



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 02:05 AM UTC

PDB ID : 6UC1 / pdb_00006uc1
Title : Crystal structure of D678A GoxA soaked in glycine at pH 7.5
Authors : Yukl, E.T.
Deposited on : 2019-09-13
Resolution : 2.19 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

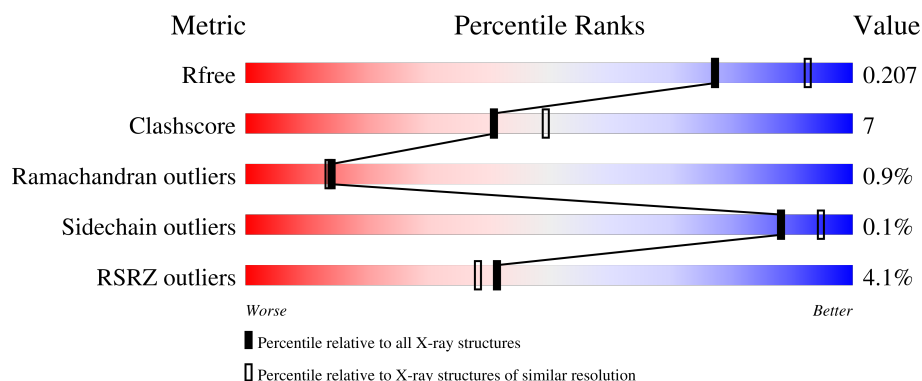
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	3% 82% 12% • 5%
1	B	816	3% 84% 10% • 5%
1	D	816	5% 82% 12% • 5%
2	C	816	4% 83% 12% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GLY	D	905	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49336 atoms, of which 23369 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 Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	776	Total	C	H	N	O	S	0	0	0
			11936	3880	5803	1044	1189	20			
1	A	776	Total	C	H	N	O	S	0	1	0
			12010	3889	5866	1044	1191	20			
1	D	776	Total	C	H	N	O	S	0	2	0
			11992	3890	5844	1047	1191	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ALA	ASP	engineered mutation	UNP A0A161XU12
A	678	ALA	ASP	engineered mutation	UNP A0A161XU12
D	678	ALA	ASP	engineered mutation	UNP A0A161XU12

- Molecule 2 is a protein called Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	777	Total	C	H	N	O	S	0	0	0
			11971	3892	5822	1046	1192	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	678	ALA	ASP	engineered mutation	UNP A0A161XU12

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

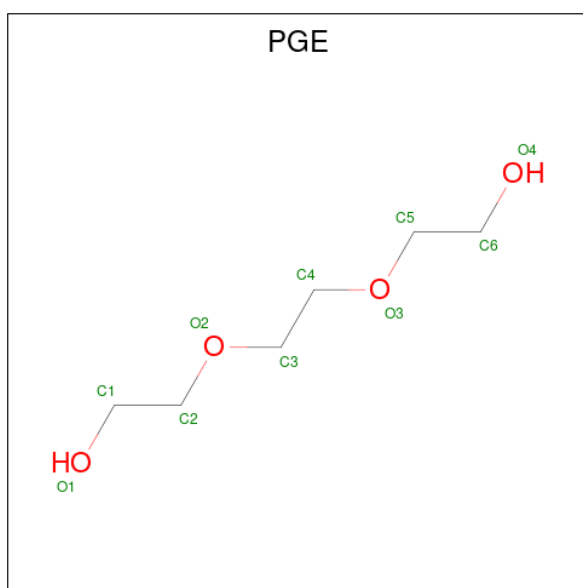


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 24 6 14 4	0	0

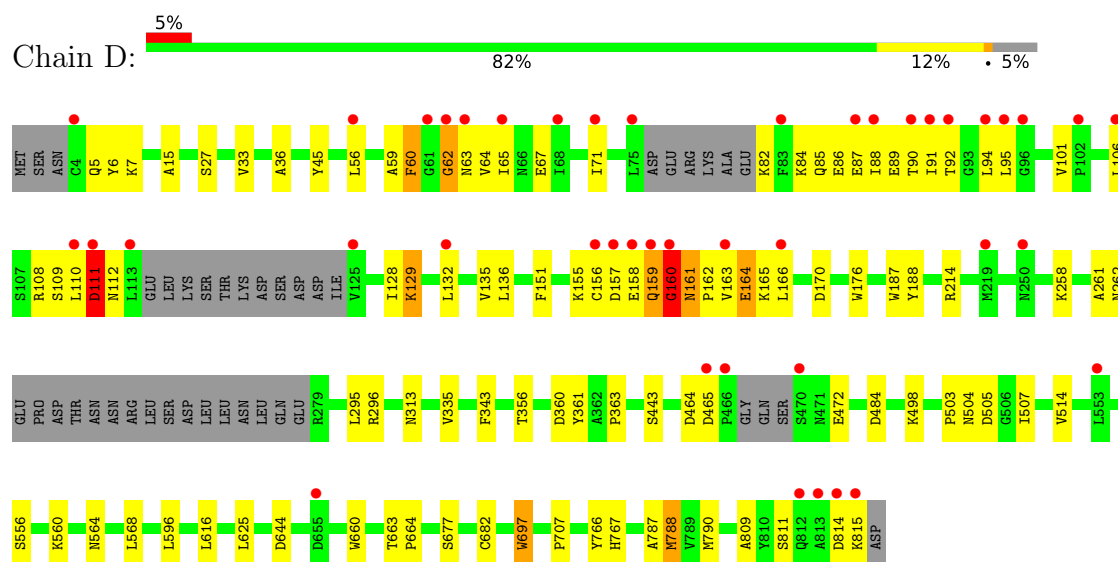
- Molecule 6 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



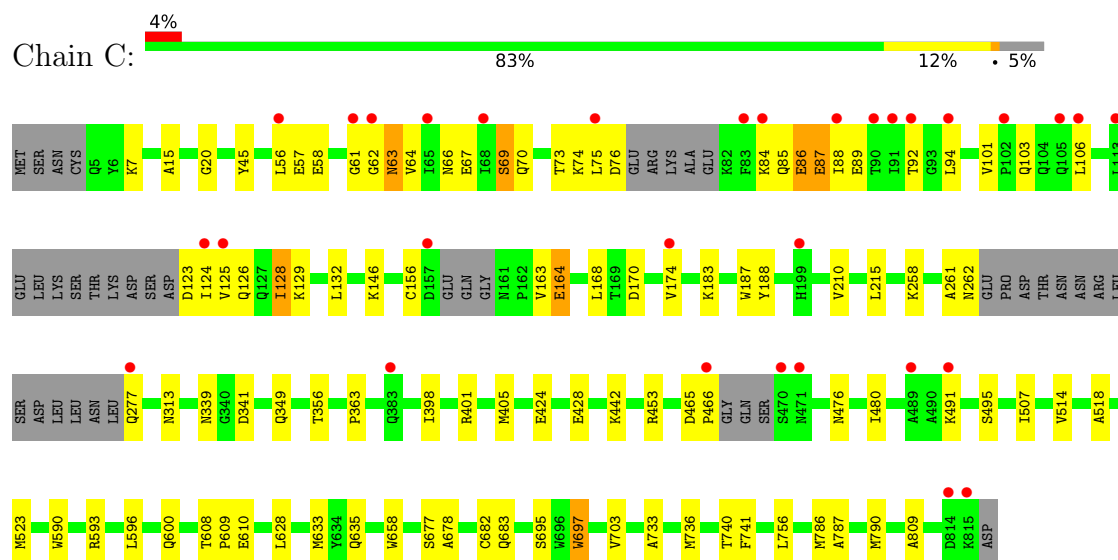
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	365	Total	O	0	1
			366	366		
7	A	288	Total	O	0	0
			288	288		
7	D	269	Total	O	0	0
			269	269		
7	C	376	Total	O	0	0
			376	376		



• Molecule 2: Uncharacterized protein GoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.21Å 93.53Å 188.33Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-2.19) 99.4 (48.38-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.169 , 0.206 0.172 , 0.207	Depositor DCC
R_{free} test set	9759 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49336	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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, TRQ, SO4, PGE, Q3P

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	0.45	2/6273 (0.0%)	0.53	0/8536
1	B	0.50	2/6264 (0.0%)	0.57	1/8526 (0.0%)
1	D	0.42	1/6279 (0.0%)	0.54	2/8546 (0.0%)
2	C	0.50	2/6265 (0.0%)	0.59	3/8526 (0.0%)
All	All	0.47	7/25081 (0.0%)	0.56	6/34134 (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	A	0	1
1	B	0	1
1	D	0	2
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	LYS	CE-NZ	-11.93	1.13	1.49
1	A	327	CYS	CB-SG	-9.27	1.50	1.81
1	D	788	MET	SD-CE	-8.57	1.58	1.79
2	C	790	MET	SD-CE	-6.91	1.62	1.79
2	C	786	MET	SD-CE	-6.82	1.62	1.79

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	LYS	CD-CE-NZ	-8.30	85.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	GLY	CA-C-N	6.34	133.11	121.70
1	D	160	GLY	C-N-CA	6.34	133.11	121.70
2	C	69	SER	CB-CA-C	-6.27	97.94	110.42
2	C	128	ILE	CB-CA-C	-5.29	105.00	112.14

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	LEU	Peptide
1	B	86	GLU	Peptide
1	D	111	ASP	Peptide
1	D	159	GLN	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	6144	5866	5918	79	1
1	B	6133	5803	5906	73	1
1	D	6148	5844	5924	88	0
2	C	6149	5822	5911	76	0
3	A	10	0	0	1	0
3	B	25	0	0	2	0
3	C	15	0	0	1	0
3	D	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	10	14	14	0	0
6	A	10	10	4	3	0
6	D	10	10	4	4	0
7	A	288	0	0	8	0
7	B	366	0	0	1	0
7	C	376	0	0	5	0
7	D	269	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25967	23369	23681	316	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 7.

The worst 5 of 316 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:B:54:GLN:NE2	1:B:58:GLU:OE1	1.84	1.09
1:D:644:ASP:OD2	7:D:1001:HOH:O	1.79	0.98
2:C:86:GLU:HB3	2:C:89:GLU:HB2	1.48	0.94
1:B:334:VAL:O	7:B:1001:HOH:O	1.86	0.91
2:C:75:LEU:HD21	2:C:87:GLU:OE1	1.71	0.90

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:B:62:GLY:N	1:A:67:GLU:OE2[1_455]	1.96	0.24

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	764/816 (94%)	719 (94%)	35 (5%)	10 (1%)	9 8
1	B	765/816 (94%)	735 (96%)	25 (3%)	5 (1%)	18 19
1	D	767/816 (94%)	726 (95%)	33 (4%)	8 (1%)	12 11
2	C	763/816 (94%)	728 (95%)	31 (4%)	4 (0%)	24 27
All	All	3059/3264 (94%)	2908 (95%)	124 (4%)	27 (1%)	14 14

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	GLY
1	B	159	GLN
1	A	94	LEU
1	D	60	PHE
1	D	111	ASP

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	673/710 (95%)	672 (100%)	1 (0%)	88	95
1	B	672/710 (95%)	670 (100%)	2 (0%)	86	93
1	D	674/710 (95%)	674 (100%)	0	100	100
2	C	673/709 (95%)	673 (100%)	0	100	100
All	All	2692/2839 (95%)	2689 (100%)	3 (0%)	88	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	159	GLN
1	B	625	LEU
1	A	814	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	231	ASN
1	D	804	ASN
2	C	785	ASN
2	C	600	GLN
1	D	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	TRQ	D	697	1	16,17,18	1.64	2 (12%)	16,24,26	0.88	0
2	TRQ	C	697	2	16,17,18	1.35	1 (6%)	16,24,26	1.16	2 (12%)
1	TRQ	B	697	1	16,17,18	1.24	3 (18%)	16,24,26	0.90	2 (12%)
2	Q3P	C	222	2	10,12,13	0.91	0	5,13,15	0.77	0
1	TRQ	A	697	1	16,17,18	1.47	1 (6%)	16,24,26	0.92	1 (6%)

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	TRQ	D	697	1	-	2/5/19/21	0/2/2/2
2	TRQ	C	697	2	-	2/5/19/21	0/2/2/2
1	TRQ	B	697	1	-	2/5/19/21	0/2/2/2
2	Q3P	C	222	2	-	2/11/12/14	-
1	TRQ	A	697	1	-	2/5/19/21	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TRQ	CD1-CG	4.17	1.44	1.38
1	A	697	TRQ	CD1-CG	4.17	1.44	1.38
2	C	697	TRQ	CD1-CG	3.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	697	TRQ	CD1-CG	3.03	1.42	1.38
1	B	697	TRQ	CB-CG	-2.60	1.45	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	TRQ	O7-CZ2-CH2	2.31	121.34	118.39
1	A	697	TRQ	O7-CZ2-CE2	2.13	125.72	120.04
2	C	697	TRQ	O7-CZ2-CH2	2.09	121.06	118.39
1	B	697	TRQ	O7-CZ2-CE2	2.08	125.59	120.04
2	C	697	TRQ	O7-CZ2-CE2	2.08	125.57	120.04

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	697	TRQ	CA-CB-CG-CD2
1	A	697	TRQ	CA-CB-CG-CD2
1	D	697	TRQ	CA-CB-CG-CD2
2	C	222	Q3P	O2-C1-C4-N5
2	C	697	TRQ	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TRQ	1	0
2	C	697	TRQ	3	0
1	B	697	TRQ	3	0
1	A	697	TRQ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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$
6	GLY	D	904	-	4,4,4	1.14	1 (25%)	3,4,4	1.58	0
6	GLY	A	904	-	4,4,4	1.14	1 (25%)	3,4,4	1.68	1 (33%)
6	GLY	D	905	-	4,4,4	1.28	1 (25%)	3,4,4	1.86	1 (33%)
3	SO4	B	901	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	D	901	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	901	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	C	902	-	4,4,4	0.30	0	6,6,6	0.08	0
6	GLY	A	905	-	4,4,4	1.06	0	3,4,4	1.40	0
3	SO4	B	905	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	B	904	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	C	903	-	4,4,4	0.29	0	6,6,6	0.20	0
5	PGE	B	907	-	9,9,9	0.40	0	8,8,8	0.25	0
3	SO4	B	903	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	C	901	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	902	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	902	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	D	902	-	4,4,4	0.27	0	6,6,6	0.14	0

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
6	GLY	D	905	-	-	2/2/2/2	-
6	GLY	A	904	-	-	0/2/2/2	-
6	GLY	A	905	-	-	2/2/2/2	-
5	PGE	B	907	-	-	2/7/7/7	-
6	GLY	D	904	-	-	1/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	905	GLY	OXT-C	-2.48	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	904	GLY	OXT-C	-2.20	1.23	1.30
6	A	904	GLY	OXT-C	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	905	GLY	OXT-C-O	-2.54	116.80	123.33
6	A	904	GLY	OXT-C-CA	2.10	121.74	113.38

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	905	GLY	O-C-CA-N
6	A	905	GLY	OXT-C-CA-N
6	D	905	GLY	O-C-CA-N
6	D	905	GLY	OXT-C-CA-N
5	B	907	PGE	O2-C3-C4-O3

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	904	GLY	3	0
6	A	904	GLY	2	0
6	D	905	GLY	1	0
3	B	901	SO4	1	0
3	A	901	SO4	1	0
6	A	905	GLY	1	0
3	B	904	SO4	1	0
3	C	901	SO4	1	0
3	D	902	SO4	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	775/816 (94%)	0.15	25 (3%)	50	47	26, 54, 123, 165	1 (0%)
1	B	775/816 (94%)	-0.08	28 (3%)	46	43	23, 42, 109, 162	0
1	D	775/816 (94%)	0.19	43 (5%)	30	27	24, 54, 132, 173	2 (0%)
2	C	775/816 (94%)	-0.04	31 (4%)	42	39	23, 42, 112, 150	0
All	All	3100/3264 (94%)	0.05	127 (4%)	41	38	23, 48, 120, 173	3 (0%)

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	814	ASP	5.8
1	A	262	ASN	4.9
1	B	466	PRO	4.7
1	D	83	PHE	4.7
1	D	466	PRO	4.6

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
2	Q3P	C	222	13/14	0.92	0.12	24,34,79,94	0
1	TRQ	A	697	16/17	0.96	0.07	28,29,36,50	0
1	TRQ	D	697	16/17	0.97	0.06	28,29,44,46	0
1	TRQ	B	697	16/17	0.97	0.05	22,23,30,36	0
2	TRQ	C	697	16/17	0.97	0.06	23,24,29,35	0

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(Å ²)	Q<0.9
3	SO4	D	902	5/5	0.74	0.12	98,104,109,120	0
3	SO4	B	905	5/5	0.76	0.11	84,96,110,113	0
3	SO4	C	903	5/5	0.77	0.12	88,97,116,126	0
3	SO4	B	904	5/5	0.82	0.11	85,89,100,112	0
3	SO4	A	902	5/5	0.82	0.10	111,115,117,121	0
3	SO4	B	901	5/5	0.83	0.13	101,107,113,116	0
3	SO4	D	901	5/5	0.86	0.15	86,100,112,116	0
3	SO4	A	901	5/5	0.86	0.14	66,91,106,112	0
3	SO4	B	903	5/5	0.86	0.12	89,92,104,105	0
5	PGE	B	907	10/10	0.86	0.20	44,93,111,121	0
3	SO4	C	901	5/5	0.89	0.11	82,82,96,110	0
3	SO4	B	902	5/5	0.91	0.08	76,78,90,109	0
3	SO4	C	902	5/5	0.91	0.09	70,76,94,100	0
6	GLY	A	904	5/5	0.92	0.12	33,45,49,63	0
6	GLY	D	905	5/5	0.93	0.14	48,79,111,111	0
6	GLY	D	904	5/5	0.95	0.11	41,53,71,71	0
4	MG	A	903	1/1	0.96	0.06	48,48,48,48	0
6	GLY	A	905	5/5	0.96	0.12	46,84,123,123	0
4	MG	B	906	1/1	0.97	0.04	32,32,32,32	0
4	MG	C	904	1/1	0.98	0.04	34,34,34,34	0
4	MG	D	903	1/1	0.98	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.