



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 08:31 AM EDT

PDB ID : 1RYI
Title : STRUCTURE OF GLYCINE OXIDASE WITH BOUND INHIBITOR GLYCOLATE
Authors : Moertl, M.; Diederichs, K.; Welte, W.; Pollegioni, L.; Molla, G.; Motteran, L.; Andriolo, G.; Pilone, M.S.
Deposited on : unknown
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

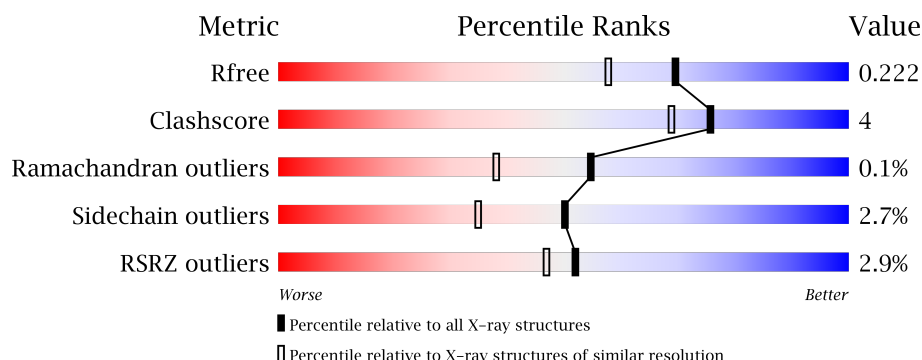
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 $\leq 5\%$. 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	382	<div> <div>3%</div> <div>84% 10% 5%</div> </div>
1	B	382	<div> <div>2%</div> <div>88% 6% 5%</div> </div>
1	C	382	<div> <div>2%</div> <div>87% 8% 5%</div> </div>
1	D	382	<div> <div>4%</div> <div>86% 9% 5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOA	A	9110	-	-	X	-
3	GOA	B	9210	-	-	X	X
3	GOA	C	9310	-	-	X	X
3	GOA	D	9410	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12720 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 GLYCINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	1	0
			2855	1826	489	523	17			
1	B	364	Total	C	N	O	S	0	2	0
			2866	1835	490	524	17			
1	C	364	Total	C	N	O	S	0	1	0
			2855	1826	489	523	17			
1	D	364	Total	C	N	O	S	0	2	0
			2866	1835	490	524	17			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP O31616
A	-11	HIS	-	EXPRESSION TAG	UNP O31616
A	-10	HIS	-	EXPRESSION TAG	UNP O31616
A	-9	HIS	-	EXPRESSION TAG	UNP O31616
A	-8	HIS	-	EXPRESSION TAG	UNP O31616
A	-7	HIS	-	EXPRESSION TAG	UNP O31616
A	-6	HIS	-	EXPRESSION TAG	UNP O31616
A	-5	MET	-	EXPRESSION TAG	UNP O31616
A	-4	ALA	-	EXPRESSION TAG	UNP O31616
A	-3	ARG	-	EXPRESSION TAG	UNP O31616
A	-2	ILE	-	EXPRESSION TAG	UNP O31616
A	-1	ARG	-	EXPRESSION TAG	UNP O31616
A	0	ALA	-	EXPRESSION TAG	UNP O31616
B	-12	MET	-	EXPRESSION TAG	UNP O31616
B	-11	HIS	-	EXPRESSION TAG	UNP O31616
B	-10	HIS	-	EXPRESSION TAG	UNP O31616
B	-9	HIS	-	EXPRESSION TAG	UNP O31616
B	-8	HIS	-	EXPRESSION TAG	UNP O31616
B	-7	HIS	-	EXPRESSION TAG	UNP O31616
B	-6	HIS	-	EXPRESSION TAG	UNP O31616
B	-5	MET	-	EXPRESSION TAG	UNP O31616

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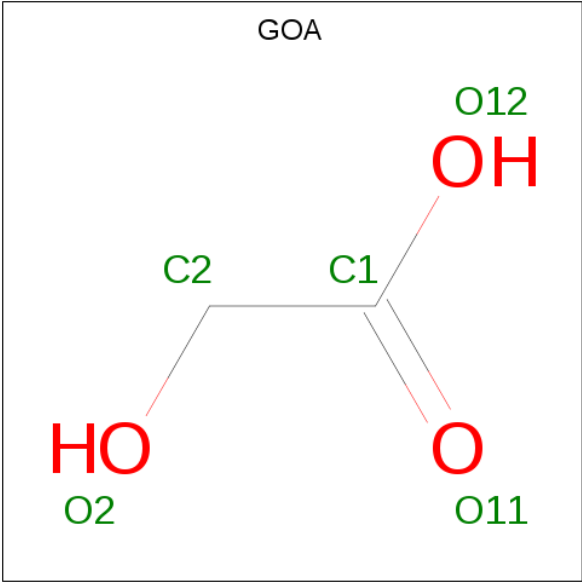
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	EXPRESSION TAG	UNP O31616
B	-3	ARG	-	EXPRESSION TAG	UNP O31616
B	-2	ILE	-	EXPRESSION TAG	UNP O31616
B	-1	ARG	-	EXPRESSION TAG	UNP O31616
B	0	ALA	-	EXPRESSION TAG	UNP O31616
C	-12	MET	-	EXPRESSION TAG	UNP O31616
C	-11	HIS	-	EXPRESSION TAG	UNP O31616
C	-10	HIS	-	EXPRESSION TAG	UNP O31616
C	-9	HIS	-	EXPRESSION TAG	UNP O31616
C	-8	HIS	-	EXPRESSION TAG	UNP O31616
C	-7	HIS	-	EXPRESSION TAG	UNP O31616
C	-6	HIS	-	EXPRESSION TAG	UNP O31616
C	-5	MET	-	EXPRESSION TAG	UNP O31616
C	-4	ALA	-	EXPRESSION TAG	UNP O31616
C	-3	ARG	-	EXPRESSION TAG	UNP O31616
C	-2	ILE	-	EXPRESSION TAG	UNP O31616
C	-1	ARG	-	EXPRESSION TAG	UNP O31616
C	0	ALA	-	EXPRESSION TAG	UNP O31616
D	-12	MET	-	EXPRESSION TAG	UNP O31616
D	-11	HIS	-	EXPRESSION TAG	UNP O31616
D	-10	HIS	-	EXPRESSION TAG	UNP O31616
D	-9	HIS	-	EXPRESSION TAG	UNP O31616
D	-8	HIS	-	EXPRESSION TAG	UNP O31616
D	-7	HIS	-	EXPRESSION TAG	UNP O31616
D	-6	HIS	-	EXPRESSION TAG	UNP O31616
D	-5	MET	-	EXPRESSION TAG	UNP O31616
D	-4	ALA	-	EXPRESSION TAG	UNP O31616
D	-3	ARG	-	EXPRESSION TAG	UNP O31616
D	-2	ILE	-	EXPRESSION TAG	UNP O31616
D	-1	ARG	-	EXPRESSION TAG	UNP O31616
D	0	ALA	-	EXPRESSION TAG	UNP O31616

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: C₂H₄O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 5 2 3	0	0
3	B	1	Total C O 5 2 3	0	0
3	C	1	Total C O 5 2 3	0	0
3	D	1	Total C O 5 2 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	267	Total O 267 267	0	0
4	B	262	Total O 262 262	0	0
4	C	298	Total O 298 298	0	0
4	D	219	Total O 219 219	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.71Å 218.76Å 217.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 1.80 19.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.92-1.80) 98.3 (19.92-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.177 , 0.214 0.189 , 0.222	Depositor DCC
R_{free} test set	8006 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12720	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% 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: GOA, FAD

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	0.51	0/2926	0.78	9/3952 (0.2%)
1	B	0.52	0/2938	0.75	5/3968 (0.1%)
1	C	0.52	0/2926	0.76	5/3952 (0.1%)
1	D	0.50	0/2938	0.74	5/3968 (0.1%)
All	All	0.51	0/11728	0.76	24/15840 (0.2%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	271	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	362	ASP	CB-CG-OD2	6.55	124.20	118.30
1	C	271	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	233	ASP	CB-CG-OD2	6.27	123.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2855	0	2803	28	0
1	B	2866	0	2811	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2855	0	2803	20	0
1	D	2866	0	2811	21	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	5	0	2	4	0
3	B	5	0	2	3	0
3	C	5	0	2	3	0
3	D	5	0	2	4	0
4	A	267	0	0	5	0
4	B	262	0	0	1	0
4	C	298	0	0	0	0
4	D	219	0	0	3	0
All	All	12720	0	11360	83	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 4.

The worst 5 of 83 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:A:302:ARG:HE	3:A:9110:GOA:H22	1.17	1.09
1:B:302:ARG:HE	3:B:9210:GOA:H22	1.23	1.03
1:D:302:ARG:HE	3:D:9410:GOA:H22	1.23	1.01
1:C:147:HIS:CD2	1:C:248:VAL:HG13	2.02	0.95
1:C:91:HIS:HB3	1:C:147:HIS:CE1	2.17	0.80

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	363/382 (95%)	353 (97%)	8 (2%)	2 (1%)	28	13
1	B	364/382 (95%)	350 (96%)	14 (4%)	0	100	100
1	C	363/382 (95%)	353 (97%)	10 (3%)	0	100	100
1	D	364/382 (95%)	350 (96%)	14 (4%)	0	100	100
All	All	1454/1528 (95%)	1406 (97%)	46 (3%)	2 (0%)	55	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	58	GLU

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	296/310 (96%)	285 (96%)	11 (4%)	39	22
1	B	297/310 (96%)	292 (98%)	5 (2%)	66	55
1	C	296/310 (96%)	287 (97%)	9 (3%)	46	30
1	D	297/310 (96%)	290 (98%)	7 (2%)	54	40
All	All	1186/1240 (96%)	1154 (97%)	32 (3%)	50	35

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	184	LEU
1	C	55	GLU
1	D	186	ILE
1	C	25	LYS
1	C	56	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	ASN
1	C	53	HIS
1	D	290	GLN
1	B	217	ASN
1	B	352	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	FAD	A	9100	-	51,58,58	1.37	7 (13%)	54,89,89	2.33	8 (14%)
3	GOA	A	9110	-	1,4,4	2.00	1 (100%)	1,4,4	1.11	0
2	FAD	B	9200	-	51,58,58	1.34	7 (13%)	54,89,89	2.01	8 (14%)
3	GOA	B	9210	-	1,4,4	2.08	1 (100%)	1,4,4	1.44	0
2	FAD	C	9300	-	51,58,58	1.33	6 (11%)	54,89,89	2.25	9 (16%)
3	GOA	C	9310	-	1,4,4	1.89	0	1,4,4	2.35	1 (100%)
2	FAD	D	9400	-	51,58,58	1.55	7 (13%)	54,89,89	2.37	8 (14%)
3	GOA	D	9410	-	1,4,4	2.25	1 (100%)	1,4,4	1.46	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
2	FAD	A	9100	-	-	0/28/50/50	0/6/6/6
3	GOA	A	9110	-	-	0/0/2/2	0/0/0/0
2	FAD	B	9200	-	-	0/28/50/50	0/6/6/6
3	GOA	B	9210	-	-	0/0/2/2	0/0/0/0
2	FAD	C	9300	-	-	0/28/50/50	0/6/6/6
3	GOA	C	9310	-	-	0/0/2/2	0/0/0/0
2	FAD	D	9400	-	-	0/28/50/50	0/6/6/6
3	GOA	D	9410	-	-	0/0/2/2	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	9410	GOA	O2-C2	-2.25	1.31	1.41
3	B	9210	GOA	O2-C2	-2.08	1.32	1.41
3	A	9110	GOA	O2-C2	-2.00	1.32	1.41
2	C	9300	FAD	C5X-N5	2.12	1.38	1.35
2	A	9100	FAD	C5X-N5	2.13	1.38	1.35

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9400	FAD	N3A-C2A-N1A	-12.52	117.95	128.86
2	C	9300	FAD	N3A-C2A-N1A	-11.09	119.20	128.86
2	A	9100	FAD	N3A-C2A-N1A	-10.36	119.83	128.86
2	B	9200	FAD	N3A-C2A-N1A	-9.37	120.69	128.86
2	A	9100	FAD	C4X-C4-N3	-3.59	118.37	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9110	GOA	4	0
3	B	9210	GOA	3	0
3	C	9310	GOA	3	0
3	D	9410	GOA	4	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	364/382 (95%)	-0.07	11 (3%) 51 45	17, 26, 50, 71	0
1	B	364/382 (95%)	-0.06	9 (2%) 58 53	17, 25, 44, 83	0
1	C	364/382 (95%)	-0.15	6 (1%) 72 69	15, 23, 44, 75	0
1	D	364/382 (95%)	0.11	16 (4%) 35 30	17, 28, 49, 83	0
All	All	1456/1528 (95%)	-0.04	42 (2%) 52 47	15, 26, 48, 83	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	CYS	12.0
1	C	56	CYS	7.9
1	B	58	GLU	7.2
1	B	56	CYS	6.7
1	D	54	ALA	5.8

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 carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOA	B	9210	5/5	0.89	0.18	3.71	26,30,36,55	0
3	GOA	C	9310	5/5	0.92	0.21	2.84	21,26,34,51	0
3	GOA	D	9410	5/5	0.94	0.17	2.19	28,29,35,41	0
3	GOA	A	9110	5/5	0.95	0.15	1.76	22,25,32,44	0
2	FAD	B	9200	53/53	0.97	0.07	-0.66	13,18,22,23	0
2	FAD	D	9400	53/53	0.97	0.07	-0.92	14,21,27,29	0
2	FAD	A	9100	53/53	0.98	0.07	-0.93	14,18,20,26	0
2	FAD	C	9300	53/53	0.98	0.07	-1.05	12,16,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.