	14,14,15	0.62	0	17,19,21	1.52	4 (23%)
2	NAG	E	1479	1	14,14,15	0.51	0	17,19,21	1.40	3 (17%)

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
2	NAG	A	1480	1	-	4/6/23/26	0/1/1/1
2	NAG	D	1480	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1480	1	-	4/6/23/26	0/1/1/1
2	NAG	E	1479	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1480	NAG	C1-O5-C5	5.25	119.30	112.19
2	A	1480	NAG	C1-O5-C5	4.76	118.64	112.19
2	B	1480	NAG	C1-C2-N2	4.15	117.57	110.49
2	A	1480	NAG	O4-C4-C5	3.42	117.78	109.30
2	E	1479	NAG	C1-O5-C5	3.27	116.62	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1480	NAG	C8-C7-N2-C2
2	A	1480	NAG	O7-C7-N2-C2
2	D	1480	NAG	C8-C7-N2-C2
2	D	1480	NAG	O7-C7-N2-C2
2	B	1480	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1480	NAG	1	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 [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	399/432 (92%)	-0.20	6 (1%) 73 71	5, 24, 42, 61	3 (0%)
1	B	397/432 (91%)	-0.08	9 (2%) 60 56	7, 28, 54, 62	6 (1%)
1	D	406/432 (93%)	-0.06	11 (2%) 54 50	9, 26, 52, 63	4 (0%)
1	E	394/432 (91%)	0.10	25 (6%) 20 16	8, 28, 66, 80	1 (0%)
All	All	1596/1728 (92%)	-0.06	51 (3%) 47 44	5, 27, 55, 80	14 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	431	THR	4.8
1	E	380	GLY	4.2
1	E	69	GLY	4.1
1	E	469	VAL	4.1
1	E	473	ALA	3.9

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 monosaccharides 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
2	NAG	E	1479	14/15	0.85	0.19	43,46,48,51	0
2	NAG	D	1480	14/15	0.90	0.12	28,32,36,36	0
2	NAG	B	1480	14/15	0.92	0.17	22,28,30,32	0
2	NAG	A	1480	14/15	0.92	0.13	20,22,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.