



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 10:44 PM EDT

PDB ID : 6VMW
Title : Crystal structure of the F316A mutant of GoxA soaked with glycine
Authors : Yukl, E.T.
Deposited on : 2020-01-28
Resolution : 1.99 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

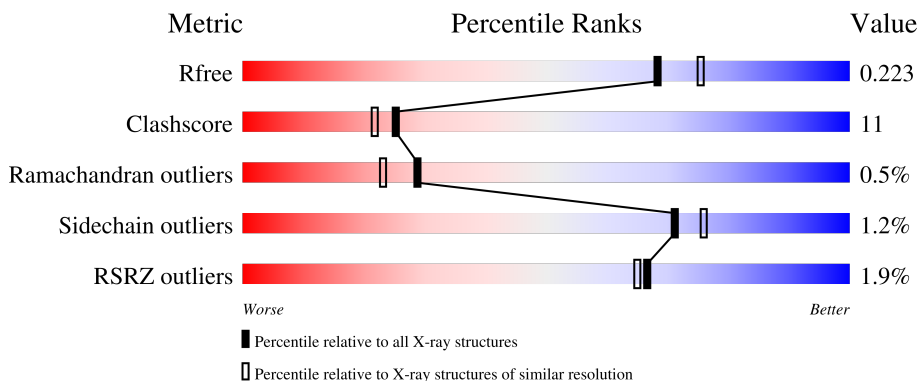
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	816	
1	B	816	
1	C	816	
1	D	816	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 27305 atoms, of which 826 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 Glycine oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	784	6460	3919	257	1056	1208	20	0	1	0
1	A	764	6138	3812	105	1029	1173	19	0	1	0
1	C	769	6305	3838	234	1032	1181	20	0	0	0
1	D	759	6240	3798	230	1025	1167	20	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	316	ALA	PHE	engineered mutation	UNP A0A161XU12
A	316	ALA	PHE	engineered mutation	UNP A0A161XU12
C	316	ALA	PHE	engineered mutation	UNP A0A161XU12
D	316	ALA	PHE	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

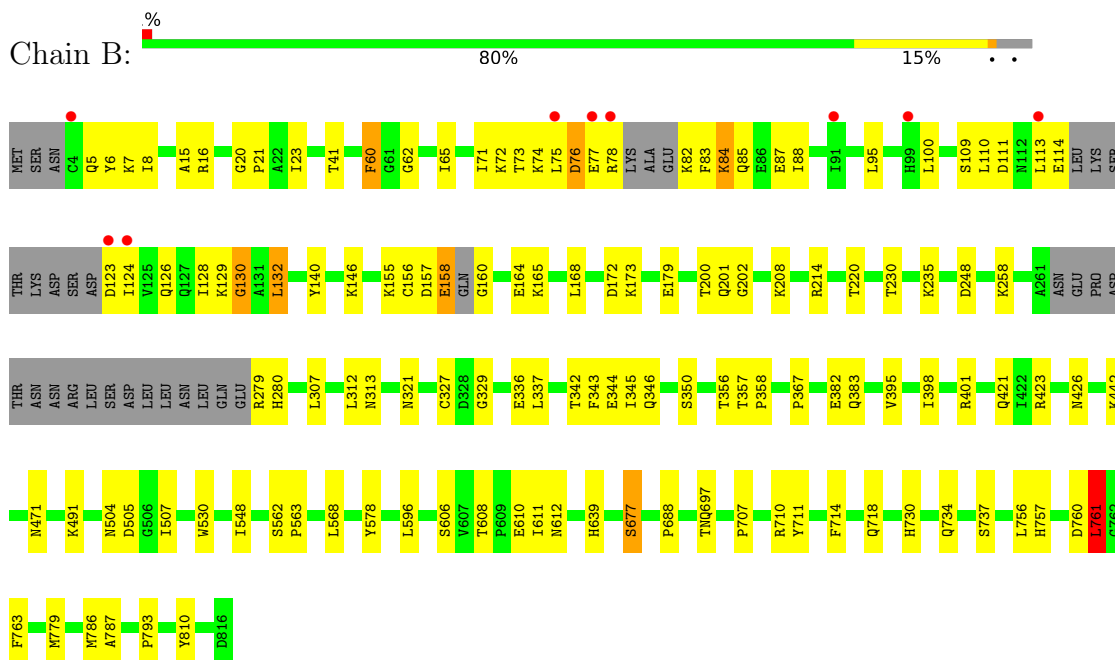
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	568	Total	O	0	0
			568	568		
4	A	562	Total	O	0	1
			563	563		
4	C	498	Total	O	0	0
			498	498		
4	D	528	Total	O	0	0
			528	528		

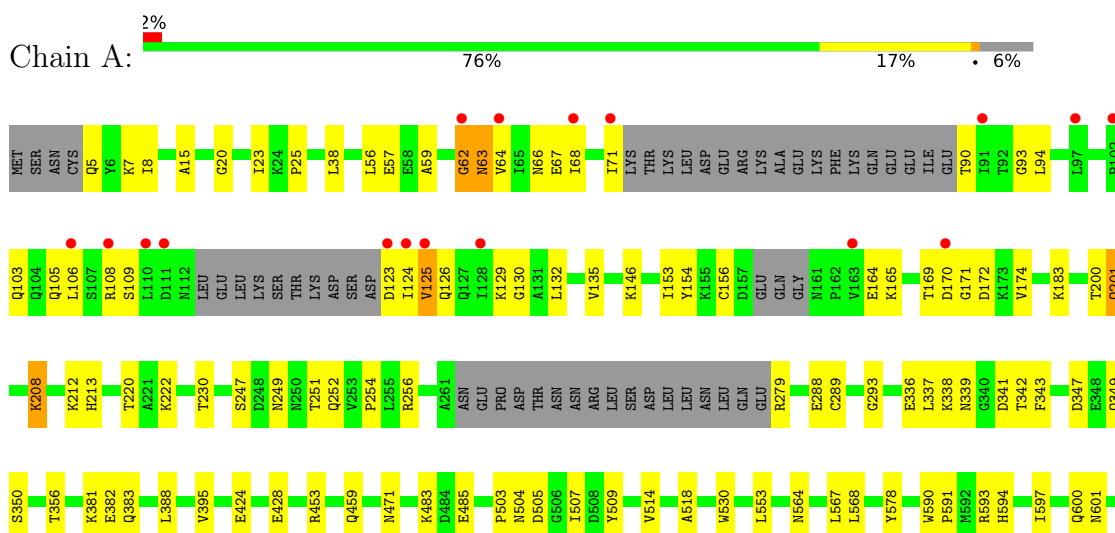
3 Residue-property plots [i](#)

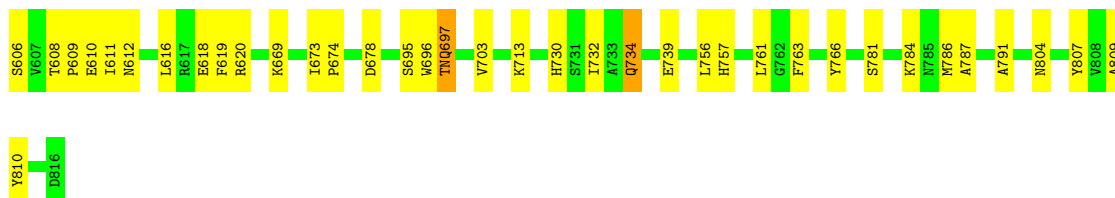
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycine oxidase

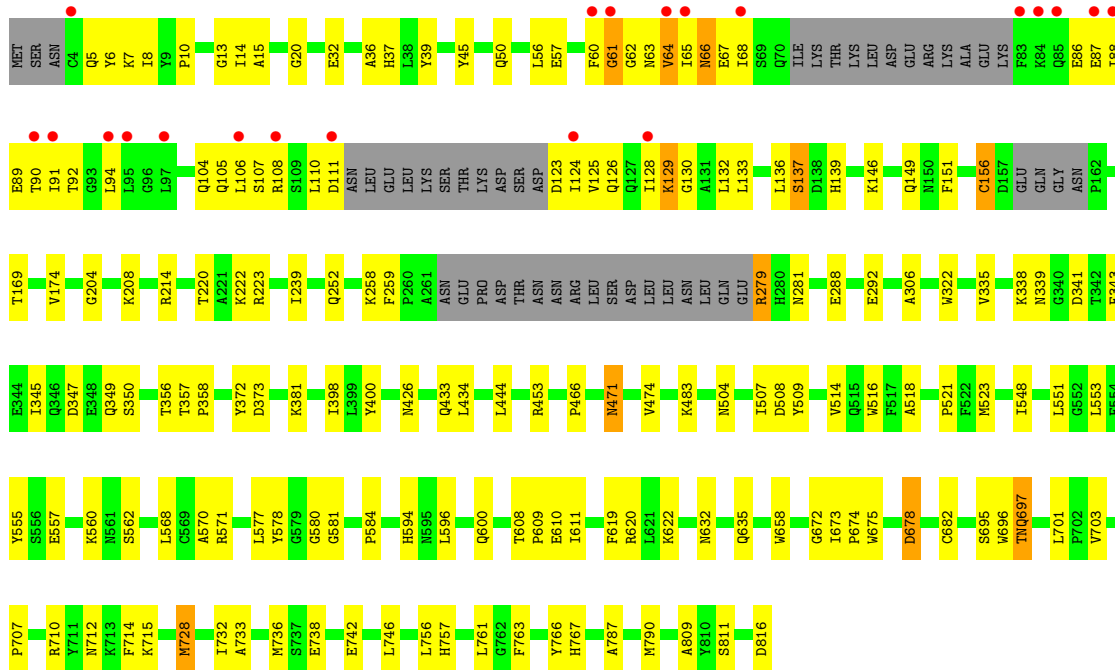
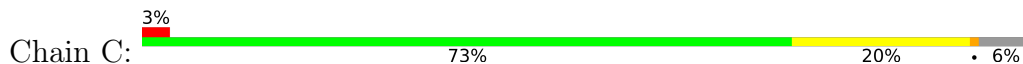


• Molecule 1: Glycine oxidase

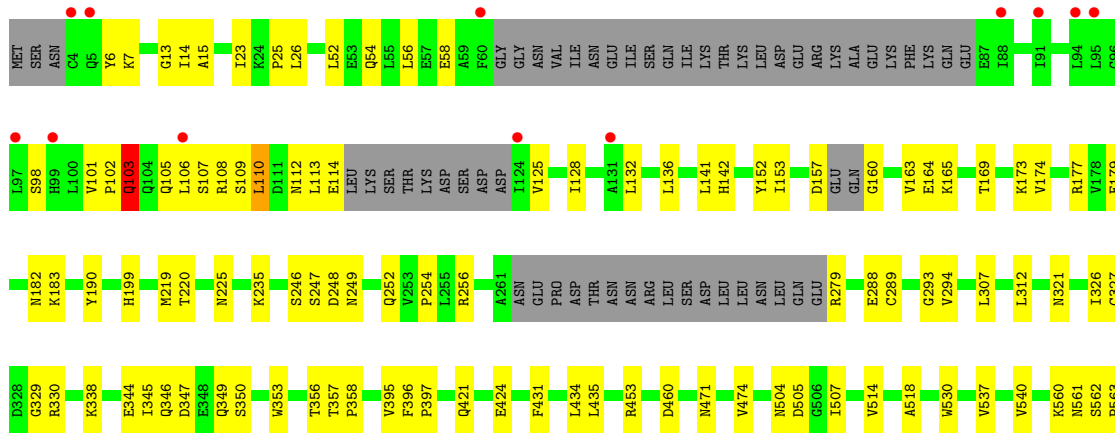
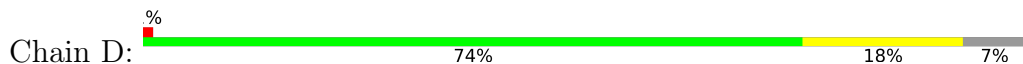




● Molecule 1: Glycine oxidase



● Molecule 1: Glycine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.61Å 91.88Å 178.79Å 90.00° 91.37° 90.00°	Depositor
Resolution (Å)	45.94 – 1.99 45.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.94-1.99) 99.1 (45.94-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.172 , 0.223 0.172 , 0.223	Depositor DCC
R_{free} test set	12078 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.172	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27305	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MG, NA, TNQ

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	0.44	1/6158 (0.0%)	0.57	0/8388
1	B	0.43	1/6329 (0.0%)	0.60	3/8613 (0.0%)
1	C	0.40	0/6197	0.56	0/8437
1	D	0.43	1/6135 (0.0%)	0.57	0/8355
All	All	0.42	3/24819 (0.0%)	0.58	3/33793 (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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	CYS	CB-SG	8.42	1.96	1.82
1	A	201	GLN	CD-NE2	7.68	1.52	1.32
1	B	327	CYS	CB-SG	6.65	1.93	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	LEU	CB-CG-CD2	-8.24	96.99	111.00
1	B	761[A]	LEU	CA-CB-CG	-6.76	99.76	115.30
1	B	761[B]	LEU	CA-CB-CG	-6.76	99.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	156	CYS	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	6033	105	5787	123	0
1	B	6203	257	5961	116	0
1	C	6071	234	5824	159	0
1	D	6010	230	5763	134	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	1	0	0	0	0
4	A	563	0	0	12	0
4	B	568	0	0	11	0
4	C	498	0	0	20	0
4	D	528	0	0	13	0
All	All	26479	826	23335	512	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 512 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:C:600:GLN:NE2	4:C:1001:HOH:O	1.83	1.10
1:A:201:GLN:NE2	1:A:381:LYS:HE3	1.75	1.02
1:C:63:ASN:HB2	1:C:94:LEU:HD21	1.45	0.97
1:B:383:GLN:OE1	4:B:1001:HOH:O	1.83	0.97
1:C:6:TYR:HB2	1:C:345:ILE:HD11	1.46	0.97

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	754/816 (92%)	721 (96%)	28 (4%)	5 (1%)	22	16
1	B	774/816 (95%)	745 (96%)	25 (3%)	4 (0%)	29	23
1	C	758/816 (93%)	725 (96%)	30 (4%)	3 (0%)	34	30
1	D	749/816 (92%)	715 (96%)	31 (4%)	3 (0%)	34	30
All	All	3035/3264 (93%)	2906 (96%)	114 (4%)	15 (0%)	29	23

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	LYS
1	A	125	VAL
1	C	64	VAL
1	D	103	GLN
1	B	76	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	661/710 (93%)	653 (99%)	8 (1%)	71	76
1	B	680/710 (96%)	671 (99%)	9 (1%)	69	74
1	C	665/710 (94%)	655 (98%)	10 (2%)	65	69
1	D	658/710 (93%)	650 (99%)	8 (1%)	71	76
All	All	2664/2840 (94%)	2629 (99%)	35 (1%)	71	74

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	177	ARG
1	D	246	SER
1	D	564[B]	ASN
1	A	279	ARG
1	A	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
1	D	99	HIS
1	D	730	HIS
1	D	539	GLN
1	D	612	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](#)

4 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	TNQ	D	697	1	18,21,22	3.15	3 (16%)	16,29,31	2.77	4 (25%)
1	TNQ	A	697	1	18,21,22	2.84	4 (22%)	16,29,31	2.57	5 (31%)
1	TNQ	B	697	1	18,21,22	2.93	3 (16%)	16,29,31	2.58	6 (37%)
1	TNQ	C	697	1	18,21,22	2.13	4 (22%)	16,29,31	1.76	4 (25%)

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	TNQ	D	697	1	-	3/9/11/13	0/2/2/2
1	TNQ	A	697	1	-	2/9/11/13	0/2/2/2
1	TNQ	B	697	1	-	2/9/11/13	0/2/2/2
1	TNQ	C	697	1	-	3/9/11/13	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TNQ	C2-N1	-11.17	1.27	1.45
1	B	697	TNQ	C2-N1	-10.69	1.28	1.45
1	A	697	TNQ	C2-N1	-9.37	1.30	1.45
1	C	697	TNQ	C2-N1	-6.58	1.35	1.45
1	A	697	TNQ	CZ2-CE2	5.54	1.52	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	697	TNQ	C1-C2-N1	7.68	125.06	110.96
1	B	697	TNQ	C1-C2-N1	6.20	122.33	110.96
1	A	697	TNQ	C1-C2-N1	6.20	122.33	110.96
1	D	697	TNQ	C2-N1-CH2	-5.89	115.53	123.98
1	B	697	TNQ	C2-N1-CH2	-5.21	116.51	123.98

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	697	TNQ	CZ2-CH2-N1-C2
1	A	697	TNQ	CZ2-CH2-N1-C2
1	D	697	TNQ	CZ3-CH2-N1-C2
1	B	697	TNQ	CZ3-CH2-N1-C2
1	A	697	TNQ	CZ3-CH2-N1-C2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TNQ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	697	TNQ	2	0
1	C	697	TNQ	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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	763/816 (93%)	-0.33	17 (2%) 62 60	12, 24, 65, 132	0
1	B	783/816 (95%)	-0.38	9 (1%) 80 79	10, 22, 65, 111	0
1	C	768/816 (94%)	-0.25	21 (2%) 54 53	15, 27, 84, 137	0
1	D	758/816 (92%)	-0.33	12 (1%) 72 70	11, 23, 65, 126	0
All	All	3072/3264 (94%)	-0.32	59 (1%) 66 65	10, 24, 70, 137	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	83	PHE	10.1
1	D	95	LEU	7.5
1	B	75	LEU	6.6
1	D	91	ILE	6.5
1	C	4	CYS	6.3

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. 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(Å ²)	Q<0.9
1	TNQ	C	697	20/21	0.96	0.10	14,25,47,62	0
1	TNQ	A	697	20/21	0.97	0.09	8,23,52,64	0
1	TNQ	B	697	20/21	0.97	0.09	9,23,42,53	0
1	TNQ	D	697	20/21	0.97	0.08	8,18,48,53	0

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(Å ²)	Q<0.9
3	NA	B	902	1/1	0.95	0.16	46,46,46,46	0
2	MG	B	901	1/1	0.98	0.06	21,21,21,21	0
2	MG	C	901	1/1	0.99	0.05	23,23,23,23	0
2	MG	D	901	1/1	0.99	0.07	21,21,21,21	0
2	MG	A	901	1/1	0.99	0.05	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.