wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 08:44 PM EDT

PDB ID	:	6VMV
Title	:	Crystal structure of the H767A mutant of GoxA soaked with glycine
Authors	:	Yukl, E.T.
Deposited on	:	2020-01-28
Resolution	:	2.20 Å(reported)

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

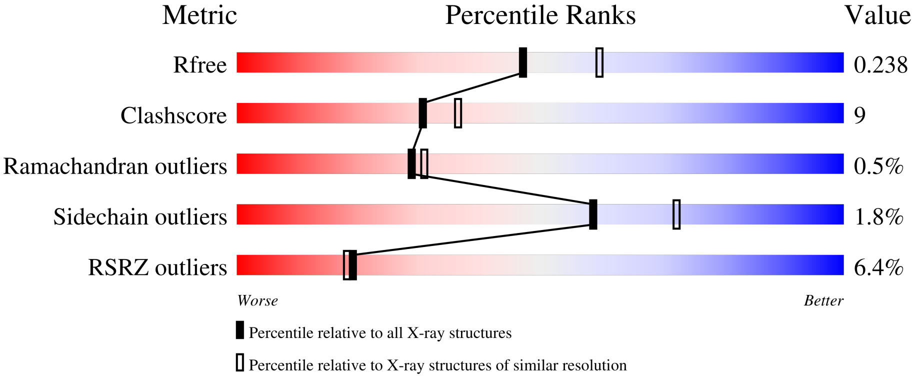
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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

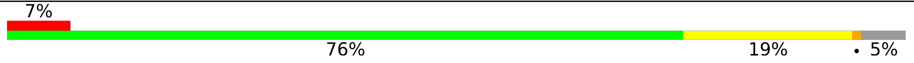
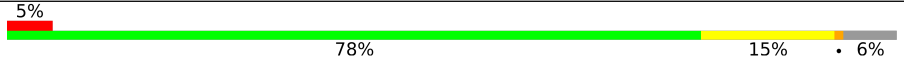
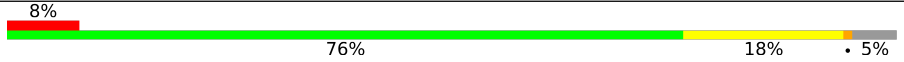
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	

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
3	SO4	A	902	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 25765 atoms, of which 43 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	A	765	6149	3880	10	1043	1196	20	0	14	0
1	B	778	6264	3947	11	1063	1222	21	0	12	0
1	C	769	6146	3884	11	1043	1188	20	0	6	0
1	D	778	6196	3908	11	1051	1206	20	0	4	0

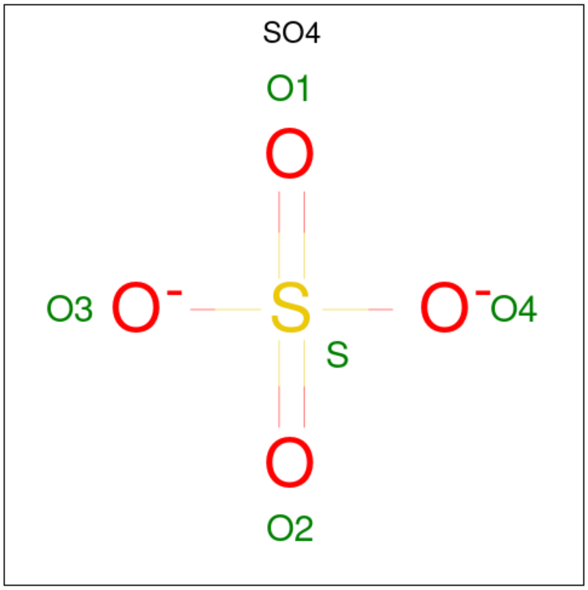
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	ALA	HIS	engineered mutation	UNP A0A161XU12
B	767	ALA	HIS	engineered mutation	UNP A0A161XU12
C	767	ALA	HIS	engineered mutation	UNP A0A161XU12
D	767	ALA	HIS	engineered mutation	UNP A0A161XU12

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	261	Total O 261 261	0	0
4	B	206	Total O 206 206	0	0
4	C	269	Total O 269 269	0	0

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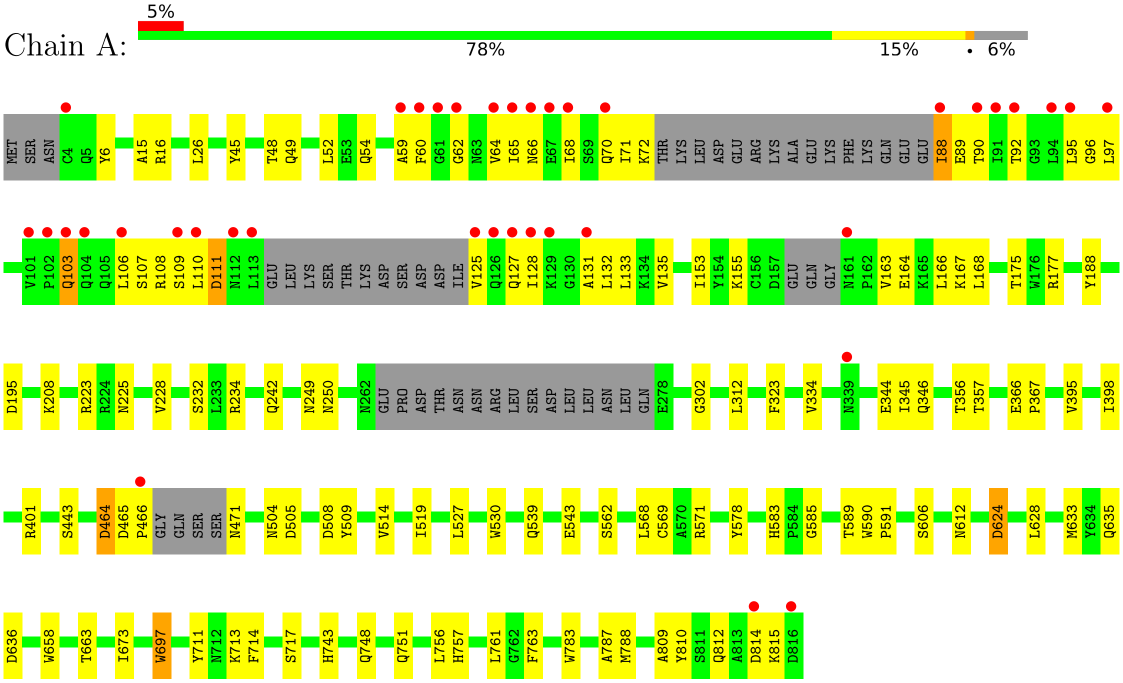
Mol	**Chain**	**Residues**	**Atoms**		**ZeroOcc**	**AltConf**
			Total	O		
4	D	225	225	225	0	0

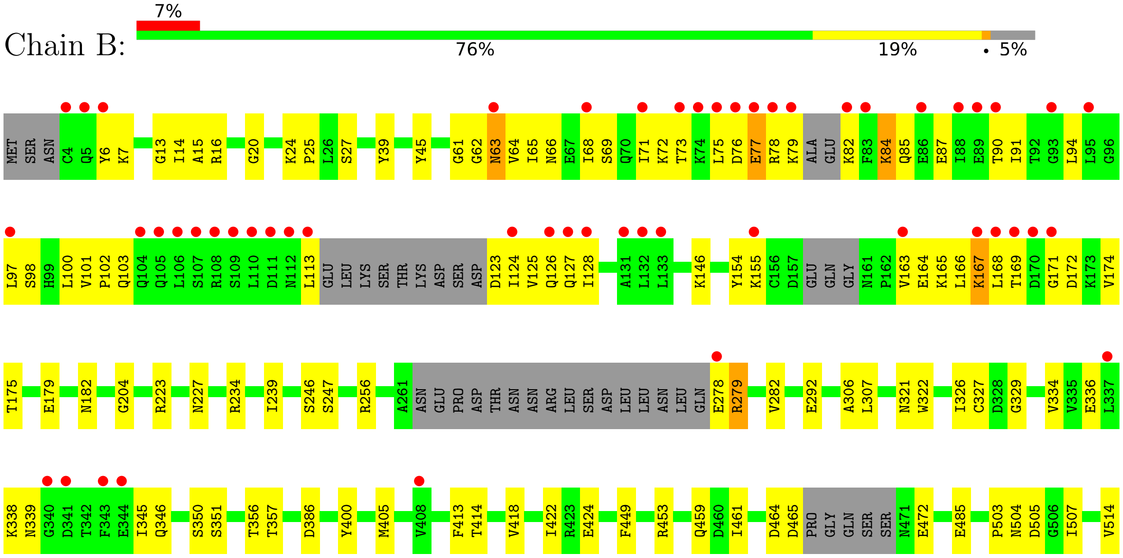
3 Residue-property plots ⓘ

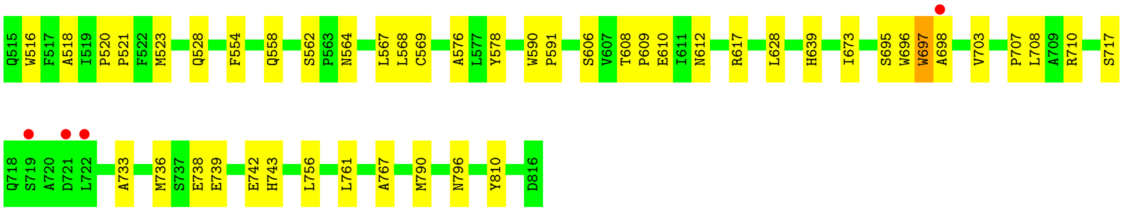
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

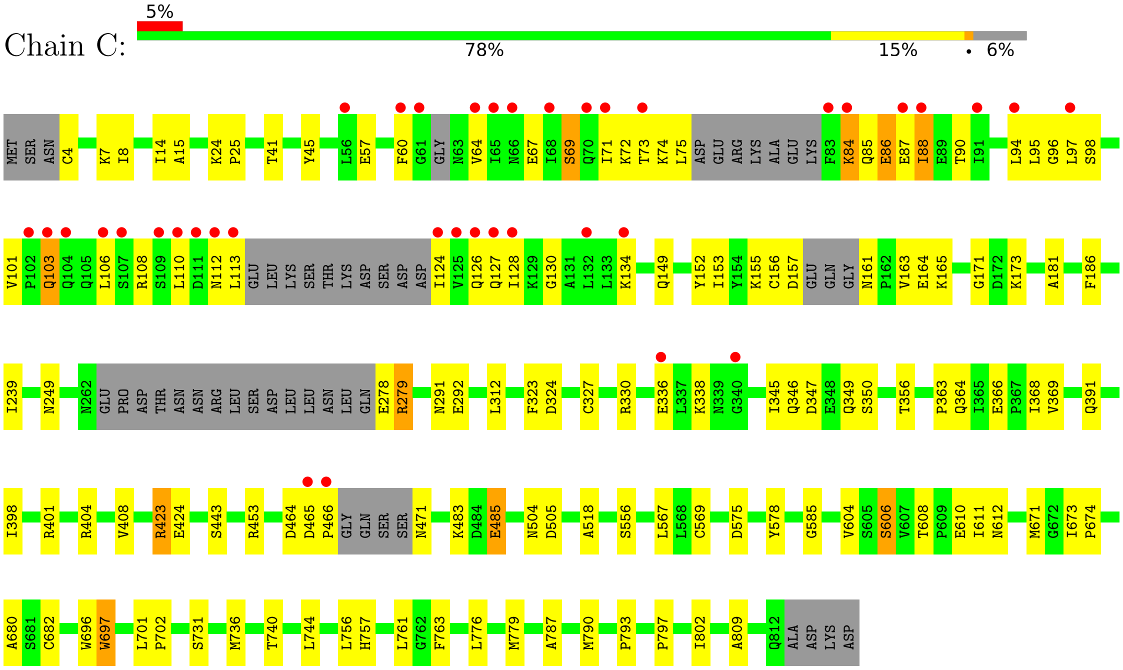


- Molecule 1: Glycine oxidase

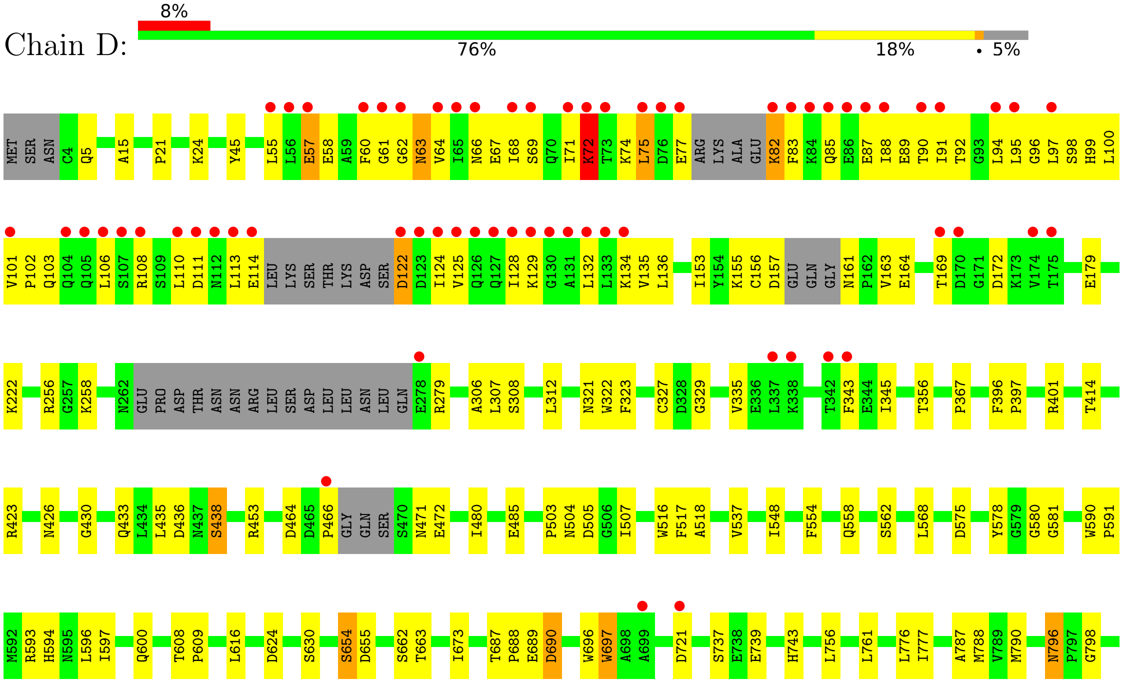


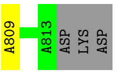


- Molecule 1: Glycine oxidase



- Molecule 1: Glycine oxidase




A809
A813
ASP
LYS
ASP

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.97Å 93.08Å 187.64Å 90.00° 95.07° 90.00°	Depositor
Resolution (Å)	48.20 – 2.20 48.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.20-2.20) 98.7 (48.20-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.238 0.187 , 0.238	Depositor DCC
R_{free} test set	1991 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25765	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, MG, TGH

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	0.63	0/6262	0.66	3/8528 (0.0%)
1	B	0.57	1/6376 (0.0%)	0.62	1/8672 (0.0%)
1	C	0.64	3/6258 (0.0%)	0.66	2/8517 (0.0%)
1	D	0.57	1/6309 (0.0%)	0.61	0/8586
All	All	0.60	5/25205 (0.0%)	0.64	6/34303 (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	2
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	CYS	CB-SG	-9.20	1.66	1.82
1	B	327	CYS	CB-SG	-8.83	1.67	1.82
1	D	327	CYS	CB-SG	-7.36	1.69	1.82
1	C	569	CYS	CB-SG	-5.28	1.73	1.81
1	C	186	PHE	CE2-CZ	5.03	1.47	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ASP	CB-CG-OD1	7.03	124.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	671	MET	CG-SD-CE	5.69	109.30	100.20
1	A	624	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	324	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	195	ASP	CB-CG-OD1	5.25	123.02	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	ILE	Peptide,Mainchain
1	C	86	GLU	Peptide
1	D	72	LYS	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	6139	10	5890	91	0
1	B	6253	11	5996	122	0
1	C	6135	11	5904	113	0
1	D	6185	11	5935	126	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	A	20	0	0	2	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	261	0	0	2	0
4	B	206	0	0	7	0
4	C	269	0	0	5	0
4	D	225	0	0	6	0
All	All	25722	43	23725	445	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 9.

The worst 5 of 445 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:64:VAL:HG12	1:C:94:LEU:HD13	1.32	1.07
1:C:71:ILE:HG23	1:C:74:LYS:HD3	1.48	0.96
1:D:67:GLU:O	1:D:71:ILE:HG13	1.67	0.92
1:D:68:ILE:HA	1:D:71:ILE:HD12	1.52	0.91
1:D:155:LYS:O	1:D:163:VAL:HG12	1.73	0.89

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	766/816 (94%)	733 (96%)	28 (4%)	5 (1%)	22	22
1	B	777/816 (95%)	750 (96%)	25 (3%)	2 (0%)	41	46
1	C	760/816 (93%)	732 (96%)	24 (3%)	4 (0%)	29	31
1	D	769/816 (94%)	734 (95%)	32 (4%)	3 (0%)	34	37
All	All	3072/3264 (94%)	2949 (96%)	109 (4%)	14 (0%)	29	31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	C	88	ILE
1	D	63	ASN
1	D	96	GLY
1	A	62	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	676/710 (95%)	670 (99%)	6 (1%)	78	88
1	B	687/710 (97%)	675 (98%)	12 (2%)	60	74
1	C	674/710 (95%)	660 (98%)	14 (2%)	53	67
1	D	679/710 (96%)	659 (97%)	20 (3%)	42	54
All	All	2716/2840 (96%)	2664 (98%)	52 (2%)	59	71

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	578	TYR
1	D	75	LEU
1	D	690	ASP
1	C	606[A]	SER
1	D	57	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	66	ASN
1	D	346	GLN
1	D	796	ASN
1	D	612	ASN
1	A	743	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TGH	D	697	1	17,22,23	2.36	7 (41%)	16,31,33	3.38	9 (56%)
1	TGH	B	697	1	17,22,23	1.76	4 (23%)	16,31,33	2.06	5 (31%)
1	TGH	A	697	1	17,22,23	1.96	5 (29%)	16,31,33	4.23	8 (50%)
1	TGH	C	697	1	17,22,23	2.01	5 (29%)	16,31,33	3.60	8 (50%)

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	TGH	D	697	1	-	3/12/14/16	0/2/2/2
1	TGH	B	697	1	-	3/12/14/16	0/2/2/2
1	TGH	A	697	1	-	3/12/14/16	0/2/2/2
1	TGH	C	697	1	-	5/12/14/16	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TGH	CE3-CZ3	5.48	1.48	1.36
1	B	697	TGH	CE3-CZ3	4.38	1.45	1.36
1	A	697	TGH	CE3-CZ3	4.28	1.45	1.36
1	D	697	TGH	CZ2-CE2	4.20	1.50	1.42
1	C	697	TGH	CE3-CZ3	4.20	1.45	1.36

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	697	TGH	CZ2-CH2-N1	9.33	126.96	117.26
1	A	697	TGH	CZ2-CH2-N1	9.19	126.81	117.26
1	A	697	TGH	CZ3-CH2-CZ2	-7.87	114.82	119.80
1	D	697	TGH	CZ3-CE3-CD2	-7.35	110.91	121.13
1	A	697	TGH	CZ3-CE3-CD2	-6.96	111.46	121.13

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	697	TGH	CZ3-CH2-N1-C2
1	C	697	TGH	CZ3-CH2-N1-C2
1	A	697	TGH	O2-C1-C2-O1
1	D	697	TGH	O2-C1-C2-O1
1	D	697	TGH	O3-C1-C2-O1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	SO4	C	903	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	D	903	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	A	902	-	4,4,4	0.12	0	6,6,6	0.25	0
3	SO4	A	905	-	4,4,4	0.22	0	6,6,6	0.27	0
3	SO4	C	902	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	A	904	-	4,4,4	0.14	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	902	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	B	902	-	4,4,4	0.12	0	6,6,6	0.36	0
3	SO4	A	903	-	4,4,4	0.17	0	6,6,6	0.11	0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	903	SO4	1	0
3	A	902	SO4	2	0

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, 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	764/816 (93%)	0.04	38 (4%)	28	27	26, 40, 96, 138	0
1	B	777/816 (95%)	0.21	57 (7%)	15	14	31, 50, 107, 160	0
1	C	768/816 (94%)	0.06	38 (4%)	29	28	26, 42, 101, 150	0
1	D	777/816 (95%)	0.19	65 (8%)	11	9	26, 48, 111, 161	0
All	All	3086/3264 (94%)	0.13	198 (6%)	19	18	26, 45, 105, 161	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	11.2
1	D	113	LEU	7.5
1	B	83	PHE	7.1
1	A	65	ILE	7.1
1	A	68	ILE	6.5

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

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	TGH	A	697	21/22	0.93	0.16	23,36,66,71	0
1	TGH	B	697	21/22	0.93	0.20	31,51,95,103	0
1	TGH	C	697	21/22	0.93	0.17	26,44,79,85	0
1	TGH	D	697	21/22	0.96	0.15	26,47,89,97	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 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	B-factors($Å^2$)	Q<0.9
3	SO4	A	904	5/5	0.83	0.28	138,139,141,144	0
3	SO4	A	903	5/5	0.87	0.28	108,112,114,115	0
2	MG	C	901	1/1	0.89	0.13	41,41,41,41	0
3	SO4	D	902	5/5	0.90	0.24	106,108,115,117	0
2	MG	B	901	1/1	0.93	0.13	52,52,52,52	0
3	SO4	C	902	5/5	0.94	0.14	102,104,105,106	0
3	SO4	B	902	5/5	0.94	0.20	91,97,99,101	0
3	SO4	D	903	5/5	0.96	0.14	101,103,105,108	0
3	SO4	C	903	5/5	0.97	0.13	75,77,85,88	0
2	MG	D	901	1/1	0.97	0.12	43,43,43,43	0
3	SO4	A	905	5/5	0.97	0.09	65,69,82,86	0
2	MG	A	901	1/1	0.98	0.12	36,36,36,36	0
3	SO4	A	902	5/5	0.98	0.12	88,92,97,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.