



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:51 am BST

PDB ID : 5VFB  
Title : 1.36 Angstrom Resolution Crystal Structure of Malate Synthase G from *Pseudomonas aeruginosa* in Complex with Glycolic Acid.  
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-04-07  
Resolution : 1.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 2.11  
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) : 2.11

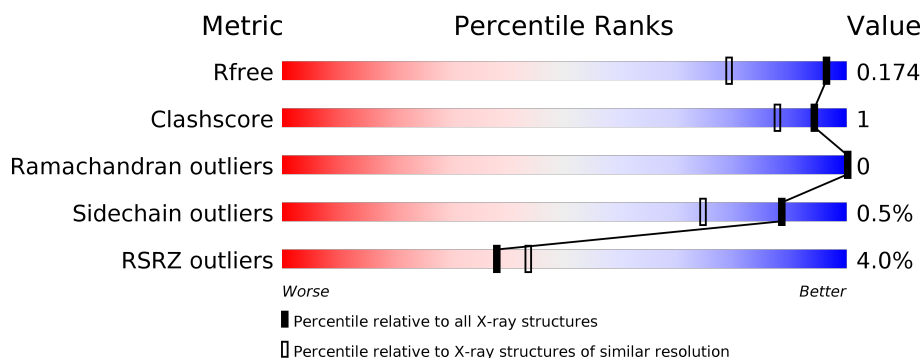
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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  $\geq 3$ , 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	728	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
1	B	728	<div> <div>5%</div> <div>97%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14296 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	53	0
			5979	3735	1069	1150	25			
1	B	724	Total	C	N	O	S	0	37	0
			5846	3649	1048	1126	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I636
A	-1	ASN	-	expression tag	UNP Q9I636
A	0	ALA	-	expression tag	UNP Q9I636
B	-2	SER	-	expression tag	UNP Q9I636
B	-1	ASN	-	expression tag	UNP Q9I636
B	0	ALA	-	expression tag	UNP Q9I636

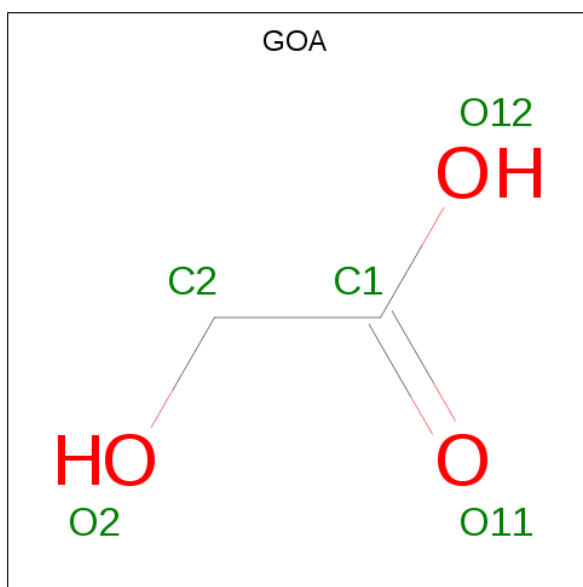
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Cl	0	0
			5	5		
3	A	5	Total	Cl	0	0
			5	5		

- Molecule 4 is GLYCOLIC ACID (three-letter code: GOA) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 2 3	0	0
4	B	1	Total C O 10 4 6	0	1

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Na 2 2	0	0

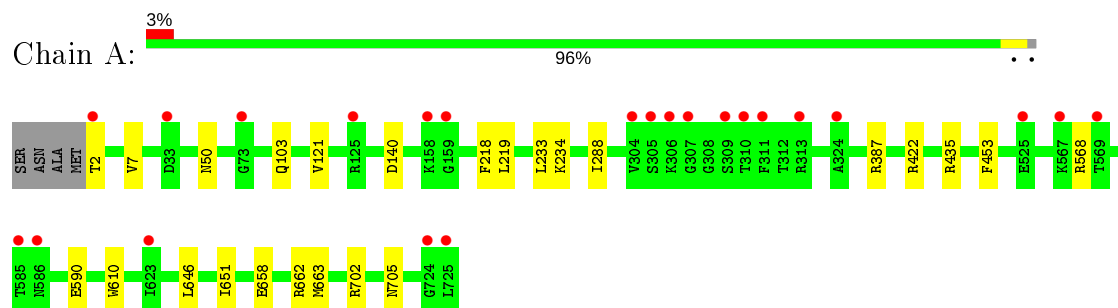
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1150	Total O 1251 1251	0	123
6	B	1097	Total O 1191 1191	0	126

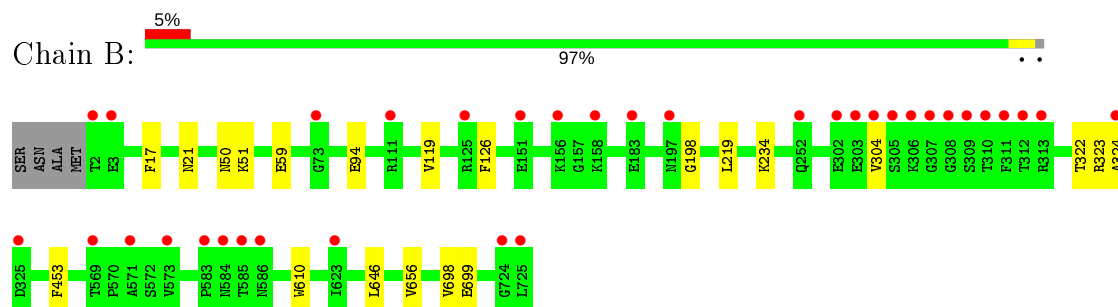
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Malate synthase G



#### • Molecule 1: Malate synthase G



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.38 Å 111.71 Å 96.95 Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	29.62 – 1.36 29.62 – 1.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.62-1.36) 99.0 (29.62-1.36)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 1.36 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.143 , 0.168 0.153 , 0.174	Depositor DCC
$R_{free}$ test set	13944 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI, CL, GOA, NA

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	0.46	0/6082	0.76	2/8226 (0.0%)
1	B	0.45	0/5946	0.74	0/8048
All	All	0.46	0/12028	0.75	2/16274 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	422	ARG	NE-CZ-NH1	6.58	123.59	120.30

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	5979	0	5909	17	1
1	B	5846	0	5774	14	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	5	0	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	5	0	0
5	B	2	0	0	0	0
6	A	1251	0	0	7	0
6	B	1191	0	0	4	0
All	All	14296	0	11690	31	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 1.

All (31) 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:198:GLY:HA2	1:B:324:ALA:HB1	1.56	0.87
1:B:219:LEU:HD21	1:B:234[B]:LYS:HE3	1.68	0.75
1:B:94[B]:GLU:OE1	6:B:901[B]:HOH:O	2.04	0.74
1:A:435[B]:ARG:HD3	6:A:1222:HOH:O	1.93	0.67
1:B:94[A]:GLU:OE1	6:B:902[A]:HOH:O	2.14	0.65
1:B:59[B]:GLU:HA	1:B:59[B]:GLU:OE1	2.03	0.59
1:A:590[B]:GLU:OE2	6:A:903:HOH:O	2.17	0.58
1:A:663[B]:MET:HE2	1:A:663[B]:MET:HA	1.86	0.56
1:A:2:THR:HG22	6:A:1699:HOH:O	2.05	0.56
1:B:646[B]:LEU:HD11	1:B:656:VAL:HG21	1.87	0.55
1:A:103[B]:GLN:NE2	6:A:904:HOH:O	2.33	0.55
1:A:705:ASN:ND2	3:A:805:CL:CL	2.75	0.55
1:A:702[A]:ARG:NH2	6:A:902:HOH:O	2.01	0.54
1:A:219:LEU:HD21	1:A:234[B]:LYS:HE3	1.91	0.52
1:B:94[A]:GLU:CD	6:B:902[A]:HOH:O	2.47	0.52
1:B:51[B]:LYS:NZ	6:B:903[B]:HOH:O	2.22	0.51
1:A:646[B]:LEU:HD23	1:A:651:ILE:HG13	1.93	0.50
1:A:658:GLU:CD	1:A:662[B]:ARG:HE	2.16	0.48
1:A:234[A]:LYS:HE3	6:A:1018[A]:HOH:O	2.15	0.47
1:A:387[B]:ARG:N	1:A:387[B]:ARG:HD3	2.30	0.47
1:A:663[B]:MET:CE	1:A:663[B]:MET:HA	2.45	0.46
1:B:17:PHE:CZ	1:B:21[B]:ASN:ND2	2.85	0.45
1:B:119[A]:VAL:CG2	1:B:126:PHE:HB3	2.47	0.44
1:B:322:THR:HG22	1:B:323:ARG:O	2.18	0.43
1:A:218:PHE:HA	1:A:233:LEU:HD23	2.00	0.43
1:A:121:VAL:CG1	1:A:288[B]:ILE:HG23	2.50	0.42
1:B:198:GLY:HA2	1:B:324:ALA:CB	2.37	0.42
1:A:7[B]:VAL:O	1:A:7[B]:VAL:HG13	2.20	0.41
1:A:234[A]:LYS:CE	6:A:1018[A]:HOH:O	2.69	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51[B]:LYS:HB2	1:B:51[B]:LYS:HE2	1.85	0.40
1:B:698[B]:VAL:HG23	1:B:699:GLU:HG2	2.03	0.40

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:A:140[A]:ASP:OD2	1:B:304:VAL:CG2[2_546]	2.14	0.06

## 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	776/728 (107%)	763 (98%)	13 (2%)	0	100	100
1	B	760/728 (104%)	750 (99%)	10 (1%)	0	100	100
All	All	1536/1456 (106%)	1513 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	628/579 (108%)	625 (100%)	3 (0%)	88	74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	614/579 (106%)	611 (100%)	3 (0%)	88	74
All	All	1242/1158 (107%)	1236 (100%)	6 (0%)	88	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	453	PHE
1	A	610	TRP
1	B	50	ASN
1	B	453	PHE
1	B	610	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	653	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	$\# Z  > 2$
4	GOA	B	809[A]	2	1,4,4	0.31	0	0,4,4	0.00	-
4	GOA	A	807	2	1,4,4	0.54	0	0,4,4	0.00	-
4	GOA	B	809[B]	2	1,4,4	0.38	0	0,4,4	0.00	-

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
4	GOA	B	809[A]	2	-	0/0/2/2	-
4	GOA	A	807	2	-	0/0/2/2	-
4	GOA	B	809[B]	2	-	0/0/2/2	-

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	724/728 (99%)	0.10	23 (3%)	47 53	5, 9, 19, 37	0
1	B	724/728 (99%)	0.19	35 (4%)	30 35	5, 10, 24, 42	0
All	All	1448/1456 (99%)	0.15	58 (4%)	38 43	5, 9, 22, 42	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	VAL	9.5
1	B	311	PHE	8.7
1	B	310	THR	8.4
1	B	308	GLY	7.2
1	B	2	THR	7.1
1	B	307	GLY	7.0
1	B	324	ALA	6.9
1	A	725	LEU	6.1
1	B	725	LEU	6.0
1	A	2	THR	5.9
1	A	569	THR	5.9
1	B	312	THR	5.3
1	A	307	GLY	5.0
1	B	306	LYS	4.9
1	A	158	LYS	4.0
1	B	302	GLU	4.0
1	A	159[A]	GLY	3.8
1	A	585	THR	3.7
1	A	73	GLY	3.6
1	B	303	GLU	3.6
1	B	73	GLY	3.4
1	B	313	ARG	3.3
1	A	304	VAL	3.3
1	A	623	ILE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	306	LYS	3.2
1	B	586	ASN	3.1
1	B	309	SER	3.1
1	B	724	GLY	3.0
1	B	156	LYS	3.0
1	A	324	ALA	2.9
1	B	584	ASN	2.9
1	B	305	SER	2.9
1	A	724	GLY	2.9
1	A	586	ASN	2.8
1	B	569	THR	2.8
1	B	151	GLU	2.8
1	B	325	ASP	2.7
1	B	585	THR	2.7
1	B	3	GLU	2.5
1	A	125	ARG	2.5
1	A	525[A]	GLU	2.5
1	A	311	PHE	2.4
1	A	305	SER	2.4
1	B	583	PRO	2.3
1	B	125	ARG	2.3
1	B	623	ILE	2.3
1	B	252	GLN	2.2
1	A	310	THR	2.2
1	A	567	LYS	2.2
1	A	309	SER	2.2
1	A	313[A]	ARG	2.2
1	B	111	ARG	2.2
1	B	571	ALA	2.1
1	B	197	ASN	2.1
1	B	183[A]	GLU	2.1
1	A	33	ASP	2.0
1	B	573	VAL	2.0
1	B	158	LYS	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CL	B	808	1/1	0.95	0.10	24,24,24,24	0
3	CL	B	806	1/1	0.96	0.14	33,33,33,33	0
3	CL	A	803	1/1	0.97	0.07	17,17,17,17	0
3	CL	B	805	1/1	0.97	0.06	19,19,19,19	0
4	GOA	B	809[A]	5/5	0.97	0.10	5,6,6,6	5
4	GOA	B	809[B]	5/5	0.97	0.10	11,11,12,12	5
5	NA	B	802	1/1	0.98	0.18	26,26,26,26	0
5	NA	B	803	1/1	0.98	0.33	28,28,28,28	0
3	CL	B	804	1/1	0.98	0.12	21,21,21,21	0
3	CL	A	804	1/1	0.99	0.09	17,17,17,17	0
3	CL	B	807	1/1	0.99	0.06	14,14,14,14	0
4	GOA	A	807	5/5	0.99	0.06	6,7,7,8	0
3	CL	A	806	1/1	0.99	0.06	14,14,14,14	0
3	CL	A	805	1/1	1.00	0.12	17,17,17,17	0
3	CL	A	802	1/1	1.00	0.10	23,23,23,23	0
2	NI	A	801	1/1	1.00	0.03	7,7,7,7	0
2	NI	B	801	1/1	1.00	0.03	7,7,7,7	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.